Contemporary Mathematicians

Manfred Denker
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Editors

Rabi N. Bhattacharya

Selected Papers

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Preface

It is our privilege and great honor to pay our tribute to our friend, collaborator, and teacher Rabi N. Bhattacharya in the form of this volume of selected papers, collecting some of his most influential papers together with commentaries of colleagues from around the world. For more than three decades, we have been able to see Rabi's knowledge, insight, and influence in probability, statistics, and their applications grow; we hope this volume will shed some light on this fact and the reader will enjoy reading about Rabi's scientific developments and the state of research his name represents.

The book is divided into three parts, *Modes of Approximation*, *Large Times for Markov Processes*, and *Stochastic Foundations in Applied Sciences*, representing the main scientific contributions of Professor Bhattacharya. It ranges from theoretical statistics via analytical probability theory, Markov processes, and random dynamics to applied topics in statistics, economics, and geophysics. Such a wide range of interests is hardly overseen by a single person, so we are especially glad that so many of our colleagues representing these fields were willing and eager to contribute to this volume. Their articles help to position Rabi's work in the light of other achievements, further developments, and directions of research. An explicit goal is to help researchers who may wish to embark on any of these many varied paths. The reader will find a list of Rabi's PhD students and scientific writings just before the table of content.

This volume would not have been put together without the help of several people and numerous publishers. First of all, Anirban DasGupta from Purdue University made an initial proposal to Springer for a volume like this one. We thank Lizhen Li from the University of Texas at Austin for her support in collecting data, and Christopher Tommich and Benjamin Levitt from Birkhäuser/Springer for their help in the editorial process. The technical support by Suresh Kumar from Birkhäuser is greatly appreciated.

We also thank the publishers *American Mathematical Society*, *World Scientific Publishing Com.*, *Institute of Mathematical Statistics*, *Society for Industrial and Applied Mathematics (SIAM)*, *János Bolyai Mathematical Society*, *Elsevier*, and *Springer Nature* for generously granting the copyrights of those articles of R.N. Bhattacharya we had chosen to be reproduced in this volume. A list of these papers is provided under Acknowledgments.

Dedicated to Random Processes

The name “Bhattacharya” is a combination of two words: Bhatta, meaning Vedic priest, generally known as sages or seers during the Vedic period, and the word Acharya, with the Sanskrit meaning of teacher. Although Rabindra Nath (Rabi) Bhattacharya has no formal religious affiliation, he exemplifies the best of the human spirit through his steadfast concern for the well-being of others throughout his career. This comes across most clearly in his professorial role via a sincere dedication to teaching, research, and service. Rabi has been a remarkable “seer” of unknown mathematical and statistical truths and always happy to share those insights with students and collaborators.

“But this can be treated as a Markov process” is a standing phrase of Rabi’s that exemplifies a fundamentally important mathematical structure that attracted Rabi’s attention shortly after completing his PhD thesis on a classic unsolved problem pertaining to rates of convergence in the central limit theorem for independent and identically distributed random vectors. An interest in Markov processes and their applications endured throughout his scientific career and is also well documented by this Selecta volume. An important part of this volume is dedicated to Rabi’s extraordinary contributions to the theory and application of Markov dynamics in their many guises, ranging from discrete parameter Markov chains and/or i.i.d. iterated random maps to continuous parameter Markov processes and diffusions.

However, this volume covers more than one or two such topics from Rabi’s work and interest in mathematics. There are two achievements connected to his name forever, the aforementioned clarification of rates of convergence to the normal distribution, the topic he started in his dissertation that made him well known immediately. This culminated in his providing the complete mathematical framework to justify the Edgeworth expansion of distributions during a collaboration with J.K. Ghosh in the 1970s. A statistician might argue that its value is overcome by computing power. In fact, Rabi and his students have substantiated this in a comparative analysis with Efron’s bootstrap method. However, the intrinsic mathematical and statistical value of Rabi’s contribution is far from being even a topic of discussion when viewed on its own right. Such results gain their importance in mathematical applications and generally serve as the final word on this question in the foundations of probability theory and mathematical statistics.

It is very hard to have a final judgment on Rabi’s more recent interest and achievements in statistics for data observed on manifolds. The absence of an obvious notion of a mean was overcome by Rabi and his former Indiana PhD student Vic Patrangenaru. Rabi had conceived of the proper formulation for statistical inference in this context as far back as the 1990s. Today, as we witness the emergence of a relatively new and deep area of statistics, it is not hard to guess that results of Rabi and his students will play an important role. The new theory and methods are supported by high computational power. We have been seeing this for quite some time in other areas of statistics as well. Rabi’s ideas follow traditional lines but also take excursions into unknown territory for statistical inference, such as data represented through the differential geometry of manifolds and cotangent spaces. As we see it today, one of the outstanding problems for statistical inference on manifolds is that of uniqueness of the Fréchet mean when there is positive curvature. Beyond Rabi’s initial proof for the case of the circle published in his monograph with his student Abhishek Bhattacharya, such results under conditions of practical value for statistics remains one of the central obstructions to the development of a proper theory of inference on manifolds having positive curvature.

It is one of Rabi's firmly held tenets that mathematics can have a significant impact on applied sciences and many other disciplines, as he has demonstrated in diverse ways. Fair play in economics is one of his beliefs, and he tried in several publications to clarify the time evolution of market data. This is mainly done in the framework of random dynamics, which may be a good approximation to observed time series data. Although we do not yet know this, it is natural to follow this mathematical path to see where it leads. Another of Rabi's main contributions from an application point of view originates in the dispersion of solutes in fluid flows. In a long-term collaboration with hydrologist Vijay Gupta, Rabi was among the first to recognize the role of central limit theorems, Brownian motion, and the role of multiple-scale hierarchies in explaining observed transport behavior from laboratory to field scales. Striking results have been achieved here which made Rabi a much cited author in hydrology, geophysics, and applied probability.

Rabindra Nath Bhattacharya was born January 11, 1937, in his ancestral home of Porgola, District of Barisal, in the present country of Bangladesh. His family was uprooted by the partition of India and moved to Calcutta in 1947, where Rabi studied in Presidency College, receiving Bachelor of Science and Master of Science degrees, respectively, in 1956 and 1959. He then secured a research scholar appointment at the Indian Statistical Institute from 1959 to 1960. Rabi joined the mathematics faculty at the University of Kalyani, teaching there from 1961 to 1964. In 1964, Rabi obtained a fellowship from the Statistics Department at the University of Chicago, where he completed his PhD in 1967 under direction of Patrick Billingsley. Upon graduation, he returned to India to marry Bathika (Gouri) Banerjee, followed by acceptance of a position as Assistant Professor in the Statistics Department at the University of California in Berkeley in 1967. Rabi and Gouri have two children and four grandchildren.

In 1972, Rabi was recruited to join the Mathematics Department at the University of Arizona as an Associate Professor and was promoted to Full Professor in 1977, where he remained until 1982. In 1982, he accepted a professorship in the Mathematics Department at Indiana University and remained there until retirement in 2002. Upon retirement from Indiana University, Rabi returned to the University of Arizona where he is once again a tenured Professor of Mathematics.

Rabi received many honors and awards during his career. Well known are his Special Invited Papers in the *Annals of Probability 1977* and the *Annals of Applied Probability 1999*. He was a specially invited lecturer at the German Mathematical Meeting 1989 and the IMS Annual Meeting 1996 in Chicago (Medallion Lecture). He received the prestigious Humboldt Senior Award in 1994/1995 and the Guggenheim Fellowship in 2002. The book *Probability, Statistics and Their Applications: Papers in Honor of Rabi Bhattacharya*[1] attests to the utmost appreciation by his friends, collaborators, and colleagues.

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[1] IMS Lecture Notes Monogr. Ser., 41, Institute of Mathematical Statistics, Beachwood, OH, 2003.

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A. American Mathematical Society
   1. Berry-Esseen bounds for the multi-dimensional central limit theorem. *Bulletin of the American Mathematical Society* 74 (1968), 285–287.
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Contents

Part I
Modes of Approximation

Chapter 1
Contributions of Rabi Bhattacharya to the Central Limit Theory and Normal Approximation

Peter Hall

Abstract Rabi Bhattacharya has made signal contributions to central limit theory and normal approximation, particularly for sums of independent random vectors. His monograph in the area (Bhattacharya and Ranga Rao 1976) has become a classic, its importance being so great that it has had significant influence on mathematical statistics as well as probability. The methods developed in that monograph led to Bhattacharya and Ghosh's (1978) seminal account of general Edgeworth expansions under the smooth function model, as it is now commonly called. That article had a profound influence on the development of bootstrap methods, not least because it provided a foundation for influential research that enabled different bootstrap methods to be compared. At a vital time in the evolution of bootstrap methods, it led to an authoritative and enduring assessment of many of the bootstrap's important contributions.

Keywords Asymptotic expansion, Berry-Esseen bound, Bootstrap, Diffusion, Edgeworth expansion, Markov model, Moment condition, Oscillation, Rates of convergence, Smooth function model, Smoothing lemma

1.1 Rates of Convergence in the Central Limit Theorem

Included among Rabi's earliest research are vital contributions to rates of convergence in the multidimensional central limit theorem. A good example is the work in Bhattacharya [3], taken from his PhD thesis, which established a Berry-Esseen type rate of convergence in the multidimensional central limit theorem under rather general moment conditions. He introduced important tools and applied them to successively more complex problems, for example in the papers Bhattacharya [4, 5, 6, 7].

P. Hall (✉)
Professor Peter Hall passed away on January 9, 2016. We are most fortunate to have his remarkably astute and insightful contribution to this volume. As a great admirer of Rabi's work, Peter was the first to contribute, and a most generous scholar to the very end of his life.

M. Denker, E.C. Waymire (eds.), *Rabi N. Bhattacharya*, Contemporary Mathematicians, DOI 10.1007/978-3-319-30190-7_1

One of Rabi's key contributions, opening up the field for considerable further work, was the development of new methods for describing distributions of sums of independent random vectors in terms of the characteristic functions of those sums. In one dimension such problems can often be solved rather simply, by invoking Esseen's [34] smoothing lemma. This result has applications well beyond the context of the central limit theorem and related expansions, but we shall state it below in that setting.

Lemma (Esseen 1945 [34]). *Let F be a nondecreasing function on the real line, and write G for the standard normal distribution function plus, if desired, terms in its Edgeworth expansion. Let $\chi_F(t) = \int e^{its}\, dF(s)$ denote the Fourier-Stieltjes transform of F, where $i = \sqrt{-1}$, and define χ_G analogously. Then, for each $c_1 > 1$ and each $T > 0$,*

$$\sup_{-\infty<x<\infty} |F(x) - G(x)| \le \frac{c_1}{2\pi} \int_{-T}^{T} \left| \frac{\chi_F(t) - \chi_G(t)}{t} \right| dt + \frac{c_2\, C}{T} \tag{1.1.1}$$

where $c_2 > 0$ depends only on c_1, and $C = \sup_x |G'(x)|$.

A closely related result had been used earlier, implicitly, by Berry [2], but was not stated formally. Esseen [34] introduced a partial extension of his smoothing lemma to the multidimensional case, but was not able to generalize directly what we know today as the Berry-Essen theorem, to the multidimensional form of that result.

Rabi showed that, when working in more than one dimension, a very different approach has to be taken, based on a careful and subtle assessment of "oscillations" of functions. As Esseen [34] had discovered, when working in multidimensional settings the case of finite fourth moments, rather than finite third moments, is from some points of view easier to treat, since it does not require such a detailed analysis of oscillations.

Next we consider an oscillation-based version of (1.1.1), appropriate in k dimensions. The oscillation of a function $f : \mathbb{R}^k \to \mathbb{R}$, on a set $\mathcal{R} \subseteq \mathbb{R}^k$, is defined by

$$\omega_f(\mathcal{R}) = \sup\{|f(y) - f(z)| : y, z \in \mathcal{R}\}\,.$$

The average oscillation of f, with respect to a bounded, positive measure Q, is given by

$$\bar{\omega}_f(2\epsilon : Q) = \int_{\mathbb{R}^k} \omega_f\{B(x, \epsilon)\}\, Q(dx)\,,$$

where $B(x, \epsilon)$ denotes the open ball in $\mathbb{R}^k$ with center $x \in \mathbb{R}^k$ and radius $\epsilon > 0$. In k-variate cases the analogue of the integrand in (1.1.1) is not necessarily integrable, and to avert the problems that this creates we smooth F, which is typically the distribution function of a k-variate random variable, by convolution with a particular probability measure K_ϵ. This leads to the following bound, in place of (1.1.1):

$$\left| \int_{\mathbb{R}^k} f\, d(F - G) \right| \le \omega_f(\mathbb{R}^k)\, \|(F - G) * K_\epsilon\| + \bar{\omega}_f(2\epsilon : |G|) \tag{1.1.2}$$

where we have written $|G|$ for the total variation measure associated with G. (We have used the same notation for the functions F and G, and their associated measures.) Result (1.1.2) plays the role of (1.1.1) in multidimensional problems, and leads to Berry-Esseen bounds and asymptotic expansions in central limit theorems in k-variate cases. The measure K_ϵ is defined by $K_\epsilon(\mathcal{R}) = K(\epsilon^{-1}\mathcal{R})$, where $\epsilon^{-1}\mathcal{R} = \{\epsilon^{-1}x : x \in \mathcal{R}\}$ for each Borel set $\mathcal{R} \subseteq \mathbb{R}$, and K is a probability measure with support confined to $B(0, 1)$ and particularly smooth on $\mathbb{R}^k$.

With characteristic generosity, Rabi discussed his oscillation arguments widely within the mathematics community, and that may have resulted in Sazanov [54] publishing the multidimensional analogue of the Berry-Esseen theorem a little ahead of him. Related work at that time included contributions by von Bahr [57, 58], who introduced bounds and short expansions in the multidimensional central limit theorem under various moment conditions; by Sadikova [51], whose convergence rates in the central limit theorem addressed the case $k = 2$ and include additional log-factors; and by Bergström [1].

Bhattacharya [6], in a contribution to the Sixth Berkeley Symposium, provided a remarkably authoritative and influential treatment of rates of convergence in the multidimensional central limit theorem under the assumption of just three moments. A particularly attractive feature of that work was his derivation of relatively small values for the constants in Berry-Esseen bounds, in cases where the components are independent, by exploiting results of Zolotarev [60].

In Bhattacharya [8], appearing in the *Annals of Probability*, he established accurate bounds for expected values of functions of sums of independent k-variate random variables with three finite moments.

1.2 Asymptotic Expansions

In the *Annals of Probability* in 1977 [9], Rabi surveyed recent developments in the area of rates of convergence and asymptotic expansions for multidimensional central limit theorems for independent and identically distributed random vectors. Writing in *Mathematical Reviews*, Julian Leslie noted of this paper that:

> The tedium and intricacy of proofs in this subject are well known; in this article the author manages to prune away unnecessary detail to reveal the essential mechanisms of these proofs.

A year earlier there had appeared the remarkably influential, and now classic, research monograph by Bhattacharya and Ranga Rao [19]. This volume set down the wealth of knowledge Rabi had acquired during about a decade of research on rates of convergence and asymptotic expansions in multidimensional central limit theorems. The book proved to be a guiding light for a generation of probabilists, and others, who worked in the area. I am proud to count myself among them. I became familiar with the volume relatively late, a little less than decade after it appeared. Indeed, I had difficulty buying it in Australia, and I recall that it was a kind and generous colleague who purchased it abroad for me. For a long time it became a close companion, sharing my bag on many travels, along with V.V. Petrov's *Sums of Independent Random Variables*.

As the quotation from Leslie's review of an earlier paper, two paragraphs above, makes clear, the field is not for the faint hearted. The book does not pull its punches; the reader has to be prepared to work hard to master the material. However, he or she is rewarded richly for the experience.

I have my copy on my desk now, as I write this. It is quite visibly water damaged. I took it on a trip one spring Saturday, some twenty years ago, into the countryside north-west of Canberra, where I wished to take some photographs. Towards the end of a very pleasant afternoon, about two hours before sunset, I realized that to get to where I wanted to go next I had to ford a stream. Judging the stream to be sandy but shallow, I drove my car rather fast down one bank in the hope of building up enough momentum to get across to the other. However, I was too timid; I should have driven faster, and my car stalled abruptly a little way up the opposite bank. My copy of Bhattacharya and Ranga Rao [19] flew off the back seat onto the floor, and water from the stream flooded in when I opened the driver's door. Fortunately the car's engine was out of the water, and by putting floor mats under the wheels, driving across them and repeating the process several times, I managed to move the car onto dry ground.

Every time I pick up that book, where the pages are still curled from the effects of water, I remember the many things I learned from it, for example while reading it out in the countryside that day. I also recall that lovely, golden evening, as the cockatoos chatted to one another before roosting in trees for the night.

1.3 Influence on Statistics

The paper by Bhattacharya and Ghosh [14], published in the *Annals of Statistics*, solved a major, long-open problem relating to the accuracy of Edgeworth expansions. It provided simple, explicit conditions under which such expansions are valid. Half a century earlier, Cramér [27, 28, Chapter VII] had given detailed, rigorous theory in the context of sums of independent and identically distributed random variables, but beyond that, even in 1978, little was known in generality, with mathematical precision and rigor.

Geary [37], Gayen [36], and Wallace [59] had discussed both particular and general expansions, but concise assumptions and general, detailed conclusions were largely absent. For example, Bergström's account of the work of Wallace [59], in *Mathematical Reviews*, described it as "an expository lecture reviewing some important problems." The research of Hsu [45] and Chibisov [23, 24, 25], in probability and statistics, and of Sargan [52, 53], in econometrics, helped significantly, but it predated the work of Bhattacharya and Ranga Rao [19], and so lacked the simultaneous rigor and sweep that was now becoming possible in the area.

Commenting on the need for general Edgeworth expansions for many different statistics, Wallace [59] lamented in the following words our lack of understanding of expansions:

> A general result would be highly desirable or else an example of a statistic, smooth enough at the population value, but for which the series is not a valid asymptotic expansion to show that the construction described is not valid as generally as appears plausible.

Bickel [20], discussing "results obtained since the general review paper by D. Wallace," also pointed to the disparate development of results on Edgeworth expansions via particular cases.

To a large extent, Bhattacharya and Ghosh [14] changed all that. They introduced what has come to be known as the "smooth function model," where a statistic, perhaps after

Studentizing, is represented as a smooth function of the components of a sum, or mean, of independent and identically distributed random vectors. By appealing to results of Bhattacharya and Ranga Rao [19], and undertaking subtle analysis to identify terms in Edgeworth expansions, Bhattacharya and Ghosh [14] introduced a theoretical approach which gave, at once, expansions for a particularly wide class of quantities of considerable statistical interest.

Almost as though by design, the work of Bhattacharya and Ghosh [14] came just in time for the development of theory for a wide variety of bootstrap methods, ushered in by Efron [32]. Efron's rather non-technical paper suggested methodology whose broad acceptance by the statistical community was to rely heavily on authoritative theoretical analysis.

Efron [33] was himself in the vanguard of those who appreciated the essential, intimate connection between theory for, and applications of, computer-intensive statistical methods:

> The need for a more flexible, realistic, and dependable statistical theory is pressing, given the mountains of data now being amassed. The prospect for success is bright, but I believe the solution is likely to lie along the lines suggested [above]—a blend of traditional mathematical thinking combined with the numerical and organizational aptitude of the computer.

The general Edgeworth expansions of Bhattacharya and Ghosh [14], and just as importantly the methods by means of which those expansions were derived, were to play a major role in establishing the credentials of the bootstrap for distribution estimation and for constructing confidence intervals and hypothesis tests. The first Edgeworth-type contributions came from Singh [56] and Bickel and Freedman [21], and over the next decade they became ubiquitous, based heavily on Bhattacharya and Ghosh's paper. For example, the work of Bhattacharya and Ghosh [14] formed the basis for the second chapter of Hall [43].

Related work of Chandra and Ghosh [22] also should be mentioned here. Those authors showed that, in the context of the smooth function model, and using arguments of Bhattacharya and Ghosh [14], statistics whose asymptotic distributions are central chi-squared have finite-sample distributions that enjoy asymptotic expansions in powers of n^{-1}, rather than $n^{-1/2}$. These results are, in a sense, two-sided analogues of one-sided properties derived by Bhattacharya and Ghosh [14].

Bhattacharya [11] showed that the smoothness assumptions in the smooth function model could be relaxed, and that ideas similar to those in Bhattacharya and Ghosh [14] could be used to develop asymptotic expansions of general moments, similar to those derived by Götze and Hipp [39].

The substantial generality of the results of Bhattacharya and Ghosh [14] can be improved somewhat in particular cases, as Bhattacharya and Ghosh [16] demonstrated. They showed that if the gradient of the function in the smooth function model has certain zero components, then moment conditions can be relaxed substantially. This generalized, in important ways, earlier work of Hall [40].

Bhattacharya [12] developed Edgeworth expansions for non-independent data, for example data from linear and nonlinear autoregressions. In that paper he also compared bootstrap distribution estimators with empirical Edgeworth expansion approximations to the same distributions. The latter estimators involve replacing population moments by the corresponding sample moments.

In a similar vein, but using theoretical arguments, Bhattacharya and Qumsiyeh [18] showed that, under the smooth-function model and moment conditions, the bootstrap enjoys greater accuracy than a two-term, empirical Edgeworth expansion. This result pointed clearly to the value of computer-intensive methods such as those based on resampling.

However, in related numerical work in a different setting, Bhattacharya and Chan [13] reached a somewhat different conclusion. They described the relative accuracy of local Edgeworth expansions, bootstrap and chi-squared approximations to probability densities, in both numerical and theoretical terms. In the cases considered, two-term Edgeworth expansions enjoy very good performance, although, as the authors acknowledged, they can be particularly difficult to evaluate in complex cases. Additionally the authors observed that, again in the cases that they consider:

> The bootstrap does quite well occasionally. Chisquare, however, seems to outperform the bootstrap in the majority of cases, symmetric or asymmetric.

The first part of the monograph by Bhattacharya and Denker [15] introduces Edgeworth expansions in a variety of settings, including that of smooth functions of means of independent and identically distributed random variables.

Rabi also has made many contributions to central limit theory for a variety of processes, including several types of diffusion. For example, Bhattacharya [10] established central limit theorems and laws of the iterated logarithm for ergodic, stationary Markov processes. Bhattacharya and Ghosh [17] derived central limit theorems for U-statistics where the kernel depends on sample size. The generality of this setting allowed the authors to establish new properties of the number of k-clusters among uniformly distributed points in the d-dimensional box $[-a, a]^d$, as a diverges.

1.4 Past, Present, and Future

To appreciate the motivation for advances that might be made in the future, let us revisit the past. The contributions to Edgeworth expansions made by Geary [37], Gayen [36], and Wallace [59], and even those of Chibisov [23, 24, 25] and Sargan [52, 53], were undertaken in an era where asymptotic theory was still the most widely used, and even the most promising, approach to approximating the distributions of estimators and related statistics. Prior to 1970, only a prescient few—for example, Simon [55], along with the early developers of bootstrap methods such as those noted by Hall [44], and perhaps Fisher [35, p. 50] and others who developed permutation methods—saw with relative clarity the computer-intensive future of statistical methods.

Against this background it comes as no surprise to learn that the early work on Edgeworth expansion, mentioned above, was designed to enhance the performance of standard asymptotic methods based on the central limit theorem. Even today statistical scientists sometimes argue that Edgeworth expansions should, or could, be pressed into use as practical statistical tools; to give a range of examples over the last 40 years we mention Pfanzagl [50], Pfaff and Pfanzagl [49], Hall [41], Contaldi et al. [26], and Gonçalvesa and Meddahia [38].

However, a distinct drawback of this approach is that it often requires a high degree of mathematical analysis in order to establish the nature of the expansion. Even with the benefit of software such as `Mathematica`, this can be quite inconvenient for practitioners of statistics. For that reason alone, even if Edgeworth approximation was particularly competitive in terms of its accuracy, which it often is not, it would face a significant obstacle to widespread use.

Similar comments apply to central limit theorems applied without Edgeworth correction. For example, those methods often require explicit computation of a variance estimator, which can be awkward in nonstandard cases (or even in standard cases, for example the correlation coefficient). One of the attractive aspects of the percentile bootstrap approach to constructing confidence intervals is that it estimates scale implicitly. If the interval is coverage-corrected using the double bootstrap, it preserves the coverage accuracy of methods that involve explicit estimation of scale.

There is both numerical and theoretical evidence that empirical Edgeworth correction is not always effective, indeed that it is inferior to the bootstrap, at least for sufficiently large samples. See, for example, Hall [42]. One reason is that Edgeworth expansions give of their best in "absolute" rather than "relative" senses, whereas bootstrap methods tend to perform well from both perspectives.

To explain this point we note that an Edgeworth expansion of the distribution of $n^{1/2}(\hat{\theta} - \theta)$, where $\hat{\theta}$ is an estimator of a parameter θ and is computed from a sample of size n, can provide accurate approximations to $P(\hat{\theta} > \theta + n^{-1/2}x)$ for fixed x, in the sense that when x is fixed, the absolute error in the approximation converges to zero at rate n^{-c}, for some $c > \frac{1}{2}$, as n diverges. However, that expansion generally does not provide an accurate approximation in a relative sense, as both x and n diverge. That is to say, the ratio of $P(\hat{\theta} > \theta + n^{-1/2}x)$ to its Edgeworth approximation typically departs quickly from 1 if x and n diverge together. That scenario often reflects accurately the context of confidence intervals in the case of small to moderate-sized samples. Good performance in a relative sense is the realm of large (or moderate) deviation expansions, rather than Edgeworth expansions.

The statistical analogues of large or moderate deviation expansions are saddlepoint approximations, and they are known to be competitive with the simulation-based bootstrap. See, for example, Davison and Hinkley [30], Daniels and Young [29], and DiCiccio et al. [31]. Innovative research on large and moderate deviations, in some ways analogous to Rabi's early work on Edgeworth expansions, is continuing at a reasonably fast pace. Qi-Man Shao and his co-authors have been major contributors; examples include the work of Jing et al. [47], Hu et al. [46], and Liu and Shao [48].

Partly for the reasons mentioned above, contributions to Edgeworth expansions, with reasonably direct statistical applications, are apparently not being pursued so actively. One could add that, in the approximately 15-year period during which bootstrap methods were being evaluated vigorously, Edgeworth expansions were used widely as a theoretical tool for explaining the effectiveness of bootstrap techniques, but were not so frequently suggested as serious, direct competitors with the bootstrap.

Thus, while there are particularly good reasons for further developing large and moderate deviation expansions, the case for Edgeworth expansions arguably is not so compelling right now. That is not to say that in the future we shall not see substantial motivation for further development of Edgeworth expansions. It's just that, today, statistical work on

Edgeworth expansions for their own sake, rather than to shed light on other techniques, appears not to be as well motivated as it was when Rabi made his crucial, and rightly influential, contributions. Rabi's work too was used not so much to develop new statistical techniques based directly on Edgeworth expansions, as to explain the effectiveness of various computer-intensive methods, such as the bootstrap and the jacknife, which, it was shown, could be interpreted as making implicit Edgeworth corrections.

As we explained in Section 1.3, Rabi's contributions to probability are linked closely to his influence on statistics. Today, however, one finds increasingly that most topics related to the central limit theorem are regarded as part of statistics, not probability. I was rather surprised to discover this recently, while serving on an IMS committee. Thus, some of the great contributors to probability and stochastic processes, including Rabi, are being seen increasingly as pioneers in statistics, quite apart from any additional statistical work they might have done.

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Chapter 2
Asymptotic Expansions for Stochastic Processes

Nakahiro Yoshida

2.1 Introduction

The central limit theorems are the basis of the large sample statistics. In estimation theory, the asymptotic efficiency is evaluated by the asymptotic variance of estimators, and in testing statistical hypotheses, the critical region of a test is determined by the normal approximation.

Though asymptotic properties of statistics are based on central limit theorems, the accuracy of their approximation is not necessarily sufficient in practice, especially in the case not many observations are available. Even then, we experienced possibility of getting more precise approximation by the asymptotic expansion methods.

The asymptotic expansion has theoretical importance. This method is today recognized as basis of various branches of theoretical statistics like higher order inferential theory, prediction, model selection, resampling methods, information geometry, and so on. For example, the Akaike Information Criterion (AIC) for statistical model selection is a statistic that incorporates higher-order behavior of the maximum log likelihood.

In the recent four decades, intensive studies have been done for statistics of semimartingales. See, e.g., Kutoyants [54, 55, 56], Basawa and Prakasa Rao [8], Küchler and Soerensen [51], and Prakasa Rao [80, 79]. Since large sample theoretical approaches are inevitable to semimartingales, the development was in exact timing interactively with that of limit theorems.

The counterpart of traditional independent observations is the class of stochastic processes with ergodic property. Laws of large numbers were often deduced from mixing properties or from ergodic theorems through Markovian structures of processes, and various central limit theorems have been produced in the mixing framework and in the martingale framework. Thus, after developments of the first order statistics, it was natural that

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a part of studies of limit theorems for stochastic processes was directed to higher-order asymptotics. This trend entailed generalization of techniques applicable to dependency.

The emphasize of this survey is put on central limit theorems and asymptotic expansion applied to statistics for semimartingales. The results can essentially apply to Markov chains, therefore so-called nonlinear time series models. On the other hand, it should be remarked that quite a few techniques invented in classical higher-order limit theorems, such as smoothing inequalities, work as fundamentals of the theory of asymptotic expansion for semimartingales.

Since non-normality of the limit distribution of statistical estimators, even in regular experiments, emerged rather early [95, 4], the non-ergodic statistics was commonly recognized and established in the 70s. There appear limit theorems that have a mixture of normal distributions as the limit distribution. Intuitively, the Fisher information or the energy of the martingale of the score function does not converge to a constant like classical statistics, but does to a random variable. Then the error becomes asymptotically conditionally normal given the random Fisher information. The non-ergodic statistics required developments in limit theorems and raises a problem about asymptotic expansion. These topics will be discussed in Section 2.5.

2.2 Refinements of Central Limit Theorems

Let $(\xi_j)_{j\in\mathbb{N}}$ be a sequence of d-dimensional independent and identically distributed (i.i.d.) random vectors with $E[\xi_1] = 0$ and $\mathrm{Cov}[\xi_1] = I_\mathsf{d}$, the identity matrix.

2.2.1 Rate of Convergence of the Central Limit Theorem

The central limit theorem states $S_n = n^{-1/2}\sum_{j=1}^n \xi_j \to^d N_\mathsf{d}(0, I_\mathsf{d})$, namely, for any bounded continuous function g on $\mathbb{R}^\mathsf{d}$, $\int_{\mathbb{R}^\mathsf{d}} gd(Q_n - \Phi) \to 0$ as $n \to \infty$, where Q_n is the distribution of S_n and $\Phi = N_\mathsf{d}(0, I_\mathsf{d})$.

Let $\beta_{s,i} = E[|\xi_1^{(i)}|^s]$ and $\beta_s = \sum_{i=1}^\mathsf{d} \beta_{s,i}$, $\xi_1^{(i)}$ being the i-th element of ξ_1. For a function g on $\mathbb{R}^\mathsf{d}$, let $\omega_g(A) = \sup\{|g(x) - g(y)|; x, y \in A\}$ and let $\omega_g(x;\epsilon) = \omega_g(B(x,\epsilon))$ for $B(x,\epsilon) = \{y; |x-y| < \epsilon\}$. The existence of third order moment gives a refinement of the central limit theorem. For example, under the assumption $\beta_3 < \infty$, it holds that for every real valued bounded measurable function g on $\mathbb{R}^\mathsf{d}$,

$$\left|\int_{\mathbb{R}^\mathsf{d}} gd(Q_n - \Phi)\right| \le c_0\omega_g(\mathbb{R}^\mathsf{d})\beta_3 n^{-1/2} + \int_{\mathbb{R}^\mathsf{d}} \omega_g(\cdot; c_2\beta_3 n^{-1/2}\log n)d\Phi \tag{2.1}$$

if $\beta_3 < c_1 n^{1/2}(\log n)^{-\mathsf{d}}$, where c_0, c_1, and c_2 are constants depending on d (Theorem 4.2 of Bhattacharya [15]). See also Bhattacharya [13, 14] for the origin of this result. Bhattacharya and Ranga Rao [20] give a comprehensive exposition and generalizations.

2.2.2 Cramér-Edgeworth Expansion

The ν-th cumulant of ξ_1 is denoted by χ_ν for a multi-index $\nu \in \mathbb{Z}_+^{\mathsf{d}}$, $\mathbb{Z}_+ = \{0, 1, \ldots\}$. That is, for the characteristic function φ_{ξ_1} of ξ_1,

$$\log \varphi_{\xi_1}(u) = \sum_{\nu:2\le|\nu|\le s} \frac{\chi_\nu}{\nu!}(iu)^\nu + o(|u|^s) \quad (u \to 0)$$

where $|\nu| = \nu_1 + \cdots + \nu_{\mathsf{d}}$ and $u^\nu = (u_1)^{\nu_1} \cdots (u_{\mathsf{d}})^{\nu_{\mathsf{d}}}$ for $\nu = (\nu_1, \ldots, \nu_{\mathsf{d}}) \in \mathbb{Z}_+^{\mathsf{d}}$ and $u = (u^1, \ldots, u^{\mathsf{d}}) \in \mathbb{R}^{\mathsf{d}}$.

Let $S_n = n^{-1/2} \sum_{j=1}^n \xi_j$. Then independency yields

$$\varphi_{S_n}(u) = e^{-|u|^2/2} \exp\Bigg[\sum_{\nu:3\le|\nu|\le s} \frac{\chi_\nu}{\nu!}(\mathtt{i}u)^\nu n^{-(|\nu|-2)/2}\Bigg] \times [1 + o(n^{-(s-2)/2})]$$

as $n \to \infty$ for every $u \in \mathbb{R}^{\mathsf{d}}$. The last expression is rewritten as

$$\varphi_{S_n}(u) = e^{-|u|^2/2}\Bigg[1 + \sum_{r=1}^{s-2} n^{-r/2} \tilde{P}_r(\mathtt{i}u)\Bigg] + o(n^{-(s-2)/2}). \tag{2.2}$$

Here each $\tilde{P}_r$ is a certain polynomial whose coefficients are written in χ_ν's. The first term on the right-hand side of (2.2) will be denoted by $\hat{P}_n$.

The $(s-2)$-th order Edgeworth expansion of the distribution of S_n is given by the Fourier inversion $p_n = \mathcal{F}^{-1}[\hat{P}_n]$ of $\hat{P}_n$. Asymptotic expansion gives higher-order approximation of the distribution of S_n. This method goes back to Tchebycheff, Edgeworth, and Cramér.

Regularity of the distribution is often supposed to obtain an asymptotic expansion of the distribution. Otherwise, this approximation is not necessarily valid. In fact, for the Bernoulli trials ξ_j ($j \in \mathbb{N}$), i.e., these random variables are independent and $P[\xi_j = -1] = P[\xi_j = 1] = 1/2$. We denote by F_n the distribution function of $n^{-1/2} \sum_{j=1}^n \xi_j$. Then for even $n \in \mathbb{N}$,

$$F_n(0) - F_n(0-) = P\Bigg[\sum_{j=1}^n \xi_j = 0\Bigg] = \binom{n}{n/2}\left(\frac{1}{2}\right)^n \sim \sqrt{2/\pi}n^{-1/2}$$

and hence for any sequence of continuous functions Φ_n,

$$\liminf_{n\to\infty} (2n)^{1/2} \sup_{x\in\mathbb{R}} \big|F_{2n}(x) - \Phi_n(x)\big| > 0.$$

Therefore the ordinary Edgeworth expansion always fails to give a first-order asymptotic expansion to F_n.

The Cramér condition

$$\limsup_{|u|\to\infty} \big|\varphi_{\xi_1}(u)\big| < 1 \tag{2.3}$$

is effective to deduce the decay of the characteristic function of S_n. If the distribution $\mathcal{L}\{\xi_1\}$ has a nonzero absolutely continuous part of the Lebesgue decomposition, then Condition (2.3) holds.

Under (2.3), combining the estimate (2.6) with (2.5) below, it is possible to evaluate the error of the asymptotic expansion. Let s be an integer greater than 2. Let $M_r(f) = \sup_{x\in\mathbb{R}^{\mathsf{d}}}(1+|x|^r)^{-1}|f(x)|$ for measurable function f on $\mathbb{R}^{\mathsf{d}}$. Let $s' \le s$. Then, under (2.3),

$$\left|\int_{\mathbb{R}^{\mathsf{d}}} f dQ_n - \int_{\mathbb{R}^{\mathsf{d}}} f p_n dx\right| \le M_{s'}(f)\epsilon_n + c(s,\mathsf{d})\int_{\mathbb{R}^{\mathsf{d}}} \omega_f(x; 2e^{-cn})\Phi(dx) \tag{2.4}$$

where c is a positive constant, $c(s,\mathsf{d})$ is a constant depending on (s,d), and $\epsilon_n = o(n^{-(s-2)/2})$ as $n\to\infty$. This result is Theorem 20.1 of Bhattacharya and Ranga Rao [20]. We refer the reader to Cramér [26], Bhattacharya [14], Petrov [75], and other papers mentioned therein for results in the early days.

2.2.3 Smoothing Inequality

The so-called smoothing inequality plays an essential role in validation of the above refinements (2.1) and (2.4) of the central limit theorem. Let p be an integer with $p \ge 3$. Consider a probability measure $\mathcal{K}$ on $\mathbb{R}^{\mathsf{d}}$ and a constant a such that $\alpha := K_\epsilon(B(0,a)) > 1/2$. The scaled measure $\mathcal{K}_\epsilon$ is defined by $\mathcal{K}_\epsilon(A) = \mathcal{K}(\epsilon^{-1}A)$ for Borel sets A. Given a finite measure P and a finite signed measure Q on $\mathbb{R}^{\mathsf{d}}$, let $\gamma_f(\epsilon) = \|f^\star\|_\infty \int_{\mathbb{R}^{\mathsf{d}}} h(|x|)|\mathcal{K}_\epsilon * (P-Q)|(dx)$, $\zeta_f(r) = \|f^\star\|_\infty \int_{\{x;|x|\ge ar\}} h(|x|)\mathcal{K}(dx)$, and $\tau(t) = \sup_{x:|x|\le ta\epsilon'} \int_{\mathbb{R}^{\mathsf{d}}} \omega_f(x+y, 2a\epsilon)Q^+(dy)$, where $f^\star(x) = f(x)/h(|x|)$, $h(r) = 1 + r^{p_0}$ ($p_0 = 2[p/2]$) and Q^+ is the positive part of Q. Among many versions, Sweeting's smoothing inequality [88] is given by

$$\left|(P-Q)[f]\right| \le \frac{1}{2\alpha-1}[A_0\gamma_f(\epsilon) + A_1\zeta_f(\epsilon'/\epsilon) + \tau(t)] + \left(\frac{1-\alpha}{\alpha}\right)^t A_2\|f^\star\|_\infty \tag{2.5}$$

for ϵ, ϵ' t satisfying $0 < \epsilon < \epsilon' < a^{-1}$ and $t \in \mathbb{N}$ ($a\epsilon' t \le 1$), where A_0, A_1, and A_2 are some constants depending on p, d, and $(P+|Q|)[h(|\cdot|)]$. See Bhattacharya [13, 14, 15] and Bhattacharya and Rao [20] for more information of smoothing inequalities.

There exists a constant C_{d} such that

$$\int_{\mathbb{R}^{\mathsf{d}}} |f(x)|dx \le C_{\mathsf{d}} \max_{\substack{n\nu\in\mathbb{Z}_+^{\mathsf{d}},\\ |\nu|=0,\mathsf{d}+1}} \int_{\mathbb{R}^{\mathsf{d}}} \left|\partial^\nu \mathcal{F}[f](u)\right| du \tag{2.6}$$

for all measurable functions $f : \mathbb{R}^{\mathsf{d}} \to \mathbb{R}$ satisfying $\int_{\mathbb{R}^{\mathsf{d}}}(1+|x|^{\mathsf{d}+1})|f(x)|dx < \infty$; see [19, 20]. Thus, the comparison between two measures comes down to the integrability of their Fourier transforms and estimation of the gap between them.

2.2.4 Applications to Statistics

Asymptotic expansion has been a basis of modern theoretical statistics. Bhattacharya and Ghosh [17] established validity of the Edgeworth expansion of functionals of independent random variables, and it was applied to various statistical problems by many authors; see Google Scholar for citing papers. The reader finds related works in Bhattacharya and Denker [11]. Bootstrap methods obtain their basis on the asymptotic expansion (Hall [36]). Information geometry introduced α-connection and gave an interpretation of the higher-order efficiency of the maximum likelihood estimators by the curvature of the fiber associated with the estimator (Amari [1]). Asymptotic expansion was also applied to construction of information criteria for model selection as well as prediction problems; e.g., Konishi and Kitagawa [50], Uchida and Yoshida [91], Komaki [49].

2.3 Asymptotic Expansion for Mixing Processes

As a generalization from independency, central limit theorems and asymptotic expansion were developed under mixing properties; Ibragimov [39] among many others for a central limit theorem. Error bounds were given in Tikhomirov [89], Stein [86], and others. Nagaev [71, 72] presented rates of convergence and asymptotic expansions for Markov chains. Doukhan [29] gives exposition of mixing properties and related central limit theorems.

The class of diffusion processes is of importance as the intersection of the Markovian processes and the processes for which the ergodicity can be successfully treated. Bhattacharya [16], Bhattacharya and Ramasubramanian [18], and Bhattacharya and Wasielak [12] provided ergodicity of multidimensional diffusion processes and related limit theorems. Also see the textbook by Meyn and Tweedie [67] for a general exposition of ergodicity, and a series of papers of Meyn and Tweedie [64, 65, 66]. Kusuoka and Yoshida discussed mixing property of possibly degenerate diffusion processes in [53]. Masuda [61] gave mixing bounds for jump diffusion processes.

Under assumption of mixing property, Götze and Hipp [34] gave asymptotic expansions for sums of weakly dependent processes that are approximated by a Markov chain. The smoothing inequality discussed in Section 2.2 was applied together with inventive estimates of the characteristic function. A Cramér type estimate was assumed for a conditional characteristic function of local increments of the process. Götze and Hipp [35] carried out their scheme for more concrete time series.

The Markovian property in practice plays an essential role in estimation of the characteristic function of an additive functional of the underlying process. Mixing property is deeply related to the ergodicity especially in Markovian contexts. Therefore it is practically natural to approach Edgeworth expansion through mixing.

Given a probability space $(\Omega, \mathcal{F}, P)$, let $Y = (Y_t)_{t\in\mathbb{R}_+}$ be a d_2-dimensional càdlàg process and let $X = (X_t)_{t\in\mathbb{R}_+}$ be a d_1-dimensional càdlàg process with independent increments in the sense that $\mathcal{B}^{X,Y}_{[0,r]}$ is independent of $\mathcal{B}^{dX}_{[r,\infty)}$ for $r \in \mathbb{R}_+$, where $\mathcal{B}^{X,Y}_{[0,r]} = \sigma[X_t, Y_t; t \in [0, r]] \vee \mathcal{N}$ and $\mathcal{B}^{dX}_I = \sigma[X_t - X_s; s, t \in I] \vee \mathcal{N}$, $I \subset \mathbb{R}_+$, with $\mathcal{N}$ being the null-σ-field. Suppose that Y is an ϵ-Markov process driven by X. That is, there exists a nonnegative constant ϵ such that Y_t is $\mathcal{B}^Y_{[s-\epsilon,s]} \vee \mathcal{B}^{dX}_{[s,t]}$-measurable for all $t \geq s \geq \epsilon$, where $\mathcal{B}^Y_I = \sigma[Y_t; t \in I] \vee \mathcal{N}$. Let $\mathcal{B}_I = \sigma[X_t - X_s, Y_t; s, t \in I] \vee \mathcal{N}$ for $I \subset \mathbb{R}_+$.

An α-mixing condition for Y is expressed by the inequality

$$E\big[\big|E_{\mathcal{B}^Y_{[s-\epsilon,s]}}[f] - E[f]\big|\big] \leq \tilde{\alpha}_Y(s,t)\|f\|_\infty$$

for $s \leq t$ and bounded $\mathcal{B}^Y_{[t,\infty)}$-measurable functions f. Let $\alpha(s,t) = \tilde{\alpha}_Y(s, t-\epsilon)$ if $s \leq t - \epsilon$ and 1 if $s > t - \epsilon$. Let $\alpha(h) = \sup_{h' \geq h, s \in \mathbb{R}_+} \alpha(s, s+h')$. we shall assume exponential rate, namely, there exists a constant $a > 0$ such that $\alpha(h) \leq a^{-1}e^{-ah}$ for all $h > 0$. This condition can be relaxed but the exponential rate is assumed for simplicity.

We consider a d-dimensional process $Z = (Z_t)_{t \in \mathbb{R}_+}$ satisfying that Z_0 is $\mathcal{B}_{[0]}$-measurable and that $Z_t - Z_s$ is $\mathcal{B}_{[s,t]}$-measurable for every $t \geq s \geq \epsilon$. Given an integer $p \geq 3$, we assume that there exists $h_0 > 0$ such that

$$E[|Z_0|^{p+1}] + \sup_{t,h: t \in \mathbb{R}_+, 0 \leq h \leq h_0} E[|Z_{t+h} - Z_t|^{p+1}] < \infty,$$

and that $E[Z_t] = 0$ for all $t \in \mathbb{R}_+$.

Suppose that there exists a sequence of intervals $I(j)=[u(j), v(j)]$ ($j=1,\ldots,n(T)$) such that $\lim_{T\to\infty} n(T)/T > 0$ and $0 < \delta \leq v(j) - u(j) \leq \bar{\delta} < \infty$ for some δ and $\bar{\delta}$, and that for each j, some σ-field $\mathcal{B}'_{[v(j)-\epsilon,v(j))}$ of $\mathcal{B}_{[v(j)-\epsilon,v(j)]}$ satisfies $E_{\mathcal{B}_{[v(j)-\epsilon,v(j)]}}[h] = E_{\mathcal{B}'_{[v(j)-\epsilon,v(j)]}}[h]$ for all bounded $\mathcal{B}_{[v(j),\infty)}$-measurable functions h. Let $\hat{C}(j) = \mathcal{B}_{[u(j)-\epsilon,u(j)]} \vee \mathcal{B}'_{[v(j)-\epsilon,v(j)]}$. Denote by Z_J the increment of Z over the interval J. Moreover, suppose that

$$\lim_{B\to\infty} \limsup_{T\to\infty} n(T)^{-1} \sum_j E\big[\sup_{u:|u|\geq B} \big|E_{\hat{C}(j)}[e^{iu\cdot Z_{I(j)}}\psi_j]\big|\big] = 0 \tag{2.7}$$

and $\liminf_{T\to\infty} n(T)^{-1}\sum_j E[\psi_j] > 0$ for some $[0,1]$-valued measurable functionals ψ_j. These conditions work as a kind of Cramér's condition. Thus, in this situation, we obtain an Edgeworth expansion of $T^{-1/2}Z_T$ as follows. The cumulant functions $\chi_{T,r}(u)$ of $T^{-1/2}Z_T$ are defined by $\chi_{T,r}(u) = (\partial_\epsilon)^r|_{\epsilon=0} \log E[\exp(i\epsilon u \cdot T^{-1/2}Z_T)]$ for $u \in \mathbb{R}^{\mathsf{d}}$. Next define $\tilde{P}_{T,r}(u)$ by the formal expansion

$$\exp\Big(\sum_{r=2}^{\infty}(r!)^{-1}\epsilon^{r-2}\chi_{T,r}(u)\Big) = \exp\big(2^{-1}\chi_{T,2}(u)\big) + \sum_{r=1}^{\infty}\epsilon^r T^{-r/2}\tilde{P}_{T,r}(u).$$

Let $\Psi_{T,p} = \mathcal{F}^{-1}[\hat{\Psi}_{T,p}]$ for $\hat{\Psi}_{T,p}(u) = \exp\big(2^{-1}\chi_{T,2}(u)\big) + \sum_{r=1}^{p-2} T^{-r/2}\tilde{P}_{T,r}(u)$. Then if the covariance matrix $\mathrm{Cov}[T^{-1/2}Z_T]$ converges to a regular matrix as $T \to \infty$, then it is possible to show that a similar estimate to (2.4), and the error $|E[f(T^{-1/2}Z_T)] - \Psi_{T,p}[f]|$ becomes $o(T^{-(p-2)/2})$ ordinarily in applications. See Kusuoka and Yoshida [53] and Yoshida [99].

In order to validate the asymptotic expansion, it suffices to find good truncation functionals ψ_j and σ-fields $\mathcal{B}'_{[v(j)-\epsilon,v(j)]}$ as well as intervals $I(j)$ for which (2.7) is satisfied. For example, we shall consider a system of stochastic integral equations

$$Y_t = Y_0 + \int_0^t A(Y_{s-})ds + \int_0^t B(Y_{s-})dw_s + \int_0^t \int C(Y_{s-}, x)\tilde{\mu}(ds, dx)$$
$$Z_t = Z_0 + \int_0^t A'(Y_{s-})ds + \int_0^t B'(Y_{s-})dw_s + \int_0^t \int C'(Y_{s-}, x)\tilde{\mu}(ds, dx)$$

where Z_0 is $\sigma[Y_0]$-measurable, $A \in C^\infty(\mathbb{R}^{d_2}; \mathbb{R}^{d_2})$, $B \in C^\infty(\mathbb{R}^{d_2}; \mathbb{R}^{d_2} \otimes \mathbb{R}^m)$, $C \in C^\infty(\mathbb{R}^{d_2} \times E; \mathbb{R}^{d_2})$, and similarly $A' \in C^\infty(\mathbb{R}^{d_2}; \mathbb{R}^{d})$, $B' \in C^\infty(\mathbb{R}^{d_2}; \mathbb{R}^{d} \otimes \mathbb{R}^m)$, $C' \in C^\infty(\mathbb{R}^{d_2} \times E; \mathbb{R}^{d})$, where w is an m-dimensional Wiener process, E is an open set in $\mathbb{R}^b$, and $\tilde{\mu}$ is a compensated Poisson random measure on $\mathbb{R}_+ \times E$ with intensity $dt \times dx$. Under standard regularity conditions, (Y_t, Z_t) can be regarded as smooth functionals over the canonical space. In this case, the process X_t can be chosen as $X_t = (w_t, \mu_t(g_i); i \in \mathbb{N})$ for a countable measure determining family over E, and Y is a 0-Markov process (i.e., a Markovian process). Though there are several versions of the Malliavin calculus for jump processes, we consider a classical version based on diffusive intensive measure for example by Bichteler et al. [22]. Then it is possible to make truncation functionals ψ_j by using local non-degeneracy of the Malliavin covariance matrix of the system. See Kusuoka and Yoshida [53] and Yoshida [99] for details of this case. The local non-degeneracy of the Malliavin covariance of the functional to be expanded plays a similar role as the Cramér condition in independent cases, assisted by the support theorem for stochastic differential equations.

Since typical statistics are expressed as a Bhattacharya-Ghosh [17] transform of a multidimensional additive functional that admits the Edgeworth expansion, it is possible to obtain Edgeworth expansions for them. This enables us to construct higher-order statistics for stochastic processes (Sakamoto and Yoshida [83, 84], Uchida and Yoshida [91]). For moment expansions, if the Fourier analytic aspect of the smoothing inequality is recalled or the Taylor expansion is applied directly, it is clearly possible to remove Cramér's type condition of the regularity of the distribution. Some refinements of the results of Götze and Hipp were given in Lahiri [57].

2.4 Asymptotic Expansion for Martingales

2.4.1 Martingale Central Limit Theorems

Suppose that, for each $n \in \mathbb{N}$, $\mathcal{B}^n = (\Omega^n, \mathcal{F}^n, \mathbf{F}^n, P^n)$ is a stochastic basis with a filtration $\mathbf{F}^n = (\mathcal{F}_t^n)_{t \in 0,1,\ldots,T_n}$. We consider a sequence of discrete-time L^2-martingales $M^n = (M_t^n)_{t=0,1,\ldots,T_n}$ $(n \in \mathbb{N})$, each M^n defined on $\mathcal{B}^n$ and $M_0 = 0$. Let $\xi_t^n = M_t^n - M_{t-1}^n$ for $t = 1, \ldots, T_n$. Then a classical martingale central limit theorem is stated as follows. Suppose that (i) $\sum_{t=1}^{T_n} E^n[(\xi_t^n)^2 | \mathcal{F}_{t-1}^n] \to^p \sigma^2$ as $n \to \infty$ for some constant σ^2, and that for $\epsilon > 0$, $\sum_{t \in =1}^{T_n} E^n[(\xi_t^n)^2 1_{\{|\xi_t^n| > \epsilon\}} | \mathcal{F}_{t-1}^n] \to^p 0$ as $n \to \infty$. Then $M_{T_n}^n \to^d N(0, \sigma^2)$ as $n \to \infty$. Here E^n denotes the expectation with respect to P^n, and the convergence $\to^p$ is naturally defined along the sequence $(P^n)_{n \in \mathbb{N}}$. For this result, see B. M. Brown [25], Dvoretsky [30], McLeish [63], Rebolledo [82], Hall and Heyde [37]. Functional type convergence results also hold.

Various extensions were made to limit theorems for semimartingales. Among them, a version of the central limit theorem for seminartingales is as follows. Consider a sequence of stochastic processes X^n, $n \in \mathbb{N}$, each of which is a semimartingale defined on a stochastic basis $\mathcal{B}^n$ with a filtration $\mathbf{F}^n = (\mathcal{F}_t^n)_{t\in\mathbb{R}_+}$, and has the local characteristics (B^n, C^n, ν^n), where B^n is the finite variation part with respect to the truncation by the function $x1_{\{|x|\leq 1\}}$, C^n is the predictable covariation process for the continuous local martingale part $X^{n,c}$ of X^n, and ν^n is the compensator of the integer-valued random measure μ^n of jumps of X^n. Denote by $M = (M_t)_{t\in\mathbb{R}_+}$ a continuous Gaussian martingale with a (deterministic) quadratic variation $\langle M\rangle$. Suppose that $X_0^n = 0$ and the following conditions are fulfilled for every $t > 0$ and $\epsilon > 0$ as $n \to \infty$: (i) $\int_0^t \int_{\{|x|>\epsilon\}} \nu^n(ds, dx) \to^p 0$, (ii) $B^{n,c} + \sum_{s\leq t} \int_{\{|x|\leq\epsilon\}} x\nu^n(\{s\}, dx) \to^p 0$, $B^{n,c}$ being the continuous part of B^n, and (iii) $C_t^n + \int_0^t \int_{\{|x|\leq\epsilon\}} x^2\nu^n(ds, dx) - \sum_{s\leq t} \left(\int_{\{|x|\leq\epsilon\}} \nu^n(\{s\}, dx)\right)^2 \to^p \langle M\rangle_t$. Then the finite-dimensional convergence $X^n \to^{d_f} M$ holds. Moreover, under (i), (iii), and (ii$^\sharp$) $\sup_{s\in[0,t]} \left|B_s^{n,c} + \sum_{s\leq t} \int_{\{|x|\leq\epsilon\}} x\nu^n(\{s\}, dx)\right| \to^p 0$ as $n \to \infty$ for every $t > 0$ and $\epsilon > 0$, in place of (ii), one has the functional convergence $X^n \to^d M$ in $\mathbb{D}(\mathbb{R}_+; \mathbb{R})$ as $n \to \infty$. See Liptser and Shiryayev [59], Jacod et al. [42], Jacod and Shiryaev [43], and Liptser and Shiryaev [60]. Developments of the central limit theorems for martingales and convergences to processes with independent increments are owed to many authors. We refer the reader to the bibliographical comments to Chapter VIII of Jacod and Shiryaev [43].

The simplest case is the central limit theorem for continuous local martingales. Let $M^n = (M_t^n)_{t\in[0,1]}$ be a continuous local martingale defined on $\mathcal{B}^n$. If $\langle M^n\rangle_1 \to^p C_\infty$ as $n \to \infty$ for some constant C_∞, then

$$M_1^n \to^d N(0, C_\infty) \quad \text{as} \quad n \to \infty. \tag{2.8}$$

For later discussions, it is worth recalling the derivation of the central limit theorem (2.8). Let $C_t^n = \langle M^n\rangle_t$. We have a trivial decomposition of the characteristic function of M_1^n:

$$E[e^{iuM_1^n}] = \mathbb{T}_0 + \mathbb{T}_1 + \mathbb{T}_2 \tag{2.9}$$

for $u \in \mathbb{R}$, where $\mathbb{T}_0 = E[e^{-2^{-1}C_\infty u^2}]$, $\mathbb{T}_1 = E[e^{iuM_1^n}(1 - e^{2^{-1}(C_1^n - C_\infty)u^2})]$ and $\mathbb{T}_2 = E[(e^{iuM_1^n + 2^{-1}C_1^n u^2} - 1)e^{-2^{-1}C_\infty u^2}]$. If necessary, we replace M^n by a suitably stopped process to validate integrability of variables. By the convergence of C_1^n, the tangent $\mathbb{T}_1$ tends to 0. Moreover, the torsion $\mathbb{T}_2$ vanishes thanks to the martingale property of the exponential martingale since C_∞ is deterministic. Thus, $E[e^{iuM_1^n}] \to E[e^{-2^{-1}C_\infty u^2}] = e^{-2^{-1}C_\infty u^2}$, which proves (2.8).

For martingales with jumps, a uniformity condition such as the conditional type Lindeberg condition is necessary to obtain central limit theorems. Otherwise, processes with independent increments can appear as the limit.

2.4.2 Berry-Esseen Bounds

Berry-Esseen type bounds are in Bolthausen [24] and Häusler [38]. Rate of convergence in the central limit theorem for semi-martingales is in Liptser and Shiryaev [58, 60]. In other frames of dependent structures, error bounds are found in Bolthausen [23] for functionals of discrete Markov chains, Bentkus, Götze, and Tikhomirov [10] for statistics of β-mixing processes, Dasgupta [28] for nonuniform estimates for some stationary m-dependent processes, and Sunklodas [87] for a lower bound for the rate of convergence in the central limit theorem for m-dependent random fields.

2.4.3 Asymptotic Expansion of Martingales

Consider a sequence of random variables $(Z_n)_{n\in\mathbb{N}}$ having a stochastic expansion

$$Z_n = M_n + r_n N_n, \tag{2.10}$$

where for each $n \in \mathbb{N}$, M_n denotes the terminal random variable M_1^n of a continuous martingale $(M_t^n)_{t\in[0,1]}$ with $M_0^n = 0$, on a stochastic basis $\mathcal{B}^n = (\Omega^n, \mathcal{F}^n, \mathbb{F}^n, P^n)$, $\mathbb{F}^n = (\mathcal{F}_t^n)_{t\in[0,1]}$. The variable N_n is a random variable on $\mathcal{B}^n$ but no specific structure like adaptiveness is assumed, and (r_n) is a sequence of positive numbers tending to zero as $n \to \infty$. Suppose that $\langle M^n\rangle_1 \to^p 1$ as $n \to \infty$ for the quadratic variation $\langle M^n\rangle$ of M^n. Then the martingale central limit theorem (2.8) ensures the convergence $M_n \to^d N(0,1)$ as $n \to \infty$.

The effect of the tangent $\mathbb{T}_1$ appears in the asymptotic expansion of the law $\mathcal{L}\{Z_n\}$. We suppose that $(M_n, \xi_n, N_n) \to^d (Z, \xi, \eta)$ as $n \to \infty$ for $\xi_n = r_n^{-1}(\langle M^n\rangle_1 - 1)$. Define the density p_n by

$$p_n(z) = \phi(z) + \frac{1}{2} r_n \partial_z^2 (E[\xi|Z = z]\phi(z)) - r_n \partial_z (E[\eta|Z = z]\phi(z)), \tag{2.11}$$

where ϕ is the standard normal density. Furthermore, we assume that each $(\Omega^n, \mathcal{F}^n, P^n)$ is equipped with a Malliavin calculus and random variables are differentiable in Malliavin's sense. Then the derivatives in (2.11) exist, and for any $\alpha \in \mathbb{Z}_+$, $p > 1$ and $q > 2/3$, we obtain the estimate

$$\left| E[f(Z_n)] - \int f(z)p_n(z)dz \right| \leq C(\|f(Z_n)\|_{L^{p'}} + \|f\|_{L^1((1+|z|^2)^{-\alpha/2}dz)}) \times (r_n^{-q} P[\sigma_{M_n} < s_n]^{1/p} + \epsilon_n)$$

for any measurable function f satisfying $E[|f(Z_n)|] < \infty$ and $\int |f(x)|p_n(z)dz < \infty$, where σ_{M_n} is the Malliavin covariance of M_n, s_n are positive smooth functionals with complete non-degeneracy $\sup_{n\in\mathbb{N}} E[s_n^{-m}] < \infty$ for any $m > 1$, $p' = p/(p-1)$, $\epsilon_n = o(r_n)$, and C is a constant independent of f. Assumption of full non-degeneracy for σ_{M_n} is not realistic in statistical applications, nor necessary in asymptotic expansion.

The central limit theorem for the functional of the form $\int_0^T T^{-1/2} a_t dw_t$ for a random process a_t is indispensable to deduce asymptotic normality of the estimators in the likelihood analysis of the drift parameter of ergodic diffusion processes. Then it is natural to seek for asymptotic expansion for martingales to formulate higher-order statistical inference for diffusion processes. As a matter of fact, the martingale expansion went ahead of the mixing method, as for semimartingales. The second-order mean-unbiased maximum likelihood estimator $\hat{\theta}_T^*$ of the drift parameter θ of an ergodic diffusion process has the Edgeworth expansion

$$P\left[\sqrt{IT}(\hat{\theta}_T^* - \theta) \leq x\right] = \Phi(x) + \frac{\Gamma^{(-1/3)}}{2I^{3/2}\sqrt{T}}(x^2-1)\phi(x) + o\left(T^{-1/2}\right)$$

where I is the Fisher information at θ and Φ is the standard normal distribution function. $\Gamma^{(-1/3)}$ is the coefficient of the Aamari-Chentsov affine α-connection for $\alpha = -1/3$ [97].

See [97] for details of this subsection. A similar asymptotic expansion formula exits for general martingales M^n with jumps. In that case, we take $\xi_n = r_n^{-1}(\Xi_n - 1)$ with $\Xi_n = \frac{1}{3}[M^n] + \frac{2}{3}\langle M^n\rangle_1$. A Malliavin calculus on Wiener-Poisson space is used to quantify the non-degeneracy of M_n [98].

Mykland [68, 69, 70] provided asymptotic expansion of moments. The author was inspired by his pioneering work.

The mixing approach gives in general more efficient way to asymptotic expansion if one treats functionals of ϵ-Markov processes with mixing property like the above example. However, the martingale approach still has advantages of wide applicability. For example, an estimator of volatility in finite time horizon, non-Gaussianity appears in the higher-order term of the limit distribution even if the statistic is asymptotically normal. Such phenomena cannot be handled by mixing approach; however, the martingale expansion still gives asymptotic expansion.

2.5 Non-ergodic Statistics and Asymptotic Expansion

2.5.1 Non-central Limit of Estimators in Non-ergodic Statistics

The non-ergodic statistics features asymptotic mixed normality of estimators. Non-normality of the maximum likelihood estimators was observed quite many years ago: White [95], Anderson [4], Rao [81], Keiding [46, 47].

Extension of the classical asymptotic decision theory was required to formulate non-ergodic statistics: Basawa and Koul [7], Basawa and Prakasa Rao [8], Jeganathan [45], and Basawa and Scott [9]. From aspects of limit theorems, the notion of stable convergence is fundamental since the Fisher information is random even in the limit. The nesting condition with Rényi mixing is a standard argument there. In this trend, Feigin [31] proved stable convergence for semimartingales.

Statistical inference for high frequency data has been attracting attention since around 1990. Huge volume of literature is available today: Prakasa Rao [77, 78], Dacunha-Castelle and Florens-Zmirou [27], Florens-Zmirou [32], Yoshida [96, 100], Genon-Catalot and Jacod [33], Bibby and Soerensen [21], Kessler [48], Andersen and Bollerslev [2], Andersen et al. [3], Barndorff-Nielsen and Shephard [5, 6], Shimizu and Yoshida [85], Uchida [90], Ogihara and Yoshida [73, 74], Uchida and Yoshida [92, 93], and Masuda [62] among many others. Recently a great interest is in estimation of volatility. The scaled error of a volatility estimator admits a stable convergence to a mixed normal distribution, that is, typically for a volatility estimator $\hat{\theta}_n$, $\sqrt{n}(\hat{\theta}_n - \theta) \to^{d_s} \Gamma^{-1/2}\zeta$ where Γ is the random Fisher information and $\zeta \sim N(0,1)$ independent of Γ. It is possible to apply the martingale problem method as in Genon-Catalot and Jacod [33], Jacod [41], or convergence of stochastic integrals in Jakubowski et al. [44] and Kurtz and Protter [52] to obtain stable convergence.

2.5.2 Non-ergodic Statistics and Martingale Expansion

To go beyond the first order[1] asymptotic statistical theory, we need to develop asymptotic expansion of functionals. However, the potential (Doléans-Dade exponential^{-1}) that makes a local martingale from $\exp(uM_1^n)$ no longer has a deterministic limit, and this breaks a usual way to asymptotic expansion. In other words, the exponential martingale in $\mathbb{T}_2$ is not a martingale under the measure $E[\cdot e^{-C_\infty u^2/2}]/E[e^{-C_\infty u^2/2}]$, and the torsion of this shift on the martingale appears in the expansion.

We will consider a d-dimensional random variable Z_n that admits the stochastic expansion (2.10) on $(\Omega, \mathcal{F}, \mathbb{F}, P)$, $\mathbb{F} = (\mathcal{F}_t)_{t\in[0,1]}$. M^n is a d-dimensional continuous local martingale with $M_0^n = 0$, and N_n is a d-dimensional random variable. Let $C_t^n = \langle M^n \rangle_t$, $\mathbb{R}^{\mathsf{d}} \otimes \mathbb{R}^{\mathsf{d}}$-valued random matrix. A d_1-dimensional reference variable is denoted by F_n. For example, F_n is the Fisher information matrix. We shall present an expansion of the joint law $\mathcal{L}\{(Z_n, F_n)\}$.

The tangent vectors are given by $\overset{\circ}{C}_n = r_n^{-1}(C_1^n - C_1^\infty)$ and $\overset{\circ}{F}_n = r_n^{-1}(F_n - F_\infty)$. Suppose that $(M^n, N_n, \overset{\circ}{C}_n, \overset{\circ}{F}_n) \to^{d_s(\mathcal{F})} (M^\infty, N_\infty, \overset{\circ}{C}_\infty, \overset{\circ}{F}_\infty)$ and $M_t^\infty \sim N_{\mathsf{d}}(0, C_t^\infty)$. These limit variables are defined on the extension $(\bar{\Omega}, \bar{\mathcal{F}}, \bar{P}) = (\Omega \times \overset{\circ}{\Omega}, \mathcal{F} \times \overset{\circ}{\mathcal{F}}, P \times \overset{\circ}{P})$ of $(\Omega, \mathcal{F}, P)$. Let $\check{\mathcal{F}} = \mathcal{F} \vee \sigma[M_1^\infty]$. Random function $\tilde{C}_\infty(z) = \tilde{C}(\omega, z)$ is a matrix-valued random function satisfying $\tilde{C}(\omega, M_1^\infty) = E[\overset{\circ}{C}_\infty | \check{\mathcal{F}}]$. Similarly, let $\tilde{F}_\infty(\omega, M_1^\infty) = E[\overset{\circ}{F}_\infty | \check{\mathcal{F}}]$ and $\tilde{N}_\infty(\omega, M_1^\infty) = E[N_\infty | \check{\mathcal{F}}]$.

To make an expansion formula, we need two kinds of random symbols: the adaptive random symbol and the anticipative random symbol. The adaptive random symbol is defined by

$$\underline{\sigma}(z, iu, iv) = \frac{1}{2}\tilde{C}_\infty(z)[(iu)^{\otimes 2}] + \tilde{N}_\infty(z)[iu] + \tilde{F}_\infty(z)[iv]$$

for $u \in \mathbb{R}^{\mathsf{d}}$ and $v \in \mathbb{R}^{\mathsf{d}_1}$. Here the brackets mean a linear functional. This random symbol is corresponding to the correction term of the classical asymptotic expansion. Let $\Psi_\infty(u, v) = \exp\big(-\frac{1}{2}C_\infty[u^{\otimes 2}] + iF_\infty[v]\big)$, $C_\infty := C_1^\infty$ and let $L_t^n(u) = \exp\big(iM_t^n[u] + \frac{1}{2}C_t^n[u^{\otimes 2}]\big) - 1$. Then the anticipative random symbol $\overline{\sigma}(iu, iv) = \sum_j c_j (iu)^{m_j} (iv)^{n_j}$ (multi-index) is specified by

$$\lim_{n\to\infty} r_n^{-1} E[L_1^n(u)\Psi_\infty(u, v)\psi_n] = E[\Psi_\infty(u, v)\overline{\sigma}(iu, iv)], \tag{2.12}$$

where $\psi_n \sim 1$ is a truncation functional a suitable choice of which reflects the local non-degeneracy of (Z_n, F_n).

[1] The order of the central limit theorem is referred to as the first order in asymptotic decision theory, differently from the numbering of terms in asymptotic expansion.

For the full random symbol $\sigma = \underline{\sigma} + \overline{\sigma}$, the asymptotic expansion formula is defined by

$$p_n(z,x) = E[\phi(z;0,C_\infty)\delta_x(F_\infty)] + r_n E[\sigma(z,\partial_z,\partial_x)^*\{\phi(z;0,C_\infty)\delta_x(F_\infty)\}],$$

where $\phi(z;0,C)$ is the normal density with mean 0 and covariance matrix C, and $\delta_x(F_\infty)$ is Watanabe's delta function; cf. Watanabe [94], Ikeda and Watanabe [40]. The adjoint $\sigma(z,\partial_z,\partial_x)^*$ is naturally defined as $\overline{\sigma}(z,\partial_z,\partial_x)^*\{\phi(z;0,C_\infty)\delta_x(F_\infty)\} = \sum_j(-\partial_z)^{m_j}(-\partial_x)^{n_j}$ $s\{c_j\phi(z;0,C_\infty)\delta_x(F_\infty)\}$ and similarly for $\underline{\sigma}$. The density formula gives a concrete expression since $E[\psi\delta_x(F)] = E[\psi|F=x]p^F(x)$ for functionals ψ and F.

Under certain non-degeneracy conditions, for any positive numbers B and γ,

$$\sup_{f\in\mathcal{E}(B,\gamma)}\left|E[f(Z_n,F_n)] - \int_{\mathbb{R}^{\mathsf{d}+\mathsf{d}_1}} f(z,x)p_n(z,x)dzdx\right| = o(r_n) \tag{2.13}$$

as $n\to\infty$, where $\mathcal{E}(B,\gamma)$ is the set of measurable functions $f:\mathbb{R}^{\mathsf{d}+\mathsf{d}_1}\to\mathbb{R}$ satisfying $|f(z,x)|\le B(1+|z|+|x|)^\gamma$ for all $(z,x)\in\mathbb{R}^{\mathsf{d}}\times\mathbb{R}^{\mathsf{d}_1}$. Details are given in [102].

The martingale expansion (2.13) was applied to the realized volatility in [101]. The martingale part M^n is a sum of double Skorokhod integrals. The anticipative random symbol $\overline{\sigma}$ specified by the integration-by-parts formula at (2.12) has expression involving the Malliavin derivatives. Recently Podolskij and Yoshida [76] obtained expansions for p-variations. Construction of higher order statistical inference is a theme of the non-ergodic statistics today.

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Chapter 3
An Introduction to Normal Approximation

Qi-Man Shao

3.1 Introduction

Normal approximation or, more generally the asymptotic theory, plays a fundamental role in the developments of modern probability and statistics. The one-dimensional central limit theorem and the Edgeworth expansion for independent real-valued random variables are well studied. We refer to the classical book by Petrov (1995). In the context of the multi-dimensional central limit theorem, Rabi Bhattacharya has made fundamental contributions to asymptotic expansions. The book by Bhattacharya and Ranga Rao (1976) is a standard reference. In this note I shall focus on two of his seminal papers (1975, 1977) on asymptotic expansions. Recent developments on normal approximation by Stein's method and strong Gaussian approximation will also be discussed.

3.2 Asymptotic Expansions

Let $\{X_n = (X_{n,1}, \cdots, X_{n,k}), n \geq 1\}$ be a sequence of independent and identically distributed (i.i.d.) random vectors with values in $\mathbb{R}^k$ and common distribution Q_1. Assume that

$$E(X_1) = 0, \ \ \mathrm{Cov} X_1 = I,$$

where I is the $k \times k$ identity matrix. Let $v = (v_1, \cdots, v_k)$ denote a multi-index and write

$$|v| = v_1 + \cdots + v_k, \ \ v! = v_1! v_2! \cdots v_k!, \ \ x^v = (x_1^{v_1}, \cdots, x_k^{v_k}) \ \text{ for } x = (x_1, \cdots, x_k) \in \mathbb{R}^k.$$

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For a positive integer s, the sth absolute moment of X_1 is

$$\rho_s = E\|X_1\|^s,$$

where $\|\cdot\|$ is the Euclidean norm. Let $\hat{Q}_1(t) = E\exp(i\langle t, X_1\rangle)$ be the characteristic function of X_1. The vth cumulant of X_1 is

$$\chi_v = i^{-|v|}(D^v \log \hat{Q}_1)(0),$$

provided $\rho_{|v|} < \infty$. Here D^v is the vth derivative, i.e.,

$$D^v = D_1^{v_1} \cdots D_k^{v_k},$$

where D_j denotes differentiation with respect to the jth coordinate variable. The Taylor expansion gives

$$\log \hat{Q}_1(t) = \sum_{2\le|v|\le s} \frac{\chi_v}{v!}(it)^v + o(\|t\|^s).$$

Let

$$\chi_r(it) = r! \sum_{|v|=r} \frac{\chi_v}{v!}(it)^v$$

and

$$\tilde{P}_r(it) = \sum_{m=1}^{r} \frac{1}{m!}\Big\{\sum{}^{*} \frac{\chi_{j_1+2}(it)}{(j_1+2)!}\frac{\chi_{j_2+2}(it)}{(j_2+2)!}\cdots\frac{\chi_{j_m+2}(it)}{(j_m+2)!}\Big\}$$

where the summation $\sum^*$ is over all m-tuples of positive integers $(j_1, \cdots, j_m)$ satisfying $\sum_{l=1}^m j_l = r$. Let

$$P_r(-\phi)(x) = \tilde{P}_r(-D)\phi(x)$$

where ϕ is the standard normal density and $\tilde{P}_r(-D)$ is the differential operator obtained by formally replacing $(it)^v$ by $(-D)^v = (-1)^{|v|}D^v$ in the polynomial expression for $\tilde{P}_r(it)$. For example,

$$\begin{aligned} P_1(-\phi)(x) = &-\frac{1}{6}\sum_{l=1}^{k} E(X_{1,l}^3)(3x_l - x_l^8) \\ &-\frac{1}{2}\sum_{1\le l\ne m\le k} E(X_{1,l}^2 X_{1,m})(x_m - x_m x_l^2) \\ &+\sum_{1\le l<m<j\le k} E(X_{1,l}X_{1,m}X_{1,j})x_l x_m x_j. \end{aligned}$$

Let Q_n denote the distribution of $n^{-1/2}(X_1 + \cdots + X_n)$. Theorem 1.2 in Bhattacharya (1977) gives the expansion for the density of Q_n.

Theorem 1. *Assume $\rho_s < \infty$ for some integer $s \geq 2$. In order for the distribution Q_n to have a density q_n satisfying*

$$\sup_{x \in \mathbb{R}^k} |x^\nu (q_n(x) - \phi(x) - \sum_{r=1}^{s-2} n^{-r/2} P_r(-\phi)(x))| = o(n^{-(s-2)/2}), \quad 0 \leq |\nu| \leq s, \tag{3.1}$$

for sufficiently large n, it is necessary and sufficient for Q_1^{*m} to have a bounded density for some positive integer m.

This is followed by an Edgeworth type expansion, see Theorem 1.5 in [4].

Theorem 2. *If $\rho_s < \infty$ for some integers $s \geq 3$ and $\hat{Q}_1$ satisfies Cramér's condition*

$$\limsup_{\|t\| \to \infty} |\hat{Q}_1(t)| < 1,$$

then for every real-valued, bounded, Borel measurable function f on $\mathbb{R}^k$ one has

$$|\int_{\mathbb{R}^k} f d[Q_n - \Phi - \sum_{r=1}^{s-2} n^{-r/2} P_r(-\Phi)]| \leq \frac{\delta_n}{n^{(s-2)/2}} \omega_f(\mathbb{R}^k) + \tilde{\omega}_f(e^{-dn}, \Phi), \tag{3.2}$$

where $P_r(-\Phi)$ is the signed measure having density $P_r(-\phi)$, $\delta_n \to 0$ as $n \to \infty$, d is a positive constant, and the quantities δ_n and d do not depend on f, $\omega_f(\mathbb{R}^k) = \sup\{|f(y) - f(z)| : \; y, z \in \mathbb{R}^k\}$, and

$$\tilde{\omega}_f(\varepsilon, \Phi) = \int_{\mathbb{R}^k} \omega_f(x, \varepsilon) \Phi(dx), \quad \omega_f(x, \varepsilon) = \sup\{|f(y) - f(z)| : \; y, z \in B(x, \varepsilon)\}.$$

A Berry-Essen type bound is also available assuming the Cramér condition; see Theorem 1.7 in [4] and Sweeting (1997).

Theorem 3. *If $\rho_3 < \infty$, then for every real-valued, bounded, Borel measurable function f on $\mathbb{R}^k$ one has*

$$|\int_{\mathbb{R}^k} f(d(Q_n - \Phi)| \leq c_{1,k}\{\omega_f(\mathbb{R}^k)\rho_3 n^{-1/2} + \tilde{\omega}_f(\varepsilon_n, \Phi)\}, \tag{3.3}$$

where $\varepsilon_n = c\rho_3 n^{-1/2}$ and $c_{1,k}$ is a constant depending only on k.

Letting f in (3.3) be the indicator function of a convex set yields for any convex set A

$$|Q_n(A) - \Phi(A)| \leq c_{2,k} \rho_3 n^{-1/2}. \tag{3.4}$$

As proved in Bentkus (2003), $c_{2,k} \leq 400k^{1/2}$.

Bhattacharya (1975) obtains a similar result as (3.3) for unbounded functions f and for independent not necessary identically distributed random vectors. In particular, for i.i.d. random vectors $X_n, n \geq 1$ in $\mathbb{R}^k$, he proved the following theorem.

Theorem 4. *Assume*

$$\rho_s < n^{(s-2)/2}/(8k)$$

for some integer $s \geq 3$. *Let* r *be a nonnegative integer,* $0 \leq r \leq s$, *and define* $r_0 = r$ *if* r *is even, and* $r_0 = r + 1$ *if* r *is odd. Then there exist constants* $c_i, 1 \leq i \leq 2$ *depending only on* k, r, s *such that the inequalities*

$$\begin{aligned} &|\int_{\mathbb{R}^k} f d(Q_n - \Phi)| \\ &\leq c_1 M_r(f) \max_{3\leq m\leq s} \rho_m n^{-(m-2)/2} + c_1 \tilde{\omega}_g(c_2 \rho_3 n^{-1/2}, \Phi_{r_0}). \end{aligned} \tag{3.5}$$

A direct consequence of (3.5) is a nonuniform Berry-Esseen type bound for the multi-dimensional central limit theorem.

The results of Theorems 2 and 3 have been extended to general independent random vectors by Sweeting (1980).

For a statistic that can be expressed as $W_n = H(\bar{X})$, where $\bar{X} = \frac{1}{n}\sum_{j=1}^{n} X_j$ is a mean of i.i.d. vectors in $\mathbb{R}^k$ and H is a smooth function in a neighborhood of $\mu = EX_1$, Bhattacharya and Ghosh (1988) give a (3.2) type Edgeworth expansion with an error $o(n^{-(s-2)/2})$. Götze and Hipp (1983) had previously obtained a useful asymptotic expansion for dependent sequences.

3.3 Normal Approximation by Stein's Method

The results presented in the previous section are mainly proved through the Fourier transform or characteristic functions. It was Stein (1972) who introduced a completely different method to determine the accuracy of the normal approximation. The method works for both independent and dependent random variables, for normal approximation and also for non-normal approximation. The method has been successfully applied to study the absolute error of approximations and the relative error as well. Using Stein's method, Chen and Shao (2001, 2004) proved the uniform and nonuniform Berry-Esseen bounds for independent as well as locally dependent random variables; Chen, Fang, and Shao (2013) obtained Cramér type moderate deviation theorems for random variables satisfying a general Stein's identity. We refer to Chen, Goldstein, and Shao (2011) for a thorough coverage of the fundamental methods, as well as recent developments in both theory and applications. We also refer to Chatterjee (2014) for "a short survey of Stein's method."

For the one-dimensional case, let W_n be the random variable of interest. One wants to prove that W_n can be approximated by a standard normal random variable Z. More specifically, for a given Borel measurable function h, one wants to estimate

$$Eh(W_n) - Eh(Z).$$

Letting $f = f_h$ be the solution to the following Stein's equation:

$$f'(w) - wf(w) = h(w) - Eh(Z),$$

one has

$$Eh(W_n) - Eh(Z) = Ef'(W_n) - EW_n f(W_n).$$

A key idea of Stein's method is to express $EW_n f(W_n)$ as close as possible to $Ef'(W_n)$.

Stein's method has also been extended to multivariate normal approximation for both smooth and non-smooth functions although the problem is much more challenging for non-smooth functions, see, e.g., Götze (1991), Chatterjee and Meckes (2008), and Reinert and Röllin (2009). Götze (1991) used Stein's method to provide an ingenious derivation of the Berry-Esseen type bound (3.4) with $c_{2,k} = O(k)$. Bhattacharya and Holmes (2010) provided a more readable account of Götze's result than given in his original work with $c_{2,k} = O(k^{3/2})$. Chen and Fang (2011) recently also recovered (3.4) with the constant $c_{2,k}$ of order of $k^{1/2}$ by developing a concentration inequality in $\mathbb{R}^k$. It would be interesting to see if the constant $c_{2,k}$ can be reduced to an order of $k^{1/4}$, as proved by Bentkus (2003).

It is also noted that the results proved by Stein's method are mainly the first order approximation. It is unclear whether Stein's method can be used to prove an Edgeworth expansion such as (3.2). If one can establish the expansion for independent random vectors, then one may also be able to obtain similar results for dependent random vectors.

3.4 Strong Gaussian Approximation

Let $X_n, n \geq 1$ be a sequence of independent random vectors in $\mathbb{R}^k$ with $EX_i = 0$ and covariance matrix $\mathrm{Cov}(X_i)$, and let $Y_n, n \geq 1$ be a sequence of independent **Gaussian** random vectors with $EY_i = 0$ and covariance matrix $\mathrm{Cov}(Y_i) = \mathrm{Cov}(X_i)$. Set

$$S_n = \sum_{i=1}^{n} X_i, \quad T_n = \sum_{i=1}^{n} Y_i.$$

The central limit theorem as well as Edgeworth expansion provides the distribution approximation between S_n and T_n. It is well known that S_n cannot be approximated by T_n in probability on the original probability space; however, the strong Gaussian approximation gives a completely new aspect. One can construct a new probability space and define a new sequence of independent random vectors $\{\tilde{X}_n, n \geq 1\}$ and a sequence of independent Gaussian random vectors $\{Y_n, n \geq 1\}$ such that

$$\tilde{X}_n \overset{d.}{=} X_n, \quad \tilde{Y}_n \overset{d.}{=} Y_n$$

and

$$\|\sum_{i=1}^{n} \tilde{X}_i - \sum_{i=1}^{n} \tilde{Y}_i\| = o(a_n) \ \ a.s. \tag{3.1}$$

where a_n tends to infinity but as slow as possible. For the sake of simplicity, the strong approximation result (3.1) will be stated as follows: *There is a construction such that*

$$\|S_n - T_n\| = o(a_n) \ \ a.s.$$

Let

$$\Delta_n(X, Y) = \max_{1\le j\le n} \|S_i - T_i\|.$$

When $k = 1$, the strong approximation theory has been well developed. Well-known results include KMT (1975, 1976)'s strong approximation theorem and the following theorem of Sakhanenko:

Theorem 5. *Let $X_n, n \ge 1$ be independent real-valued random variables with $EX_n = 0$ and $E|X_n|^p < \infty$ for $p > 2$. Then there is a construction such that*

$$E\Delta_n(X, Y)^p \le Cp^{2p} \sum_{i=1}^{n} E|X_i|^p,$$

where C is an absolute constant.

For the multi-dimensional case, Zaitsev (2007) gives a similar result as Theorem 5. For bounded random variables, Zaitsev (1987) obtained the following result.

Theorem 6. *Assume that $\|X_i\| \le M$. Then there is a construction such that for $x > 0$*

$$P(\Delta_n(X, Y) \ge x) \le c_{1,k} \exp(-c_{2,k}x/M).$$

where $c_{1,k}$ and $c_{2,k}$ are positive constants depending only on k.

A weaker result, but with a more precise convergence rate, has been established in Lin and Liu (2009). Let N be a centered normal random vector with covariance matrix I_k. Let $|\cdot|$ denote the spectral norm for a matrix and $|\cdot|_k$ denote $|z|_k = \min\{|z_1|, \ldots, |z_k|\}$ for $z = (z_1, \ldots, z_k) \in \mathbb{R}^k$.

Theorem 7. *Assume that $\|X_i\| \le c_n B_n^{1/2}$, $1 \le i \le n$, for some $c_n \to 0$ and $B_n \to \infty$ and that*

$$\left|B_n^{-1} Cov(S_n) - I_k\right| \le b_n \tag{3.2}$$

for some $1 \ge b_n \to 0$. Suppose that $\beta_n := B_n^{-3/2} \sum_{i=1}^{n} E\|X_i\|^3 \le a_n$ for some $a_n \to 0$. Let $d_n > 0$ be any sequence satisfying $d_n^2/|\beta_n^2 \log\beta_n| \to \infty$. Then, there exists a number n_0 determined by the sequences $\{a_n, b_n, c_{n1}, d_n\}$ such that for all $n \ge n_0$,

$$|P(|S_n|_k \ge x) - P(|N|_k \ge xB_n^{-1/2})| \le A_{n1}P(|N|_k \ge x/B_n^{1/2}) + A_{n2}$$

for all $0 \le x \le c_{1,k} \min\{c_n^{-1}, d_n^{-1}, \beta_n^{-1/3}\}B_n^{1/2}$, where

$$\begin{aligned} A_{n1} &= c_{2,k}(\beta_n t_n^3 + d_n(1 + x/\sqrt{B_n})), \\ A_{n2} &= 7\exp\Big(-c_{3,k}t_n^2\Big) + 3\exp\Big(\frac{c_{3,k}d_n^2}{\beta_n^2 \log\beta_n}\Big) \\ &\quad +3\exp\Big(-c_{3,k}c_n^{-1}b_n^{-1}d_n\Big) + 3\exp\Big(-c_{3,k}b_n^{-2}d_n^2\Big), \end{aligned}$$

$c_{1,k}$, $c_{2,k}$ and $c_{3,k}$ are positive constants depending only on k, and t_n is any positive number satisfying $4x/B_n^{1/2} + 1 \le t_n \le \min\{c_n^{-1}, \beta_n^{-1/3}\}$.

Theorems 6 and 7 have been applied to derive various asymptotic results. For example, Liu and Shao (2013) establish a Cramér type moderate deviation theorem for Hotelling's T^2 statistics.

There has been an increasing interest in the case of k tending to infinity along with n. Write

$$S_n = (S_{n,1}, \cdots, S_k) \quad \text{and} \quad T_n = (T_{n,1}, \cdots, T_{n,k}).$$

Chernozhukov, Chetverikov, and Kato (2014) prove that

Theorem 8. *There is a construction such that*

$$\begin{aligned} &P(|\max_{1\le i\le k} S_{n,i} - \max_{1\le i\le k} T_{n,i}| \ge x) \\ &\le C(x^{-2}B_1 + x^{-3}B_2 \log(kn)) \log(kn) + Cn^{-1}\log n, \end{aligned} \tag{3.3}$$

where $C > 0$ is an absolute constant and

$$B_1 = E \max_{1\le j,l\le k} \Big| \sum_{i=1}^n \{X_{ij}X_{il} - E(X_{ij}X_{il})\} \Big|,$$

$$B_2 = E \max_{1\le j\le k} \sum_{i=1}^n |X_{ij}|^3 + \sum_{i=1}^n E \max_{1\le j\le k} |X_{i,j}|^3 I\{\max_{1\le j\le k} |X_{i,j}| \ge x/(\log(kn)\}.$$

Other related results can be found in Chernozhukov, Chetverikov, and Kato (2013). It would be interesting to improve their results.

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Chapter 4
Reprints: Part I

R.N. Bhattacharya and Coauthors

Berry-Essen bounds for the multi-dimensional central limit theorem. Bull. Amer. Math. Society. 74 (1968), 285–287. © 1968 American Mathematical Society.

Rates of weak convergence and asymptotic expansions for classical central limit theorems. The Annals of Mathematical Statistics. 42 (1971), 241–259. ©1971 Institute of Mathematical Statistics.

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4.1 "Berry-Essen bounds for the multi-dimensional central limit theorem"

Berry-Essen bounds for the multi-dimensional central limit theorem. Bull. Amer. Math. Society. 74 (1968), 285–287.

BERRY-ESSEEN BOUNDS FOR THE MULTI-DIMENSIONAL CENTRAL LIMIT THEOREM[1]

BY R. N. BHATTACHARYA

Communicated by P. R. Halmos, September 21, 1967

1. Introduction. Let $\{X_n\}$ be a sequence of independent and identically distributed random variables each with mean zero, variance unity, and finite absolute third moment β_3. Let F_n denote the distribution function of $(X_1+\cdots+X_n)/(n)^{1/2}$. Berry [2] and Esseen [4] have proved that

$$(1)\quad \sup_{x\in R_1} \left| F_n(x) - \frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{x} e^{-y^2/2}dy \right| \leqq c\beta_3/n^{1/2}, \qquad n = 1, 2, \cdots,$$

where c is a universal constant. Consider now a sequence $\{X(n) = (X_1^{(n)}, \cdots, X_k^{(n)})\}$ of independent and identically distributed random vectors in R_k each with mean vector $(0, \cdots, 0)$ and covariance matrix I, the $k\times k$ identity matrix. If P_n denotes the probability distribution of $(X^{(1)}+\cdots+X^{(n)})/n^{1/2}$ and Φ is the standard k-dimensional normal distribution, then it is well known that P_n converges weakly to Φ as $n\to\infty$. Bergström [1] has extended (1) to this case, assuming finiteness of absolute third moments of the components of $X^{(1)}$. Since weak convergence of a sequence Q_n of probability measures to Φ means that $Q_n(B)\to\Phi(B)$ for every Borel set B satisfying $\Phi(\partial B)=0$, ∂B being the boundary of B, it seems natural to seek bounds of $|P_n(B)-\Phi(B)|$ for such sets B (called *Φ-continuity sets*). Let $\mathfrak{A}$ be a class of Borel sets such that, whatever be the sequence Q_n converging weakly to Φ, $Q_n(B)\to\Phi(B)$ as $n\to\infty$ uniformly for all $B\in\mathfrak{A}$. Such a class is called a *Φ-uniformity* class. By a theorem of Billingsley and Topsoe [3], a class $\mathfrak{A}$ is a Φ-uniformity class if and only if $\sup\{\Phi(\partial B)^\epsilon; B\in\mathfrak{A}\}\downarrow 0$ as $\epsilon\downarrow 0$, where $(\partial B)^\epsilon$ is the ϵ-neighborhood of ∂B. This leads one naturally to consider the class $\mathfrak{A}_1(d, \epsilon_0)$ of all Borel sets B for which $\Phi(\partial B)^\epsilon \leqq d\epsilon$ for $0<\epsilon<\epsilon_0$, d and ϵ_0 being any two given positive constants. One may also consider the class $\mathfrak{A}_1^*(d, \epsilon_0)$, which is the largest translation-invariant subclass of $\mathfrak{A}_1(d, \epsilon_0)$; this means that $B\in\mathfrak{A}_1^*(d, \epsilon_0)$ if and only if all translates of B belong to $\mathfrak{A}_1(d, \epsilon_0)$.

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2. **Results**. We shall write $\beta_s = \sum_{i=1}^k E|X_i^{(1)}|^s$ for $s>0$. Also c's will denote constants. For example, $c_1(k, \delta)$, $c_2(k)$, and c_4 will stand for a constant depending only on k and δ, a constant depending on k alone, and a universal constant, respectively.

THEOREM 1. *Suppose* $\beta_{3+\delta} < \infty$ *for some* $\delta > 0$. *Then, for all* n,

$$\sup |P_n(B) - \Phi(B)| \leqq n^{-1/2}\{c_1(k, \delta)\beta_{3+\delta}^{3(1+\delta)/(3+\delta)} + [c_2(k)d + c_3(k)/\epsilon_0]\beta_{3+\delta}^{3/(3+\delta)}\},$$

where the supremum extends over all B *in* $\mathcal{A}_1^*(d, \epsilon_0)$.

We shall state two applications of Theorem 1.

EXAMPLE 1. Let $\mathcal{C}$ be the class of all measurable convex sets in R_k. It follows from certain results of Ranga Rao [5] that $\mathcal{C} \subset \mathcal{A}_1^*(d(k), \epsilon_0)$ for every $\epsilon_0 > 0$, $d(k)$ being an appropriate constant depending on k. Hence

$$\sup_{C \in \mathcal{C}} |P_n(C) - \Phi(C)| \leqq n^{-1/2}\{c_1(k, \delta)\beta_{3+\delta}^{3(1+\delta)/(3+\delta)} + c_2(k)d(k)\beta_{3+\delta}^{3/(3+\delta)}\}$$

for all n. This is an improvement on a result of Ranga Rao [6].

EXAMPLE 2. Let $\mathcal{F}(l)$ be the class of all measurable sets in R_2 each of whose boundaries is contained in a rectifiable curve of length not exceeding l. It may be shown (cf. [3]) that $\mathcal{F}(l) \subset \mathcal{A}_1^*(4\pi l + 8\pi, 1)$. Hence Theorem 1 applies. In fact, in this case it suffices to assume that $\beta_3 < \infty$, so that we have

$$\sup_{F \in \mathcal{F}(l)} |P_n(F) - \Phi(F)| \leqq n^{-1/2}\{(c_4 l^2 + c_5 l + c_6)\beta_3\}, \quad n = 1, 2, \cdots.$$

THEOREM 2. *Suppose* $\beta_{3+\delta} < \infty$ *for some* $\delta > 0$. *Then, for all* n,

$$\sup |P_n(B) - \Phi(B)| \leqq n^{-1/2}\{c_7(k, \delta)\beta_{3+\delta}^{6/(3+\delta)} + c_8(k)[d + 1/\epsilon_0]\beta_{3+\delta}^{3/(3+\delta)} \log(n+1)\},$$

where the supremum extends over all B *in* $\mathcal{A}_1(d, \epsilon_0)$.

The methods used in proving Theorems 1 and 2 enable one to obtain bounds for general Φ-uniformity classes, and, in particular, for any Φ-continuity set.

An asymptotic expansion holds for the class $\mathcal{A}_1(d, \epsilon_0)$ under the assumption that

$$\limsup_{|t| \to \infty} |f(t)| < 1,$$

where f is the characteristic function of $X^{(1)}$. If $\beta_s < \infty$ for some integer $s \geqq 3$, then $P_n(B)$ may be estimated by this expansion with an error $O(n^{-(s-2)/2} \cdot [\log n]^{k/2})$ uniformly for all $B \in \mathcal{A}_1(d, \epsilon_0)$.

EXTENSIONS. Theorems 1 and 2 may be extended to the following cases: (1) $\{X^{(n)}\}$ is not identically distributed, but $\sup_n \sum_{i=1}^k E|X_i^{(n)}|^{3+\delta} < \infty$ for some $\delta > 0$; (2) $\{X^{(n)}\}$ has a common nonsingular covariance matrix perhaps different from I.

In proving Theorem 1 we look at the convolution $(P_n - \Phi)^* \Gamma_n$, where Γ_n is a probability measure having a characteristic function which vanishes everywhere outside a sphere, and Γ_n converges weakly to the probability measure degenerate at $(0, \cdots, 0)$. Theorem 2 is obtained by sharpening a technique of Esseen [4] and Ranga Rao [5].

The details and proofs of these results, which are part of the author's doctoral dissertation, submitted to the University of Chicago, will appear elsewhere.

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4.2 "Rates of weak convergence and asymptotic expansions for classical central limit theorems"

Rates of weak convergence and asymptotic expansions for classical central limit theorems. The Annals of Mathematical Statistics. 42 (1971), 241–259.

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RATES OF WEAK CONVERGENCE AND ASYMPTOTIC EXPANSIONS FOR CLASSICAL CENTRAL LIMIT THEOREMS[1]

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0. Introduction and summary. Let $Q_n(n = 1, 2, \cdots)$, Q be probability measures on the Borel σ-field of R^k. The sequence $\{Q_n\}$ *converges weakly* to Q if for every real-valued, bounded, almost surely (Q) continuous function g on R^k the convergence

$$\lim_n \int g\, dQ_n = \int g\, dQ \tag{0.1}$$

holds (cf. [9], Chapter 1). Such functions g are called *Q-continuous*. If the indicator function I_A of the set A is Q-continuous, then A is also called *Q-continuous*. If $\mathscr{F}$ is a class of Q-continuous functions g over which the convergence (0.1) is uniform for every sequence $\{Q_n\}$ converging weakly to Q, then $\mathscr{F}$ is called a *Q-uniformity class*. A class of sets is called a *Q-uniformity class* if the indicator functions of the sets of this class form a Q-uniformity class of functions. A systematic study of Q-uniformity (in separable metric spaces) was initiated by Ranga Rao [21], who obtained a number of nice results. His studies were carried further in a very useful manner by Billingsley and Topsøe [10].

In this article the error of normal approximation $|\int g\, d(Q_n - \Phi)|$ is estimated for arbitrary Φ-continuous g, Φ being the k-dimensional standard normal distribution and Q_n the distribution of the appropriately normalised nth partial sum of a sequence of independent k-dimensional random vectors $\{X^{(r)}; r = 1, 2, \cdots\}$. The classical central limit theorems assert weak convergence of $\{Q_n\}$ to Φ under certain moment conditions. It is shown here (Theorem 1, Section 3) that for an arbitrary real-valued, bounded, measurable g on R^k one has

$$\left|\int g\, d(Q_n - \Phi)\right| \leqq c(k, \delta)\omega_g(R^k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)} n^{-\frac{1}{2}} + \int \omega_g(S(x, \varepsilon_n))\, d\Phi(x), \tag{0.2}$$

where δ is any positive number; $\rho_{3+\delta,n}$ is defined by (1.4), and

$$\omega_g(A) = \sup\{|g(x) - g(y)|; x, y \in A\}, S(x, \varepsilon) = \{y; |x - y| < \varepsilon\}, \tag{0.3}$$
$$\varepsilon_n = c(k)\rho_{3+\delta,n}^{3/(3+\delta)} n^{-\frac{1}{2}} \log n,$$

$c(k)$, $c(k, \delta)$ being positive constants depending only on their respective arguments. If ε_n goes to zero as n goes to infinity, then the right side of (0.2) goes to zero for every Φ-continuous g. For the rest of this section let us assume that $\{\rho_{3+\delta,n}\}$ is bounded. By (0.2), if $\int \omega_g(S(x, \varepsilon))\, d\Phi(x) = O(\varepsilon)$ as ε goes to zero, then the error of approximation is $O(n^{-\frac{1}{2}} \log n)$. One may also use (0.2) to obtain uniform upper

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bounds for errors of approximation over arbitrary Φ-uniformity classes. In particular,

$$(0.4) \qquad \sup\{|\int g\, d(Q_n-\Phi)|;\, g\in \mathscr{F}_1(\Phi; c, d, \varepsilon_0)\} = O(n^{-\frac{1}{2}}\log n),$$

where

$$(0.5) \quad \mathscr{F}_1(\Phi; c, d, \varepsilon_0) = \{g; \omega_g(R^k) \leqq c,\ \int\omega_g(S(\cdot,\varepsilon))\, d\Phi \leqq \varepsilon \text{ for } 0<\varepsilon \leqq \varepsilon_0\},$$

c, d, ε_0 being arbitrary positive constants. For the largest translation-invariant subclass of this class a sharper bound $O(n^{-\frac{1}{2}})$, which is best possible, was obtained in [3]; [5], (cf. [4]). A similar result (in the i.i.d. case) has been independently obtained by Von Bahr [22]. As applications one obtains precise bounds for many interesting classes of sets and functions. However, there are Φ-continuous functions and Φ-uniformity classes of functions for which the technique used in [5] or [22] is not effective. An example in Section 3 shows that there are Borel sets A such that the upper bound for $|Q_n(A)-\Phi(A)|$ as provided by [5] (Theorem 1) is $O(1)$, while (0.2) provides the bound $O(n^{-\frac{1}{2}}\log n)$. A modification of the bound (0.2) when applied to $g = I_A$ for an arbitrary Borel set A enables one to show that the Prokhorov distance between Q_n and Φ is $O(n^{-\frac{1}{2}}\log n)$. It is not known whether the factor $\log n$ in the expression for ε_n in (0.3) (and, hence, in (0.4) and in the estimate of Prokhorov's distance) may be dispensed with or not. However, under Cramér's condition (3.42) $\log n$ may be replaced by one.

The remaining theorems are proved for the i.i.d. case, partly for the sake of simplicity and partly because of the non-availability in the existing literature of complete proofs for some of the expansions related to the characteristic function of Q_n in the non-identically distributed case. Theorem 2 provides an asymptotic expansion for $\int g\, dQ_n$ with a remainder term which is $o(n^{-(s-2)/2})$ uniformly over all g in $\mathscr{F}_1{}^*(\Phi; c, d, \varepsilon_0)$, the largest translation-invariant subclass of $\mathscr{F}_1(\Phi; c, d, \varepsilon_0)$, when $E|X^{(1)}|^s < \infty$ for some integer s not smaller than three and the characteristic function of $X^{(1)}$ obeys Cramér's condition (3.42)′. Applications to the class $\mathscr{C}$ of all measurable convex sets, the class $L(c, d)$ (see (3.54)) of bounded Lipschitzian functions, etc., are immediate. Theorem 3 gives an asymptotic expansion for $\int g\, dQ_n$ for a very special class of functions g when no restriction like (3.42)′ is imposed. Theorem 4 provides some classes of functions g (under varying restrictions on the distribution of $X^{(1)}$) for which the error of approximation $|\int g\, d(Q_n-\Phi)|$ is of the order $O(n^{-1})$.

Section 1 introduces notation to be used throughout the article. Section 2 provides basic lemmas for proving the results (outlined above) of Section 3.

1. Notation. All probability measures here are defined over the Borel σ-field $\mathscr{B}^k$, unless otherwise specified. Let $\{X^{(r)} = (X_1{}^{(r)}, \cdots, X_k{}^{(r)});\, r = 1, 2, \cdots\}$ be a sequence of independent random vectors in R^k, the rth vector $X^{(r)}$ having distribution $Q^{(r)}$ and characteristic function $f^{(r)}$. It will be assumed that

$$(1.1) \qquad E(X_i{}^{(r)}) = 0, \qquad i = 1, \cdots, k; \quad r = 1, 2, \cdots,$$

$$\operatorname{Cov} X^{(r)} = D^{(r)}, \qquad r = 1, 2, \cdots,$$

$D^{(r)}$ being a positive definite covariance matrix. The same symbol will be used for a linear operator on R^k and its matrix relative to the standard Euclidean basis. Thus Bx denotes the image of x under the map B. Let B_n, B_n' denote a non-singular matrix and its transpose, respectively, such that

$$B_n'B_n = n(\textstyle\sum_{r=1}^n D^{(r)})^{-1}. \tag{1.2}$$

Let

$$Y_n = n^{-\frac{1}{2}}B_n \textstyle\sum_{r=1}^n X^{(r)}; \qquad Q_n(A) = \text{Probability}\,(Y_n \in A), \qquad A \in \mathscr{B}^k; \tag{1.3}$$

$$f_n(t) = \textstyle\prod_{r=1}^n f^{(r)}(n^{-\frac{1}{2}}B_n't), \qquad t \in R^k.$$

Thus Q_n is the distribution of Y_n and f_n its characteristic function. The covariance matrix of Y_n is, by (1.2), the identity matrix. We write

$$\begin{aligned} &\mu_s^{(r)} = \textstyle\sum_{j=1}^k E(X_j^{(r)})^s, && \mu_{s,n} = (\textstyle\sum_{r=1}^n \mu_s^{(r)})/n, \\ &\beta_s^{(r)} = \textstyle\sum_{j=1}^k E\,|X_j^{(r)}|^s, && \beta_{s,n} = (\textstyle\sum_{r=1}^n \beta_s^{(r)})/n, \\ &\rho_{s,n} = (\textstyle\sum_{r=1}^n E\,|B_n X^{(r)}|^s)/n, && \lambda_{s,n}(u) = (\textstyle\sum_{r=1}^n \lambda_s^{(r)}(u))/n, \qquad u \in R^k, \end{aligned} \tag{1.4}$$

where $|x| = (\sum_{j=1}^k x_j^2)^{\frac{1}{2}}$, $(x, y) = \sum_{j=1}^k x_j y_j$ for $x = (x_1, \cdots, x_k)$, and $y = (y_1, \cdots, y_k)$ belonging to R^k, and $\lambda_s^{(r)}(u)$ is the cumulant of order s of the random variable $(u, X^{(r)})$. The expressions in (1.4) are, of course, defined for appropriate values of s. Let $P_j(u)$, $j = 0, 1, 2, \cdots$, be polynomials in $u = (u_1, \cdots, u_k)$ defined purely formally by equating coefficients of $n^{-j/2}$ on both sides of

$$\exp\,[\textstyle\sum_{j=3}^\infty n^{-(j-2)/2}\lambda_{j,n}(u)/j!] = \textstyle\sum_{j=0}^\infty n^{-j/2}P_j(u). \tag{1.5}$$

Thus what P_j's are meaningfully defined depends on the set of moments which are assumed finite. One has

$$P_0(u) = 1, \qquad P_1(u) = \lambda_{3,n}(u)/6, \qquad P_2(u) = \lambda_{4,n}(u)/24 + \lambda_{3,n}^2(u)/72. \tag{1.6}$$

We shall denote by $P_j(-\varphi)$ the function on R^k whose Fourier transform has the value $P_j(it)\exp(-|t|^2/2)$ at t. Note that since the relation

$$\begin{aligned} &(it_1)^{s_1} \cdots (it_k)^{s_k} \exp(-|t|^2/2) \\ &\quad = (-1)^{s_1 + \cdots + s_k} \int \exp\,[i(t, x)]\, \frac{\partial^{s_1 + \cdots + s_k}}{\partial x_1^{s_1} \cdots \partial x_k^{s_k}}\, \varphi(x)\, dx, \end{aligned} \tag{1.7}$$

where φ is the standard normal density, $\varphi(x) = (2\pi)^{-k/2}\exp(-|x|^2/2)$, holds for every k-tuple of nonnegative integers (this may be proved by repeated integration by parts), $P_j(-\varphi)(x)$ may be obtained from the expression $P_j(it)\exp(-|t|^2/2)$ by replacing each term $(it_1)^{s_1} \cdots (it_k)^{s_k} \exp(-|t|^2/2)$ by $(-\partial/\partial x_1)^{s_1} \cdots (-\partial/\partial x_k)^{s_k}\varphi(x)$. The finite signed measure with density $P_j(-\varphi)$ is denoted by $P_j(-\Phi)$. The distribution function corresponding to the measure Φ will also be denoted by Φ.

The topological boundary of any subset A of R^k will be denoted by ∂A. Also the *ε-neighborhood* A^ε of A is defined by

$$A^\varepsilon = \{x; |x - y| < \varepsilon \text{ for some } y \text{ in } A\}, \qquad \varepsilon > 0. \tag{1.8}$$

For ease of reference the definitions (0.3) of the sphere $S(x, \varepsilon)$ and the oscillation $\omega_g(A)$ are repeated here.

$$S(x,\varepsilon) = \{y; y \in R^k, |x-y| < \varepsilon\}, \qquad x \in R^k, \varepsilon > 0; \tag{1.9}$$

$$\omega_g(A) = \sup\{|g(x)-g(y)|; x, y \in A\}, \qquad A \subset R^k,$$

g being a given real-valued function on R^k. Often times we shall deal with the *oscillation function* $\omega_g(S(x, \varepsilon))$ on R^k into the nonnegative reals for a given positive ε.

A probability measure P will be said to have *support* in a set B if $P(B) = 1$.

CONVENTION. Throughout c's will denote constants, either absolute or depending on the indicated arguments.

2. Some lemmas. We shall prove five lemmas in this section. Lemma 1 gives a type of inequality first obtained by Cramér [11] (page 72, Lemma 2).

LEMMA 1. *If* $\rho_{3+\delta,n} < \infty$ *for some* δ, $0 < \delta \leqq 1$, *and* $|t| \leqq n^{\frac{1}{2}}/(2\rho_{3+\delta,n}^{1/(3+\delta)})$, *then*

$$\begin{aligned}&|f_n(t) - (1+n^{-\frac{1}{2}}P_1(it))\exp(-|t|^2/2)| \\ &\quad \leqq (5/2)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)} n^{-(1+\delta)/2}(|t|^{3+\delta} + |t|^{3(1+\delta)})\exp(-|t|^2/2).\end{aligned} \tag{2.1}$$

PROOF. We first prove the lemma for $k = 1$. In this case

$$B_n = \mu_{2,n}^{-\frac{1}{2}}, \qquad \rho_{3+\delta,n} = \mu_{2,n}^{-(3+\delta)/2}\beta_{3+\delta,n}. \tag{2.2}$$

Let

$$g(r,t) = f^{(r)}(n^{-\frac{1}{2}}\mu_{2,n}^{-\frac{1}{2}}t), \qquad U(r,t) = g(r,t) - 1. \tag{2.3}$$

By Taylor expansion (cf. [18], page 199),

$$\begin{aligned} g(r,t) = {}& 1 - \mu_2^{(r)}t^2/(2n\mu_{2,n}) + \mu_3^{(r)}(it)^3/(6n^{\frac{3}{2}}\mu_{2,n}^{\frac{3}{2}}) \\ &+ \theta 2^{1-\delta}\beta_{3+\delta}^{(r)}|t|^{3+\delta}/[(1+\delta)(2+\delta)(3+\delta)n^{(3+\delta)/2}\mu_{2,n}^{(3+\delta)/2}], \end{aligned} \tag{2.4}$$

where θ is used here and elsewhere for a complex number, not always the same, of magnitude not exceeding one. In the given range of t,

$$|U(r,t)| < \tfrac{3}{16}, \qquad |\log(1+U(r,t)) - U(r,t)| \leqq |U(r,t)|^2. \tag{2.5}$$

Hence from (2.4) one gets

$$\begin{aligned} \log g(r,t) = {}& -\mu_2^{(r)}t^2/(2n\mu_{2,n}) + (\tfrac{1}{6})\mu_3^{(r)}(it)^3/(n\mu_{2,n})^{\frac{3}{2}} \\ &+ \theta(\tfrac{1}{3})\beta_{3+\delta}^{(r)}|t|^{3+\delta}/(n\mu_{2,n})^{(3+\delta)/2} + \theta[\mu_2^{(r)}t^2/(2n\mu_{2,n}) \\ &+ (\tfrac{1}{6})\beta_3^{(r)}|t|^3/(n\mu_{2,n})^{\frac{3}{2}} + (\tfrac{1}{3})\beta_{3+\delta}^{(r)}|t|^{3+\delta}/(n\mu_{2,n})^{(3+\delta)/2}]^2. \end{aligned} \tag{2.6}$$

We now note that for $2 \leqq s \leqq 3+\delta$ one has

$$\beta_s^{(r)} \leqq (\beta_{3+\delta}^{(r)})^{s/(3+\delta)}, \qquad \textstyle\sum_{r=1}^n (\beta_s^{(r)})^2 \leqq (n\beta_{3+\delta,n})^{2s/(3+\delta)}. \tag{2.7}$$

Summing both sides of (2.6) over $r = 1, \cdots, n$, and using (2.7) one obtains after elementary calculations (note that for any three complex numbers a, b, c, $|a+b+c|^2 \leqq 3(|a|^2+|b|^2+|c|^2)$)

$$\log f_n(t) = -t^2/2+\mu_{3,n}(it)^3/(6n^{\frac{1}{2}}\mu_{2,n}^{\frac{3}{2}}) + \theta(\tfrac{29}{24})\beta_{3+\delta,n}|t|^{3+\delta}/(n^{(1+\delta)/2}\mu_{2,n}^{(3+\delta)/2}) = -t^2/2+V, \tag{2.8}$$

say, so that

$$f_n(t)-\exp(-t^2/2) = [\exp(V)-1]\exp(-t^2/2). \tag{2.9}$$

Clearly,

$$\exp(V)-1 = V+(\theta/2)|V|^2\exp(|V|). \tag{2.10}$$

Also simple calculations show that in the given range of t

$$|V| < \tfrac{1}{5}, \qquad |V|^2 \leqq \beta_{3+\delta,n}^{3(1+\delta)/(3+\delta)}|t|^{3(1+\delta)}/(n^{(1+\delta)/2}\mu_{2,n}^{3(1+\delta)/2}). \tag{2.11}$$

Using (2.10) and (2.11) in (2.9) one obtains

$$\begin{aligned} &|f_n(t)-[1+n^{-\frac{1}{2}}\mu_{3,n}\mu_{2,n}^{-\frac{3}{2}}(it)^3/6]\exp(-t^2/2)| \\ &\quad \leqq (\tfrac{5}{2})\beta_{3+\delta,n}^{3(1+\delta)/(3+\delta)}\mu_{2,n}^{-3(1+\delta)/2}n^{-(1+\delta)/2}(|t|^{3+\delta}+|t|^{3(1+\delta)})\exp(-|t|^2/2) \end{aligned} \tag{2.12}$$

for $|t| \leqq n^{\frac{1}{2}}/(2\rho_{3+\delta,n}^{1/(3+\delta)})$. This proves the lemma for $k = 1$. Note that in this case $P_1(it) = \lambda_{3,n}(it)/6 = \mu_{3,n}\mu_{2,n}^{-\frac{3}{2}}(it)^3/6$. For the general case, define, for a non-zero t in R^k,

$$Z^{(r)} = (t, B_n X^{(r)})/|t|. \tag{2.13}$$

Then $\{Z^{(r)}\}$ is a sequence of independent random variables centered at expectations, and

$$\begin{aligned} &(\textstyle\sum_{r=1}^n E(Z^{(r)})^2)/n = 1, \qquad (i|t|)^3(\textstyle\sum_{r=1}^n E(Z^{(r)})^3)/(6n) = P_1(it), \\ &(\textstyle\sum_{r=1}^n E|Z^{(r)}|^s)/n \leqq \rho_{s,n}, \qquad s \geqq 0. \end{aligned} \tag{2.14}$$

Applying (2.1) (for $k = 1$) to the characteristic function g_n, say, of $(\sum_{r=1}^n Z^{(r)})/n^{\frac{1}{2}}$ and using (2.14) one gets the inequality

$$\begin{aligned} &|g_n(v)-[1+n^{-\frac{1}{2}}(iv)^3(\textstyle\sum_{r=1}^n E(Z^{(r)})^3)/(6n)]\exp(-v^2/2)| \\ &\quad \leqq (\tfrac{5}{2})\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-(1+\delta)/2}(|v|^{3+\delta}+|v|^{3(1+\delta)})\exp(-v^2/2) \end{aligned} \tag{2.15}$$

for $|v| \leqq n^{\frac{1}{2}}/(2\rho_{3+\delta,n}^{1/(3+\delta)})$. Take $v = |t|$ in (2.15). Since $g_n(|t|) = f_n(t)$, (2.15) reduces to (2.1). □

LEMMA 2. *If $\rho_{3+\delta,n} < \infty$ for some δ, $0 < \delta \leqq 1$, and $|t| \leqq n^{\frac{1}{2}}/(4\rho_{3+\delta,n}^{3/(3+\delta)})$, then*

$$|f_n(t)| \leqq \exp(-|t|^2/3). \tag{2.16}$$

PROOF. For $k = 1$ and $\delta = 0$ this is a result of Cramér [11] (page 75, Lemma 3). Since $\rho_{3,n} \leqq \rho_{3+\delta,n}^{3/(3+\delta)}$ for $\delta \geqq 0$, (2.16) holds in the given range of t, for the case $k = 1$. The multi-dimensional case is proved by applying the one-dimensional inequality to the characteristic function g_n defined above. □

The next two lemmas estimate the effect of smoothing by convolution. We denote by μ^+, μ^-, $|\mu|$, the positive, negative, and total variations, respectively, of a finite signed measure μ ($\mu = \mu^+ - \mu^-$, $|\mu| = \mu^+ + \mu^-$). The symbol '$*$' denotes the operation of convolution. For a bounded, real-valued function g on R^k and a positive number ε, we define (see (1.9))

$$g^{s,\varepsilon}(x) = \sup\{g(y); y \in S(x,\varepsilon)\},\qquad (2.17)$$
$$g^{i,\varepsilon}(x) = \inf\{g(y); y \in S(x,\varepsilon)\}.$$

Note that $g^{s,\varepsilon}$ is lower semi-continuous and $g^{i,\varepsilon}$ is upper semi-continuous because of the (readily verified) equalities

$$\{x; g^{s,\varepsilon}(x) > c\} = \bigcup\{S(x,\varepsilon); g(x) > c\}, \qquad c \in R^1; \qquad (2.18)$$
$$g^{i,\varepsilon} = -(-g)^{s,\varepsilon}.$$

In particular, $g^{s,\varepsilon}$, $g^{i,\varepsilon}$, $\omega_g(S(\cdot,\varepsilon)) = g^{s,\varepsilon} - g^{i,\varepsilon}$ are all Borel measurable (whether or not g is measurable).

LEMMA 3. *Let G_ε be a probability measure with support in $S(0,\varepsilon)$, P an arbitrary probability measure, and Q a finite signed measure. For a real-valued, bounded, Borel measurable function g on R^k, define*

$$\gamma(\varepsilon) = \max\left\{\int g^{s,\varepsilon}\, d(P-Q) * G_\varepsilon, -\int g^{i,\varepsilon}\, d(P-Q) * G_\varepsilon\right\}, \qquad (2.19)$$
$$\tau(\varepsilon) = \max\left\{\int (g^{s,2\varepsilon} - g)\, dQ^+, \int (g - g^{i,2\varepsilon})\, dQ^+\right\}.$$

Then, for every positive ε,

$$\left|\int g\, d(P-Q)\right| \leqq \gamma(\varepsilon) + \tau(\varepsilon). \qquad (2.20)$$

PROOF. By definitions (2.19),

$$\begin{aligned}
\gamma(\varepsilon) &\geqq \int g^{s,\varepsilon}\, d(P-Q) * G_\varepsilon \\
&= \int_{|x|<\varepsilon} \left[\int g^{s,\varepsilon}(y+x)\, d(P-Q)(y)\right] dG_\varepsilon(x) \\
&= \int_{|x|<\varepsilon} \Big[\int g^{s,\varepsilon}(y+x)\, dP(y) - \int g(y)\, dQ(y) \\
&\qquad\qquad - \int (g^{s,\varepsilon}(y+x) - g(y))\, dQ(y)\Big]\, dG_\varepsilon(x) \\
&\geqq \int_{|x|<\varepsilon} \left[\int g(y)\, dP(y) - \int g(y)\, dQ(y) - \int (g^{s,\varepsilon}(y+x) - g(y))\, dQ^+(y)\right] dG_\varepsilon(x) \\
&\geqq \int_{|x|<\varepsilon} \left(\int g\, d(P-Q)\right) dG_\varepsilon(x) - \int_{|x|<\varepsilon} \left[\int (g^{s,2\varepsilon}(y) - g(y))\, dQ^+(y)\right] dG_\varepsilon(x) \\
&= \int g\, d(P-Q) - \int (g^{s,2\varepsilon} - g)\, dQ^+ \geqq \int g\, d(P-Q) - \tau(\varepsilon).
\end{aligned} \qquad (2.21)$$

Similarly,

$$\begin{aligned}
-\gamma(\varepsilon) &\leqq \int g^{i,\varepsilon}\, d(P-Q) * G_\varepsilon = \int_{|x|<\varepsilon} \left[\int g^{i,\varepsilon}(y+x)\, d(P-Q)(y)\right] dG_\varepsilon(x) \\
&= \int_{|x|<\varepsilon} \Big[\int g^{i,\varepsilon}(y+x)\, dP(y) - \int g(y)\, dQ(y) \\
&\qquad\qquad + \int (g(y) - g^{i,\varepsilon}(y+x))\, dQ(y)\Big]\, dG_\varepsilon(x) \\
&\leqq \int g\, d(P-Q) + \int (g - g^{i,2\varepsilon})\, dQ^+ \leqq \int g\, d(P-Q) + \tau(\varepsilon).
\end{aligned} \qquad (2.22)$$

If $\int g\, d(P-Q) \geqq 0$, (2.21) yields (2.20); if $\int g\, d(P-Q) < 0$, then (2.20) follows from (2.22). □

COROLLARY. *Under the hypothesis of Lemma* 3, *the following inequality holds*:

$$(2.23) \qquad \left|\int g\, d(P-Q)\right| \leqq \left|\int g\, d(P-Q) * G_\varepsilon\right| + \int \omega_g(S(\cdot, \varepsilon))\, d\left|(P-Q) * G_\varepsilon\right| + \int \omega_g(S(\cdot, 2\varepsilon))\, d|Q|.$$

If, further $(P-Q) * G_\varepsilon(R^k) = 0$, *then*

$$(2.24) \qquad \left|\int g\, d(P-Q)\right| \leqq \omega_g(R^k)\left|(P-Q) * G_\varepsilon\right|(R^k) + \int \omega_g(S(\cdot, 2\varepsilon))\, d|Q|.$$

PROOF. It is easy to see that

$$(2.25) \qquad \gamma(\varepsilon) \leqq \left|\int g\, d(P-Q) * G_\varepsilon\right| + \int \omega_g(S(\cdot, \varepsilon))\, d\left|(P-Q) * G_\varepsilon\right|,$$

and that

$$(2.26) \qquad \tau(\varepsilon) \leqq \int \omega_g(S(\cdot, 2\varepsilon))\, d|Q|.$$

Using these estimates in Lemma 3 one gets (2.23). If $(P-Q) * G_\varepsilon(R^k) = 0$, then from the definition of $\gamma(\varepsilon)$ it follows that

$$(2.27) \qquad \gamma(\varepsilon) \leqq \omega_g(R^k)\left|(P-Q) * G_\varepsilon\right|(R^k).$$

Inequalities (2.26), (2.27) yield (2.24). □

The next lemma is similar to Lemma 3 in content. Given any probability measure G we denote by G_ε the distribution of the random vector εX, X having distribution G. In this notation G_ε of Lemma 3 may be regarded as arising from a G with support in the unit sphere. Given any real-valued function g on R^k we denote by g_u the translate of g by u, i.e.,

$$(2.28) \qquad g_u(x) = g(x+u).$$

For a given probability measure G, and a constant α' satisfying

$$(2.29) \qquad \tfrac{1}{2} < \alpha' < 1,$$

one can find a constant α such that

$$(2.30) \qquad \int_{|x| < \alpha\varepsilon} dG_\varepsilon(x) = \int_{|x| < \alpha} dG(x) \geqq \alpha'.$$

LEMMA 4. *Let P be a probability measure and Q a finite signed measure. For a real-valued, bounded, Borel measurable function g on R^k, define*

$$(2.31) \quad \gamma_1(\varepsilon) = \sup\{\max(\left|\int g_u^{s,\alpha\varepsilon}\, d(P-Q) * G_\varepsilon\right|, \left|\int g_u^{i,\alpha\varepsilon}\, d(P-Q) * G_\varepsilon\right|); u \in R^k\},$$

$$\tau_1(\varepsilon) = \sup\left[\max\{\int (g_u^{s,2\alpha\varepsilon} - g_u)\, d|Q|, \int (g_u - g_u^{i,2\alpha\varepsilon})\, d|Q|\}; u \in R^k\right],$$

where G is any probability measure, α is chosen to satisfy (2.30). *Then one has, for every positive* ε,

$$(2.32) \qquad \left|\int g\, d(P-Q)\right| \leqq (2\alpha'-1)^{-1}[\gamma_1(\varepsilon) + \tau_1(\varepsilon)].$$

This lemma and the following corollary are proved in [5] (Lemma 8 and relation (2.27)).

COROLLARY. *Under the hypothesis of Lemma* 4 *one has*

$$(2.33)\quad \left|\int g\, d(P-Q)\right| \leqq (2\alpha'-1)^{-1}[\sup\{\left|\int g_u\, d(P-Q)*G_\varepsilon\right| + \int \omega_{g_u}(S(\cdot,\alpha\varepsilon)) \cdot d\left|(P-Q)*G_\varepsilon\right|; u\in R^k\} + \sup\{\int \omega_{g_u}(S(\cdot,2\alpha\varepsilon))\, d\left|Q\right|; u\in R^k\}].$$

Lastly, we shall need the following lemma.

LEMMA 5. *There exists a probability measure H_1 with support in $S(0,1)$ and having a characteristic function ζ satisfying*

$$(2.34)\qquad \left|\zeta(t)\right| \leqq \alpha(k)\exp(-\left|t\right|^{\frac{1}{2}}), \qquad t\in R^k.$$

PROOF. By a result of Ingham [17], there exists a probability measure H on $\mathscr{B}^1$ such that

$$(2.35)\qquad \int_{-k^{-1/2}}^{k^{-1/2}} dH = 1, \qquad \left|\int \exp(itx)\, dH(x)\right| \leqq \alpha(k)\exp(-\left|t\right|^{\frac{1}{2}}), \qquad t\in R^1.$$

Let H_1 be the product measure on $(R^k, \mathscr{B}^k)$, each coordinate measure being H. □

3. Main results. We continue to use the notation of Section 1.

THEOREM 1. *If $\rho_{3+\delta,n} < \infty$ for some $\delta > 0$, then for any bounded, Borel measurable function g on R^k, the inequality*

$$(3.1)\quad \left|\int g\, d(Q_n-\Phi)\right| \leqq c(k,\delta)\omega_g(R^k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)} n^{-\frac{1}{2}} + \int \omega_g(S(\cdot,\varepsilon_n))\, d\Phi$$

holds with $\varepsilon_n = c(k)\rho_{3+\delta,n}^{3/(3+\delta)} n^{-\frac{1}{2}}\log n$.[2]

PROOF. Without loss of generality we assume $0<\delta\leqq 1$. Let Z be a random vector with distribution H_1 of Lemma 5. Let H_η denote the distribution of ηZ for positive η. In Lemma 3 take $P = Q_n$, $Q = \Phi$, $\varepsilon = p\eta$, $G_\varepsilon = H_\eta{}^{*p}$, where p is a positive integer and $H_\eta{}^{*p}$ is the p-fold convolution of H_η. Since $(Q_n-\Phi)*G_\varepsilon(R^k) = 0$, one has, by (2.24) (corollary to Lemma 3),

$$(3.2)\qquad \left|\int g\, d(Q_n-\Phi)\right| \leqq \omega_g(R^k)\left|(Q_n-\Phi)*G_\varepsilon\right|(R^k) + \int \omega_g(S(\cdot,2\varepsilon))\, d\Phi.$$

Now

$$(3.3)\quad \left|(Q_n-\Phi)*G_\varepsilon\right|(R^k) \leqq \left|(Q_n-\Phi-n^{-\frac{1}{2}}P_1(-\Phi))*G_\varepsilon\right|(R^k) + n^{-\frac{1}{2}}\left|P_1(-\Phi)\right|(R^k).$$

One can show (cf. [5], Lemma 7) that

$$(3.4)\qquad \left|P_1(-\Phi)\right|(R^k) \leqq h(k)\rho_{3,n}.$$

We now estimate $\left|\mu_n\right|(R^k)$, where

$$(3.5)\qquad \mu_n = (Q_n-\Phi-n^{-\frac{1}{2}}P_1(-\Phi))*G_\varepsilon.$$

---

[2] One may take $\delta = 0$ if $k = 1$ or 2 (see [5]). This is true for all k if $\{X^{(r)}\}$ is i.i.d. This and some other recent results in the i.i.d. case are contained in the author's article "Recent results on refinements of the central limit theorem" in the forthcoming *Proc. Sixth Berkeley Symp. Math. Statist. Prob.*

For $r > 0$,

(3.6) $$|\mu_n|(R^k) = |\mu_n|(S(0,r)) + |\mu_n|(R^k - S(0,r)).$$

Now

(3.7) $$|\mu_n|(R^k - S(0,r)) \leqq (Q_n * H_\eta^{*p} + \Phi * H_\eta^{*p})(R^k - S(0,r)) + n^{-\frac{1}{2}}|P_1(-\Phi)| * H_\eta^{*p}(R^k).$$

We shall later choose r, p, and η so as to satisfy

(3.8) $$r > 2p\eta,$$

and, consequently,

(3.9) $$H_\eta^{*p}(R^k - S(0, r/2)) = 0.$$

Therefore,

(3.10) $$Q_n * H_\eta^{*p}(R^k - S(0,r)) \leqq Q_n(R^k - S(0, r/2)),$$
$$\Phi * H_\eta^{*p}(R^k - S(0,r)) \leqq \Phi(R^k - S(0, r/2)).$$

Now it is easy to show that

(3.11) $$\Phi(R^k - S(0, r/2)) \leqq (c_1(k)\exp(-r^2/8k))/r.$$

Also one can show (cf. [5], relation (2.48)) by using the Berry–Esseen theorem (cf. [14], page 43, Theorem 1) that

(3.12) $$Q_n(R^k - S(0, r/2)) \leqq (c_1(k)\exp(-r^2/8k))/r + c_2(k)\rho_{3,n} n^{-\frac{1}{2}}.$$

Using these estimates and (3.4) in (3.7) one obtains

(3.13) $$|\mu_n|(R^k - S(0,r)) \leqq (2c_1(k)\exp(-r^2/8k))/r + c_2(k)\rho_{3,n} n^{-\frac{1}{2}} + h(k)\rho_{3,n} n^{-\frac{1}{2}}.$$

It remains to estimate $|\mu_n|(S(0,r))$. Now μ_n has an integrable Fourier transform ξ_n given by

(3.14) $$\xi_n(t) = (f_n(t) - [1 + n^{-\frac{1}{2}}P_1(it)]\exp(-|t|^2/2))\zeta^p(\eta t), \qquad t \in R^k,$$

where ζ is the characteristic function of H_1. By the Fourier inversion theorem μ_n has a density q_n given by

(3.15) $$q_n(x) = (2\pi)^{-k}\int \exp[-i(t,x)]\cdot \xi_n(t)\,dt, \qquad x \in R^k.$$

Hence

(3.16) $$|\mu_n|(S(0,r)) = \int_{|x|<r} |q_n(x)|\,dx \leqq c_3(k)r^k(I_1 + I_2 + I_3),$$

where

$$I_1 = \int_{\{|t| \leqq n^{1/6}/(2\rho_{3+\delta,n}^{1/(3+\delta)})\}} |f_n(t) - [1 + n^{-\frac{1}{2}}P_1(it)]\exp(-|t|^2/2)|\,dt,$$

(3.17) $$I_2 = \int_{\{|t| > n^{1/6}/(2\rho_{3+\delta,n}^{1/(3+\delta)})\}} |f_n(t)\zeta^p(\eta t)|\,dt,$$

$$I_3 = \int_{\{|t| > n^{1/6}/(2\rho_{3+\delta,n}^{1/(3+\delta)})\}} |1 + n^{-\frac{1}{2}}P_1(it)|\exp(-|t|^2/2)\,dt.$$

By Lemma 1,

$$I_1 \leqq c_4(k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-(1+\delta)/2}. \tag{3.18}$$

Since one may assume that

$$n^{\frac{1}{2}}/(2\rho_{3+\delta,n}^{1/(3+\delta)}) \geqq 1 \tag{3.19}$$

(in the contrary case (3.1) is trivially true), one easily obtains

$$I_3 \leqq c_5(k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-(1+\delta)/2}. \tag{3.20}$$

By Lemma 2,

$$I_2 \leqq \int_{\{|t|>n^{1/6}/(2\rho_{3+\delta,n}^{1/(3+\delta)})\}} \exp(-|t|^2/3)\,dt + \int_{\{|t|\geqq n^{1/2}/(4\rho_{3+\delta,n}^{3/(3+\delta)})\}} |f_n(t)\zeta^p(\eta_t)|\,dt. \tag{3.21}$$

The first integral is smaller than

$$c_6(k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-(1+\delta)/2}, \tag{3.22}$$

and the second is, by Lemma 5, smaller than

$$I_4 = \int_{\{|t|\geqq n^{1/2}/(4\rho_{3+\delta,n}^{3/(3+\delta)})\}} \alpha^p(k)\exp(-|\eta t|^{\frac{1}{2}}p)\,dt. \tag{3.23}$$

We now choose

$$\eta = 16(\log\alpha(k)+k)^2\rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}, \tag{3.24}$$
$$p = [\log n]+1,$$

where $[x]$ denotes the integer part of x. Elementary calculations now yield

$$I_4 \leqq c_7(k)n^{-k/2}\log^{-2k} n. \tag{3.25}$$

Using estimates (3.22) and (3.25) in (3.21) one obtains

$$I_2 \leqq c_6(k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-(1+\delta)/2} + c_7(k)n^{-k/2}\log^{-2k} n. \tag{3.26}$$

The estimates (3.18), (3.20) and (3.26), when used in (3.16), give

$$|\mu_n|(S(0,r)) \leqq c_8(k,\delta)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}r^k n^{-\frac{1}{2}}\log^{-2k} n. \tag{3.27}$$

Now choose

$$r = (8k\log(n+1))^{\frac{1}{2}}. \tag{3.28}$$

Then (3.13) and (3.27) give

$$|\mu_n|(R^k) \leqq c_9(k,\delta)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}. \tag{3.29}$$

Finally, making use of (3.29) in (3.2) one obtains (via (3.3) and (3.4)) the desired inequality (3.1). Note that $\varepsilon = p\eta \doteqdot c(k).\ \rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}\log n$ by the choice of η and p in (3.24). □

REMARK 1. If g in Theorem 1 is such that

$$\int \omega_g(S(\cdot,\varepsilon))\,d\Phi = O(\varepsilon), \qquad \varepsilon \to 0, \tag{3.30}$$

then

$$\left|\int g\,d(Q_n-\Phi)\right| \leqq c(k,\delta)\omega_g(R^k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}+c_{10}(k,g)\rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}\log n. \tag{3.31}$$

For the Φ-uniformity class $\mathscr{F}_1(\Phi;\, c,\, d,\, \varepsilon_0)$ defined by (0.5) one has

$$\begin{aligned}\sup\{\left|\int g\,d(Q_n-\Phi)\right|;\, g\in\mathscr{F}_1(\Phi;c,d,\varepsilon_0)\}\\ \leqq c(k,\delta)c\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}+c(k)(d+c/\varepsilon_0)\rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}\log n.\end{aligned} \tag{3.32}$$

The term involving ε_0 is introduced to take care of those integers for which $\varepsilon_n > \varepsilon_0$; note that $\left|\int g\,d(Q_n-\Phi)\right| \leqq c$ for all g in the class $\mathscr{F}_1(\Phi;\, c,\, d,\, \varepsilon_0)$. If we denote by $\mathscr{A}_1(\Phi;\, d,\, \varepsilon_0)$ the class of all Borel sets A satisfying (cf. [5], Section 1)

$$\Phi((\partial A)^{\varepsilon}) \leqq d\varepsilon, \qquad 0<\varepsilon\leqq\varepsilon_0, \tag{3.33}$$

∂A denoting the boundary of A, then the class of all indicator functions of sets in this class is contained in $\mathscr{F}_1(\Phi;\, 1,\, d,\, \varepsilon_0)$.
Hence

$$\begin{aligned}\sup\{|Q_n(A)-\Phi(A)|;\, A\in\mathscr{A}_1(\Phi;d,\varepsilon_0)\}\\ \leqq c(k,\delta)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}+c(k)(d+1/\varepsilon_0)\rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}\log n.\end{aligned} \tag{3.34}$$

For suitable c and d these two classes include most functions and sets of interest. But (3.1) provides an upper bound for every Φ-continuous g. By a variant of a characterization of uniformity classes of functions due to Billingsley and Topsøe [8] (also see [5]), $\mathscr{F}$ is a Φ-uniformity class of functions if and only if

$$\begin{aligned}&\text{(i)}\quad \sup\{\omega_g(R^k);\, g\in\mathscr{F}\}<\infty,\\ &\text{(ii)}\quad \limsup_{\varepsilon\downarrow 0}\{\int\omega_g(S(\cdot,\varepsilon))\,d\Phi;\, g\in\mathscr{F}\}=0.\end{aligned} \tag{3.35}$$

Hence (3.1) provides effective uniform upper bounds to errors of normal approximation over arbitrary Φ-uniformity classes.

REMARK 2. An error bound different from (3.1) is given in [5] (Theorem 1). According to this

$$\begin{aligned}\left|\int g\,d(Q_n-\Phi)\right| \leqq c'(k,\delta)\omega_g(R^k)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}\\ +c'(k)\sup\{\int\omega_{g_u}(S(\cdot,\alpha_n))\,d\Phi;\, u\in R^k\},\end{aligned} \tag{3.36}$$

where $\alpha_n = c''(k)\rho_{3+\delta,n}^{3/(3+\delta)}n^{-\frac{1}{2}}$. Although (3.36) provides a precise upper bound $O(n^{-\frac{1}{2}})$ (if $\{\rho_{3+\delta,n}\}$ is bounded) for several interesting classes of functions and sets (cf. [5], [20]), we shall show by an example now that there are Borel sets A for which $\Phi((\partial A)^{\varepsilon}) = O(\varepsilon)$ as ε goes to zero, while $\sup\{\Phi((\partial(A-u))^{\varepsilon});\, u\in R^k\} = 1$ for every positive ε; thus for such a set A, (3.36) is useless, while (3.1) provides an upper bound $O(\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)}n^{-\frac{1}{2}}\log n)$.

EXAMPLE. In R^1 let

$$A = \bigcup_{r=1}^{\infty} \bigcup_{i=1}^{[(r-1)/2]} \{[r+2i/r, r+(2i+1)/r]\}, \tag{3.37}$$

where $[(r-1)/2]$ is the integer part of $(r-1)/2$. It is easy to see that for every positive ε

$$\sup\{\Phi((\partial(A-u))^{\varepsilon}); u \in R^k\} = 1, \quad \text{but} \tag{3.38}$$

$$\Phi((\partial A)^{\varepsilon}) \leqq \varepsilon(2\pi)^{-\frac{1}{2}} \textstyle\sum_{r=1}^{\infty} r \exp(-r^2/2) = d\varepsilon, \quad \text{say.} \tag{3.39}$$

REMARK 3. It is clear that if g has a compact support, then one may take $\delta = 0$, in Theorem 1. For this case one will have to replace (3.2) by (see (2.23))

$$\left|\int g\, d(Q_n - \Phi)\right| \leqq \left|\int g\, d(Q_n - \Phi) * G_{\varepsilon}\right| + \int \omega_g(S(\cdot, \varepsilon))\, d\left|(Q_n - \Phi) * G_{\varepsilon}\right| + \int \omega_g(S(\cdot, 2\varepsilon))\, d\Phi, \tag{3.40}$$

and (3.27) by (use Lemma 1 and Lemma 2 with $\delta = 0$)

$$|\mu_n|(S(0,r)) \leqq c_{11}(k, g)\rho_{3,n} n^{-\frac{1}{2}}, \tag{3.41}$$

where r is such that g vanishes outside $S(0,r)$. A similar remark applies to the inequality (3.36). It is not known however, whether the factor $\log n$ in the expression for ε_n in Theorem 1 may be removed or not. If the sequence of characteristic functions $\{f^{(r)}\}$ obeys *Cramér's condition: for all positive* η

$$\sup\{|f^{(r)}(t)|; |t| > \eta, r = 1, 2, \cdots\} < 1, \tag{3.42}$$

then even without the factor $\log n$ in ε_n (i.e., with $p = 1$ in (3.24)) one may easily show that I_2, defined by (3.17), is of the smaller order of $1/n$ as n goes to infinity, so that one obtains (3.1) with $\varepsilon_n = c(k)\rho_{3+\delta,n}^{3/(3+\delta)} n^{-\frac{1}{2}}$. Consequently, $\log n$ may be removed from the expressions (3.31), (3.32), and (3.34). For the independent and identically distributed case (3.42) is equivalent to:

$$\limsup_{|t| \to \infty} |f^{(1)}(t)| < 1. \tag{3.42$'$}$$

REMARK 4. There are several well-known metrics which metrize the topology of weak convergence of probability measures on $(R^k, \mathscr{B}^k)$. We mention here the Lévy distance d_L, the Prokhorov distance d_P, and the bounded Lipschitzian distance d_{BL} defined by

$$\begin{aligned} d_L(Q, Q') &= \inf\{\varepsilon; \varepsilon > 0, F_Q(x - \varepsilon e) - \varepsilon \leqq F_{Q'}(x) \\ &\qquad \leqq F_Q(x + \varepsilon e) + \varepsilon \text{ for all } x \text{ in } R^k\}, \\ d_P(Q, Q') &= \inf\{\varepsilon; \varepsilon > 0, Q(A) \leqq Q'(A^{\varepsilon}) + \varepsilon \text{ and} \\ &\qquad Q'(A) \leqq Q(A^{\varepsilon}) + \varepsilon \text{ for all Borel sets } A\}, \\ d_{BL}(Q, Q') &= \sup\{|\textstyle\int g\, d(Q - Q')|; g, |g(x) - g(y)| \leqq |x - y| \text{ for all} \\ &\qquad x, y \text{ in } R^k, \omega_g(R^k) \leqq 1\}, \end{aligned} \tag{3.43}$$

where F_Q, $F_{Q'}$ are the distribution functions corresponding to Q, Q', respectively, and $e = (1, 1, \cdots, 1)$ is the unit vector in R^k. The fact that d_L metrizes the topology of weak convergence of probability measures in R^1 is proved in [16] (page 33, Theorem 1); the proof for R^k is entirely analogous. A proof of the corresponding assertion for d_P (in a separable metric space) may be found in [9] (page 237–238). Dudley [12] (Theorem 12) shows that d_{BL} also metrizes this topology (in a separable metric space). We now estimate these distances between Q_n and Φ. Note that in view of Bergström's extension (cf. [1]) to R^k of the Berry–Esseen theorem, one has

$$d_L(Q_n, \Phi) \leqq \sup\{|F_{Q_n}(x) - \Phi(x)|; x \in R^k\} = O(n^{-\frac{1}{2}}), \qquad n \to \infty, \tag{3.44}$$

if $\{\rho_3^{(r)}\}$ is a bounded sequence. This estimate is precise. The estimate (3.44) may also be obtained under weaker hypotheses (cf. [5], (3.19)). It has been shown in [5] (Section 3, Application 2) that under the hypothesis of Theorem 1,

$$d_{BL}(Q_n, \Phi) = O(n^{-\frac{1}{2}}), \qquad n \to \infty. \tag{3.45}$$

To estimate d_P we note that (cf. [13], Proposition 1)

$$d_P(Q, Q') = \inf\{\varepsilon; \varepsilon > 0, Q(A) \leqq Q'(A^{\varepsilon}) + \varepsilon \text{ for all Borel sets } A\}. \tag{3.46}$$

Also, note that, by (2.21), for every bounded Borel measurable g,

$$\int g\, d(Q - Q') \leqq \int g^{s,\varepsilon} d(Q - Q') * G_\varepsilon + \int (g^{s,2\varepsilon} - g)\, dQ', \tag{3.47}$$

for probability measures Q, Q'. Taking $g = I_A$, where A is a Borel set, one obtains

$$Q(A) - Q'(A) \leqq (Q - Q') * G_\varepsilon(A^\varepsilon) + Q'(A^{2\varepsilon} - A). \tag{3.48}$$

Now take $Q = Q_n$, $Q' = \Phi$, and G_ε as in Theorem 1. From the estimates obtained in the course of proving Theorem 1, one now has, for every Borel set A,

$$Q_n(A) - \Phi(A) \leqq c_{12}(k, \delta)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)} n^{-\frac{1}{2}} + \Phi(A^{\varepsilon_n} - A), \tag{3.49}$$

where ε_n is as in Theorem 1. Let $c_{13}(k, \delta) = \max\{c(k), c_{12}(k, \delta)\}$.
Then

$$Q_n(A) - \Phi(A) \leqq \varepsilon_n' + \Phi(A^{\varepsilon_n'} - A), \qquad \text{where} \tag{3.50}$$

$$\varepsilon_n' = c_{13}(k, \delta)\rho_{3+\delta,n}^{3(1+\delta)/(3+\delta)} n^{-\frac{1}{2}} \log n. \tag{3.51}$$

It now follows from (3.46) and (3.50) that

$$d_P(Q_n, \Phi) \leqq \varepsilon_n'. \tag{3.52}$$

The next theorem provides an asymptotic expansion for a large class of functions under Cramér's condition (3.42)'. For a given triplet (c, d, ε_0) of positive numbers, we define

$$\begin{aligned} \mathscr{F}_1^*(\Phi; c, d, \varepsilon_0) &= \{g; g_u \in \mathscr{F}_1(\Phi; c, d, \varepsilon_0) \text{ for all } u \in R^k\} \\ &= \{g; \omega_g(R^k) \leqq c, \textstyle\int \omega_{g_u}(S(\cdot, \varepsilon))\, d\Phi \leqq d\varepsilon \text{ for all } \varepsilon \text{ in} \\ &\qquad (0, \varepsilon_0] \text{ and for all } u \text{ in } R^k\}. \end{aligned} \tag{3.53}$$

Thus $\mathscr{F}_1{}^*(\Phi; c, d, \varepsilon_0)$ is the largest translation-invariant subclass of $\mathscr{F}_1(\Phi; c, d, \varepsilon_0)$. We consider a few examples.

EXAMPLES. Let $\mathscr{C}$ be the class of all measurable convex sets of R^k. For a suitable constant d depending on k (cf. [20], Appendix A, or [5], Application 1), the class of all indicator functions of members of $\mathscr{C}$ is contained in $\mathscr{F}_1{}^*(\Phi; 1, d, \varepsilon_0)$ for every positive ε_0. The bounded Lipschitz class $L(c, d)$ of all functions g satisfying

$$(3.54) \qquad \omega_g(R^k) \leqq c, \qquad |g(x)-g(y)| \leqq d\,|x-y| \text{ for all } x \text{ and } y \text{ in } R^k,$$

is contained in $\mathscr{F}_1{}^*(\Phi; c, 2d, \varepsilon_0)$. The class of all indicator functions of sets in R^2, each with a boundary contained in a rectifiable curve of length not exceeding a given number l, is contained in $\mathscr{F}_1{}^*(\Phi; 1, 2l+4, 1)$ in R^2 (cf. [10], Section 9, Example 7).

The proof of the theorem below makes use of Lemma 4 and an important estimate of Bikjalis [8]. We shall consider only the identically distributed case. The symbol Φ_ε will denote the distribution of εZ, where Z_1 has distribution Φ.

THEOREM 2. *Let $\{X^{(r)}\}$ be a sequence of independent and identically distributed k-dimensional random vectors each with a zero mean vector, a covariance matrix I (the $k \times k$ identity matrix), and a finite moment $\rho_s = E|X^{(1)}|^s$, s being an integer not smaller than three. If Q_n denotes the distribution of $(\sum_{r=1}^n X^{(r)})/n^{\frac{1}{2}}$, then for every triplet of positive numbers (c, d, ε_0),*

$$(3.55) \qquad \sup\{|\textstyle\int g\, d[Q_n - \sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)]|; g \in \mathscr{F}_1{}^*(\Phi; c, d, \varepsilon_0)\} = o(n^{-(s-2)/2}), \qquad n \to \infty,$$

provided $X^{(1)}$ obeys Cramér's condition: $\limsup_{|t|\to\infty} |f^{(1)}(t)| < 1$.

PROOF. It has been shown by Bikjalis [8] (relations (15), (16), (22), (28), (29) combined) that

$$(3.56) \qquad |[Q_n - \textstyle\sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)] * \Phi_\varepsilon|(R^k) = o(n^{-(s-2)/2}), \qquad n \to \infty$$

for a suitable ε satisfying

$$(3.57) \qquad \varepsilon = o(n^{-(s-2)/2}), \qquad n \to \infty.$$

By Lemma 4, for every bounded Borel measurable g,

$$(3.58) \qquad |\textstyle\int g\, d[Q_n - \sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)]| \leqq (2\alpha'-1)^{-1}[\gamma_1(\varepsilon) + \tau_1(\varepsilon)],$$

where, denoting by ν_n the signed measure $\sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)$, one has

$$(3.59) \qquad \gamma_1(\varepsilon) = \sup\{\max(|\textstyle\int g_u{}^{s,\alpha\varepsilon}\, d(Q_n - \nu_n) * \Phi_\varepsilon|); u \in R^k\} \leqq \omega_g(R^k)\,|(Q_n - \nu_n) * \Phi_\varepsilon|(R^k) = o(n^{-(s-2)/2}), \qquad n \to \infty,$$

by (3.56). The inequality in (3.59) holds because

$$(3.60) \qquad (Q_n - \nu_n)(R^k) = 0.$$

Also,

(3.61) $\tau_1(\varepsilon) = \sup[\max\{\int(g_u^{s,2\alpha\varepsilon} - g_u)\,d|v_n|, \int(g_u - g_u^{i,2\alpha\varepsilon})\,d|v_n|\}; u \in R^k]$,

so that, for $g \in \mathscr{F}_1^*(\Phi; c, d, \varepsilon_0)$, one has

$$(3.62)\qquad \tau_1(\varepsilon) \leqq \sup\{\int \omega_{g_u}(S(\cdot, 2\alpha\varepsilon))\,d(\Phi + \textstyle\sum_{j=1}^{s-2} n^{-j/2}|P_j(-\Phi)|); u \in R^k\}$$
$$\leqq 2\,d\alpha\varepsilon + \sup\{\int \omega_{g_u}(S(\cdot, 2\alpha\varepsilon))\,d(\textstyle\sum_{j=1}^{s-2} n^{-j/2}|P_j(-\Phi)|); u \in R^k\}.$$

Now (see the definition of $P_j(-\Phi)$ in Section 1) for $r = (3s\log n)^{\frac{1}{2}}$,

$$(3.63)\qquad \int_{S(0,r)} \omega_{g_u}(S(\cdot, 2\alpha\varepsilon))\,d(\textstyle\sum_{j=1}^{s-2} n^{-j/2}|P_j(-\Phi)|)$$
$$\leqq c_{14}(k) n^{-\frac{1}{2}} \rho_s (1 + r^{3(s-2)}) \int \omega_{g_u}(S(\cdot, 2\alpha\varepsilon))\,d\Phi \leqq c_{15}(k)\rho_s d\varepsilon,$$

and

$$(3.64)\qquad \int_{R^k - S(0,r)} \omega_{g_u}(S(\cdot, 2\alpha\varepsilon))\,d(\textstyle\sum_{j=1}^{s-2} n^{-j/2}|P_j(-\Phi)|)$$
$$\leqq \omega_g(R^k) \textstyle\sum_{j=1}^{s-2} n^{-j/2}|P_j(-\Phi)|(R^k - S(0,r)) = o(n^{-s/2}), \qquad n \to \infty.$$

Hence

$$(3.65)\qquad \tau_1(\varepsilon) = o(n^{-(s-2)/2}), \qquad n \to \infty.$$

One now obtains (3.55) by using (3.59) and (3.65) in (3.58). □

REMARK 1. As an application of Theorem 2 one has

$$(3.66)\qquad \sup\{|Q_n(C) - \textstyle\sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)(C)|; C \in \mathscr{C}\} = o(n^{-(s-2)/2}), \qquad n \to \infty,$$

under the hypothesis of Theorem 2. This is an improvement on a previous result of Ranga Rao [20] (Theorem 5.3.2). A result similar to Theorem 2 for indicator functions has been proved by Von Bahr [22] (Theorem 3(b)) under more restrictive assumptions. When applied to distribution functions (i.e., taking the supremum in (3.66) over the subclass of infinite rectangles), one obtains a previous result due to Bikjalis [8] (Teorema 2) and Von Bahr [22] (Theorem 2). The present author has now been able to prove that one may replace $\mathscr{F}_1^*(\Phi; c, d, \varepsilon_0)$ by the larger class $\mathscr{F}_1(\Phi; c, d, \varepsilon_0)$ in Theorem 2. The proof, however, is based on somewhat different techniques, and will be given elsewhere.

REMARK 2. If $X^{(1)}$ has a distribution with a non-zero absolutely continuous (with respect to Lebesgue measure) component, then Cramér's condition is satisfied. However, in this case the following much stronger inequality holds under the same moment conditions as in Theorem 2:

$$(3.67)\qquad |Q_n - \textstyle\sum_{j=0}^{s-2} n^{-j/2} P_j(-\Phi)|(R^k) = o(n^{-(s-2)/2}), \qquad n \to \infty.$$

For $k = 1$, this was proved simultaneously by Petrov [19] (Theorem 5) and Bikjalis [6] (Teorema 1). For arbitrary k it has been proved by Bikjalis [8] (Teorema 3).

Theorem 2 obviously holds (and so does Theorem 1) if we allow g to be complex-valued, and redefine $\mathscr{F}_1^*(\Phi; c, d, \varepsilon_0)$ appropriately. In particular, if one takes $g(x) = \exp[i(t, x)]$, $x \in R^k$, then one obtains

$$(3.68)\qquad |f_n(t) - [\textstyle\sum_{j=0}^{s-2} n^{-j/2} P_j(it)]\exp(-|t|^2/2)| = o(n^{-(s-2)/2}), \qquad n \to \infty,$$

for all t in R^k. However, much more refined expansions of the characteristic function $f_n(t)$ are available (cf. [16], page 204, Theorem 1 for $k = 1$, and [20], Theorem 5.4.1 for arbitrary k), under the same moment conditions as in Theorem 2, and without the assumption of Cramér's condition (such expansions are, in fact, used to prove (3.56); note also that Lemma 1 of Section 1 is an expansion of this kind). It is, therefore, natural to seek out functions g for which asymptotic expansions hold whatever be the type of distribution of $X^{(1)}$. The theorem below is only a preliminary result in this direction. It does not imply (3.68).

THEOREM 3. *Let $\{X^{(r)}\}$ be a sequence of independent and identically distributed k-dimensional random vectors, each with a zero mean vector, a covariance matrix I (the $k \times k$ identity matrix), and a finite moment $\rho_s = E|X^{(1)}|^s$ for some integer s not smaller than three. Let Q_n be the distribution of $(\sum_{r=1}^n X^{(r)})/n^{\frac{1}{2}}$. Then for a real-valued, integrable function g on R^k whose Fourier transform Ψ satisfies*

(3.69) $$\int |t|^{s-2}|\Psi(t)|\,dt < \infty,$$

the asymptotic expansion

(3.70) $$\int g\,d[Q_n - \textstyle\sum_{j=0}^{s-2} n^{-j/2}P_j(-\Phi)] = o(n^{-(s-2)/2}), \qquad n \to \infty$$

holds.

PROOF. We need the following lemma (cf. [20], Theorem 5.4.1).

LEMMA 6. *For $|t| \leqq n^{\frac{1}{2}}(1/8s)\rho_s^{-3/s}$, the characteristic function f_n of Q_n satisfies*

(3.71) $$|f_n(t) - (\textstyle\sum_{j=0}^{s-2} n^{-j/2}P_j(it))\exp(-|t|^2/2)| \leqq c_{16}(k,s)\,\delta(n)n^{-(s-2)/2}\rho_s^{3(s-2)/s}(|t|^s + |t|^{3(s-2)})\exp(-|t|^2/4),$$

where $\delta(n)$ goes to zero as n goes to infinity. Now by Parseval's formula

(3.72) $$\int g\,d[Q_n - \textstyle\sum_{j=0}^{s-2} n^{-j/2}P_j(-\Phi)] = (2\pi)^{-k}\int \Psi(-t)[f_n(t) - (\sum_{j=0}^{s-2} n^{-j/2}P_j(it))\exp(-|t|^2/2)]\,dt.$$

The integral on the right is estimated first over the region $\{|t| \leqq n^{\frac{1}{2}}(1/8s)\rho_s^{-3/s}\}$ by Lemma 6. This is of the order $o(n^{-(s-2)/2})$. Over the complement of this region it is bounded above in absolute value by

(3.73) $$(2\pi)^{-k}\int_{\{|t| > n^{1/2}(1/8s)\rho_s^{-3/s}\}} |\Psi(t)|\,dt + (2\pi)^{-k}\int_{\{|t| > n^{1/2}(1/8s)\rho_s^{-3/s}\}} |\textstyle\sum_{j=0}^{s-2} n^{-j/2}P_j(it))|\exp(-|t|^2/2)\,dt.$$

The first integral is $o(n^{-(s-2)/2})$ because of (3.69), while the second integral is $o(n^{-(s-2)/2})$ because of the presence of the exponential term. □

REMARK. Condition (3.69) implies that g has bounded, continuous derivatives of all orders up to (and including) $s-2$.

EXAMPLES. The functions $g_1(x) = \exp[-\sum_{i,j=1}^k a_{ij}(x_i - m_i)(x_j - m_j)]$ where $A = ((a_{ij}))$ is a positive definite symmetric matrix and $m = (m_1, \cdots, m_k)$ is a given vector in R^k, $g_2(x) = \prod_{i=1}^k (1+x_i^2)^{-1}$, and any function whose Fourier transform has a compact support (e.g., $\prod_{i=1}^k (\sin^2 x_i)/x_i^2$) meet the requirement (3.69).

Before stating the final result let us observe that one cannot expect the error $|\int g\, d(Q_n - \Phi)|$ to be of order $o(n^{-\frac{1}{2}})$ if the second term $n^{-\frac{1}{2}} \int g\, dP_1(-\Phi)$ in the asymptotic expansion (whenever appropriate) does not vanish. It does vanish, however, if g is symmetric (about zero) in each co-ordinate for every set of values of the remaining co-ordinates, in which case we shall say that g is *symmetric.* It also vanishes if the third order moments of $X^{(1)}$ (i.e., $E(X_i^{(1)} X_j^{(1)} X_l^{(1)})$ for all i, j, l) vanish (e.g., if $X^{(1)}$ and $-X^{(1)}$ have the same distribution). Esseen [14] (Theorem 1, page 92) has shown that the error is of the order $O(n^{-k/(k+1)})$ uniformly over all indicator functions of spheres centered at the origin provided $E|X^{(1)}|^4$ is finite. Theorem 4 below provides some classes of functions (under varying restrictions on $\{X^{(r)}\}$) for which the error of normal approximation is $O(n^{-1})$.

THEOREM 4. *Let $\{X^{(r)}\}$ be a sequence of independent and identically distributed k-dimensional random vectors each being centered at expectation, and having the covariance matrix I and a finite fourth moment $\rho_4 = E|X^{(1)}|^4$. Let g be a real-valued, bounded, Borel measurable function on R^k. Let also the following hypothesis (H) hold: either g is symmetric, or all the third order moments of $X^{(1)}$ are equal to those of Φ. Then each of the conditions* (a), (b), (c) *below implies*

$$|\textstyle\int g\, d(Q_n - \Phi)| = O(n^{-1}), \qquad n \to \infty. \tag{3.74}$$

(a) *g is integrable and has an integrable Fourier transform Ψ satisfying*

$$\int_{\{|t| > c\}} |t| \cdot |\Psi(t)|\, dt = O(c^{-1}), \qquad c \to \infty. \tag{3.75}$$

(b) *Cramér's condition* (i.e., $\limsup_{|t| \to \infty} |f^{(1)}(t)| < 1$) *holds, and*

$$\sup\{\textstyle\int \omega_{g_u}(S(\cdot, \varepsilon))\, d\Phi; u \in R^k\} = O(\varepsilon), \qquad \varepsilon \downarrow 0. \tag{3.76}$$

(c) *The distribution of the random vector $X^{(1)}$ has a non-zero absolutely continuous component.*

PROOF. (a) By the hypothesis (H) and Parseval's formula,

$$\begin{aligned}\int g\, d(Q_n - \Phi) &= \int g\, d(Q_n - \Phi - n^{-\frac{1}{2}} P_1(-\Phi)) \\ &= (2\pi)^{-k} \int \Psi(-t)[f_n(t) - (1 + n^{-\frac{1}{2}} P_1(it)) \exp(-|t|^2/2)]\, dt.\end{aligned} \tag{3.77}$$

Over the region $\{|t| \leq n^{\frac{1}{2}}(1/32)\rho_4^{-\frac{3}{4}}\}$ the last integral is of the order $O(n^{-1})$, by Lemma 6. Over the complement of this region it is bounded above in absolute value by

$$\begin{aligned}&(2\pi)^{-k} \int_{\{|t| > n^{1/2}(1/32)\rho_4^{-3/4}\}} |\Psi(t)|\, dt \\ &\quad + (2\pi)^{-k} \int_{\{|t| > n^{1/2}(1/32)\rho_4^{-3/4}\}} |1 + n^{-\frac{1}{2}} P_1(it)| \exp(-|t|^2/2)\, dt.\end{aligned} \tag{3.78}$$

The first integral is of the order $O(n^{-1})$ because of (3.75), and the second integral is of the order $o(n^{-1})$ because of the presence of the exponential term.

(b) In this case (3.74) is a consequence of Theorem 2 and the first equality in (3.77).

(c) In this case (3.74) follows from the first equality in (3.77) and Remark 2 following Theorem 2. □

REMARK 1. If one assumes, instead of (H), that all moments of order s and less (s is an integer larger than two) of $X^{(1)}$ coincide with the corresponding moments of Φ, then under the condition (b) one has, by Theorem 2,

$$\sup\{|\int g\,d(Q_n-\Phi)|;g\in\mathscr{F}_1{}^*(\Phi;c,d,\varepsilon_0)\}=o(n^{-(s-2)/2}), \tag{3.79}$$

since the polynomials $P_j(it)$ (see (1.5) and remember that every cumulant of Φ of order three or more is zero), and, hence, the corresponding signed measures $P_j(-\Phi)$, vanish identically for $j=1,2,\cdots,s-2$. If, in this case, (c) holds, then (by (3.67),

$$|Q_n-\Phi|(R^k)=o(n^{-(s-2)/2}). \tag{3.80}$$

REMARK 2. All the results in this article may be stated for convergence to a normal distribution Φ_Σ with an arbitrary positive definite covariance matrix Σ. This may be done directly by using expansions of characteristic functions in terms of the characteristic function of such a normal distribution (cf. Bikjalis [7]), or by noting that (cf. [5], Section 4) if $\{Q_n\}$ converges weakly to Φ_Σ, then for every bounded, measurable g, one has

$$\int g\,d(Q_n-\Phi_\Sigma)=\int gT^{-1}\,d(P_n-\Phi), \tag{3.81}$$

where $\{P_n\}$ converges weakly to Φ, and $gT^{-1}(x)=g(T^{-1}(x))$, T being a linear operator satisfying

$$T'T=\Sigma^{-1}. \tag{3.82}$$

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4.3 "On errors of normal approximation"

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ON ERRORS OF NORMAL APPROXIMATION

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Let Q_n be the distribution of the normalized sum of n independent random vectors with values in R^k, and Φ the standard normal distribution in R^k. In this article the error $|\int f d(Q_n - \Phi)|$ is estimated (for essentially) all real-valued functions f on R^k which are integrable with respect to Q_n when sth moments are finite, and for which the error may be expected to go to zero. When specialized to known examples, the (main) error bound provides precise rates of convergence.

0. Introduction and summary. In this article we study rates of convergence for the classical central limit theorem. For the sake of simplicity let us assume in this section that $\{X_n : n \geqq 1\}$ is a sequence of i.i.d. random vectors with values in $R^k (k \geqq 1)$ and that

$$(0.1) \qquad EX_1 = 0\,, \qquad \text{Cov}\, X_1 = I\,, \qquad \rho_3 \equiv E\|X_1\|^3 < \infty\,.$$

Here I is the identity matrix. The classical central limit theorem asserts that the distribution Q_n of $n^{-\frac{1}{2}}(X_1 + \cdots + X_n)$ converges weakly to the standard normal distribution Φ on R^k, as $n \to \infty$. This means that

$$(0.2) \qquad \lim_{n\to\infty} |\textstyle\int_{R^k} f d(Q_n - \Phi)| = 0$$

for every bounded measurable real-valued function f on R^k whose points of discontinuity form a Φ-null set. It is reasonable to expect that the rate of convergence in (0.2) will depend on the range $M_0(f)$ of f (see (1.6)) and on the average oscillation function (see (1.3))

$$(0.3) \qquad \bar{\omega}_f(\varepsilon : \Phi) = \textstyle\int_{R^k} \omega_f(x, \varepsilon)\Phi(dx) \quad (\varepsilon > 0)\,.$$

Indeed, a variant of a general theorem due to Billingsley and Topsøe [9] (Theorem 1) proved in [3] (Theorem 1′) shows that in order that the relation

$$(0.4) \qquad \lim_n \sup_{f\in\mathscr{F}} |\textstyle\int_{R^k} f d(P_n - \Phi)| = 0$$

be satisfied for a given class $\mathscr{F}$ of bounded Borel measurable functions on R^k and for every sequence of probability measures $\{P_n : n \geqq 1\}$ converging weakly to Φ, it is necessary as well as sufficient that one has

$$(0.5) \qquad \sup_{f\in\mathscr{F}} M_0(f) < \infty\,, \qquad \lim_{\varepsilon\downarrow 0} \sup_{f\in\mathscr{F}} \bar{\omega}_f(\varepsilon : \Phi) = 0\,.$$

The second inequality (1.11) in our theorem implies, when specialized to $r = 0$,

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$s = 3$, that one has

$$(0.6) \qquad |\textstyle\int_{R^k} f d(Q_n - \Phi)| \leqq c_1' M_0(f) \rho_3 n^{-\frac{1}{2}} + c_2' \bar{\omega}_f(c_3' \rho_3 n^{-\frac{1}{2}} \log n : \Phi) .$$

Thus it provides an effective bound for every bounded almost surely (w.r.t. Φ) continuous f (uniformly over every class $\mathscr{F}$ satisfying (0.5)). Further, (1.10) shows that the factor $\log n$ in (0.6) may be removed if one replaces $\bar{\omega}_f$ by the function (of ε)

$$(0.7) \qquad \tilde{\omega}_f(\varepsilon : \Phi) \equiv \sup_{y \in R^k} \omega_{f_y}(\varepsilon : \Phi) ,$$

where f_y is the translate of f by y (see (1.5)), so that one obtains the important inequality

$$(0.8) \qquad |\textstyle\int_{R^k} f d(Q_n - \Phi)| \leqq c_1 M_0(f) \rho_3 n^{-\frac{1}{2}} + c_2 \tilde{\omega}_f(c_3 \rho_3 n^{-\frac{1}{2}} : \Phi) .$$

The applications (2.1), (2.5) follow from (0.8). The inequality (0.6) is still useful in estimating some elusive quantities like the Prokhorov distance between Q_n and Φ (see [5], Application 4.3, pages 472–473), and error bounds for functions f for which $\bar{\omega}_f$ is small and $\tilde{\omega}_f$ is large. As special cases of (0.6), (0.8) (or (2.1), (2.5)) one can obtain virtually all known 'uniform' or Berry–Esseen type bounds. Because $M_0(f) = \infty$ if f is unbounded (and so may be $\tilde{\omega}_f(\varepsilon : \Phi)$), (0.6), (0.8) are unsuitable for unbounded f. It turns out that the proper things to look at are $M_r(f)$, $\tilde{\omega}_g(\varepsilon : \Phi_{r_0})$ defined by (1.4), (1.6), (1.7), (1,9) and (1.13), and one obtains the very general inequalities (1.10), (1.11). This takes care of all functions which are integrable with respect to Q_n under the given moment condition. Application 2 provides the simplest examples of unbounded functions (namely those which are Lipschitzian) to which (1.10) may be applied; however, the same inequality (2.7) would hold if $\tilde{\omega}_g(\varepsilon : \Phi_{r_0}) \leqq d_1 \varepsilon^\alpha (\varepsilon > 0)$, where g, Φ_{r_0} are defined by (1.13), (1.7). Perhaps of greater significance is the fact that (even for bounded f) (1.10) uses different features (of growth and average smoothness) of f for different values of r. This enables one to obtain the very general inequality (2.13). In turn this inequality yields essentially all known 'nonuniform' rates (e.g., (2.16), (2.17)) and the 'mean central limit theorem' (2.18).

References to some earlier work are given in Section 2. It should be mentioned, however, that even for the i.i.d. case and bounded f the present results are significant extensions of corresponding results in [5] (Theorems 4.1, 4.2). For general non-identically distributed random vectors the theorem improves earlier investigations [2]–[4] of the author in two directions. First, with $s = 3$, it relaxes the moment condition assumed earlier (namely, $\rho_{3+\delta} < \infty$ for some $\delta > 0$). Secondly, of course, it is much more general in scope, being able to deal with all integrable functions and yielding existing as well as new nonuniform rates.

The proof of (1.10) is based on a number of technical lemmas which are stated in Section 3 without proof. Some of these are either available in the current literature or easily deduced from them. The other lemmas are new. Detailed proofs of all lemmas will appear in [6]. To facilitate comprehension of the proof of the theorem we briefly sketch the main ideas here. If the distribution Q_1 of X_1 has an integrable characteristic function (ch. f.) $\hat{Q}_1$, then the ch. f. $\hat{Q}_n$ of Q_n is integrable for all n, and one can use Fourier inversion to obtain the density of the signed measure $Q_n - \Phi$ in terms of $\hat{Q}_n - \hat{\Phi}$. To get an estimate of the variation norm $||Q_n - \Phi||$ one may integrate the bound of the density so obtained over R^k. Although precise estimates of $\hat{Q}_n - \hat{\Phi}$ are available, integration over the unbounded domain R^k results in a loss of precision; to overcome this one also incorporates estimates of $D^\alpha(\hat{Q}_n - \hat{\Phi})$ (where α is a nonnegative integer vector and D^α is the αth derivative) in this scheme and uses the powerful Lemma 8. Since this Lemma can be used only if $\int ||x||^{k+1}Q_n(dx)$ is finite, one has to resort to truncation. Lemmas 1, 5, and 6 allow one to take care of the perturbation due to truncation, and a fairly precise estimate of $||Q_n - \Phi||$ is obtained. For integration of unbounded functions, however, one needs to estimate $\int ||x||^r|Q_n - \Phi|(dx)$, where $|Q_n - \Phi|$ is the total variation (measure) of $Q_n - \Phi$. The procedure for this is similar; one looks at the signed measure $||x||^{r_0}(Q_n - \Phi)(dx)$, where r_0 is defined by (1.9), instead of $Q_n - \Phi$. We use r_0 instead of r because $||x||^r$ is not a polynomial for odd r and the Fourier–Stieltjes transform of $||x||^r(Q_n - \Phi)(dx)$ for an odd r is not nearly as well-behaved as that for an even integer r. However, this change from r to r_0 does not entail any essential loss of generality; for one merely changes Φ_r to Φ_{r_0} (see (1.7)) and, the normal density being rapidly decreasing at infinity, this change is insignificant. In the general case (i.e., when X_1 does not have a density) we smoothen Q_n by convolving it with a smooth kernel K_ε, apply the above argument to $(Q_n - \Phi) * K_\varepsilon$ and, for final accounting, use the general Lemma 7. Although in the actual proof one uses expansions of $\hat{Q}_n$ (and $D^\alpha\hat{Q}_n$) beyond the first term $\hat{\Phi}$ for greater precision, the ideas are quite similar to those explained above.

It is noteworthy that the present method allows one to obtain analogous significant extensions of existing results on asymptotic expansions in case Q_1 has a density (as given in Bikjalis [7], Theorem 3) or when Q_1 satisfies the so-called *Cramér's condition* (as given in Bhattacharya [5], Theorem 4.3). Indeed, the derivation of such an extension in the first case using Lemma 3 is simpler (than the present proof), since, as indicated in the sketch above, the smoothing by convolution in the last step may be avoided. These new results and details of their derivations will appear in [6] and will not be discussed any further here.

1. Notation and the main result. Let $X_1, \cdots, X_n$ be n independent random vectors with values in R^k. Throughout this article we assume, without any essential loss of generality,

$$EX_j = 0 \quad (1 \leqq j \leqq n), \qquad n^{-1} \sum_{j=1}^n \operatorname{Cov} X_j = I \tag{1.1}$$

where EX_j is the expectation (vector) and Cov X_j the covariance matrix of X_j, and I is the $k \times k$ identity matrix. We write

$$\rho_{s,j} = E||X_j||^s \quad (1 \leqq j \leqq n), \qquad \rho_s = n^{-1} \sum_{j=1}^n \rho_{s,j} \quad (s > 0), \tag{1.2}$$

where $||\cdot||$ denotes Euclidean norm in R^k. Let f be a real-valued Borel measurable function on R^k. We define

$$\omega_f(x, \varepsilon) = \sup\{|f(y) - f(x)| : y \in R^k, ||y - x|| < \varepsilon\} \quad (x \in R^k, \varepsilon > 0) . \tag{1.3}$$

For a given measure ν on R^k (measures and signed measures are defined on the Borel sigma-field) define

$$\begin{aligned} \bar{\omega}_f(\varepsilon : \nu) &= \textstyle\int_{R_k} \omega_f(x, \varepsilon)\nu(dx) , \\ \tilde{\omega}_f(\varepsilon : \nu) &= \sup_{y \in R^k} \bar{\omega}_{f_y}(\varepsilon : \nu) , \end{aligned} \tag{1.4}$$

where the translate f_y of f is defined by

$$f_y(x) = f(x + y) \qquad x \in R^k . \tag{1.5}$$

For a given nonnegative integer r define

$$\begin{aligned} M_r(f) &= \sup_{x \in R^k} (1 + ||x||^r)^{-1}|f(x)| , \qquad r > 0 , \\ M_0(f) &= \sup\{|f(x) - f(y)| : x, y \in R^k\} . \end{aligned} \tag{1.6}$$

For a given finite (signed) measure ν on R^k and for a given $r_0 \geqq 0$, define a new (signed) measure ν_{r_0} by

$$\begin{aligned} \nu_{r_0}(dx) &= (1 + ||x||^{r_0})\nu(dx) , \qquad r_0 > 0 , \\ \nu_0 &= \nu . \end{aligned} \tag{1.7}$$

Let Q_n denote the distribution of $n^{-\frac{1}{2}} \sum_{j=1}^n X_j$ and let Φ denote the standard normal distribution on R^k. Our main result is the following.

THEOREM. *Assume*

$$\rho_s < n^{(s-2)/2}/(8k) \tag{1.8}$$

for some integer $s \geqq 3$. *Let* r *be a nonnegative integer,* $0 \leqq r \leqq s$, *and define*

$$\begin{aligned} r_0 &= r \qquad \textit{if } r \textit{ is even,} \\ &= r + 1 \qquad \textit{if } r \textit{ is odd.} \end{aligned} \tag{1.9}$$

There exist constants c_i, c_i' $(i = 1, 2, 3)$ *depending only on* k, r, s, *such that the inequalities*

$$\begin{aligned} |\textstyle\int_{R^k} f d(Q_n - \Phi)| \leqq{}& c_1 M_r(f) \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} \\ &+ c_2 \tilde{\omega}_g(c_3 \rho_3 n^{-\frac{1}{2}} : \Phi_{r_0}) , \end{aligned} \tag{1.10}$$

and

$$\begin{aligned} |\textstyle\int_{R^k} f d(Q_n - \Phi)| \leqq{}& c_1' M_r(f) \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} \\ &+ c_2' \bar{\omega}_f(c_3' \rho_3 n^{-\frac{1}{2}} \log n : \Phi) \end{aligned} \tag{1.11}$$

hold for every real-valued Borel measurable function f *on* R^k *satisfying*

$$M_r(f) < \infty . \tag{1.12}$$

Here

$$g(x) = (1 + ||x||^{r_0})^{-1} f(x) \quad \text{if} \quad r > 0\,, \qquad = f(x) \quad \text{if} \quad r = 0\,. \tag{1.13}$$

Assumption (1.8) *may be replaced simply by*

$$\rho_3 < \infty\,, \tag{1.14}$$

if $r = 0$.

2. Applications.

2.1. Let A be a Borel subset of R^k. Take $r = 0$, $s = 3$, $f = I_A$ (the indicator function of A) in the theorem. Inequality (1.10) then reduces to

$$|Q_n(A) - \Phi(A)| \leqq c_1 \rho_3 n^{-\frac{1}{2}} + c_2 \sup_{y \in R^k} \Phi((\partial A)^{\varepsilon'} + y)\,, \tag{2.1}$$

where

$$\varepsilon' = c_3 \rho_3 n^{-\frac{1}{2}}\,, \tag{2.2}$$

∂A is the topological *boundary* of A and $(\partial A)^{\varepsilon'}$ is the set of all points whose distances from ∂A are less than ε'. This follows from

$$M_0(I_A) = 1\,, \qquad \omega_{I_A}(x, \varepsilon) = I_{(\partial A)^\varepsilon}(x)\,, \qquad x \in R^k\,. \tag{2.3}$$

Denoting by $\mathscr{A}_\alpha^*(d : \Phi)$ the *class of all Borel sets A satisfying*

$$\sup_{y \in R^k} \Phi((\partial A)^\varepsilon + y) \leqq d\varepsilon^\alpha\,, \qquad \varepsilon > 0\,, \tag{2.4}$$

for a given pair of positive numbers α, d, one has (from (2.1))

$$\sup_{A \in \mathscr{A}_\alpha^*(d:\Phi)} |Q_n(A) - \Phi(A)| \leqq c_1 \rho_3 n^{-\frac{1}{2}} + c_2 d(c_3 \rho_3 n^{-\frac{1}{2}})^\alpha\,, \tag{2.5}$$

whenever (1.14) holds. Examples of various classes of sets A satisfying (2.4) uniformly for $\alpha = 1$ and some d are given in [3]. Among these is the class $\mathscr{C}$ *of all Borel measurable convex subsets of* R^k. Inequalities similar to (2.1), (2.5) were first obtained independently by Von Bahr [14] and Bhattacharya [2] under somewhat more stringent moment conditions. For the special class $\mathscr{C}$ (replacing $\mathscr{A}_\alpha^*$ by $\mathscr{C}$ and α by 1) inequality (2.5) was also obtained by Sazonov [13] in the i.i.d. case.

2.2. An immediate application of (1.10) is to a function f satisfying

$$|f(x) - f(y)| \leqq d_1 ||x - y||^\alpha\,, \qquad M_r(f) < \infty\,, \qquad x, y \in R^k\,, \tag{2.6}$$

for some α, $0 < \alpha \leqq 1$, some $d_1 > 0$, and some integer r, $0 \leqq r \leqq s$. For such a function (1.10) yields

$$|\textstyle\int_{R^k} f d(Q_n - \Phi)| \leqq c_1 M_r(f) \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} + c_2 d_1 (c_3 \rho_3 n^{-\frac{1}{2}})^\alpha\,. \tag{2.7}$$

2.3. For an application of a different nature, let A be a Borel set and define

$$f(x) = (1 + d^s(0, \partial A)) I_{A'}(x)\,, \qquad x \in R^k\,, \tag{2.8}$$

where

$$A' = A \quad \text{if} \quad 0 \notin R^k, \qquad = R^k \backslash A \quad \text{if} \quad 0 \in R^k, \tag{2.9}$$

and $d(0, \partial A)$ is the *Euclidean distance between* 0 (the origin) *and* ∂A. Note that

$$M_s(f) \leqq 1 . \tag{2.10}$$

Taking $r = s$ in the theorem, one has

$$\begin{aligned} |g(x+y+z) - g(x+y)| &\leqq (1 + \|x+y\|^{s_0})^{-1}|f(x+y+z) - f(x+y)| + c_5\varepsilon \\ &\leqq (1 + \|x+y\|^{s_0})^{-1}(1 + d^s(0, \partial A))I_{(\partial A)^\varepsilon}(x+y) + c_5\varepsilon \\ &\leqq (1 + [d(0, \partial A) - \varepsilon]^{s_0})^{-1}(1 + d^s(0, \partial A))I_{(\partial A)^\varepsilon}(x+y) + c_5\varepsilon \\ &\leqq c_6 I_{(\partial A)^\varepsilon}(x+y) + c_5\varepsilon , \qquad \|z\| < \varepsilon,\ 0 < \varepsilon < c_7 , \end{aligned} \tag{2.11}$$

for a suitable constant c_7. The constants c_5, c_6, c_7 as well as c_8—c_{13} below depend only on s and k. On integration with respect to Φ_{s_0}, (2.11) yields

$$\bar{\omega}_g(\varepsilon : \Phi_{s_0}) \leqq c_6 \sup_{y \in R^k} \Phi_{s_0}((\partial A)^\varepsilon + y) + c_8\varepsilon . \tag{2.12}$$

Hence (1.10) reduces to

$$\begin{aligned} (1 + d^s(0, \partial A))|Q_n(A) - \Phi(A)| &= |\textstyle\int_{R^k} f d(Q_n - \Phi)| \\ &\leqq c_1 \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} + c_9 \sup_{y \in R^k} \Phi_{s_0}((\partial A)^{\varepsilon'} + y) , \end{aligned} \tag{2.13}$$

where

$$\varepsilon' = c_{10}\rho_3 n^{-\frac{1}{2}} . \tag{2.14}$$

For the class $\mathscr{C}$ of convex sets one has (see von Bahr [14], Lemmas 8, 9)

$$\sup_{C \in \mathscr{C}} \Phi_{s_0}((\partial C)^{\varepsilon'} + y) \leqq c_{11}\varepsilon' . \tag{2.15}$$

Using (2.15) in (2.13) one obtains a result announced in Rotar' [12] (Theorem 2):

$$\sup_{C \in \mathscr{C}} (1 + d^s(0, \partial C))|Q_n(C) - \Phi(C)| \leqq c_{12} \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} . \tag{2.16}$$

Taking $C = (-\infty, x]$, $x \in R^k$, one obtains

$$\begin{aligned} |F_n(x) - \Phi(x)| &\leqq c_{13}(1 + \min\{|x_i|^s : i = 1, \cdots, k\})^{-1} \\ &\quad \times \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} , \qquad x = (x_1, \cdots, x_k) \in R^k , \end{aligned} \tag{2.17}$$

where $F_n(\cdot)$ and $\Phi(\cdot)$ are the distributions of Q_n and Φ, respectively. For $k = 1$, (2.17) was proved by Nagaev [11] in the i.i.d. case. For $k = 1$, (2.17) immediately yields the so-called *mean central limit theorem*:

$$\begin{aligned} \|F_n - \Phi\|_p &\equiv (\textstyle\int_{R^1} |F_n(x) - \Phi(x)|^p)^{1/p} \\ &\leqq c_{14} \max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\} \end{aligned} \tag{2.18}$$

for all $p > 1/s$. Here c_{14} depends only on s and p. Inequalities like (2.18) were first obtained by Agnew [1] and Esseen [10].

3. Proof of the theorem. We shall only give a detailed proof of inequality (1.10), and outline the modifications necessary to prove (1.11). Note that all the applications above stem from (1.10).

We need some additional notation. Let $\chi_{r,j}(t)$ denote the rth *cumulant* of the random variable $\langle t, X_j \rangle$, where $\langle\ ,\ \rangle$ denotes Euclidean inner product, $t \in R^k$, and r is a positive integer. Define

$$\chi_r(it) = n^{-1} i^r \sum_{j=1}^n \chi_{r,j}(t) , \tag{3.1}$$
$$\tilde{P}_r(it) = \sum_{m=1}^r \frac{1}{m!} \left\{ \sum{}^* \frac{\chi_{r_1+2}(it)}{(r_1+2)!} \cdots \frac{\chi_{r_m+2}(it)}{(r_m+2)!} \right\} ,$$

where the summation $\sum^*$ is over all m-tuples of positive integers $(r_1, \cdots, r_m)$ satisfying

$$\sum_{l=1}^m r_l = r . \tag{3.2}$$

Associated with the polynomials $\tilde{P}_r$ are the functions P_r defined by

$$P_r(x) = (2\pi)^{-k} \int_{R^k} \exp\{-i\langle t, x\rangle - \tfrac{1}{2}||t||^2\} \tilde{P}_r(it)\, dt . \tag{3.3}$$

It is easy to show that P_r is a linear combination of the standard normal density on R^k and some of its derivatives. For convenience we write

$$\tilde{P}_0(it) \equiv 1 , \qquad t \in R^k , \tag{3.4}$$
$$P_0(x) = (2\pi)^{-k/2} \exp\{-\tfrac{1}{2}||x||^2\} , \qquad x \in R^k .$$

We also define *truncated* random vectors

$$\begin{aligned} Y_j &= X_j \quad \text{if} \quad ||X_j|| \leqq n^{\frac{1}{2}} \\ &= 0 \quad \text{if} \quad ||X_j|| > n^{\frac{1}{2}} , \\ Z_j &= Y_j - EY_j , \qquad 1 \leqq j \leqq n . \end{aligned} \tag{3.5}$$

Write

$$D = n^{-1} \sum_{j=1}^n \operatorname{Cov} Z_j , \qquad a_n = n^{-\frac{1}{2}} \sum_{j=1}^n EY_j , \tag{3.6}$$

and define *polynomials* $\tilde{P}_r'$ as in (3.1) with $\chi_{r,j}(t)$ replaced by the rth cumulant of $\langle t, Z_j \rangle$. If D is nonsingular, define functions P_r' by

$$P_r'(x) = (2\pi)^{-k} \int_{R^k} \exp\{-i\langle t, x\rangle - \tfrac{1}{2}\langle t, Dt\rangle\} \tilde{P}_r'(it)\, dt , \qquad r > 0 , \tag{3.7}$$
$$P_0'(x) = (2\pi)^{-k/2} (\operatorname{Det} D)^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}\langle x, D^{-1}x\rangle\} , \qquad x \in R^k .$$

Let Q_n', Q_n'' denote the distributions of $n^{-\frac{1}{2}}(Z_1 + \cdots + Z_n)$ and $n^{-\frac{1}{2}}(Y_1 + \cdots + Y_n)$, respectively. We also write

$$\rho_r' = n^{-1} \sum_{j=1}^n E||Z_j||^r . \tag{3.8}$$

Finally, if D is nonsingular we let B denote the unique symmetric positive definite matrix satisfying

$$B^2 = D^{-1} . \tag{3.9}$$

The following series of lemmas will be needed. Detailed proofs of these will appear in the forthcoming monograph [6], although some of them are essentially proved in the literature.

LEMMA 1. *Let $\rho_s < \infty$ for some integer $s > 3$. Then one has*

$$(3.10) \qquad ||a_n|| \leqq k^{\frac{1}{2}} n^{-(s-2)/2} \rho_s\,, \qquad |\langle t, Dt\rangle - ||t||^2| \leqq 2kn^{-(s-2)/2}\rho_s \qquad t \in R^k\,,$$

and

$$(3.11) \qquad \begin{aligned} \rho_r' &\leqq 2^r \rho_r & &\text{if } 2 \leqq r \leqq s\,, \\ &\leqq 2^r n^{(r-s)/2} \rho_s & &\text{if } r > s\,. \end{aligned}$$

This type of estimate was earlier obtained by Bikjalis [7] (pages 411–412), [8] (Lemma 10).

LEMMA 2. *Let m be an integer not smaller than three. For every integer $r \leqq m$ and every nonnegative integer vector $\alpha = (\alpha_1, \cdots, \alpha_k)$ satisfying $\alpha_1 + \cdots + \alpha_k \leqq 3r$, one has*

$$|(D^\alpha \tilde{P}_r')(it)| \leqq c_{15}(1 + \rho_2'^{r(m-3)/(m-2)})(1 + ||t||^{3r-\alpha_1-\cdots-\alpha_k}) \cdot \rho_m'^{r/(m-2)}$$

where $D^\alpha = (\partial/\partial t_1)^{\alpha_1} \cdots (\partial/\partial t_k)^{\alpha_k}$ and c_{15} depends only on r, m, k, and α. If $\alpha_1 + \cdots + \alpha_k > 3r$, then $D^\alpha \tilde{P}_r'$ is identically zero.

A special case of Lemma 2 appears in Bikjalis [8] (Lemma 17).

LEMMA 3. *Suppose D is nonsingular. Let*

$$(3.12) \qquad \eta_r \equiv n^{-1} \sum_{j=1}^n E||BZ_j||^r\,.$$

Let m be an integer not smaller than three. Then there exist two positive numbers c_{16}, c_{17} depending only on m and k such that if

$$(3.13) \qquad ||t|| \leqq c_{16} n^{(m-2)/2m} / \eta_m^{1/m}\,,$$

then

$$(3.14) \qquad \begin{aligned} &|D^\alpha[\textstyle\prod_{j=1}^n E(\exp\{\langle iBt, n^{-\frac{1}{2}}X_j\rangle\}) - \sum_{r=0}^{m-3} n^{-r/2}\tilde{P}_r'(iBt) \cdot \exp\{-\frac{1}{2}||t||^2\}]| \\ &\quad \leqq c_{17}\eta_m n^{-(m-2)/2}[||t||^{m-\alpha_1-\cdots-\alpha_k} + ||t||^{3(m-2)+\alpha_1+\cdots+\alpha_k}] \cdot \exp\{-\tfrac{1}{4}||t||^2\}\,, \end{aligned}$$

for every nonnegative integer vector $\alpha = (\alpha_1, \cdots, \alpha_k)$ satisfying $\alpha_1 + \cdots + \alpha_k \leqq m$.

Special cases of this lemma appear in Bikjalis [7] (Lemma 8), [8] (Lemma 16).

LEMMA 4. *Suppose (1.8) holds for some integer $s \geqq 3$. Let $\hat{Q}_n'$ denote the characteristic function of Q_n'. If*

$$(3.15) \qquad ||t|| \leqq n^{\frac{1}{2}}/(16\rho_3)\,,$$

then

$$|(D^\alpha \hat{Q}_n')(t)| \leqq c_{18}(1 + ||t||^{\alpha_1+\cdots+\alpha_k}) \exp\{-\tfrac{5}{24}||t||^2\}$$

for every nonnegative integer vector $\alpha = (\alpha_1, \cdots, \alpha_k)$. Here c_{18} depends only on α and k.

This result is essentially due to Rotar' [12] (Lemma 7).

LEMMA 5. *Suppose* (1.8) *holds for some integer* $s \geqq 3$. *Then* D *is nonsingular, and for every integer* r, $0 \leqq r \leqq s-2$, *one has*

$$n^{-r/2}|P_r(x) - P_r'(x)| \leqq c_{19}\rho_s n^{-(s-2)/2}(1 + ||x||^{3r+2}) \exp\{-\tfrac{1}{6}||x||^2 + ||x||\},$$

$$(3.16) \qquad n^{-r/2}|P_r(x + a_n) - P_r(x)| \leqq c_{20}\rho_s n^{-(s-2)/2}(1 + ||x||^{3r+1}) \cdot \exp\left\{-\tfrac{1}{2}||x||^2 + \frac{1}{8k^{\frac{1}{2}}}||x||\right\} \qquad x \in R^k,$$

where c_{19}, c_{20} *depend only on* r, s, k.

LEMMA 6. *Assume* (1.8) *for some integer* $s \geqq 3$. *Recall that* Q_n'' *is the distribution of* $n^{-\frac{1}{2}}(Y_1 + \cdots + Y_n)$. *For every integer* r, $0 \leqq r \leqq s$, *there is a positive number* c_{21} *(depending only on* s, k, *and* r*) such that*

$$\int_{R^k} ||x||^r |Q_n - Q_n''|(dx) \leqq c_{21}\rho_s n^{-(s-2)/2},$$

where $|\mu|$ *denotes the total variation (measure) of a finite signed measure* μ.

LEMMA 7. *Let* μ *be a finite measure and* ν *a finite signed measure on* R^k. *Let* ε *be a positive number and* K_ε *a probability measure on* R^k *satisfying*

$$(3.17) \qquad \beta \equiv K_\varepsilon(\{x : ||x|| < \varepsilon\}) > \tfrac{1}{2}.$$

Then for each real-valued, Borel measurable bounded function f *on* R^k *one has*

$$|\int_{R^k} f d(\mu - \nu)| \leqq (2\beta - 1)^{-1}[||f||_\infty ||(\mu - \nu) * K_\varepsilon|| + \bar{\omega}_f(2\varepsilon : |\nu|)],$$

where $||f||_\infty = \sup\{|f(x)| : x \in R^k\}$, $|\nu|$ *is the total variation of* ν, *and* $*$ *denotes convolution.*

This is proved in [5] (Lemma 2.2, inequality (2.14)). Finally one has

LEMMA 8. *Let* h *be integrable with respect to Lebesgue measure on* R^k *and satisfy*

$$\int_{R^k} ||x||^{k+1}|h(x)|\, dx < \infty.$$

Then there exists a positive constant c_{22} *depending only on* k *such that*

$$||h||_1 \leqq c_{22} \max\{||D^\beta \hat{h}||_1 : 0 \leqq \beta_1 + \cdots + \beta_k \leqq k + 1\},$$

where $||\ ||_1$ *denotes* L^1*-norm,* $\hat{h}$ *is the Fourier transform of* h *and* $\beta = (\beta_1, \cdots, \beta_k)$ *is a nonnegative integer vector.*

The above lemma is perhaps well known to analysts.

After these preliminaries we proceed to prove (1.10). The constants c_{23}—c_{47} below do not depend on anything other than r, s, k. The symbol $\int h\, d\mu$ denotes integration of h with respect to μ over the whole space R^k. The characteristic function of a probability measure Q is denoted by $\hat{Q}$.

PROOF OF INEQUALITY (1.10). Let Φ', Φ'' denote normal distributions on R^k, Φ' having mean zero and covariance D while Φ'' has mean $-a_n$ and covariance I. One has

$$(3.18) \qquad |\int f d(Q_n - \Phi)| \leqq |\int f d(Q_n - Q_n'')| + |\int f d(Q_n'' - \Phi)|.$$

By Lemma 6,

$$(3.19)\qquad |\textstyle\int fd(Q_n - Q_n'')| \leqq M_r(f) \int (1 - ||x||^r)|Q_n - Q_n''|(dx) \leqq 2c_{23} M_r(f)\rho_s n^{-(s-2)/2} .$$

Also,

$$(3.20)\qquad |\textstyle\int fd(Q_n'' - \Phi)| = |\int f_{a_n} d(Q_n' - \Phi'')| \leqq |\int f_{a_n} d(Q_n' - \Phi')| + |\int f_{a_n} d(\Phi' - \Phi)| + |\int f_{a_n} d(\Phi - \Phi'')| .$$

But, by Lemma 5 (with $r = 0$),

$$(3.21)\qquad \begin{aligned} |\textstyle\int f_{a_n} d(\Phi' - \Phi)| &\leqq M_r(f) \textstyle\int (1 + ||x + a_n||^r)|\Phi' - \Phi|(dx) \\ &\leqq M_r(f) \textstyle\int (1 + 2^r||a_n||^r + 2^r||x||^r)|\Phi' - \Phi|(dx) \\ &\leqq M_r(f)[||\Phi' - \Phi|| + 2^r||a_n||^r||\Phi' - \Phi|| \\ &\qquad + 2^r \textstyle\int ||x||^r|\Phi' - \Phi|(dx)] \leqq c_{24} M_r(f)\rho_s n^{-(s-2)/2} , \\ |\textstyle\int f_{a_n} d(\Phi - \Phi'')| &\leqq M_r(f)[||\Phi - \Phi''|| + 2^r||a_n||^r||\Phi - \Phi''|| \\ &\qquad + 2^r \textstyle\int ||x||^r|\Phi - \Phi''|(dx)] \leqq c_{25} M_r(f)\rho_s n^{-(s-2)/2} . \end{aligned}$$

Note that $||a_n|| \leqq \rho_s n^{-(s-2)/2} \leqq 1/(8k)$ (by Lemma 1 and (1.8)). Hence (3.18) reduces to

$$(3.22)\qquad |\textstyle\int fd(Q_n - \Phi)| \leqq c_{26} M_r(f)\rho_s n^{-(s-2)/2} + |\int f_{a_n} d(Q_n' - \Phi')| .$$

To estimate the second term on the right side of (3.22) we introduce a kernel probability measure K on R^k satisfying

$$(3.23)\qquad K(\{x : ||x|| < 1\}) \geqq \tfrac{3}{4} , \qquad \textstyle\int ||x||^{k+s+2} K(dx) < \infty , \qquad \hat{K}(t) = 0 \quad \text{if} \quad ||t|| \geqq c_{27} , \qquad t \in R^k .$$

One construction of such a probability measure is given in [5] (Lemma 3.10). For $\varepsilon > 0$ define the probability measure K_ε by

$$(3.24)\qquad K_\varepsilon(B) = K(\varepsilon^{-1}B) \qquad B \in \mathscr{B}^k,\ \varepsilon^{-1}B \stackrel{-}{=} \{\varepsilon^{-1}x : x \in B\} .$$

Then one has, by (3.23),

$$(3.25)\qquad K_\varepsilon(\{x : ||x|| < \varepsilon\}) \geqq \tfrac{3}{4} , \qquad \hat{K}_\varepsilon(t) = 0 \quad \text{if} \quad ||t|| \geqq c_{27}/\varepsilon .$$

Now

$$\begin{aligned} &|\textstyle\int f_{a_n} d(Q_n' - \Phi')| \\ &\quad = |\textstyle\int (1 + ||x + a_n||^{r_0})^{-1} f(x + a_n) \cdot (1 + ||x + a_n||^{r_0})(Q_n' - \Phi')(dx)| \\ &\quad \leqq |\textstyle\int (1 + ||x + a_n||^{r_0})^{-1} f(x + a_n)(1 + ||x||^{r_0})(Q_n' - \Phi')(dx)| \\ &\qquad + M_{r_0}(f) \textstyle\int |\,||x + a_n||^{r_0} - ||x||^{r_0}|(Q_n' + \Phi')(dx) , \end{aligned}$$

$$(3.26)\qquad \begin{aligned} &\textstyle\int |\,||x + a_n||^{r_0} - ||x||^{r_0}|(Q_n' + \Phi')(dx) \\ &\quad \leqq r_0||a_n|| \textstyle\int (||x||^{r_0-1} + ||a_n||^{r_0-1})(Q_n' + \Phi')(dx) \\ &\quad \leqq r_0\rho_s n^{-(s-2)/2}[E||n^{-\frac{1}{2}}(Z_1 + \cdots + Z_n)||^{r_0-1} + (8k)^{-r_0+1} \\ &\qquad + \textstyle\int (||x||^{r_0-1} + (8k)^{-r_0+1})\Phi(dx) \\ &\qquad + \textstyle\int (||x||^{r_0-1} + (8k)^{-r_0+1})|\Phi' - \Phi|(dx)] \leqq c_{28}\rho_s n^{-(s-2)/2} , \end{aligned}$$

using Lemmas 1, 4, 5 and inequality (1.8). Hence

$$(3.27)\qquad |\textstyle\int f d(Q_n - \Phi)| \leqq c_{29}(M_r(f) + M_{r_0}(f))\rho_s n^{-(s-2)/2} + |\textstyle\int g_{a_n}(x)(1 + ||x||^{r_0})(Q_n' - \Phi')(dx)|$$

where $g_{a_n}(x) = g(x + a_n)$. By Lemma 7,

$$(3.28)\qquad |\textstyle\int g_{a_n}(x)(1 + ||x||^{r_0})(Q_n' - \Phi')(dx)| \leqq 2(\sup_{x \in R^k} |g(x)|)||(Q_n' - \Phi')_{r_0} * K_\varepsilon|| + 2\tilde{\omega}_g(2\varepsilon : \Phi'_{r_0}),$$

where

$$(3.29)\qquad (Q_n' - \Phi')_{r_0}(dx) = (1 + ||x||^{r_0})(Q_n' - \Phi')(dx).$$

Choose

$$(3.30)\qquad \varepsilon = 16 c_{27} \rho_3 n^{-\frac{1}{2}}.$$

By Lemma 8, writing $|\alpha|$ for the sum of the coordinates of a vector α,

$$(3.31)\qquad ||(Q_n' - \Phi')_{r_0} * K_\varepsilon|| \leqq c_{30} \sum_{|\beta_1+\beta_2| \leqq k+r_0+1} \textstyle\int |D^{\beta_1}(\hat{Q}_n' - \hat{\Phi}')(t) D^{\beta_2}\hat{K}_\varepsilon(t)|\, dt.$$

Since $D^{\beta_2}\hat{K}_\varepsilon(t) = 0$ if $||t|| > n^{\frac{1}{2}}/(16\rho_3)$, and

$$(3.32)\qquad |D^{\beta_2}\hat{K}_\varepsilon(t)| \leqq \textstyle\int \varepsilon^{|\beta_2|}|x^{\beta_2}| K(dx) \leqq c_{31},$$

where one has $x^\alpha = x_1^{\alpha_1} \cdots x_k^{\alpha_k}$ for a nonnegative integer vector $\alpha = (\alpha_1, \cdots, \alpha_k)$,

$$(3.33)\qquad \textstyle\int |D^{\beta_1}(\hat{Q}_n' - \hat{\Phi}')(t) \cdot D^{\beta_2}\hat{K}_\varepsilon(t)|\, dt \leqq c_{31} \int_{\{||t|| \leqq n^{\frac{1}{2}}/(16\rho_3)\}} |D^{\beta_1}(\hat{Q}_n' - \Phi')(t)|\, dt.$$

Now

$$(3.34)\qquad \begin{aligned} &\textstyle\int_{\{||t|| \leqq n^{\frac{1}{2}}/(16\rho_3)\}} |D^{\beta_1}(\hat{Q}_n' - \hat{\Phi}')(t)|\, dt \\ &\quad \leqq \textstyle\int_{\{||t|| \leqq A_n\}} |D^{\beta_1}[\hat{Q}_n'(t) - \sum_{r'=0}^{k+s-1} n^{-r'/2}\tilde{P}'_{r'}(it)\exp\{-\frac{1}{2}\langle t, Dt\rangle\}]|\, dt \\ &\qquad + \textstyle\int |D^{\beta_1}[\sum_{r'=1}^{k+s-1} n^{-r'/2}\tilde{P}'_{r'}(it)\exp\{-\frac{1}{2}\langle t, Dt\rangle\}]|\, dt \\ &\qquad + \textstyle\int_{\{A_n < ||t|| \leqq A_n'\}} |D^{\beta_1}\hat{Q}_n'(t)|\, dt + \int_{\{A_n < ||t|| \leqq A_n'\}} |D^{\beta_1}\hat{\Phi}'(t)|\, dt \\ &\quad = I_1 + I_2 + I_3 + I_4, \end{aligned}$$

say, where (using Lemma 1)

$$(3.35)\qquad \begin{aligned} A_n &\equiv c_{32}(n^{(k+s)/2}/\rho'_{k+s+2})^{1/(k+s+2)} \geqq c_{32}(n^{(k+s)/2-(k+2)/2}/\rho_s 2^{k+s+2})^{1/(k+s+2)} \\ &= c_{33}(n^{(s-2)/2}/\rho_s)^{1/(k+s+2)}, \\ A_n' &\equiv n^{\frac{1}{2}}/(16\rho_3). \end{aligned}$$

The positive constant c_{32} is so chosen as to satisfy

$$(3.36)\qquad ||D||^{\frac{1}{2}} A_n \leqq c_{16}[n^{(k+s)/2}/(||B||^{k+s+2}\rho'_{k+s+2})]^{1/(k+s+2)}.$$

Since $||D|| \leqq \frac{5}{4}$ and $||B||^2 = ||D^{-1}|| \geqq \frac{2}{3}$ by (3.10) and (3.11), such a choice is possible (take $c_{32} = (\frac{4}{5})(\frac{2}{3})c_{16}$). By Lemma 3 we then have (using Lemma 1)

$$(3.37)\qquad I_1 \leqq c_{34}||B||^{k+s+2}\rho'_{k+s+2} n^{-(k+s)/2} \leqq c_{35}\rho_s n^{-(s-2)/2}.$$

By Lemmas 1, 2,

$$(3.38)\qquad \textstyle\int |D^{\beta_1}[n^{-r'/2}\tilde{P}'_{r'}(it)\exp\{-\frac{1}{2}\langle t, Dt\rangle\}]|\, dt \leqq c_{36} n^{-r'/2}\rho'_{r'+2} \leqq c_{36} 2^{r'+2} n^{-r'/2}\rho_{r'+2}$$

if $1 \leqq r' \leqq s-2$. If $s-2 < r' < k+s$, then

(3.39) $$\int |D^{\beta_1}[n^{-r'/2}\tilde{P}'_{r'}(it)\exp\{-\tfrac{1}{2}\langle t, Dt\rangle\}]|\,dt \leqq c_{37}n^{-r'/2}\rho'_{r'+2}$$
$$\leqq c_{37}2^{r'+2}n^{-r'/2+(r'+2-s)/2}\rho_s = c_{38}n^{-(s-2)/2}\rho_s\,.$$

Hence

(3.40) $$I_2 \leqq c_{39}\max\{\rho_m n^{-(m-2)/2} : m = 3, \cdots, s\}\,.$$

By Lemma 4 and (3.35)

(3.41) $$\begin{aligned} I_3 &= \int_{\{A_n < ||t|| \leqq A_n'\}} |D^{\beta_1}\hat{Q}_n'(t)|\,dt \\ &\leqq c_{40}\int_{\{||t||>A_n\}} (1+||t||^{|\beta_1|})\exp\{-\tfrac{5}{24}||t||^2\}\,dt \\ &\leqq c_{40}A_n^{-(k+s+2)}\int (1+||t||^{|\beta_1|})||t||^{(k+s+2)})\exp\{-\tfrac{5}{24}||t||^2\}\,dt \\ &\leqq c_{41}\rho_s n^{-(s-2)/2}\,. \end{aligned}$$

Finally, again using Lemma 1,

(3.42) $$\begin{aligned} I_4 &= \int_{\{A_n < ||t|| \leqq A_n'\}} |D^{\beta_1}\hat{\Phi}'(t)|\,dt \\ &\leqq c_{42}\int_{\{||t||>A_n\}} (1+||t||^{|\beta_1|})\exp\{-\tfrac{3}{8}||t||^2\}\,dt \\ &\leqq c_{42}A_n^{-(k+s+2)}\int (1+||t||^{|\beta_1|})||t||^{k+s+2}\exp\{-\tfrac{3}{8}||t||^2\}\,dt \\ &\leqq c_{43}\rho_s n^{-(s-2)/2}\,. \end{aligned}$$

It follows that

(3.43) $$||(Q_n' - \Phi')^*K_\varepsilon|| \leqq c_{44}\max\{\rho_{m+2}n^{-m/2} : m = 1, \cdots, s-2\}\,.$$

Next observe that by Lemma 5,

(3.44) $$\begin{aligned} &|\tilde{\omega}_g(2\varepsilon : \Phi'_{r_0}) - \tilde{\omega}_g(2\varepsilon : \Phi_{r_0})| \\ &\qquad \leqq \sup_{y\in R^k}\int \omega_{g_y}(x, 2\varepsilon)|\Phi'_{r_0} - \Phi_{r_0}|(dx) \\ &\qquad \leqq 2M_{r_0}(f)||\Phi'_{r_0} - \Phi_{r_0}|| \leqq c_{45}M_{r_0}(f)\rho_s n^{-(s-2)/2}\,. \end{aligned}$$

Using (3.43), (3.44) in (3.28) and noting that

(3.45) $$\begin{aligned} M_{r_0}(f) &= \sup_{x\in R^k}(1+||x||^{r_0})^{-1}|f(x)| \\ &\leqq M_r(f)\cdot\sup_{x\in R^k}\frac{1+||x||^r}{1+||x||^{r_0}} \leqq 2M_r(f)\,, \end{aligned}$$

we get the desired inequality (1.10). □

The proof of (1.11) differs from that of (1.10) principally in the choice of a kernel probability measure. For (1.11) one needs to choose a probability measure K' (in place of K) with compact support (i.e., assigning probability one to a compact set). This rules out the possibility of $\hat{K}'$ having a compact support (i.e., vanishing outside a compact set). However, it is necessary that $\hat{K}'$ vanishes at infinity rapidly. For such a choice see [5] (Corollary 3.1). By a different smoothing inequality than the one used to obtain (2.12) one obtains (see [5], Corollary 2.1, whose proof extends almost word for word to the present case)

(3.46) $$\begin{aligned} &\left|\int_{R^k} f_{a_n}\,d(Q_n' - \Phi')\right| \\ &\qquad \leqq \int_{R^k}(|f_{a_n}| + \omega_{f_{a_n}}(\cdot, \varepsilon))\,d|(Q_n' - \Phi') * K_\varepsilon'| + \tilde{\omega}_{f_{a_n}}(2\varepsilon : \Phi')\,, \end{aligned}$$

where K_ε' is obtained on replacing K in (3.24) by K'. One now chooses $\varepsilon = c_{46}\rho_3 n^{-\frac{1}{2}} \log n$ and proceeds with the estimation much the same way as above. One important difference is that $(\hat{Q}_n' - \hat{\Phi}')\hat{K}_\varepsilon'$ does not vanish outside $B_n = \{t : ||t|| \leq c_{47}n^{\frac{1}{2}}/\rho_3\}$, and since the estimates of $D^\beta(\hat{Q}_n' - \hat{\Phi}')$ are available only in B_n, one has to do some extra estimation outside B_n. It is here that the fast rate of convergence to zero of $\hat{K}'$ at infinity is made use of (see [5], proof of Theorem 4.2, to get an idea of this).

REMARK. By a fairly straightforward truncation argument one can extend the theorem to the case when only ρ_2 is assumed to be finite. This leads to multidimensional extensions and refinements of Liapounov's and Lindeberg's central limit theorems. Although these refinements are new we have not derived them here for fear of overburdening the notation, particularly since the bound would then have to be expressed in terms of the tail behavior of X_j's. This will appear in [6].

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SPECIAL INVITED PAPER

REFINEMENTS OF THE MULTIDIMENSIONAL CENTRAL LIMIT THEOREM AND APPLICATIONS[1]

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This is an expository survey of recent developments in the field of rates of convergence and asymptotic expansions in the context of the multidimensional central limit theorem. A number of applications are discussed. One of them deals with normal approximations and expansions of distribution functions of a class of statistics which includes functions of sample moments.

0. Introduction and summary. The problem of estimating the error of normal approximation in the central limit theorem is an old one. Among important early work we cite Liapounov [28], Cramér [19], [20], Khinchin [26], Berry [6], Esseen [21], and Bergström [5]. The present article emphasises those developments which have taken place since the appearance of Ranga Rao's work [36], [37]. Since the detailed proofs given in the literature may often appear to be long and somewhat cumbersome, the statements of results in this survey are generally accompanied by sketches of main ideas underlying the proofs.

In order to motivate the discussion we consider a sequence of probability measures $\{Q_n : n \geqq 1\}$ on R^k converging weakly to a probability measure Q. This means

$$\int_{R^k} f\, dQ_n \to \int f\, dQ \qquad n \to \infty \tag{0.1}$$

for every real-valued, bounded Borel measurable function f on R^k whose points of discontinuity form a Q-null set. Equivalently, (0.1) holds if f is bounded and the *oscillation*

$$\omega_f(x : \varepsilon) \equiv \sup\{|f(y) - f(z)| : y, z \in B(x : \varepsilon)\} \tag{0.2}$$

of f on the open ball $B(x : \varepsilon)$ with center x and radius ε goes to zero as $\varepsilon \downarrow 0$ for almost every $x(Q)$. In turn this means that (0.1) holds if

$$\begin{aligned} \omega_f(R^k) &\equiv \sup\{|f(y) - f(z)| : y, z \in R^k\} < \infty\,, \\ \bar{\omega}_f(\varepsilon : Q) &\equiv \int_{R^k} \omega_f(x : \varepsilon) Q(dx) \downarrow 0 \qquad \text{as} \quad \varepsilon \downarrow 0\,. \end{aligned} \tag{0.3}$$

We say $\omega_f(R^k)$ is the *total oscillation of f and $\bar{\omega}_f(\varepsilon : Q)$* is the *average modulus of oscillation of f with respect to Q.*

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A variant of a theorem due to Billingsley and Topsøe [14] says that in order that the convergence (0.1) be uniform over a class of functions $\mathscr{F}$, irrespective of the sequence $\{Q_n : n \geqq 1\}$ converging weakly to Q, it is necessary as well as sufficient that (0.3) holds uniformly over $\mathscr{F}$. Hence if $\{Q_n : n \geqq 1\}$ converges weakly to Q, then it should be possible to bound $|\int f dQ_n - \int f dQ|$ by an expression which depends on f only via $\omega_f(R^k)$ and the function $\varepsilon \to \bar{\omega}_f(\varepsilon : Q)$. Note that if I_A denotes the indicator function of a Borel set A, then

$$\text{(0.4)} \qquad \begin{aligned} &\omega_{I_A}(R^k) = 1 \qquad \text{if} \quad A \neq R^k , \quad A \neq \phi , \\ &\bar{\omega}_{I_A}(\varepsilon : Q) = Q((\partial A)^\varepsilon) , \end{aligned}$$

where ∂A is the *topological boundary of* A and $(\partial A)^\varepsilon$ is the *set of all points at distances less than* ε *from* ∂A. One also defines another related average modulus of oscillation, namely,

$$\text{(0.5)} \qquad \omega_f{}^*(\varepsilon : Q) \equiv \sup_{y \in R^k} \bar{\omega}_{f_y}(\varepsilon : Q) ,$$

where f_y is the *translate of* f by y, i.e.,

$$\text{(0.6)} \qquad f_y(x) = f(x + y) \qquad\qquad x, y \in R^k .$$

Again note that if A is a Borel set, then

$$\text{(0.7)} \qquad \omega_{I_A}^*(\varepsilon : Q) = \sup_{y \in R^k} Q((\partial(A + y))^\varepsilon) ,$$

where $A + y = \{x + y : x \in A\}$. Let now $\{X_n : n \geqq 1\}$ be a sequence of i.i.d. k-dimensional random vectors each with mean zero, covariance $I = ((\delta_{ij}))$ ($k \times k$ *identity matrix*), and finite sth absolute moment for some integer $s \geqq 3$. Let Q_n denote the distribution of $n^{-\frac{1}{2}}(X_1 + \cdots + X_n)$, and let Φ be the standard normal distribution on R^k. Theorem 1.7 estimates the error $\int f dQ_n - \int f d\Phi$ in terms of $\omega_f(R^k)$ and $\omega_f{}^*(\varepsilon_n : \Phi)$ where $\varepsilon_n = O(n^{-\frac{1}{2}})$. Theorem 1.5 provides an asymptotic expansion of $\int f dQ_n$ with an error term $o(n^{-(s-2)/2})$ for all f satisfying

$$\text{(0.8)} \qquad \omega_f(R^k) < \infty , \qquad \bar{\omega}_f(\varepsilon : \Phi) = o((-\log \varepsilon)^{-(s-2)/2}) \qquad \varepsilon \downarrow 0 ,$$

if Cramér's condition (1.36) holds. The condition (0.8) is very mild. Both these theorems have appropriate extensions to unbounded f. In case X_1 has a density, Theorem 1.2 provides an asymptotic expansion for the density of Q_n. Under the assumption that X_1 has a nonzero absolutely continuous component, Theorem 1.3 implies that the variation norm of the difference between Q_n and its asymptotic expansion is $o(n^{-(s-2)/2})$. If X_1 has a lattice distribution then a precise expansion of the point masses of Q_n (Theorem 2.1) may be used in conjunction with a multidimensional generalization of the Euler-Maclaurin sum formula to yield an asymptotic expansion of probabilities of rectangles properly aligned with the lattice (Theorem 2.2). This restriction on the type of sets for which one has computable expansions in the lattice case is rather severe. The source of difficulty here lies fairly deep. An indication of the nature of this problem is afforded by a discussion of its relationship with the lattice point problem of analytic number theory (Section 3). The usefulness of Theorem 3.1 and its extension

(3.12) to special convex sets A may be viewed in this context. Section 4 is devoted to another application. Here one finds precise error bounds and asymptotic expansions of distribution functions of a class of statistics. This class includes those statistics which are functions of sample moments. With the help of the expansions of Section 4 we are also able to resolve an old conjecture concerning the validity of the formal Edgeworth expansion using the so-called *delta method* for computation of approximate moments and cumulants. To keep the presentation simple, proofs (of the results of Section 4) are merely outlined leaving the details to a future publication. The final section briefly discusses some other applications.

The recent monograph [11] gives a comprehensive account of the theory of rates of convergence and asymptotic expansions in the context of the central limit theorem. Details of proofs of the results in Sections 1 and 2 (excepting Lemma 1.4) may be found there. However, applications are not dealt with in [11]. The present article is intended not only to provide an easy access to some of the main results of the theory but also to introduce the reader to some areas of fruitful applications. Bearing statistical applications (especially, robustness) in mind, an attempt has been made to specify (see, e.g., remarks following (1.50) and (1.64)) the nature of dependence of the error in asymptotic expansions not only on the function, whose integral one approximates, but also on the underlying distribution. In addition, Lemma 1.4 serves to clarify the role of Cramér's condition (1.36) in applications.

For ease of reference we list here some of the main notation used in this article. We deal with sequences of i.i.d. random vectors $\{X_n : n \geqq 1\}$ (or $\{Y_n : n \geqq 1\}$, $\{Z_n : n \geqq 1\}$). The nth normalized partial sum is $n^{-\frac{1}{2}}(X_1 + \cdots + X_n)$ if $EX_1 = 0$; its distribution is Q_n and characteristic function $\hat{Q}_n$. The Fourier transform of a function f is $\hat{f}$, and the Fourier–Stieltjes transform of a finite signed measure G is $\hat{G}$. The standard normal distribution on R^k is Φ and its density is ϕ, while Φ_V, ϕ_V denote the distribution and density of a normal random vector with mean zero and covariance V. Thus $\Phi = \Phi_I$, where I is the identity matrix. The Cramér–Edgeworth polynomials $\tilde{P}_r$, $r \geqq 1$, are defined by (1.16), (1.21). The function $P_r(-\phi_V)$ is defined by (1.24) (on replacing ϕ by the more general ϕ_V). In other words, $P_r(-\phi_V)$ is the function (ϕ_V times a polynomial) whose Fourier transform is $(\tilde{P}_r \cdot \hat{\Phi}_V)(t) = \tilde{P}_r(it)\exp\{-\frac{1}{2}\langle t, Vt\rangle\}$. The signed measure having density $P_r(-\phi_V)$ is $P_r(-\Phi_V)$.

1. The Cramér-Edgeworth expansions and rates of convergence. Consider a sequence of independent and identically distributed (i.i.d.) random vectors $\{X_n = (X_n^{(1)}, \cdots, X_n^{(k)}) : n \geqq 1\}$ with values in R^k and common distribution Q_1. Unless otherwise specified we assume (without essential loss of generality)

$$(1.1) \qquad EX_1 = 0\,, \qquad \operatorname{Cov} X_1 = I\,,$$

where EX_1, $\operatorname{Cov} X_1$ are, respectively, the *mean vector* and *covariance matrix of* X_1, and I is the $k \times k$ *identity matrix*. Let $\nu = (\nu^{(1)}, \cdots, \nu^{(k)})$ denote a *multiindex*, i.e., a k-tuple of nonnegative integers, and write

$$|\nu| = \nu^{(1)} + \cdots + \nu^{(k)}, \qquad \nu! = \nu^{(1)}!\,\nu^{(2)}! \cdots \nu^{(k)}!, \tag{1.2}$$
$$x^\nu = (x^{(1)})^{\nu^{(1)}} \cdots (x^{(k)})^{\nu^{(k)}} \qquad x = (x^{(1)}, \cdots, x^{(k)}) \in R^k .$$

The νth *moment of* X_1 (or of Q_1) is

$$\mu_\nu = EX_1^\nu = \int_{R^k} x^\nu Q_1(dx) , \tag{1.3}$$

provided the integral is convergent. For a positive integer s the sth *absolute moment of* X_1 (or of Q_1) is

$$\rho_s = E||X_1||^s = \int_{R^k} ||x||^s Q_1(dx) , \tag{1.4}$$

where $||\cdot||$ is *Euclidean norm*. If G is a finite signed measure on (the Borel sigma field of) R^k, then the *Fourier–Stieltjes transform* (or *characteristic function* (ch.f.) in case G is a probability measure) *of* G is

$$\hat{G}(t) = \int_{R^k} \exp\{i\langle t, x\rangle\} G(dx) \qquad t \in R^k , \tag{1.5}$$

where $\langle\ ,\ \rangle$ denotes *Euclidean inner product*. Since a Taylor expansion and (1.1) yields

$$|\hat{Q}_1(t) - 1| \leqq \frac{||t||^2}{2} \qquad t \in R^k , \tag{1.6}$$

the range of $\hat{Q}_1$ on the unit ball $\{||t|| < 1\}$ is contained in the disc $D(1:\frac{1}{2}) \equiv \{z \in \mathbb{C} : |z-1| < \frac{1}{2}\}$ of the complex plane. Since *log*, the principal branch of the logarithm, is analytic in $D(1:\frac{1}{2})$, $\log \hat{Q}_1$ has continuous derivatives of all orders up to s (if $\rho_s < \infty$) in a neighborhood of the origin. The νth *cumulant of* X_1 (or of Q_1) is

$$\chi_\nu = i^{-|\nu|}(D^\nu \log \hat{Q}_1)(0) , \tag{1.7}$$

provided $\rho_{|\nu|} < \infty$. Here D^ν is the νth derivative, i.e.,

$$D^\nu = D_1^{\nu^{(1)}} \cdots D_k^{\nu^{(k)}} , \tag{1.8}$$

where D_j denotes differentiation with respect to the jth coordinate variable. Since $\chi_\nu = \mu_\nu = 0$ if $|\nu| = 1$, a comparison of the Taylor-expansions

$$\hat{Q}_1(t) = 1 + \sum_{2\leq|\nu|\leq s} \frac{\mu_\nu}{\nu!}(it)^\nu + o(||t||^s) , \tag{1.9}$$
$$\log \hat{Q}_1(t) = \sum_{2\leq|\nu|\leq s} \frac{\chi_\nu}{\nu!}(it)^\nu + o(||t||^s) \qquad t \to 0 ,$$

leads to the formal identity

$$\sum_{2\leq|\nu|<\infty} \frac{\chi_\nu}{\nu!}(it)^\nu = \sum_{m=1}^\infty \frac{(-1)^{m+1}}{m}\left[\sum_{2\leq|\nu|<\infty} \frac{\mu_\nu}{\nu!}(it)^\nu\right]^m . \tag{1.10}$$

By equating coefficients of $(it)^\nu$ from the two sides of (1.10) one may express cumulants in terms of moments. In particular, if $s \geqq 3$ then (1.10) implies

$$\chi_\nu = \mu_\nu \qquad \text{if} \quad |\nu| = 2, 3 . \tag{1.11}$$

Now the distribution of $X_1 + \cdots + X_n$ is the *n-fold convolution* Q_1^{*n} and its ch.f. is $\hat{Q}_1^n$. Let Q_n denote the *distribution of* $n^{-\frac{1}{2}}(X_1 + \cdots + X_n)$. The νth cumulant of Q_n is $i^{-|\nu|}$ times

$$(1.12)\qquad D^\nu(\log \hat{Q}_n)(0) = D^\nu[\log \hat{Q}_1^n(\cdot/n^{\frac{1}{2}})](0) = n^{-(|\nu|-2)/2}\chi_\nu i^{|\nu|},$$

if $\rho_{|\nu|} < \infty$. This relation makes an asymptotic expansion of $\hat{Q}_n$ in powers of $n^{-\frac{1}{2}}$ possible. To see this assume $\rho_s < \infty$ for some $s \geqq 2$ and use the second relation in (1.9) to obtain

$$(1.13)\qquad \log \hat{Q}_n(t) = -\frac{||t||^2}{2} + \sum_{3\leqq|\nu|\leqq s} \frac{\chi_\nu}{\nu!}(it)^\nu n^{-(|\nu|-2)/2} + n\cdot o(||t/n^{\frac{1}{2}}||^s)$$
$$= -\frac{||t||^2}{2} + \sum_{3\leqq|\nu|\leqq s} \frac{\chi_\nu}{\nu!}(it)^\nu n^{-(|\nu|-2)/2} + o(n^{-(s-2)/2}),\quad n\to\infty .$$

Hence for all $t \in R^k$

$$(1.14)\qquad \hat{Q}_n = \exp\{-||t||^2/2\}\cdot\exp\left\{\sum_{3\leqq|\nu|\leqq s}\frac{\chi_\nu}{\nu!}(it)^\nu n^{-(|\nu|-2)/2}\right\}$$
$$\times[1 + o(n^{-(s-2)/2})] \qquad n\to\infty .$$

If one takes $s = 2$ in (1.14) and uses the Cramér–Lévy continuity theorem ([20], page 106) then one arrives at the classical multidimensional central limit theorem: *If* $\rho_2 < \infty$, *then* $\{Q_n : n \geqq 1\}$ *converges weakly to the standard normal distribution* Φ. If $s \geqq 3$, then expanding the second exponential in (1.14) and collecting together terms involving the same power of $n^{-\frac{1}{2}}$ one has

$$(1.15)\qquad \exp\left\{\sum_{3\leqq|\nu|\leqq s}\frac{\chi_\nu}{\nu!}(it)^\nu n^{-(|\nu|-2)/2}\right\} = 1 + \sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(it) + o(n^{-(s-2)/2}) .$$

More precisely, replacing $n^{-\frac{1}{2}}$ by the real variable u one obtains a Taylor expansion of the exponential as a function of u. The sum $1 + \sum_{r=1}^{s-2} u^r\tilde{P}_r(it)$ is this Taylor expansion, i.e.,

$$(1.16)\qquad \frac{d^r}{du^r}\left[\exp\left\{\sum_{3\leqq|\nu|\leqq s}\frac{\chi_\nu}{\nu!}(it)^\nu u^{|\nu|-2}\right\}\right](0) = r!\,\tilde{P}_r(it) .$$

Combining (1.14) and (1.15) one gets

$$(1.17)\qquad \hat{Q}_n(t) = \exp\left\{-\frac{||t||^2}{2}\right\}\cdot[1 + \sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(it)] + o(n^{-(s-2)/2}) .$$

By carefully estimating the remainders in the two Taylor expansions (1.13) and (1.15) one may obtain the following result.

THEOREM 1.1. *Suppose* $\rho_s < \infty$ *for some integer* $s \geqq 3$. *There exist two positive constants* $c_1(k, s)$, $c_2(k, s)$ *depending only on k and s such that if* $||t|| \leqq c_1(k, s)n^{\frac{1}{2}} \div \rho_s^{1/(s-2)}$ *then*

$$(1.18)\qquad |D^\nu[\hat{Q}_n(t) - \{1 + \sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(it)\}\exp\{-||t||^2/2\}]|$$
$$\leqq \frac{\delta_n}{n^{(s-2)/2}}[||t||^{s-|\nu|} + ||t||^{3(s-2)+|\nu|}]\exp\{-||t||^2/4\} \qquad |\nu| \leqq s ,$$

where $\delta_n \to 0$ *as* $n \to \infty$ *and* $\delta_n \leqq c_2(k, s)\rho_s$ *for all n.*

The first result of this type was obtained for $k = 1$ by Cramér [20] (page 72). Many authors have refined Cramér's result and the present version is proved in [11] (Theorem 9.12).

To obtain a more computable expression for $\tilde{P}_r(it)$ it is convenient to define

$$(1.19)\qquad \chi_r(t) = r!\,\sum_{|\nu|=r} \frac{\chi_\nu}{\nu!}\, t^\nu\,, \qquad \chi_r(it) = i^r\chi_r(t) = r!\,\sum_{|\nu|=r} \frac{\chi_\nu}{\nu!}\,(it)^\nu\,.$$

It is not difficult to check that $\chi_r(t)$ is the rth cumulant of the random variable $\langle t, X_1\rangle$. Now (1.15) reduces to

$$(1.20)\qquad \exp\left\{\sum_{3\le r\le s} \frac{\chi_r(it)}{r!}\, n^{-(r-2)/2}\right\} = 1 + \sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(it) + o(n^{-(s-2)/2})\,.$$

From this one obtains

$$(1.21)\qquad \tilde{P}_r(it) = \sum_{m=1}^{r} \frac{1}{m!}\left\{\sum{}^{*} \frac{\chi_{j_1+2}(it)}{(j_1+2)!}\,\frac{\chi_{j_2+2}(it)}{(j_2+2)!}\cdots\frac{\chi_{j_m+2}(it)}{(j_m+2)!}\right\}$$

where the summation $\sum^*$ is over all m-tuples of positive integers $(j_1, \cdots, j_m)$ satisfying

$$(1.22)\qquad \sum_{l=1}^{m} j_l = r\,.$$

For example,

$$(1.23)\qquad \begin{aligned} \tilde{P}_1(it) &= \frac{\chi_3(it)}{3!} = \frac{i^3}{3!}\,\chi_3(t) = \sum_{|\nu|=3} \frac{\chi_\nu}{\nu!}\,(it)^\nu\,,\\ \tilde{P}_2(it) &= \frac{\chi_4(it)}{4!} + \frac{\chi_3^2(it)}{2!\,(3!)^2}\,,\\ \tilde{P}_3(it) &= \frac{\chi_5(it)}{5!} + \frac{\chi_4(it)\chi_3(it)}{4!\,3!} + \frac{\chi_3^3(it)}{(3!)^4}\,.\end{aligned}$$

For a smooth function f rapidly decreasing at infinity the function $t \to (it)^\nu \hat{f}(t)$ is the Fourier transform of $(-1)^{|\nu|}D^\nu f$. Hence the function $t \to \tilde{P}_r(it)\exp\{-\|t\|^2/2\}$ is the Fourier transform of the function

$$(1.24)\qquad P_r(-\phi)(x) \equiv \tilde{P}_r(-D)\phi(x) \qquad x \in R^k\,,$$

where ϕ is the *standard normal density*, i.e.,

$$(1.25)\qquad \phi(x) = (2\pi)^{-k/2}\exp\{-\|x\|^2/2\} \qquad x \in R^k\,,$$

and $\tilde{P}_r(-D)$ is the differential operator obtained by formally replacing $(it)^\nu$ by $(-D)^\nu = (-1)^{|\nu|}D^\nu$ (for each multiindex ν) in the polynomial expression (1.21) for $\tilde{P}_r(it)$. For example,

$$(1.26)\qquad \begin{aligned} P_1(-\phi)(x) = &-\tfrac{1}{6}\sum_{l=1}^{k} E(X_1^{(l)})^3[3x^{(l)} - (x^{(l)})^3]\\ &- \tfrac{1}{2}\sum_{1\le l\ne m\le k} E[(X_1^{(l)})^2X_1^{(m)}][x^{(m)} - x^{(m)}(x^{(l)})^2]\\ &+ \sum_{1\le l<m<p\le k} E(X_1^{(l)}X_1^{(m)}X_1^{(p)})x^{(l)}x^{(m)}x^{(p)}\\ &\qquad x = (x^{(1)}, \cdots, x^{(k)}) \in R^k\,.\end{aligned}$$

The finite signed measure having density $P_r(-\phi)$ will be denoted by $P_r(-\Phi)$.

Note that $\phi + \sum_{r=1}^{s-2} n^{-r/2}P_r(-\phi)$ is a polynomial times ϕ, and that (1.18) implies (on taking the derivative at $t = 0$)

$$(1.27) \qquad \int_{R^k} x^\nu Q_n(dx) = (-i)^{|\nu|}(D^\nu \hat{Q}_n)(0) = \int_{R^k} x^\nu[\phi(x) + \sum_{r=1}^{s-2} n^{-r/2}P_r(-\phi)(x)]\, dx \qquad 0 \leqq |\nu| \leqq s\,.$$

However, the relations (1.27) do not uniquely determine this polynomial (multiple of ϕ). The reason for this is that the polynomial is of degree $3(s-2) > s$, if $s > 3$.

Let us assume now that $\hat{Q}_1$ is integrable. Then $\hat{Q}_n$ is integrable and Q_n has a density q_n. By Fourier inversion

$$(1.28) \qquad h_\nu(x) \equiv x^\nu[q_n(x) - \phi(x) - \sum_{r=1}^{s-2} n^{-r/2}P_r(-\phi)(x)] = (2\pi)^{-k} \int_{R^k} \exp\{-i\langle t, x\rangle\}\hat{h}_\nu(t)\, dt \qquad x \in R^k\,,$$

where

$$(1.29) \qquad \hat{h}_\nu(t) = (-i)^{|\nu|}D^\nu\left[\hat{Q}_n(t) - \{1 + \sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(it)\} \exp\left\{-\frac{\|t\|^2}{2}\right\}\right].$$

By Theorem 1.1

$$(1.30) \qquad \int_{\{\|t\| \leq c_1(k,s)n^{\frac{1}{2}}/\rho_s^{1/(s-2)}\}} |\hat{h}_\nu(t)|\, dt = o(n^{-(s-2)/2})\,.$$

Also, since $|\hat{Q}_1(t)| < 1$ for $t \neq 0$ and $|\hat{Q}_1(t)| \to 0$ as $\|t\| \to \infty$ (by the Riemann–Lebesgue lemma)

$$(1.31) \qquad \delta \equiv \sup\{|\hat{Q}_1(t)|;\ \|t\| > c_1(k, s)/\rho_s^{1(s-2)}\} < 1\,.$$

By repeated use of the Leibnitz rule for differentiation of a product of functions it may be shown that

$$(1.32) \qquad |D^\nu \hat{Q}_n(t)| = |D^\nu \hat{Q}_1^n(t/n^{\frac{1}{2}})| \leqq n^{|\nu|/2}\rho_{|\nu|}|\hat{Q}_1(t/n^{\frac{1}{2}})|^{n-|\nu|}\,.$$

Therefore,

$$(1.33) \qquad \begin{aligned} &\int_{\{\|t\| > c_1(k,s)n^{\frac{1}{2}}/\rho_s^{1/(s-2)}\}} |D^\nu \hat{Q}_n(t)|\, dt \\ &\leqq n^{|\nu|/2}\rho_{|\nu|}\delta^{n-|\nu|-1} \int_{R^k} |\hat{Q}_1(t/n^{\frac{1}{2}})|\, dt \\ &= n^{(|\nu|+k)/2}\delta^{n-|\nu|-1} \int_{R^k} |\hat{Q}_1(t)|\, dt = o(n^{-(s-2)/2})\,. \end{aligned}$$

Since the remaining terms in $\hat{h}_\nu$ possess an exponential factor it follows from (1.28), (1.30), and (1.33) that

$$(1.34) \qquad \sup_{x \in R^k} |x^\nu[q_n(x) - \phi(x) - \sum_{r=1}^{s-2} n^{-r/2}P_r(-\phi)(x)]| = o(n^{-(s-2)/2}) \qquad 0 \leqq |\nu| \leqq s\,.$$

Taking $\nu = 0$ in (1.34) one arrives at a *uniform local expansion* of q_n. It may be noted that the proof undergoes only minor modification if one assumes that $|\hat{Q}_1|^m$ is integrable for some $m \geqq 1$. It is also fairly simple to show that the last condition is equivalent to saying that Q_1^{*m} has a bounded density for some positive integer m. Thus one has

THEOREM 1.2. *Assume $\rho_s < \infty$ for some integer $s \geqq 2$. In order that for sufficiently large n the distribution Q_n may have a density q_n satisfying* (1.34) *it is necessary as well as sufficient that Q_1^{*m} has a bounded density for some positive integer m.*

One dimensional versions of this theorem may be found in Gnedenko and Kolmogorov [22] (page 228) and in Petrov [32]. The present version is proved in [11] (Theorems 19.1, 19.2). If $s > k+1$, then on integration over R^k the relation (1.34) yields an estimate $o(n^{-(s-2)/2})$ for the *variation norm* $\|Q_n - \Phi - \sum_{r=1}^{s-2} n^{-r/2}P_r(-\Phi)\|$. However, for this there is a better result. We denote by $|G|$ the *total variation* (measure) *of a finite signed measure* G.

THEOREM 1.3. *Suppose* $\rho_s < \infty$ *for some integer* $s \geqq 2$. *In order that the relation*

$$(1.35) \qquad \int_{R^k} (1 + \|x\|^s)|Q_n - \Phi - \sum_{r=1}^{s-2} n^{-r/2}P_r(-\Phi)|(dx) = o(n^{-(s-2)/2})$$

may hold it is necessary as well as sufficient that Q_1^{*m} *has a nonzero absolutely continuous component for some positive integer* m.

If the integrand $(1 + \|x\|^s)$ in (1.35) is replaced by 1, then one arrives at the variation norm estimate mentioned above. This estimate is due to Bikjalis [13]. The present stronger result is useful (e.g., in estimating moments of a function of $\bar{X} = n^{-1}(X_1 + \cdots + X_n)$) and a detailed proof is given in [11] (Theorem 19.5). It should be noted that the hypothesis of Theorem 1.3 is less restrictive than that of Theorem 1.2. Thus if one is interested only in estimating $\int f\,dQ_n$ for Borel measurable functions f (or probabilities $Q_n(B)$ for Borel sets B), then Theorem 1.3 is a more useful result than Theorem 1.2.

A hypothesis less restrictive than those used in the preceding theorems was introduced by Cramér ([20], page 82). This is the so-called *Cramér's condition*:

$$(1.36) \qquad \limsup_{\|t\|\to\infty} |\hat{Q}_1(t)| < 1 .$$

In view of the Riemann–Lebesgue lemma, it Q_1 has a nonzero absolutely continuous component then $\hat{Q}_1$ satisfies (1.36). There are, however, many singular measures satisfying Cramér's condition. The following lemma provides a class of examples which are used in Section 4.

LEMMA 1.4. *Let* X *be a random vector with values in* R^m *whose distribution has a nonzero absolutely continuous component* H (*relative to Lebesgue measure on* R^m). *Let* f_i, $1 \leq i \leq k$, *be Borel measurable real-valued functions on* R^m. *Assume that there exists an open ball* B *of* R^m *in which the density of* H *is positive almost everywhere and in which* f_i*'s are continuously differentiable. If in* B *the functions* 1, $f_1, \cdots, f_k$ *are linearly independent, then the distribution* Q_1 *of* $(f_1(X), \cdots, f_k(X))$ *satisfies Cramér's condition* (1.36).

PROOF. Let $\theta_0 = (\theta_0^{(1)}, \cdots, \theta_0^{(k)}) \in R^k$, $\theta_0 \neq 0$. The assumption of linear independence implies that there is a j $(1 \leqq j \leqq m)$ and an $x_0 \in B$ such that $(\sum_{l=1}^k \theta_0^{(l)} D_j f_l)(x_0) \neq 0$. Without loss of generality we may take $j = 1$ and assume that $(\sum_{l=1}^k \theta^{(l)} D_1 f_l)(x) > \delta > 0$ for all $x \in B$ and all θ in the open ball $B(\theta_0 \colon \varepsilon)$ with center θ_0 and radius $\varepsilon > 0$. Here δ is an appropriate positive number. Consider the function

$$g(\theta, x) = (\theta, x') ,$$
$$x' = (\textstyle\sum_{l=1}^k \theta^{(l)} f_l(x), x^{(2)}, \cdots, x^{(m)}) \qquad x = (x^{(1)}, \cdots, x^{(m)}) \in R^m ,$$

on $B(\theta_0 : \varepsilon) \times B$. Since the Jacobian of this map is $\sum_{l=1}^k \theta^{(l)} D_1 f_l$, which is positive on $B(\theta_0 : \varepsilon) \times B$, one may use the inverse function theorem to assert (by reducing ε and B is necessary) that g defines a diffeomorphism between $B(\theta_0 : \varepsilon) \times B$ and its image under g. It follows that for each $\theta \in B(\theta_0 : \varepsilon)$ the map $g_\theta(x) = (\sum_{l=1}^k \theta^{(l)} f_l(x), x^{(2)}, \cdots, x^{(m)})$ is a diffeomorphism between B and $g_\theta(B)$. Let H_0 denote the restriction of H to B. Then the measure $H_0 \circ g_\theta^{-1}$ induced on $g_\theta(B)$ by the map g_θ has a density given by

$$h_\theta(z) = \frac{h(g_\theta^{-1}(z))}{\sum_{l=1}^k \theta^{(l)}(D_1 f_l)(g_\theta^{-1}(z))} \qquad z \in g_\theta(B) ,$$

where h is the density of H_0. Extend h to all of R^m by setting it equal to zero outside $g_\theta(B)$. Then for all $z \in R^m$, $z \notin \partial g_{\theta_0}(B)$, $h_\theta(z) \to h_{\theta_0}(z)$ as $\theta \to \theta_0$. Write

$$h_{\theta,1}(z^{(1)}) = \int_{R^{m-1}} h_\theta(z)\, dz^{(2)} \cdots dz^{(m)} \qquad z^{(1)} \in R^1 .$$

Since the m-dimensional Lebesgue measure of $\partial g_{\theta_0}(B)$ is zero,

$$\text{(1.37)} \qquad \int_{R^1} |h_{\theta,1}(u) - h_{\theta_0,1}(u)|\, du \leqq \int_{R^m} |h_\theta(z) - h_{\theta_0}(z)|\, dz \to 0 \qquad \theta \to \theta_0 .$$

Now suppose (1.36) does not hold. Then there exists a sequence $\{t_n : n \geqq 1\}$ such that $||t_n|| \to \infty$ and

$$\text{(1.38)} \qquad |\hat{Q}_1(t_n)| \to 1 \qquad \text{as} \quad n \to \infty .$$

Let $\theta_n = t_n/||t_n||$. Restricting to a subsequence if necessary, we assume that $\{\theta_n\}$ converges to some θ_0. Let G_n be the distribution of the random variable $\sum_{l=1}^k \theta_n^{(l)} f_l(X)$ for $n = 0, 1, 2, \cdots$. Write

$$\text{(1.39)} \qquad G_n = G_{n,1} + G_{n,2} ,$$

where $G_{n,2}$ has density $h_{\theta_n,1}$. Then

$$\text{(1.40)} \qquad |\hat{Q}_1(t_n)| = |\hat{G}_n(||t_n||)| \leqq |\hat{G}_{n,1}(||t_n||)| + |\hat{G}_{n,2}(||t_n||)| .$$

But $||G_{n,2} - G_{0,2}|| \to 0$ as $n \to \infty$ by (1.37). Hence $\hat{G}_{n,2}(u)$ converges to $\hat{G}_{0,2}(u)$ uniformly in u. Also by the Riemann–Lebesgue lemma $\hat{G}_{0,2}(||t_n||) \to 0$ as $n \to \infty$. Therefore, $|\hat{G}_{n,2}(||t_n||)| \to 0$. Using this and (1.40) one has

$$\limsup_{n\to\infty} |\hat{Q}_1(t_n)| \leqq \limsup_{n\to\infty} |\hat{G}_{n,1}(||t_n||)| \leqq \limsup_{n\to\infty} ||G_{n,1}|| = 1 - \int_{R^1} h_{\theta_0,1}(u)\, du < 1 .$$

This contradicts (1.38). □

To appreciate the significance of this result take $m = 1$, $k > 1$. Then $x \to (f_1(x), \cdots, f_k(x))$ is a curve in R^k, and the distribution Q_1 of the random vector $(f_1(X), \cdots, f_k(X))$ is clearly singular (with respect to Lebesgue measure on R^k).

It has been shown by Yurunskii [44] that if the f_i's in Lemma 1.4 are analytic then there exists an integer m such that Q_1^{*m} has a nonzero absolutely continuous component.

It is clear that if Q_1^{*n} is, for all n, singular (with respect to Lebesgue measure on R^k), then there exists a Borel set A such that $Q_n(A) = 1$ for all n and $\Phi(A) = 0$.

Thus convergence in variation norm is ruled out and we fall back on weak convergence. Recall the definitions of the total oscillation $\omega_f(R^k)$ and the average modulus of oscillation $\bar{\omega}_f(\varepsilon : \Phi)$ (see (0.2), (0.3)). The following expansion holds.

THEOREM 1.5. *If $\rho_s < \infty$ for some integer $s \geqq 3$ and $\hat{Q}_1$ satisfies Cramér's condition* (1.36), *then for every real-valued, bounded, Borel measurable function f on R^k one has*

$$(1.41)\qquad |\textstyle\int_{R^k} f d[Q_n - \Phi - \sum_{r=1}^{s-2} n^{-r/2} P_r(-\Phi)]| \leqq \dfrac{\delta_n}{n^{(s-2)/2}}\, \omega_f(R^k) + \bar{\omega}_f(e^{-dn} : \Phi)\,,$$

where $\delta_n \to 0$ as $n \to \infty$, d is a positive constant, and the quantities δ_n and d do not depend on f.

A detailed proof of this theorem may be found in [8] (Theorem 4.3). However, the main ideas underlying the proof may be stated rather simply. In the present case $\hat{Q}_n$ is not necessarily integrable. Therefore, one chooses a kernel probability measure K whose support is contained in the closed unit ball of R^k, and whose characteristic function satisfies

$$(1.42)\qquad |D^\nu \hat{K}(t)| = O(\exp\{-||t||^{\frac{1}{2}}\}) \qquad ||t|| \to \infty\,,$$

for all multiindices ν. The existence of such a kernel follows from a result of Ingham (see [8], Corollary 3.1). For $\varepsilon > 0$ define the probability measure K_ε by

$$(1.43)\qquad K_\varepsilon(A) = K(\varepsilon^{-1}A) \quad (A \text{ Borel set; } \varepsilon^{-1}A = \{\varepsilon^{-1}x : x \in A\})\,.$$

The effect of smoothing by convolution with K_ε is provided by the following lemma (see [8], Corollary 2.1).

LEMMA 1.6. *Let G be a finite measure and H a finite signed measure such that $G(R^k) = H(R^k)$, and let K be a probability measure on R^k. If*

$$(1.44)\qquad K(B(0:1)) = 1 \qquad (B(0:1) = \{||x|| < 1\})\,,$$

then for every $\varepsilon > 0$ and every real-valued, bounded, Borel measurable function f on R^k one has

$$(1.45)\qquad |\textstyle\int_{R^k} f\, d(G - H)| \leqq \omega_f(R^k)||(G - H) * K_\varepsilon|| + \bar{\omega}_f(2\varepsilon : |H|)$$

where $|H|$ is the total variation of H.

In this lemma let $G = Q_n$, $H = \Phi + \sum_{r=1}^{s-2} n^{-r/2} P_r(-\Phi)$ and K as specified earlier. The optimum ε is of the order e^{-dn} where d is a positive constant satisfying

$$(1.46)\qquad 0 < d < -\frac{1}{k} \log \theta\,, \qquad \theta = \sup\{|\hat{Q}_1(t)| : ||t|| > (16\rho_3)^{-1}\}\,.$$

Cramér's condition (1.36) ensures that $\theta < 1$ and that, consequently, such a choice of d is possible. Since $(\hat{G} - \hat{H}) \cdot \hat{K}_\varepsilon$ is integrable, one may use Fourier inversion and Theorem 1.1 to estimate the variation norm $||(G - H) * K_\varepsilon||$. Integrability of $\hat{K}_\varepsilon$ and the fact that $\sup\{|\hat{Q}_n(t)| : ||t|| > n^{\frac{1}{2}}/(16\rho_3)\} = \theta^n$ makes an adequate estimation of the tail integral of $(\hat{G} - \hat{H}) \cdot \hat{K}_\varepsilon$ possible.

To apply Theorem 1.5 note that the right side in (1.41) is $o(n^{-(s-2)/2})$ if (0.8) holds. For example, consider the class of Borel sets

$$\mathscr{A}_\alpha(a:\Phi) = \{A: A \text{ Borel set, } \Phi((\partial A)^\varepsilon) \leqq a\varepsilon^\alpha \text{ for } \varepsilon > 0\}, \tag{1.47}$$

where α and a are specified positive numbers. Then one has

$$\sup_{A\in\mathscr{A}_\alpha(a:\Phi)} |Q_n(A) - \Phi(A) - \textstyle\sum_{r=1}^{s-2} n^{-r/2}P_r(-\Phi)(A)| = o(n^{-(s-2)/2}). \tag{1.48}$$

It was first shown by Ranga Rao [36] and later by von Bahr [2] that for the *class $\mathscr{C}$ of all Borel measurable convex subsets* of R^k one has (a complete proof may be found in [11], Corollary 3.2)

$$\sup_{C\in\mathscr{C}} \Phi((\partial C)^\varepsilon) \leqq a(k)\varepsilon \qquad \varepsilon > 0. \tag{1.49}$$

It follows from (1.48), (1.49) that

$$\sup_{C\in\mathscr{C}} |Q_n(C) - \Phi(C) - \textstyle\sum_{r=1}^{s-2} n^{-r/2}P_r(-\Phi)(C)| = o(n^{-(s-2)/2}). \tag{1.50}$$

We make two more observations on Theorem 1.5. First, suppose $\mathscr{P}$ is a relatively *norm compact* class of probability measures Q_1 satisfying, in addition to the hypothesis of Theorem 1.5, the condition

$$\sup_{Q_1\in\mathscr{P}} \int_{R^k} ||x||^{s+1}Q_1(dx) < \infty. \tag{1.51}$$

It is then simple to show, using norm compactness, that on $\mathscr{P}$ the quantity θ defined in (1.46) is bounded away from one. Hence (1.41) and, therefore, (1.48), (1.50) hold uniformly over such a class $\mathscr{P}$. The second remark concerns the extension of (1.41) to unbounded f. Such an extension is possible if

$$M_s(f) \equiv \sup_{x\in R^k} (1 + ||x||^s)^{-1}|f(x)| < \infty. \tag{1.52}$$

Indeed, if $M_r(f) < \infty$ for some integer r, $0 \leqq r \leqq s$, then (1.41) holds (see [11], Theorem 20.1) with $\omega_f(R^k)$ replaced by

$$M_r^*(f) \equiv 2 \inf_{c\in R^1} M_r(f - c). \tag{1.53}$$

Observe that if $M_s(f) = \infty$, then $\int f\,dQ_n$ may not exist.

Theorem 1.5 still leaves out the entire class of discrete probability measures as well as many nonatomic singular distributions. If Q_1 is of the lattice type, then $|\hat{Q}_1|$ is periodic and, consequently, the lim sup of $|\hat{Q}_1(t)|$ as $||t|| \to \infty$ is one. For an arbitrary discrete Q_1, the ch.f. $\hat{Q}_1$ is a uniform limit of trigonometric polynomials and is, therefore, *almost periodic* in the sense of Bohr; hence $\limsup |\hat{Q}_1(t)| = |\hat{Q}_1(0)| = 1$. Now it is possible to show ([11], Theorem 17.5), no matter what the type of the distribution Q_1 is, that an affine subspace of dimension m $(0 \leqq m < k)$ has Q_n measure at most $O(n^{-(k-m)/2})$ provided $\rho_3 < \infty$. If Q_1 is of the lattice type, then this bound is actually attained, and it follows that the distribution function F_n of Q_n has jumps of order $O(n^{-\frac{1}{2}})$. But $\Phi + \sum_{r=1}^{s-2} n^{-r/2}P_r(-\Phi)$ is absolutely continuous. Thus Theorem 1.5 can not be true in the lattice case. However, because of the lattice structure a different expansion of $Q_n(A)$ for special rectangles A may be given. This is discussed in Section 2. If no assumption is made on the type of Q_1 one may still estimate $\int f\,d(Q_n - \Phi)$.

THEOREM 1.7. *If $\rho_3 < \infty$, then for every real-valued, bounded, Borel measurable function f on R^k one has*

$$(1.54) \qquad |\textstyle\int_{R^k} f\, d(Q_n - \Phi)| \leqq c_4(k)\omega_f(R^k)\rho_3 n^{-\frac{1}{2}} + c_5(k)\omega_f^*(\varepsilon_n : \Phi) ,$$

where $\varepsilon_n = c_5'(k)\rho_3 n^{-\frac{1}{2}}$.

To prove this one chooses, as in the proof of Theorem 1.5, a smoothing kernel K. However, this time the probability measure K is chosen so that $\hat{K}$ vanishes outside a compact set. This rules out the possibility of K having a compact support. Instead one requires

$$(1.55) \qquad \gamma \equiv K(\{\|x\| < 1\}) > \tfrac{1}{2}, \qquad \textstyle\int_{R^k} \|x\|^{k+1} K(dx) < \infty .$$

Define K_ε by (1.43). Then one has, instead of Lemma 1.6 (see [8], Corollary 2.2),

LEMMA 1.8. *If G is a finite measure and H is a finite signed measure such that $G(R^k) = H(R^k)$, and if K_ε is as above, then*

$$(1.56) \quad |\textstyle\int_{R^k} f\, d(G - H)| \leqq (2\gamma - 1)^{-1}[\tfrac{1}{2}\omega_f(R^k)\|(G - H) * K_\varepsilon\| + \omega_f^*(2\varepsilon : |H|)] ,$$

for every bounded measurable f.

One also needs the analytical result (see [11], Lemma 11.6)

LEMMA 1.9. *There exists a positive constant $c_6(k)$ such that if g satisfies*

$$(1.57) \qquad \textstyle\int_{R^k} (1 + \|x\|^{k+1})|g(x)|\, dx < \infty ,$$

then

$$(1.58) \qquad \|g\|_1 \equiv \textstyle\int_{R^k} |g(x)|\, dx \leqq c_6(k) \max_{|\nu|=0,k+1} \|D^\nu \hat{g}\|_1 .$$

Write $G = Q_n$, $H = \Phi$, $\varepsilon = c_7(k)\rho_3 n^{-\frac{1}{2}}$, and let g be the density of $(G - H) * K_\varepsilon$. Assume $\rho_{k+1} < \infty$, so that (1.58) may apply. Note that $D^\nu[(\hat{G} - \hat{H}) \cdot \hat{K}_\varepsilon](t)$ vanishes outside a sphere of radius $O(n^{\frac{1}{2}})$. Thus Theorem 1.1 is adequate in showing that the right side in (1.58) is $O(n^{-\frac{1}{2}})$. Now use Lemma 1.8 to complete the proof of Theorem 1.7 in the case $\rho_{k+1} < \infty$. Finiteness of ρ_{k+1} is assured by the hypothesis of the theorem if $k = 1$ or 2. For $k > 2$ one uses truncation (see [9] or [11]).

Letting f in (1.54) be the indicator function of a Borel set A one gets

$$(1.59) \qquad |Q_n(A) - \Phi(A)| \leqq c_8(k)\rho_3 n^{-\frac{1}{2}} + c_8'(k) \sup_{y \in R^k} \Phi((\partial A)^{\varepsilon_n} + y) .$$

In view of (1.49) and the fact that $\mathscr{C}$ is translation invariant, it follows that

$$(1.60) \qquad \sup_{C \in \mathscr{C}} |Q_n(C) - \Phi(C)| \leqq c_9(k)\rho_3 n^{-\frac{1}{2}} .$$

The inequality (1.60) is an improvement of an earlier result of Ranga Rao [37]. Inequalities (1.59) and (1.60) were proved independently by von Bahr [2] and the present author [7] under slightly more stringent moment conditions (e.g., in [7] it is assumed that $\rho_{3+\delta} < \infty$ for some $\delta > 0$). Later the present form of (1.60) was obtained by Sazonov [38]. Theorem 1.7 is due to the author [9]. An extension to unbounded f and applications to nonuniform rates of convergence and mean central limit theorems may also be found in [9].

Although Theorem 1.7 seems adequate for most applications in which no assumption is made on the type of distribution Q_1, it is still important to know if ω_f^* may be replaced by $\bar{\omega}_f$ in (1.54). Very recently, Sweeting [41] has settled this important issue by proving that this is indeed possible. That this is possible if ε_n is also replaced by $\varepsilon_n' = \varepsilon_n \log n$ was shown earlier in [7], [8].

The next theorem of this section provides a limited expansion under a relaxation of Cramér's condition (1.36). To state this we define a *strongly nonlattice* probability measure Q_1 to be one for which

$$(1.61) \qquad |\hat{Q}_1(t)| < 1 \qquad \text{for all} \quad t \neq 0 .$$

It is easy to show that in one dimension the terms *nonlattice* and *strongly nonlattice* are equivalent. This is not the case in higher dimensions. Indeed, given a real c and a nonzero vector t_0 one may easily construct a nonlattice (or even nondiscrete) probability measure Q_1 which concentrates all its mass on the countable set of hyperplanes $\{x: \langle t_0, x\rangle = c + 2n\pi\}$, $n = 0, \pm 1, \pm 2, \cdots$. Clearly $|\hat{Q}_1(t_0)| = 1$, so that $\hat{Q}_1$ is *not* strongly nonlattice.

THEOREM 1.10. *If Q_1 is strongly nonlattice and $\rho_3 < \infty$, then the relation*

$$(1.62) \qquad \int_{R^k} f\, d[Q_n - \Phi - n^{-\frac{1}{2}} P_1(-\Phi)] = o(n^{-\frac{1}{2}})$$

holds uniformly for every class $\mathscr{F}$ of functions satisfying

$$(1.63) \qquad \sup_{f\in\mathscr{F}} \omega_f(R^k) < \infty , \qquad \sup_{f\in\mathscr{F}} \omega_f^*(\varepsilon : \Phi) = O(\varepsilon) \quad as \quad \varepsilon \downarrow 0 .$$

The proof of Theorem 1.10 is analogous to that of Theorem 1.7. Let η be any small number, and let $\varepsilon = n^{-\frac{1}{2}}\eta$. In Lemma 1.8 take $G = Q_n$, $H = \Phi + n^{-\frac{1}{2}}P_1(-\Phi)$, and let K_ε be as in the proof of Theorem 1.7. To estimate $\|(G - H) * K_\varepsilon\|$ use Lemma 1.8 with the density of $(G - H) * K_\varepsilon$ as g, and then apply Theorem 1.1 to estimate the integral of $|D^\nu \hat{g}| = |D^\nu[\hat{Q}_n - \hat{\Phi} - n^{-\frac{1}{2}}\hat{P}_1(-\Phi)\hat{K}_\varepsilon]|$ over a ball of radius $c_1' n^{\frac{1}{2}}$, say. This estimate is $\omega_f(R^k) \cdot o(n^{-\frac{1}{2}})$. Since $\hat{K}_\varepsilon(t) = 0$ for $\|t\| > n^{\frac{1}{2}}/\eta$, one needs to estimate the integral also over the set $B_n = \{c_1' n^{\frac{1}{2}} < \|t\| \leq n^{\frac{1}{2}}/\eta\}$. Since Q_1 is strongly nonlattice, one has

$$(1.64) \qquad \delta(u) \equiv \sup_{c' < \|t\| < u} |\hat{Q}_1(t)| < 1 \qquad u > c_1' ,$$

and $|\hat{Q}_n(t)| = |\hat{Q}_1(t/n^{\frac{1}{2}})|^n \leqq (\delta(\eta^{-1}))^n$ on B_n. But $(\delta(\eta^{-1}))^n$ goes to zero exponentially fast as $n \to \infty$, and the estimation is complete. It is also clear that a detailed knowledge of the asymptotic behavior of $\delta(\cdot)$ at infinity would enable one to refine (1.62). For example, if $\rho_4 < \infty$ and $\delta(u) = O(1 - u^{-1})$ as $u \to \infty$, then by taking one more term in the asymptotic expansion one may replace the remainder $o(n^{-\frac{1}{2}})$ by $O(n^{-1})$ in (1.62). The relation (1.62) is also uniform over every relatively norm compact class of probability measures Q_1 (strongly nonlattice and normalized) whose fourth moments are bounded away from infinity.

In many applications one needs to estimate the probability $Q_n(\{\|x\| > a_n\})$ where $a_n \to \infty$ as $n \to \infty$. The estimation (1.60) is usually not adequate for this purpose. In case the *Laplace–Stieltjes transform* $\lambda \to \int \exp\{\langle \lambda, x\rangle\} Q_1(dx)$ is finite in a neighborhood of the origin, precise estimates may be given, provided $a_n = o(n^{\frac{1}{2}})$. In one dimension this was done by Khinchin [26] in a special case and Cramér [19] in the general case. For a multidimensional extension we refer to von Bahr [3]. We shall not discuss this *large deviations* theory here. For applications discussed in this article the following result (due to von Bahr [1]) is adequate.

THEOREM 1.11. *If $\rho_s < \infty$ for some integer $s \geqq 3$, then for each $\delta > 0$ one has*

$$(1.65) \qquad \sup_{a \geqq (((s-2)+\delta)\log n)^{\frac{1}{2}}} a^s Q_n(\{||x|| \geqq a\}) = \theta_n n^{-(s-2)/2}$$

where θ_n goes to zero as $n \to \infty$.

To prove this we need to apply Lemma 1.6 to $G = Q_n$, $H = \Phi + \sum_{r=1}^{s-2} n^{-r/2} P_r(-\Phi)$, K_ε as used in the proof of Theorem 1.5, and the function

$$f(x) = 0 \quad \text{if} \quad ||x|| < a$$
$$= a^s \quad \text{if} \quad ||x|| \geqq a\,.$$

Also the quantity $\omega_f(R^k)$ in the bound (1.45) has to be replaced by $M_s(f)$ defined by (1.52). In this case $M_s(f) = a^s/(1 + a^s) < 1$, and $\bar{\omega}_f(2\varepsilon : |H|) = a^s|H|(\{a - 2\varepsilon < ||x|| < a + 2\varepsilon\})$. Since a is large, the average modulus of oscillation is small (namely, $o(n^{-(s-2)/2})$ if $\varepsilon = n^{-\frac{1}{2}} \log n$). The variation norm $||(G - H) * K_\varepsilon||$ is estimated as usual by appealing to Theorem 1.1 and doing a separate estimation of the integral of $D^\nu[(\hat{G} - \hat{H}) \cdot \hat{K}_\varepsilon](t)$ over the region $\{||t|| > n^{\frac{1}{2}}\}$. This last integration is facilitated by our choice of the kernel K (whose Fourier transform goes to zero fast at infinity).

2. Asymptotic expansion in the lattice case. A discrete subgroup L of R^k is a *lattice* if it is of rank k, i.e., if L has a representation

$$(2.1) \qquad L = \mathbb{Z} \cdot \xi_1 + \cdots + \mathbb{Z} \cdot \xi_k = \{\textstyle\sum_{l=1}^k m_l \xi_l : m_1, \cdots, m_k \in \mathbb{Z}\}\,.$$

Here $\xi_1, \cdots, \xi_k$ are k linearly independent vectors of R^k which are said to form a *basis of* L, and $\mathbb{Z}$ is the set of all integers. A probability measure Q on R^k is *of the lattice type* (or, simply, *lattice*) if there exist a lattice L and a vector x_0 such that

$$(2.2) \qquad Q(\{x_0 + L\}) = 1\,.$$

A *lattice random vector* is one whose distribution is of the lattice type. If Q is lattice and *nondegenerate* (i.e., no hyperplane carries the entire mass of Q), then there exists a smallest lattice L_0, called the *minimal lattice of* Q, such that (2.2) holds with $L = L_0$ and some x_0 (see [11], Lemma 21.4). It is obvious that if Q has finite second moments then it is nondegenerate if and only if its covariance matrix is nonsingular. If the *standard Euclidean basis* $\{e_1, \cdots, e_k\}$ is a basis of a lattice L, then $L = \mathbb{Z}^k$. For the sake of simplicity we assume below that Q_1 has a nondegenerate lattice distribution with minimal lattice $\mathbb{Z}^k$. Suppose X_1 has a nondegenerate lattice distribution whose minimal lattice has a basis $\{\xi_1, \cdots, \xi_k\}$.

Note that if T is the linear transformation mapping $\xi_1, \cdots, \xi_k$ into $e_1, \cdots, e_k$, then the random vector $Y_1 = TX_1$ has minimal lattice $\mathbb{Z}^k$. Since such a transformation changes the covariance matrix, we must now deal with an arbitrary covariance matrix V instead of the identity I. In addition, it would be convenient to take $x_0 = 0$ in (2.2). However, in order that one does not lose generality, one should then deal with an arbitrary mean vector. Throughout this section, therefore, we require that the lattice random vector Y_1 has a distribution Q with minimal lattice $\mathbb{Z}^k$ and that

$$EY_1 = \mu\,, \qquad \operatorname{Cov} Y_1 = V\,, \tag{2.3}$$

where V is nonsingular. Let then $\{Y_n : n \geqq 1\}$ be a sequence of i.i.d. lattice random vectors with Y_1 as specified. Let Q_n denote the distribution of $(Y_1 + \cdots + Y_n - n\mu)/n^{\frac{1}{2}}$. Write

$$\begin{aligned} y_{\alpha,n} &= \frac{\alpha - n\mu}{n^{\frac{1}{2}}}\,, \\ p_n(\alpha) &= \Pr(Y_1 + \cdots + Y_n = \alpha) = Q_n(\{y_{\alpha,n}\}) \qquad \alpha \in \mathbb{Z}^k\,, \\ q_{n,s}(x) &= n^{-k/2}[\phi_V(x) + \textstyle\sum_{r=1}^{s-1} n^{-r/2} P_r(-\phi_V)(x)]\,. \end{aligned} \tag{2.4}$$

Here ϕ_V is the *normal density* on R^k *having zero mean and covariance matrix* V, and $P_r(-\phi_V)$ is obtained by replacing ϕ by ϕ_V in (1.24). The polynomials $\tilde{P}_r$ are the same as before with the understanding that the cumulants χ_ν are now those of $Y_1 - \mu$.

THEOREM 2.1. *If* $\rho_s \equiv E\|Y_1 - \mu\|^s < \infty$ *for some integer* $s \geqq 2$, *then*

$$\begin{aligned} &\sup_{\alpha \in \mathbb{Z}^k} (1 + \|y_{\alpha,n}\|^s)|p_n(\alpha) - q_{n,s}(y_{\alpha,n})| = o(n^{-(k+s-2)/2})\,, \\ &\textstyle\sum_{\alpha \in \mathbb{Z}^k} |p_n(\alpha) - q_{n,s}(y_{\alpha,n})| = o(n^{-(s-2)/2}) \qquad n \to \infty\,. \end{aligned} \tag{2.5}$$

In order to prove (2.5) first note that the ch.f. $\hat{Q}^n$ of $Y_1 + \cdots + Y_n$ is the multiple Fourier series

$$\hat{Q}^n(t) = \textstyle\sum_{\alpha \in \mathbb{Z}^k} \exp\{i\langle t, \alpha\rangle\} p_n(\alpha) \qquad t \in R^k\,, \tag{2.6}$$

so that

$$\begin{aligned} p_n(\alpha) &= (2\pi)^{-k} \textstyle\int_{(-\pi,\pi]^k} \hat{Q}^n(t) \exp\{-i\langle t, \alpha\rangle\}\, dt \\ &= (2\pi)^{-k} n^{-k/2} \textstyle\int_{(-n^{\frac{1}{2}}\pi, n^{\frac{1}{2}}\pi]^k} \exp\{-i\langle \tau, y_{\alpha,n}\rangle\} \hat{Q}_n(\tau)\, d\tau\,, \end{aligned} \tag{2.7}$$

changing variables $t \to \tau = n^{\frac{1}{2}} t$ in the second step. Now approximate $\hat{Q}_n$ in (2.7) by its asymptotic expansion (a change of variables will convert Theorem 1.1 into the needed expansion corresponding to an arbitrary covariance matrix V) and compare the resulting expression with

$$\begin{aligned} q_{n,s}(y_{\alpha,n}) = (2\pi)^{-k} n^{-k/2} \textstyle\int_{R^k} &\exp\{-i\langle \tau, y_{\alpha,n}\rangle\} \\ &\times [1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2} \tilde{P}_r(i\tau)] \exp\{-\frac{1}{2}\langle \tau, V\tau\rangle\}\, d\tau\,. \end{aligned} \tag{2.8}$$

Similarly $y^\nu_{\alpha,n} p_n(\alpha)$ and $y^\nu_{\alpha,n} q_{n,s}(\alpha)$ are compared by inverting derivatives of $\hat{Q}_n$ and those of its expansion. The first relation in (2.5) is obtained in this way; the second follows from the first on summing over α.

The local expansion (2.5) is precise. The next problem is to find a method for summing up these approximations of point masses over sets. In one dimension Esseen [21] adapted the classical Euler–Maclaurin sum formula for this purpose. Ranga Rao [36], [37] proved a generalization of this summation formula in multidimension and used it to obtain expansions of Q_n. To explain this we introduce a sequence of functions S_j $(j = 0, 1, 2, \cdots)$ on R^1 which are periodic with period one, differentiable at all nonintegral points, and satisfy

$$(2.9) \qquad S_0 \equiv 1 , \qquad \frac{d}{dx} S_{j+1}(x) = S_j(x) \quad \text{for all} \quad x \quad \text{if} \quad j \geqq 1 ,$$
$$\frac{d}{dx} S_1(x) = 1 \quad \text{for nonintegral} \quad x .$$

Assume also that S_1 is right continuous. These conditions completely specify the sequence. For example,

$$(2.10) \qquad S_1(x) = x - \tfrac{1}{2} , \qquad S_2(x) = \tfrac{1}{2}(x^2 - x + \tfrac{1}{6}) ,$$
$$S_3(x) = \tfrac{1}{6}(x^3 - \tfrac{3}{2}x^2 + \tfrac{1}{2}x) , \qquad 0 \leqq x < 1 .$$

For $j \geqq 2$ the functions S_j are absolutely continuous on R^1, while S_1 has jumps -1 at all integral points. Let now f be an arbitrary real-valued function on R^1 having continuous and integrable derivatives $D^j f$, $0 \leqq j \leqq r$. Write

$$(2.11) \qquad F(x) = \int_{-\infty}^{x} f(t)\, dt ,$$
$$F_r(x) = \sum_{j=0}^{r} (-1)^j S_j(x) D^j F(x) + (-1)^{r+1} \int_{-\infty}^{x} S_r(t) D^{r+1} F(t)\, dt .$$

Then F_r is the distribution function of a finite signed measure and an integration by parts yields

$$(2.12) \qquad \sum_{m \leq x} f(m) = F_r(x) \qquad x \in R^1 .$$

The summation on the left is over integers m. To extend (2.12) to multidimension consider a function f on R^k having continuous and integrable derivatives $D^\nu f$, $0 \leqq |\nu| \leqq r$. Define

$$(2.13) \qquad F(x) = \int_{-\infty}^{x^{(1)}} \cdots \int_{-\infty}^{x^{(k)}} f(y)\, dy \qquad x = (x^{(1)}, \cdots, x^{(k)}) \in R^k .$$

Define operators $I_{r,j}$, $T_{r,j}$ acting on such functions F by

$$(2.14) \qquad \begin{aligned} I_{r,j}(F)(x) &= \int_{-\infty}^{x^{(j)}} S_r(t)(D_j^{r+1}F)(x^{(1)}, \cdots, x^{(j-1)}, t, x^{(j+1)}, \cdots, x^{(k)})\, dt \\ &= \int_{-\infty}^{x^{(1)}} \cdots \int_{-\infty}^{x^{(k)}} S_r(y^{(j)}) D_j^r f(y)\, dy \qquad x = (x^{(1)}, \cdots, x^{(k)}) , \\ T_{r,j}(F) &= (1 - S_1(x^{(j)})D_j + \cdots + (-1)^r S_r(x^{(j)}) D_j^r \\ &\quad + (-1)^{r+1} I_{r,j})(F) . \end{aligned}$$

Since the operators $T_{r,j}$ are associative and commutative one may define

$$(2.15) \qquad \begin{aligned} F_r(x) &= \left(\prod_{j=1}^{k} T_{r,j}\right)(F)(x) \\ &= \prod_{j=1}^{k} \{1 - S_1(x^{(j)})D_j + \cdots + (-1)^r S_r(x^{(j)}) D_j^r \\ &\quad + (-1)^{r+1} I_{r,j}\}(F)(x) \qquad x = (x^{(1)}, \cdots, x^{(k)}) . \end{aligned}$$

Again one may show that F_r is of bounded variation; and an induction on k using (2.12) yields

$$\sum_{\{\alpha^{(1)}\leq x^{(1)},\cdots,\alpha^{(k)}\leq x^{(k)}\}} f(\alpha) = F_r(x) \qquad x = (x^{(1)}, \cdots, x^{(k)})\,. \tag{2.16}$$

The summation on the left is over integral vectors $\alpha = (\alpha^{(1)}, \cdots, \alpha^{(k)})$. To apply this result to our specific situation define

$$f(x) = q_{n,s}\left(\frac{x - n\mu}{n^{\frac{1}{2}}}\right) \qquad x \in R^k\,, \tag{2.17}$$

and obtain (taking $r = s - 1$ in (2.16))

$$\begin{aligned}\sum_{\{\alpha:\alpha\leq n^{\frac{1}{2}}x+n\mu\}} q_{n,s}\left(\frac{\alpha - n\mu}{n^{\frac{1}{2}}}\right) = \prod_{j=1}^{k}\{1 &- S_1(n\mu^{(j)} + n^{\frac{1}{2}}x^{(j)})D_j + \cdots \\ &+ (-1)^{s-1}S_{s-1}(n\mu^{(j)} + n^{\frac{1}{2}}x^{(j)})D_j^{s-1} \\ &+ (-1)^s I_{s-1,j}\}(F)(n^{\frac{1}{2}}x + n\mu)\,.\end{aligned} \tag{2.18}$$

By expanding the product in (2.18) and omitting terms of order $O(n^{-j/2})$, $j \geq s - 1$, one has

$$\begin{aligned}&\sum_{\{\alpha\leq n^{\frac{1}{2}}x+n\mu\}} q_{n,s}\left(\frac{\alpha - n\mu}{n^{\frac{1}{2}}}\right) \\ &\quad= \sum_{|\nu|\leq s-2} n^{-|\nu|/2}(-1)^{|\nu|}S_\nu(n\mu + n^{\frac{1}{2}}x)D^\nu\Phi_V(x) \\ &\qquad+ n^{-\frac{1}{2}}\sum_{|\nu|\leq s-3} n^{-|\nu|/2}(-1)^{|\nu|}S_\nu(n\mu + n^{\frac{1}{2}}x)D^\nu P_1(-\Phi_V)(x) + \cdots \\ &\qquad+ n^{-(s-2)/2}P_{s-2}(-\Phi_V)(x) + o(n^{-(s-2)/2})\end{aligned} \tag{2.19}$$

uniformly for $x \in R^k$. Here for each multiindex $\nu = (\nu^{(1)}, \cdots, \nu^{(k)})$

$$S_\nu(x) = S_{\nu^{(1)}}(x^{(1)}) \cdots S_{\nu^{(k)}}(x^{(k)}) \qquad x = (x^{(1)}, \cdots, x^{(k)})\,. \tag{2.20}$$

Combining (2.5) and (2.19) one has

THEOREM 2.2. *If $\rho_s < \infty$ for some integer $s \geq 3$ and F_n denotes the distribution function of Q_n, then*

$$\begin{aligned}\sup_{x\in R^k}|F_n(x) &- \sum_{|\nu|\leq s-2} n^{-|\nu|/2}(-1)^{|\nu|}S_\nu(n\mu + n^{\frac{1}{2}}x)D^\nu\Phi_V(x) \\ &- n^{-\frac{1}{2}}\sum_{|\nu|\leq s-3} n^{-|\nu|/2}(-1)^{|\nu|}S_\nu(n\mu + n^{\frac{1}{2}}x)D^\nu P_1(-\Phi_V)(x) - \cdots \\ &- n^{-(s-2)/2}P_{s-2}(-\Phi_V)(x)| = o(n^{-(s-2)/2})\,.\end{aligned} \tag{2.21}$$

Note that if μ_n denotes the signed measure whose distribution function appears on the right side of (2.18), then (by virtue of (2.18) and (2.5))

$$|Q_n(A) - \mu_n(A)| = o(n^{-(s-2)/2}) \tag{2.22}$$

uniformly over all Borel sets A. Unfortunately, it has not been possible so far to obtain computable expressions of $\mu_n(A)$ for sets A other than rectangles whose sides are parallel to the hyperplanes $\{x^{(j)} = 0\}$, $1 \leq j \leq k$. In case Y_1 has a minimal lattice with basis $\{\xi_1, \cdots, \xi_k\}$, Theorem 2.2 is easily modified to apply to rectangles whose sides are parallel to the hyperplanes $\{x \equiv \sum_1^k y^{(j)}\xi_j : y^{(l)} = 0\}$, $1 \leq l \leq k$. The difficulty is caused by the presence of terms involving S_1. One of the most outstanding problems in the subject is to obtain "good" estimations of $Q_n(A)$ in the lattice case for sets A other than rectangles properly aligned with the lattice. Perhaps the nature of the problem is best appreciated by linking it with the lattice point problem of analytic number theory. We do this in the following section.

3. The lattice point problem. Confining ourselves to the standard lattice $\mathbb{Z}^k$, we define a *lattice-point* as a point in $\mathbb{Z}^k$. Let V be a positive definite symmetric matrix and consider the ellipsoids

$$E(c: V) = \{x \in R^k : \langle x, V^{-1}x \rangle \leqq c\} \qquad c > 0 . \tag{3.1}$$

Let $N(c: V)$ denote the number of lattice points in $E(c: V)$. An important problem in analytic number theory is to obtain asymptotic estimates of $N(c: V)$ as $c \to \infty$. If no further specification is made on k and V, then the best known result is that of Landau, namely,

$$|N(c: V) - \text{volume of } E(c: V)| = O(c^{k/2 - k/k+1}) \qquad c \to \infty . \tag{3.2}$$

Esseen [21] showed that (3.2) is essentially equivalent to the following theorem specialized to lattice random vectors.

THEOREM 3.1. *If* $\{Y_n : n \geqq 1\}$ *is a sequence of* i.i.d. *random vectors each with mean* μ, *covariance matrix* V, *and a finite fourth absolute moment, then*

$$\sup_{a \geqq 0} |Q_n(E(a: V)) - \Phi_V(E(a: V))| = O(n^{-k/(k+1)}) , \tag{3.3}$$

where Q_n *is the distribution of* $n^{-\frac{1}{2}} \sum_{j=1}^{n} (Y_j - \mu)$.

The proof of Theorem 3.1 is rather long and is given in [21]. We shall only give a sketch of Esseen's argument linking (3.2) and (3.3). Note that the right side in (3.3) goes to zero faster than $n^{-\frac{1}{2}}$ if $k > 1$. If the distribution Q_1 satisfies Cramér's condition (1.36), then a faster rate of convergence (with an error $O(n^{-1})$) may be obtained from (1.50) with $s = 4$. Here one uses the fact that $P_1(-\phi_V)$ is an odd function and, therefore,

$$P_1(-\Phi_V)(E(a: V)) = P_1(-\Phi)(E(a: I)) = 0 . \tag{3.4}$$

The strength of Esseen's result lies, however, in its generality. For example, suppose Y_1 in the theorem is lattice having $\mathbb{Z}^k$ as its minimal lattice. Without loss of generality assume $\Pr(Y_1 \in \mathbb{Z}^k) = 1$. The local expansion (2.5) with $s = 4$ yields (we take $\mu = 0$ for simplicity)

$$\begin{aligned} \sup_{a \geqq 0} \Big| Q_n(E(a: V) &- (\det V)^{-\frac{1}{2}} (2\pi n)^{-k/2} \\ &\times \textstyle\sum_{\{\alpha \in \mathbb{Z}^k : \langle \alpha - n\mu, V^{-1}(\alpha - n\mu)\rangle \leqq an\}} \exp\left\{-\frac{1}{2n} \langle \alpha - n\mu, V^{-1}(\alpha - n\mu)\rangle\right\}\Big| \\ &= O(n^{-1}) , \end{aligned} \tag{3.5}$$

again because $P_1(-\phi_V)$ is an odd function and the set of vectors $y_{\alpha,n} = (\alpha - n\mu)/n^{\frac{1}{2}}$ over which $P_1(-\phi_V)(y_{\alpha,n})$ is to be summed is symmetric. Combining (3.3) and (3.5) one gets

$$\begin{aligned}(3.6)\qquad &\sup_{a\geq 0}\Big|(\det V)^{-\frac{1}{2}}(2\pi n)^{-k/2}\\ &\quad\times \sum_{\{\langle\alpha-n\mu,V^{-1}(\alpha-n\mu)\rangle\leq an\}}\exp\left\{-\frac{1}{2n}\langle\alpha-n\mu,\ V^{-1}(\alpha-n\mu)\rangle\right\}\\ &\quad-(\det V)^{-\frac{1}{2}}(2\pi)^{-k/2}\int_{\{\langle x,V^{-1}x\rangle\leq a\}}\exp\{-\tfrac{1}{2}\langle x,\ V^{-1}x\rangle\}\,dx\Big|\\ &\quad= O(n^{-k/(k+1)})\,.\end{aligned}$$

Now write $N(u)$ for the number of lattice points in $E(u: V)+n\mu=\{x: \langle x-n\mu, V^{-1}(x-n\mu)\rangle\leq u\}$, $u>0$. Also write $B(u)$ for the volume of $E(u: V)$, and let

$$(3.7)\qquad R(u)=N(u)-B(u)\,.$$

Then (3.6) reduces to

$$(3.8)\qquad \sup_{a\geq 0}\left|(\det V)^{-\frac{1}{2}}(2\pi n)^{-k/2}\int_{[0,an]}\exp\left\{-\frac{u}{2n}\right\}dR(u)\right| = O(n^{-k/(k+1)})\,.$$

An integration by parts immediately gives

$$\begin{aligned}(3.9)\qquad &\sup_{a\geq 0}\left|(\det V)^{-\frac{1}{2}}(2\pi n)^{-k/2}\left[e^{-a/2n}R(an)+\frac{1}{2n}\int_{[0,an]}e^{-u/2n}R(u)\,du\right]\right|\\ &\quad= O(n^{-k/(k+1)})\,.\end{aligned}$$

Since $(an)^{-1}\int_{[0,an]}|R(u)|\,du$ is of order not larger than that of $|R(an)|$, (3.9) leads to

$$(3.10)\qquad R(an)=O(n^{k/2-k/(k+1)})$$

for all $a>0$. Landau's result (3.2) follows from (3.10). Conversely, on retracing the steps one can deduce (3.3) for lattice random vectors from (3.2). More precisely, it has been shown by Yarnold [43] using the expansion in Section 2 that in the lattice case one has

$$\begin{aligned}(3.11)\qquad &\sup_{a\geq 0}|Q_n(E(a: V))-\Phi_V(E(a: V))-R(an)e^{-a/2}(2\pi n)^{-k/2}(\det V)^{-\frac{1}{2}}|\\ &\quad= O(n^{-1})\,.\end{aligned}$$

It is a simple consequence of (3.2) that the number of lattice points on the surface $\{x: \langle x, V^{-1}x\rangle = c\}$ is of the order $O(c^{k/2-k/(k+1)})$ as $c\to\infty$. Also observe that we can derive a weaker estimate $O(c^{(k-1)/2})$ for this as well as for the remainder in (3.2) more simply from the inequality (1.60) without appealing to Theorem 3.1 or the material in Section 2.

The foregoing discussion virtually rules out the possibility of obtaining computable expansions of $Q_n(A)$ in the lattice case except for sets A properly aligned with the lattice. Under the circumstances perhaps the best one can hope for is an extension of Theorem 3.1. Of course, for sets A which are not symmetric the analogue of (3.3) is

$$(3.12)\qquad |Q_n(A)-\Phi_V(A)-n^{-\frac{1}{2}}P_1(-\Phi_V)(A)| = O(n^{-k/(k+1)})\,.$$

Recently, Matthes [30] proved this for a class of convex bodies A having sufficiently smooth surfaces whose Gaussian curvatures are bounded away from zero and infinity. The result is delicate. Note that it does not hold for rectangles. It would appear that (3.12) will not hold if ∂A contains too many points of the lattice $n^{-k/2}\mathbb{Z}^k$. Technically, the proof by Matthes uses an estimate of Esseen [21] on the value distribution of $|\hat{Q}_1|$ and a result of Herz [23] asserting

$$|\hat{I}_A(t)| = O(\|t\|^{-(k+1)/2}) \qquad \|t\| \to \infty \tag{3.13}$$

for the convex sets A discussed by Matthes. Since convexity is a bothersome restriction, it would be useful to extend the result of Matthes by proving (3.13) for other smooth sets A.

The lattice point problem is intimately related to the asymptotic distribution of eigenvalues of self adjoint elliptic operators in the theory of partial differential equations. For a delightful discussion of this we refer to Courant and Hilbert [18] (pages 429–445).

4. Asymptotic distributions of a class of statistics. In this section we briefly sketch the derivation of normal approximations and asymptotic expansions of a class of statistics commonly used for purposes of statistical inference. Simplest examples of such statistics are functions of sample moments. Detailed proofs will appear elsewhere. Theorem 4.1 is based on joint work with J. K. Ghosh. Theorem 4.2 and the expansion (4.15) were obtained by Chibisov [15] under more restrictive assumptions on the functions f_i $(1 \leqq i \leqq k)$ below using different methods. While we merely require differentiability, Chibisov [15] assumes analyticity of these functions, but obtains estimates of the variation norm.

Let $\{Y_n \equiv (Y_n^{(1)}, \cdots, Y_n^{(m)}) : n \geqq 1\}$ be a sequence of i.i.d. random vectors with values in R^m $(m \geqq 1)$. Let G denote their common distribution. We introduce real-valued, Borel measurable functions $f_1, \cdots, f_k$ on R^m and assume

A_1: *$E|f_i(Y_1)|^s < \infty$, $1 \leqq i \leqq k$. Here s is a positive integer, $s \geqq 3$.*

A_2: *H is a real-valued Borel measurable function defined on a neighborhood N of*

$$\mu \equiv (Ef_1(Y_1), \cdots, Ef_k(Y_1)) . \tag{4.1}$$

H has bounded and continuous derivatives of order p_0 or less in some neighborhood $M(\subset N)$ of μ. Here $p_0 \geqq 2$. Also,

$$(\text{grad } H)(\mu) \equiv (D_1 H, \cdots, D_k H)(\mu) \neq 0 . \tag{4.2}$$

The derivatives of H at μ are denoted by

$$\begin{aligned} l_j &= (D_j H)(\mu) \qquad (1 \leqq j \leqq k), \quad l = (l_1, \cdots, l_k) ; \\ l_{i_1 \cdots i_p} &= (D_{i_1} \cdots D_{i_p} H)(\mu) \quad (1 \leqq i_1, \cdots, i_p \leqq k; p \leqq p_0) . \end{aligned} \tag{4.3}$$

Also write

$$\begin{aligned} Z_n &= (f_1(Y_n), \cdots, f_k(Y_n)) , \qquad \bar{Z} = \frac{1}{n} \textstyle\sum_{i=1}^n Z_i , \\ W_n &= n^{1/2}[H(\bar{Z}) - H(\mu)] , \end{aligned} \tag{4.4}$$

and introduce the function

$$g_n(z) = n^{\frac{1}{2}}\left[H\left(\mu + \frac{z}{n^{\frac{1}{2}}}\right) - H(\mu)\right]. \tag{4.5}$$

By extending H, if necessary, arbitrarily (but measurably) over all of R^k we make W_n and g_n well defined. Note that $\{Z_n : n \geqq 1\}$ is an i.i.d. sequence, $EZ_1 = \mu$. Let

$$V = \operatorname{Cov} Z_1 . \tag{4.6}$$

It is easy to see that V is singular if and only if the functions $1, f_1, \cdots, f_k$ are linearly dependent on the support of G, i.e., if and only if there exist $\theta^{(1)}, \cdots, \theta^{(k)}$, $c \in R^1$, not all zero, such that

$$G(\{y : \textstyle\sum_{i=1}^k \theta^{(i)} f^{(i)}(y) = c\}) = 1 . \tag{4.7}$$

Let λ, Λ *denote the smallest and largest eigenvalues of* V, respectively. Recall that ϕ_V is the normal density on R^k with mean zero and covariance V. The following result holds.

THEOREM 4.1. *If* A_1 *holds with* $s = 3$, A_2 *holds with* $p_0 = 2$, *and if* V *is nonsingular, then*

$$\sup_{u \in R^1} |\Pr(W_n \leqq u) - \textstyle\int_{\{g_n(z) \leqq u\}} \phi_V(z)\, dz| \leqq dn^{-\frac{1}{2}} , \tag{4.8}$$

where d *depends only on the moments of* Z_1 *of orders three or less and on the first order derivatives of* H *on* M.

In order to prove this theorem one cannot appeal to (1.59) directly, since, in general, V is not the identity matrix. But transforming the random vectors $Z_1, \cdots, Z_n$, by a nonsingular linear transformation one easily obtains (from (1.59))

$$\begin{aligned} |Q_n(A) - \Phi_V(A)| &\leqq c_8(k)\lambda^{-\frac{3}{2}} E\|Z_1 - \mu\|^3 n^{-\frac{1}{2}} \\ &\quad + c_8'(k) \sup_{y \in R^k} \Phi_V((\partial A)^\eta + y) , \\ \eta &= c_6(k)\lambda^{-\frac{3}{2}} E\|Z_1 - \mu\|^3 n^{-\frac{1}{2}} , \end{aligned} \tag{4.9}$$

where Q_n is the distribution of $n^{-\frac{1}{2}}(Z_1 + \cdots + Z_n - n\mu)$. To apply (4.9) one may take $A = \{z \in R^k : g_n(z) \leqq u\}$ or, in view of Theorem 1.11, its restriction to the set $\{\|z\| \leqq ((s-1)\Lambda \log n)^{\frac{1}{2}}\}$. A fairly straightforward computation yields

$$\sup_{y \in R^k} \Phi_V((\partial A)^\varepsilon + y) \leqq d'\varepsilon \qquad \varepsilon > 0 , \tag{4.10}$$

uniformly in u, and (4.8) follows from (4.9) and (4.10).

To obtain asymptotic expansions going beyond (4.8) we assume

A_3: *The distribution* G *of* Y_1 (*or* G^{*r} *for some positive integer* r) *has a nonzero absolutely continuous component* H. *Further, there exists a nonempty open set* B *of* R^m *on which the density of* H *is positive and the functions* $1, f_1, \cdots, f_k$ *are continuously differentiable and linearly independent.*

Note that if A_3 holds, then by Lemma 1.4 the distribution of $Z_1 - \mu$ satisfies Cramér's condition (1.36). Theorem 1.5 then implies (by a linear transformation of Z_j's)

THEOREM 4.2. *Assume* A_1, A_2, A_3 *hold with* $p_0 = s \geq 3$. *Then*

$$(4.11)\qquad \sup_{u\in R^1} \left|\Pr(W_n \leq u) - \int_{\{g_n(z)\leq u\}} [\phi_V(z) + \sum_{r=1}^{s-2} n^{-r/2} P_r(-\phi_V)(z)]\,dz\right| = o(n^{-(s-2)/2}) \qquad n \to \infty .$$

Since the domain of integration $\{g_n(z) \leq u\}$ is not simple to deal with we now provide a more computable expression for the expansion. For this we first introduce the function

$$(4.12)\qquad h_{s-1}(z) = \sum_{j=1}^{k} l_j z^{(j)} + \frac{1}{2n^{\frac{1}{2}}} \sum_{1\leq i,j\leq k} l_{ij} z^{(i)} z^{(j)} + \cdots + \frac{1}{(s-1)!\, n^{(s-2)/2}} \sum_{1\leq i_1,\cdots,i_{s-1}\leq k} l_{i_1\cdots i_{s-1}} z^{(i_1)} \cdots z^{(i_{s-1})}$$

and note that h_{s-1} is a Taylor expansion of g_n and, therefore, for all constants $c > 0$,

$$(4.13)\qquad \sup_{\{\|z\|<c \log^{\frac{1}{2}} n\}} |g_n(z) - h_{s-1}(z)| = O(n^{-(s-1)/2} \log^{s/2} n) .$$

In view of (4.13) and Theorem 1.11 one may replace g_n by h_{s-1} and the random variable W_n by

$$(4.14)\qquad W_n' \equiv h_{s-1}(n^{-\frac{1}{2}}(Z_1 + \cdots + Z_n - n\mu)) .$$

The next task is to derive the expansion

$$(4.15)\qquad \int_{\{h_{s-1}(z)\leq u\}} \psi(z)\,dz = \int_{\{\sum_1^k l_j z^{(j)}\leq u\}} [\psi(z) + \sum_{r=1}^{s-2} n^{-r/2} \psi_r(z)]\,dz + O(n^{-(s-1)/2}) ,$$

where $\psi, \psi_1, \cdots, \psi_r$ are polynomial multiples of ϕ_V whose coefficients do not depend on n. This may be done by an appropriate change of variables; but we omit the details. For example, one may easily show (assuming $l_k \neq 0$)

$$(4.16)\qquad \int_{\{h_2(z)\leq u\}} \psi(z)\,dz = \int_{\{\sum l_j z^{(j)}\leq u\}} \left[\psi(z)\left(\left(1 - \frac{\sum_j l_{kj} z^{(j)}}{l_k n^{\frac{1}{2}}}\right) - (D_k\psi)(z) \frac{\sum_{i,j} l_{ij} z^{(i)} z^{(j)}}{2 l_k n^{\frac{1}{2}}}\right)\right] dz + O(n^{-1}) .$$

Applying (4.13) and (4.16) in Theorem 4.1 one obtains

$$(4.17)\qquad \sup_{u\in R^1} \left|\Pr(W_n \leq u) - \int_{-\infty}^{u} \phi_{\tilde{\sigma}^2}(v)\,dv\right| \leq d' n^{-\frac{1}{2}} ,$$

where d' is a positive constant and

$$(4.18)\qquad \tilde{\sigma}^2 = \langle l, Vl\rangle , \qquad \phi_{\tilde{\sigma}^2}(v) = \frac{1}{(2\pi)^{\frac{1}{2}}\tilde{\sigma}} \exp\left\{-\frac{v^2}{2\tilde{\sigma}^2}\right\} .$$

Similarly from Theorem 4.2 one gets

$$(4.19)\qquad \sup_{u\in R^1} \left|\Pr(W_n \leq u) - \int_{\{\langle l,z\rangle\leq u\}} \left[\phi_V(z)\left(1 - \frac{1}{l_k n^{\frac{1}{2}}} \sum_j l_{kj} z^{(j)}\right) - \frac{1}{2 l_k n^{\frac{1}{2}}} (\sum_{i,j} l_{ij} z^{(i)} z^{(j)})(D_k\phi_V)(z) + \frac{1}{n^{\frac{1}{2}}} P_1(-\phi_V)(z)\right] dz\right| = O(n^{-1}) ,$$

if A_1, A_2, A_3 hold with $p_0 = s = 4$.

By a linear transformation $z \to x$, with $x^{(1)}(z) = \langle l, z\rangle$, the right side of (4.15) may be reduced by integration to yield

$$(4.20) \qquad \int_{\{h_{s-1}(z)\le u\}} \{\phi_V(z) + \sum_{r=1}^{s-1} n^{-r/2}P_r(-\phi_V)(z)\}\, dz - \int_{-\infty}^{u} [1 + \sum_{r=1}^{s-2} n^{-r/2}q_r(v)]\phi_{\tilde\sigma^2}(v)\, dv = O(n^{-(s-1)/2}) ,$$

where $q_1, \cdots, q_{s-2}$ are polynomials whose coefficients do not depend on n. To identify the polynomials q_j's we describe another formal procedure for expanding the distribution function of W_n. Since W_n may not have finite moments of orders up to s, a formal method for computing "approximate cumulants" of W_n is used. This is the so-called *delta method*. Assume, for the sake of simplicity, that Z_1 has finite moments of all orders. Since h_{s-1} is a polynomial of degree $s-1$, the moments and cumulants of W_n' can be computed in terms of those of $Z_1 - \mu$ either directly (algebraically), or using Theorem 1.5 with $f = h_{s-1}$, or using Theorem 1.1. One may show

$$(4.21) \qquad j\text{th cumulant of} \quad W_n' = K_{j,n} + o(n^{-(s-2)/2}) ,$$

where

$$(4.22) \qquad \begin{aligned} K_{1,n} &= \sum_{i=1}^{s-2} n^{-i/2} b_{1i} , \\ K_{j,n} &= n^{-(j-2)/2}K_j + \sum_{j-1}^{s-2} n^{-i/2} b_{ji} \qquad j \geqq 2 , \\ K_j &= j\text{th cumulant of} \quad \langle l, Z_1 - \mu\rangle , \end{aligned}$$

and b_{ji}'s depend only on cumulants of $Z_1 - \mu$ of orders s^2 and less. Also note that $K_2 = \tilde\sigma^2$. Now write

$$(4.23) \qquad \exp\left\{itK_{1,n} + \frac{(it)^2}{2}(K_{2,n} - \tilde\sigma^2) + \sum_{r=3}^{s} \frac{(it)^r}{r!} K_{r,n}\right\} = 1 + \sum_{r=1}^{s-2} n^{-r/2}\Pi_r(it) + o(n^{-(s-2)/2}) \qquad t \in R^1 ,$$

where Π_r's are polynomials whose coefficients depend only on the cumulants of $Z_1 - \mu$ of orders s and less. One would then expect (as in the case of the Edgeworth expansion in Section 1)

$$(4.24) \qquad \Pr(W_n \leqq u) = \int_{-\infty}^{u} [1 + \sum_{r=1}^{s-2} n^{-r/2}\Pi_r(-D)]\phi_{\tilde\sigma^2}(v)\, dv + o(n^{-(s-2)/2}) ,$$

where $\Pi_r(-D)$ is the differential operator obtained by formally substituting $(-1)^j D^j$ for $(it)^j$ in the polynomial $\Pi_r(it)$, $j \geqq 0$. The integrands on the right sides of (4.20) and (4.24) are identical, i.e.,

$$(4.25) \qquad q_r(v) = \phi_{\tilde\sigma^2}^{-1}(v) \cdot \Pi_r(-D)\phi_{\tilde\sigma^2}(v) \qquad r \geqq 1 .$$

One proves this by showing that the two densities under the integral signs in (4.20) and (4.24) have the same moments of all orders.

We refer to Wallace [42] for a description of the original conjecture about the validity of an expansion analogous to (4.24) using $n^{-(j-2)/2}K_j$ instead of $K_{j,n}$. In [12] Bickel modified this conjecture essentially in its present form. We do emphasize, however, that the moments and cumulants of W_n are not quite relevant for the above expansion; for the asymptotic distribution of W_n depends only on the local behavior of H at μ. Bickel [12] also discusses the possibility of applying the above expansion to other types of statistics. The main problem, of course, is to prove that there exists an expansion.

The results of this section extend in a fairly straightforward way to vector-valued functions H, and to probabilities of other sets of interest (not merely intervals or rectangles).

5. Other applications, extensions. A number of applications other than those discussed in Sections 3, 4 are listed below.

(a) *U-statistics.* Suppose $\{X_n : n \geqq 1\}$ is a sequence of i.i.d. observations with values in some space S. Let ψ be a real or vector-valued function on $S \times S$ such that $\psi(x, y) = \psi(y, x)$. The function $U_n = \binom{n}{2}^{-1} \sum_{1 \leqq i < j \leqq n} \psi(X_i, X_j)$ is a *U-statistic with kernel* ψ. Subtracting the expectation if necessary, we assume that $E\psi(X_1, X_2) = 0$. Also suppose $E\|\psi(X_1, X_2)\|^2 < \infty$. Let $\psi_1(x) = E\psi(X_1, x)$; then $\{\psi_1(X_n) : n \geqq 1\}$ is an i.i.d. sequence. By comparing U_n with $S_n = n^{-1} \sum_1^n \psi_1(X_i)$, Höeffding (see [35], page 58) showed that as $n \to \infty$ the statistic $n^{\frac{1}{2}} U_n$ converges in distribution to Φ_V, where $V = \operatorname{Cov} \psi_1(X_1)$. By an attractive argument Bickel [12] has recently shown that if ψ is real-valued and bounded, then

$$\sup_{u \in R^1} \left| \Pr(n^{\frac{1}{2}} U_n \leqq u) - \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} \int_{-\infty}^{u} e^{-v^2/2\sigma^2}\, dv \right| = O(n^{-\frac{1}{2}}), \tag{5.1}$$

where $\sigma^2 = E\psi_1^2(X_1)$. It would be useful to relex Bickel's assumption of boundedness of ψ, to extend (5.1) to vector-valued ψ, and, more importantly, to obtain an asymptotic expansion under appropriate assumptions. There are similar important problems concerning the so-called *rank statistics* (see [12]).

(b) *Maximum likelihood estimators.* Let $[X_n : n \geqq 1\}$ be a sequence of i.i.d. observations from a distribution with a strictly positive density $f(x; \theta)$ (relative to some σ-finite measure), where the *parameter* θ lies in an open subset of R^k (or, more generally, in a k-dimensional manifold). Assume that f is twice differentiable in θ and that the *likelihood equations* (in θ)

$$\sum_{i=1}^{n} \frac{\partial \log f(X_i; \theta)}{\partial \theta^{(j)}} = 0 \qquad 1 \leqq j \leqq k \tag{5.2}$$

have a unique solution $\hat{\theta}_n$, the *maximum likelihood estimator of* θ. If the *information matrix* $I(\theta) = -((E_\theta D_i D_j \log f(X_1, \theta)))$ is nonsingular, then under regularity assumptions one shows that $T_n = n^{\frac{1}{2}}(\hat{\theta}_n - \theta)$ is asymptotically normal Φ_V, where $V = I^{-1}(\theta)$. For the case $k = 1$ Berry–Esseen bounds and asymptotic expansions of the distribution function of T_n have been obtained by Linnik and Mitrofanova [29] and Pfanzagl [34]. A complete derivation for multidimensional parameters is still not available.

An entirely analogous problem arises in mathematical economics [10]. Here the summands in (5.2) are *excess demands* of individuals, θ is the (normalized) price vector. The solution $\hat{\theta}_n$ is the *equilibrium price.* One is interested in the asymptotic behavior of $\hat{\theta}_n$ when n, the number of agents in the economy, is large.

(c) *Law of the iterated logarithm.* The classical law of the iterated logarithm (LIL) is essentially tied up with the central limit theorem. Indeed, a very useful method of proving LIL's is by using the classical Berry–Esseen theorem. This method is originally due to Chung [16] (also see [17] pages 231–237) and was later rediscovered by Petrov [33]. It can be used to derive classical as well as Strassen type LIL's for independent as well as dependent random variables with the help of such Berry–Esseen type bounds as obtained by Statulevicius [39] and Stein [40]. This method is comparable in effectiveness with that using the Skorokhod representation (of successive partial sums of a sequence of random variables as values of the Brownian path at appropriately defined successive stopping times).

(d) *Statistical mechanics.* In his important works on the mathematical foundations of classical statistical mechanics Khinchin [27] used (his own) results on refinements of the central limit theorem to provide an analytical derivation of the Gibbs canonical ensemble and the laws of classical thermodynamics. Khinchin's book [27] is still one of the most penetrating studies on the foundations of equilibrium statistical mechanics of ideal gasses.

We conclude this article with a few additional remarks. First, the main theorems of Sections 1 and 2 have appropriate analogs in the non-i.i.d. case; these analogs may be found in the cited references. Secondly, note that if $\{X_n : n \geqq 1\}$ is an i.i.d. sequence of k-dimensional random vectors such that X_1 has independent coordinates, then obtaining rates of convergence and asymptotic expansions of the distribution Q_n (of the normalized partial sum) reduces to a one-dimensional problem. This is obvious if one is approximating the distribution function of Q_n; but even for more general sets (e.g., the class $\mathscr{C}$ of Borel measurable convex sets) one only needs to use the classical Berry–Esseen theorem and the Fubini theorem. Thus one can easily show (see [8], Theorem 4.7)

$$(5.3) \qquad \sup_{C \in \mathscr{C}} |Q_n(C) - \Phi(C)| \leqq 2c_0 (\textstyle\sum_{i=1}^{k} E|X_1^{(i)}|^3) n^{-\frac{1}{2}} ,$$

where the universal constant c_0 is the one appearing in the Berry–Esseen bound (see Van Beek [4] for an estimation $c_0 = .7975$). Thus, in our context, the complexity of higher dimensionality arises only through the dependence among coordinate variables.

As a third remark it may be mentioned that errors of normal approximation have also been estimated by methods different from the Fourier analytic method used here (e.g., see [5], [31], [38], [41]). Because these methods are somewhat more direct it is possible that they will yield better estimates of constants involved in the bounds. However, none of these other methods have been successful in providing asymptotic expansions. Our final remark concerns the moment condition "$\rho_3 < \infty$" in Theorem 1.7. Rates of convergence can be obtained when $\rho_{2+\delta}$ is assumed finite for some δ, $0 \leqq \delta < 1$ (see, e.g., Section 18 in [11]). For distribution functions in one dimension definitive results have been obtained in this case by Heyde [24] and Ibragimov [25].

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4.5 "On the validity of the formal Edgeworth expansion"

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ON THE VALIDITY OF THE FORMAL EDGEWORTH EXPANSION

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Let $\{Y_n\}_{n\geq 1}$ be a sequence of i.i.d. m-dimensional random vectors, and let $f_1, \cdots, f_k$ be real-valued Borel measurable functions on R^m. Assume that $Z_n = (f_1(Y_n), \cdots, f_k(Y_n))$ has finite moments of order $s \geq 3$. Rates of convergence to normality and asymptotic expansions of distributions of statistics of the form $W_n = n^{\frac{1}{2}}[H(\bar{Z}) - H(\mu)]$ are obtained for functions H on R^k having continuous derivatives of order s in a neighborhood of $\mu = EZ_1$. This asymptotic expansion is shown to be identical with a formal Edgeworth expansion of the distribution function of W_n. This settles a conjecture of Wallace (1958). The class of statistics considered includes all appropriately smooth functions of sample moments. An application yields asymptotic expansions of distributions of maximum likelihood estimators and, more generally, minimum contrast estimators of vector parameters under readily verifiable distributional assumptions.

1. Introduction. Consider a sequence of independent and identically distributed m-dimensional random vectors $\{Y_n\}_{n\geq 1}$. Let $f_1, \cdots, f_k$ be real-valued Borel measurable functions on R^m. Consider the statistic

$$W_n = n^{\frac{1}{2}}(H(\bar{Z}) - H(\mu)) \tag{1.1}$$

where H is a real-valued Borel measurable function on R^k, and

$$Z_n = (f_1(Y_n), \cdots, f_k(Y_n)), \qquad \bar{Z} = \frac{1}{n}\sum_{i=1}^n Z_i, \qquad \mu = EZ_n. \tag{1.2}$$

Note that all functions of sample moments are of the form $H(\bar{Z})$. For example, $H(\bar{Z})$ becomes the bivariate sample correlation coefficient if one takes $m = 2$, $k = 5$, $f_1(y) = y^{(1)}$, $f_2(y) = y^{(2)}$, $f_3(y) = (y^{(1)})^2$, $f_4(y) = (y^{(2)})^2$, $f_5(y) = y^{(1)}y^{(2)}$ (for $y = (y^{(1)}, y^{(2)})$), $H(z) = (z^{(5)} - z^{(1)}z^{(2)})(z^{(3)} - (z^{(1)})^2)^{-\frac{1}{2}}(z^{(4)} - (z^{(2)})^2)^{-\frac{1}{2}}$ for $z = (z^{(1)}, \cdots, z^{(5)})$ belonging to a neighborhood N of $\mu = (EY_1^{(1)}, EY_1^{(2)}, E(Y_1^{(1)})^2, E(Y_1^{(2)})^2, (EY_1^{(1)}Y_1^{(2)}))$ contained in the set $\{z \in R^5 : z^{(3)} > (z^{(1)})^2, z^{(4)} > (z^{(2)})^2, -1 < H(z) < 1\}$; H may be defined arbitrarily outside N.

It is well known (see Cramér (1946), page 366, and Wilks (1962), page 260) that if Z_1 has finite second moments and H is continuously differentiable in a neighborhood of μ, then W_n has a limiting normal distribution with mean zero

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and variance

(1.3) $$\sigma^2 = \sum_{i,j=1}^{k} v_{ij} l_i l_j$$

where $V = ((v_{ij}))$ is the *dispersion matrix* of Z_1 and

(1.4) $$l_i = (D_i H)(\mu) = \frac{\partial H(z)}{\partial z^{(i)}}\bigg|_{z=\mu} \qquad 1 \leqq i \leqq k;\ z = (z^{(1)}, \cdots, z^{(k)})\,.$$

Throughout this article *it is assumed that σ^2 is positive.* As a first refinement of asymptotic normality one has

THEOREM 1. *If Z_1 has finite third moments and if all third order derivatives of H are continuous in a neighborhood of $\mu = EZ_1$, then*

(1.5) $$\sup_{B\in\mathscr{B}} |\text{Prob}\,(W_n \in B) - \textstyle\int_B \phi_{\sigma^2}(v)\,dv| = O(n^{-\frac{1}{2}})$$

for every class $\mathscr{B}$ of Borel sets satisfying

(1.6) $$\sup_{B\in\mathscr{B}} \textstyle\int_{(\partial B)^\varepsilon} \phi_{\sigma^2}(v)\,dv = O(\varepsilon) \quad (\varepsilon \downarrow 0)\,.$$

Here ∂B is the boundary of B, $(\partial B)^\varepsilon$ is the ε-neighborhood of B, and

(1.7) $$\phi_{\sigma^2}(v) = (2\pi\sigma^2)^{-\frac{1}{2}} \exp\{-v^2/(2\sigma^2)\} \qquad -\infty < v < \infty\,.$$

It is important to note that the mean $H(\mu)$ and the variance σ^2/n of the asymptotic distribution of $H(\bar{Z})$ are *not* the mean and variance of $H(\bar{Z})$. Indeed, in many common examples (e.g., the t-statistic, the sample correlation) the mean and higher moments of $H(\bar{Z})$ may not even be finite. This feature of the problem shows up in a more serious manner when one attempts an asymptotic expansion going beyond (1.5). It is common practice among applied statisticians to calculate "approximate moments" of W_n by expanding $H(\bar{Z})$ around μ, keeping a certain number of terms, raising to an appropriate power and taking expectations term by term. This is the so-called *delta method.* These "approximate moments" are sometimes used to obtain a formal Edgeworth expansion of the distribution function of W_n. It was conjectured by Wallace (1958) (also see Bickel (1974)) that such a formal expansion would be valid if suitable assumptions were made. One of the principal aims in this article is to prove that a more precisely formulated version of this conjecture, as described in the following paragraphs, is valid. As pointed out by Wallace, such a formal expansion is easier to compute compared to the alternative procedure of reducing a multivariate Edgeworth expansion to a univariate one.

Denote the derivatives of H at μ by

(1.8) $$l_{i_1,\ldots,i_p} = (D_{i_1} D_{i_2} \cdots D_{i_p} H)(\mu) \qquad 1 \leqq i_1, \cdots, i_p \leqq k\,,$$

where D_i denotes *differentiation with respect to the* ith *coordinate.* A Taylor expansion of W_n yields the statistic

(1.9) $$W_n' = n^{\frac{1}{2}}\{\textstyle\sum_{i=1}^k l_i(\bar{Z}^{(i)} - \mu^{(i)}) + \frac{1}{2}\sum_{i,j} l_{i,j}(\bar{Z}^{(i)} - \mu^{(i)})(\bar{Z}^{(j)} - \mu^{(j)}) + \cdots + \frac{1}{(s-1)!}\sum l_{i_1,\ldots,i_{s-1}}(\bar{Z}^{(i_1)} - \mu^{(i_1)}) \cdots (\bar{Z}^{(i_{s-1})} - \mu^{(i_{s-1})})\}\,.$$

Since $W_n - W_n' = o_p(n^{-(s-2)/2})$, one may expect that an asymptotic expansion of the distribution function of W_n' may coincide with that of W_n. Also, it is easy to check that (if Z_1 has sufficiently many finite moments) the jth *cumulant* $\kappa_{j,n}$ of W_n' is given by

$$\kappa_{j,n} = \tilde{\kappa}_{j,n} + o(n^{-(s-2)/2}) \qquad j \geq 1\,, \tag{1.10}$$

where

$$\begin{aligned} \tilde{\kappa}_{j,n} &= \textstyle\sum_{i=1}^{s-2} n^{-i/2} b_{j,i} && \text{if } \ j \neq 2\,, \\ &= \sigma^2 + \textstyle\sum_{i=1}^{s-2} n^{-i/2} b_{2,i} && \text{if } \ j = 2\,, \end{aligned} \tag{1.11}$$

and $b_{j,i}$'s depend only on appropriate moments of Z_1 and on derivatives of H at μ of orders $s-1$ and less. We refer to $\tilde{\kappa}_{j,n}$ as "*approximate cumulants*" of W_n' (or W_n). The expression

$$\exp\left\{it\tilde{\kappa}_{1,n} + \frac{(it)^2}{2}(\tilde{\kappa}_{2,n} - \sigma^2) + \textstyle\sum_{j=3}^{s} \frac{(it)^j}{j!}\tilde{\kappa}_{j,n}\right\}\exp\{-\sigma^2 t^2/2\} \tag{1.12}$$

is an approximation of the characteristic function of W_n' (or W_n). Expanding the first exponential factor one may reduce (1.12) to

$$\begin{aligned} \exp\{-\sigma^2 t^2/2\}[1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2}\pi_r(it)] + o(n^{-(s-2)/2}) \\ = \hat{\psi}_{s,n}(t) + o(n^{-(s-2)/2})\,, \end{aligned} \tag{1.13}$$

say, where π_r's are polynomials whose coefficients do not depend on n. The *formal Edgeworth expansion* $\Psi_{s,n}$ of the distribution function of W_n is defined by

$$\begin{aligned} \psi_{s,n}(v) &= \left[1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2}\pi_r\left(-\frac{d}{dv}\right)\right]\phi_{\sigma^2}(v)\,, \\ \Psi_{s,n}(u) &= \textstyle\int_{-\infty}^{u} \psi_{s,n}(v)\,dv\,. \end{aligned} \tag{1.14}$$

Note that the Fourier-Stieltjes transform of $\Psi_{s,n}$ is $\hat{\psi}_{s,n}$.

To state the next result let $|\cdot|$, $\langle\ ,\ \rangle$ denote *Euclidean norm* and *inner product*, respectively.

THEOREM 2. *Assume that, for some integer $s \geq 3$, all the derivatives of H of orders s and less are continuous in a neighborhood of $\mu = EZ_1$ and that $E|Z_1|^s$ is finite.*

(a) *If, in addition,* (i) *the distribution of Y_1 has a nonzero absolutely continuous component (with respect to Lebesgue measure on R^m) and* (ii) *the density of this component is strictly positive on some nonempty open set U on which $f_1, \cdots, f_k$ are continuously differentiable and $1, f_1, \cdots, f_k$ are linearly independent (as elements of the vector space of continuous functions on U), then*

$$\sup_B |\text{Prob}\,(W_n \in B) - \textstyle\int_B \psi_{s,n}(v)\,dv| = o(n^{-(s-2)/2})\,, \tag{1.15}$$

where the supremum is over all Borel sets B.

(b) *If, instead of* (a), *it is merely assumed that*

$$\limsup_{|t|\to\infty} |E(\exp\{i\langle t, Z_1\rangle\})| < 1\,, \tag{1.16}$$

then the relation

$$\sup_{B \in \mathscr{B}} |\text{Prob}\,(W_n \in B) - \textstyle\int_B \psi_{s,n}(v)\,dv| = o(n^{-(s-2)/2}) \tag{1.17}$$

holds uniformly over every class $\mathscr{B}$ of Borel sets satisfying (1.6).

REMARK 1.1. Theorems 1 and 2 extend in a straightforward manner to vector-valued $H(z) = (H_1(z), \cdots, H_p(z))$ provided that the dispersion matrix $M = \Sigma V \Sigma'$ of $(\langle Z_1, \text{grad}\, H_1(\mu)\rangle, \cdots, \langle Z_1, \text{grad}\, H_p(\mu)\rangle)$ is nonsingular. Here Σ is the $p \times k$ matrix whose rth row is grad $H_r(\mu) = (D_1 H_r(\mu), \cdots, D_k H_r(\mu))$. In this case one must replace $\psi_{s,n}$ by

$$[1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2} \tilde{\pi}_r(-D)]\phi_M(x) \qquad x \in R^p\,, \tag{1.18}$$

where ϕ_M is the normal density on R^p with mean zero and dispersion M, $\tilde{\pi}_r$ is a polynomial in p variables (whose coefficients do not depend on n), and $-D = (-D_1, \cdots, -D_p)$. There is virtually no difference in the proofs for vector-valued H, apart from an additional complexity in notation.

REMARK 1.2. Let G denote the distribution of Y_1. If the density g, say, of the absolutely continuous part of G is such that $U_1 \equiv \{y : g(y) > 0\}$ is open and $G(U_1) = 1$, then one may replace (ii) in the statement of Theorem 2(a) by (ii)′: $f_1, \cdots, f_k$ *are continuously differentiable* on U_1. For, in this case, the functions $1, f_1, \cdots, f_k$ are linearly dependent as continuous functions on U_1 if and only if $1, f_1(Y_1), \cdots, f_k(Y_1)$ are linearly dependent as elements of the L^2 space of random variables, and, as explained in the first paragraph of Section 2, one may always replace $\{1, f_1, \cdots, f_k\}$ by a maximal linearly independent set $\{1, f_{i_1}, \cdots, f_{i_{k'}}\}$ $(1 \leqq k' \leqq k)$.

REMARK 1.3. Assuming, in addition to the hypothesis of Theorem 2(a), that f_i's are analytic, Chibishov (1972) proved that an asymptotic expansion

$$\text{Prob}\,(W_n \in C) - \textstyle\int_C [1 + \sum_{r=1}^{s-2} n^{-r/2} q_r(x)]\phi_M(x)\,dx = o(n^{-(s-2)/2})$$

holds uniformly over all measurable convex sets C (intervals, in case H is real). For the special case of polynomial H he was able to prove that this expansion was uniform over all Borel sets. For many applications (see, e.g., Theorem 3) analyticity of f_i's is a severe restriction. Also, he was not concerned with the problem of identifying this expansion with the formal Edgeworth expansion.

REMARK 1.4. Note that in Theorem 2 we only require $E|Z_1|^s < \infty$, whereas an algebraic computation of the moments of W_n' yields expressions for $\kappa_{j,n}$ $(1 \leqq j \leqq s)$ as polynomials in $n^{-\frac{1}{2}}$ whose coefficients are (polynomial) functions of moments of Z_1 of orders up to $s(s-1)$. This apparent anomaly is resolved by the fact that the "approximate cumulants" $\tilde{\kappa}_{j,n}$, $1 \leqq j \leqq s$, only involve moments (of Z_1) of orders s and less so that (1.14) is well defined. In the course of proving Theorem 2 it is first shown that under the hypothesis of Theorem 2(b) there exists an asymptotic expansion of the distribution function of W_n in the form

$$(1.19)\qquad \begin{aligned} &F_n(u) + o(n^{-(s-2)/2}) ,\\ &F_n(u) = \textstyle\int_{-\infty}^{u} [1 + \sum_{r=1}^{s-2} n^{-r/2} q_r(v)] \phi_{\sigma^2}(v)\, dv , \end{aligned}$$

where q_r's are polynomials. The coefficients of q_r $(1 \leqq r \leqq s-2)$ are polynomials in the moments of Z_1 of orders s and less, and the coefficients of these last polynomials are constants which do not depend on the distribution of Z_1. It is next shown that, in case Z_1 has finite moments of all orders,

$$(1.20)\qquad q_r(v)\phi_{\sigma^2}(v) = \pi_r\left(-\frac{d}{dv}\right)\phi_{\sigma^2}(v) \qquad 1 \leqq r \leqq s-2 .$$

It follows that π_r's $(1 \leqq r \leqq s-2)$ depend only on those moments of Z_1 which are of orders s and less, and the same is, therefore, true of $\tilde{\kappa}_{j,n}$ $(1 \leqq j \leqq s)$. In view of (1.11)—(1.13), and (1.21) below, the jth moment of $\Psi_{s,n}$ $(j \geqq 0)$ differs from that computed from $\tilde{\kappa}_{j,n}$ (using the familiar relations between moments and cumulants) by $o(n^{-(s-2)/2})$. In other words, under the hypothesis of Theorem 2(b) it is a valid procedure to compute moments of the asymptotic expansion by the so-called *delta method* in which W_n' is raised to a power, expectations taken term by term (formally) and terms of order $o(n^{-(s-2)/2})$ neglected. Expansions of moments as well as expectations of other smooth functions of W_n' (and of W_n, if it has enough moments) are valid *solely* under moment conditions on Z_1 (see Götze and Hipp (1977)), and these expansions may be obtained by integrating the smooth function with respect to the formal Edgeworth expansion $\Psi_{s,n}$, *even when the distribution function of W_n does not admit an expansion.* Finally, the proof of the identification (1.20) depends crucially on the following important combinatorial result of James (1955), (1958), and James and Mayne (1962):

$$(1.21)\qquad \kappa_{j,n} = O(n^{-(j-2)/2}) \qquad j \geqq 3 ,$$

which holds if $E|Z_1|^{j(s-1)} < \infty$. There may, however, be statistics whose cumulants satisfy (1.10), (1.11), but not (1.21). Consider such a statistic T_n, assume (for simplicity) that it has finite moments of all orders, and define, for each $r \geqq 3$, the polynomials $\pi_{j,r}$ by

$$(1.22)\qquad \begin{aligned} &\exp\left\{it\tilde{\kappa}_{1,n} + \frac{(it)^2}{2}(\tilde{\kappa}_{2,n} - \sigma^2) + \textstyle\sum_{j=3}^{r} \frac{(it)^j}{j!}\tilde{\kappa}_{j,n}\right\} \exp\{-\sigma^2 t^2/2\} \\ &\quad = \exp\{-\sigma^2 t^2/2\}[1 + \textstyle\sum_{j=1}^{s-2} n^{-j/2}\pi_{j,r}(it)] + o(n^{-(s-2)/2}) \\ &\quad = \hat{\psi}_{s,r,n}(t) + o(n^{-(s-2)/2}) , \end{aligned}$$

say. Define the *formal Edgeworth expansion of type* (r, s) by

$$(1.23)\qquad \Psi_{s,r,n}(u) = \int_{-\infty}^{u}\left[1 + \textstyle\sum_{j=1}^{s-2} n^{-j/2}\pi_{j,r}\left(-\frac{d}{dv}\right)\right]\phi_{\sigma^2}(v)\, dv .$$

It is easy to see from (1.22) that the polynomials $\pi_{j,r}$ have no constant terms, and

$\hat{\psi}_{s,r,n}(0) = 1$. It follows that there exists a *smallest integer* r_0 such that

$$\frac{d^j}{dt^j} \log \hat{\psi}_{s,r,n}(t)\Big|_{t=0} = o(n^{-(s-2)/2}) \qquad \text{if} \quad j > r_0 . \tag{1.24}$$

If now the distribution function of the statistic T_n has a valid asymptotic expansion given by (1.19), then the same procedure as used in verifying (1.20) leads to the conclusion: $F_n = \Psi_{s,r,n}$ *if and only if* $r \geqq r_0$.

REMARK 1.5. Theorem 2, incidentally, justifies the remark made in Ghosh and Subramanyam (1974), page 356, that their $E^U(T_n - \theta_0)^2$ is the second moment of an Edgeworth expansion.

AN APPLICATION. We now apply Theorem 2(a) for vector-valued H (see Remark 1.1) to obtain asymptotic expansions of distributions of a class of statistics including *maximum likelihood estimators* and the so-called *minimum contrast estimators* for vector parameters.

Let $\{Y_n\}_{n\geq 1}$ be a sequence of i.i.d. m-dimensional random vectors whose common distribution G_θ is parametrized by $\theta = (\theta^{(1)}, \cdots, \theta^{(p)})$ belonging to an open subset Θ of R^p. For each θ let $f(y; \theta)$ be an extended real-valued Borel measurable function on R^m. For nonnegative integral vectors $\nu = (\nu^{(1)}, \cdots, \nu^{(p)})$ write $|\nu| = \nu^{(1)} + \cdots + \nu^{(p)}$, $\nu! = \nu^{(1)}! \cdots \nu^{(p)}!$, and let $D^\nu = (D_1)^{\nu^{(1)}} \cdots (D_p)^{\nu^{(p)}}$ denote the νth *derivative with respect to* θ. We shall write P_θ to denote the product probability measure on the space of all sequences in R^m and regard Y_n's as coordinate maps on this space. Expectation with respect to P_θ will be denoted by E_θ. The following assumptions will be made:

(A_1) There is an open subset U of R^m such that (i) for each $\theta \in \Theta$ one has $G_\theta(U) = 1$, and (ii) for each ν, $1 \leqq |\nu| \leqq s + 1$, $f(y; \theta)$ has a νth derivative $D^\nu f(y; \theta)$ with respect to θ on $U \times \Theta$.

(A_2) For each compact $K \subset \Theta$ and each ν, $1 \leqq |\nu| \leqq s$, $\sup_{\theta_0 \in K} E_{\theta_0}|D^\nu f(Y_1; \theta_0)|^{s+1} < \infty$; and for each compact K there exists $\varepsilon > 0$ such that $\sup_{\theta_0 \in K} E_{\theta_0}(\max_{|\theta-\theta_0|\leq\varepsilon} |D^\nu f(Y_1; \theta)|)^s < \infty$ if $|\nu| = s + 1$.

(A_3) For each $\theta_0 \in \Theta$, $E_{\theta_0} D_r f(Y_1; \theta_0) = 0$ for $1 \leqq r \leqq p$, and the matrices

$$\begin{aligned} I(\theta_0) &= ((-E_{\theta_0} D_i D_r f(Y_1; \theta_0))) , \\ D(\theta_0) &= ((E_{\theta_0}(D_i f(Y_1; \theta_0) \cdot D_r f(Y_1; \theta_0)))) \end{aligned} \tag{1.25}$$

are nonsingular.

(A_4) The functions $I(\theta)$, $E_\theta(D^\nu f(Y_1; \theta) \cdot D^{\nu'} f(Y_1; \theta))$, $1 \leqq |\nu|, |\nu'| \leqq s$, are continuous on Θ.

(A_5) The map $\theta \to G_\theta$ on Θ into the space of all probability measures on (the Borel sigma field of) R^m is continuous when the latter space is given the (variation) norm topology.

(A_6) For each $\theta \in \Theta$, G_θ has a nonzero absolutely continuous component (with respect to Lebesgue measure) whose density has a version $g(y; \theta)$ which is strictly positive on U. Also, for each θ and each ν, $1 \leqq |\nu| \leqq s$, $D^\nu f(y; \theta)$ is continuously differentiable in y on U.

Now write

$$(1.26)\qquad L_n(\theta) = \sum_{j=1}^{n} f(Y_j;\theta)\,, \qquad L_1(\theta) = f(Y_1;\theta)\,,$$

and consider the p equations

$$(1.27)\qquad 0 = \frac{1}{n} D_r L_n(\theta_0) + \frac{1}{n} \sum_{i=1}^{p} (\theta^{(i)} - \theta_0^{(i)}) D_i D_r L_n(\theta_0) + \cdots$$
$$+ \frac{1}{n} \sum_{|\nu|=s-1} \frac{(\theta-\theta_0)^\nu}{\nu!} D^\nu D_r L_n(\theta_0) + R_{n,r}(\theta)$$
$$= \frac{1}{n} D_r L_n(\theta)\,, \qquad 1 \leqq r \leqq p\,,$$

where $x^\nu = (x^{(1)})^{\nu(1)} \cdots (x^{(p)})^{\nu(p)}$ for $x = (x^{(1)}, \cdots, x^{(p)}) \in R^p$, and $R_{n,r}(\theta)$ is the usual remainder in the Taylor expansion, so that

$$(1.28)\qquad |R_{n,r}(\theta)| \leqq \frac{c(s,p)}{n} |\theta - \theta_0|^s \max_{|\nu|=s+1} \sup_{|\theta'-\theta_0| \leqq |\theta-\theta_0|} |D^\nu L_n(\theta')|\,.$$

The statistics $\hat\theta_n$ considered below are measurable maps on the probability space into some compactification of Θ.

THEOREM 3.

(a) *Assume* (A_1)—(A_4) *hold for some* $s \geqq 3$. *There exists a sequence of statistics* $\{\hat\theta_n\}_{n\geqq 1}$ *such that for every compact* $K \subset \Theta$

$$(1.29)\qquad \inf_{\theta_0 \in K} P_{\theta_0}(|\hat\theta_n - \theta_0| < d_0 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}},\ \hat\theta_n \text{ solves } (1.27))$$
$$= 1 - o(n^{-(s-2)/2})\,,$$

where d_0 *is a constant which may depend on* K.

(b) *If* (A_1)—(A_6) *hold, then there exist polynomials* q_{r,θ_0} *(in* p *variables), not depending on* n*, such that for every sequence* $\{\hat\theta_n\}_{n\geqq 1}$ *satisfying* (1.29) *and every compact* $K \subset \Theta$ *one has the asymptotic expansion*

$$(1.30)\qquad \sup_{\theta_0 \in K} |P_{\theta_0}(n^{\frac{1}{2}}(\hat\theta_n - \theta_0) \in B) - \int_B [1 + \sum_{r=1}^{s-2} n^{-r/2} q_{r,\theta_0}(x)] \phi_M(x)\, dx|$$
$$= o(n^{-(s-2)/2})$$

uniformly over every class $\mathscr{B}$ *of Borel sets of* R^p *satisfying*

$$(1.31)\qquad \sup_{\theta_0 \in K} \sup_{B \in \mathscr{B}} \int_{(\partial B)^\varepsilon} \phi_M(x)\, dx = O(\varepsilon) \qquad as \quad \varepsilon \downarrow 0\,.$$

Here $M = I^{-1}(\theta_0) D(\theta_0) I^{-1}(\theta_0)$, *where* $I(\theta_0)$, $D(\theta_0)$ *are defined by* (1.25). *Also, the coefficients of the polynomials* q_{r,θ_0} *are themselves polynomials in the moments of* $D^\nu L_1(\theta_0)$, $1 \leqq |\nu| \leqq s$, *under* P_{θ_0}, *and are consequently bounded on compacts.*

REMARK 1.6. Theorem 3 is actually proved under the weaker hypothesis (A_1)—(A_5) and (in place of (A_6)) $(A_6)'$: *the distribution of* Z_1 *under* P_θ *satisfies Cramér's condition* (1.16), *for each* θ. Under this latter condition, and for one-dimensional parameters, relations similar to (1.30) were established (with analogous regularity assumptions) for the class of intervals, in place of general $\mathscr{B}$

satisfying (1.31), by Pfanzagl (1973b, Theorem 1) and Chibishov (1973b). Pfanzagl also provided a verifiable condition (see [21], page 1012) under which his distributional assumption may be checked. The situation is more complex in the multiparameter case. For this case Chibishov (1972, 1973a) was able to prove a result analogous to (1.30) for the special class of all measurable convex sets (which, of course, satisfies (1.31); see [4], page 24) under the additional assumption that $D^\nu f(y;\theta)$, $1 \leqq |\nu| \leqq s$, be analytic in y. In the present context this assumption is severely restrictive. Note that assumption (A_6) provides a simple verifiable sufficient condition for the validity of $(A_6)'$ (see Lemma 2.2 and Remark 1.2). Finally, it is also possible (see the proof in Section 2) to replace the continuity conditions in (A_4) by 'boundedness' conditions (as, e.g., in Pfanzagl (1973a)).

REMARK 1.7. Under assumptions (A_1)—(A_4) with $s = 3$ one may easily prove (using Theorem 1 for vector H, instead of Theorem 2) that the error of normal approximation is $O(n^{-\frac{1}{2}})$ uniformly over every compact $K \subset \Theta$ and every class $\mathscr{B}$ satisfying (1.31). However, for the special class of all Borel measurable convex sets such a result has been proved by Pfanzagl (1973b).

REMARK 1.8. Assume that for some $s \geqq 2$ one has (A_1), (A_3), $E_{\theta_0}|D^\nu f(Y_1;\theta_0)|^s < \infty$ for $1 \leqq |\nu| \leqq s$, and $E_{\theta_0}(\max_{|\theta-\theta_0|\leqq\varepsilon} |D^\nu f(Y_1;\theta)|)^s < \infty$ for some $\varepsilon > 0$ and all ν with $|\nu| = s+1$. Then one may prove using (1.27), (1.28) and the law of the iterated logarithm that there exists an a.s. (P_{θ_0}) finite integer-valued random variable $N(\cdot)$ such that with P_{θ_0}- probability one for $n > N(\cdot)$ one has

$$\left|\frac{1}{n} D_r L_n(\theta_0)\right| \leqq d_1 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}, \tag{1.32}$$

$$\left|\frac{1}{n} D^\nu L_n(\theta_0) - E_{\theta_0} D^\nu f(Y_1;\theta_0)\right| \leqq d_1 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}} \qquad 2 \leqq |\nu| \leqq s,$$

$$|R_{n,r}(\theta)| \leqq |\theta-\theta_0|^s\{d_3 + d_1 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}\}$$
$$\text{for all} \quad \theta \quad \text{satisfying} \quad |\theta-\theta_0| \leqq \varepsilon \qquad 1 \leqq r \leqq p,$$

for any positive constant d_1 and a suitable constant d_3. Using the Brouwer fixed point theorem, as in the proof of Theorem 3(a), one can then show that there exists a sequence of statistics $\{\hat\theta_n\}_{n\geq 1}$ such that for every $d > 0$ with P_{θ_0}- probability one

$$|\hat\theta_n - \theta_0| < dn^{-\frac{1}{2}}(\log n)^{\frac{1}{2}} \quad \text{and} \quad \hat\theta_n \quad \text{solves (1.27) if} \quad n > N(\cdot). \tag{1.33}$$

If, due to some additional structure (e.g., convexity or concavity of $L_n(\theta)$ as a function θ for every n, a.s. (P_{θ_0})), the equations (1.27) have at most one solution for each n (a.s. (P_{θ_0})), then of course one may define $\hat\theta_n$ to be this solution when it exists and arbitrarily (measurably) if it does not, and such a $\hat\theta_n$ will satisfy (1.33) with P_{θ_0}- probability one (*strong consistency*) and, under the hypothesis (A_1)—(A_6) will also admit the asymptotic expansion (1.30). Finally, we consider the so-called minimum contrast estimators (see Pfanzagl (1973b)). It is known (see [21], Lemma 3, which admits extension to $p > 1$) that for such estimators $\hat{\theta}_n$, say, one has, under certain regularity conditions,

$$\sup_{\theta_0 \in K} P_{\theta_0}(|\hat{\theta}_n - \theta_0| > d'(\theta_0)n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}) = o(n^{-(s-2)/2}) \tag{1.34}$$

for every compact $K \subset \Theta$. Here d' is bounded on compacts. Since $\hat{\theta}_n$ minimizes (or maximizes) $L_n(\theta)$ it follows that (1.29) holds. Augmenting these regularity conditions, if necessary, so that (A_1)—(A_6) hold one has (1.30). Conditions not significantly different from (A_1)—(A_6) are generally included among these regularity conditions. Finally, the reason for not restricting the context of Theorem 3 to minimum contrast estimators is that in its present from this theorem also applies to problems, e.g., in mathematical economics (see Bhattacharya and Majumdar (1973)), in which $\hat{\theta}_n$ is not a statistical estimator.

Among the earliest results on asymptotic expansion of some special functions of sample moments we refer to Hsu (1945) who obtained an asymptotic expansion for the sample variance.

For relations with questions concerning asymptotic efficiencies of statistical estimators we refer to Pfanzagl (1973a), Ghosh and Subramanyam (1974), and Ghosh, Sinha and Wieand (1977).

Some of the results of this article in weaker form were announced earlier in Bhattacharya (1977). It may be noted that the entire Section 4 of that article ([2]) was based on joint work by the authors.

2. Proofs. For proving Theorems 1 and 2 it will be assumed, without any essential loss of generality, that the *dispersion matrix* V of Z_n *is nonsingular*. For, if V is singular, then $1, f_1(Y_n), \cdots, f_k(Y_n)$ are linearly dependent when considered as elements of the L^2 space of random variables. Then there exist a maximal integer k' and distinct indices $i_1, \cdots, i_{k'}$ among $1, 2, \cdots, k$ such that $1, f_{i_1}, \cdots, f_{i_{k'}}$ are linearly independent. Defining $\tilde{Z}_n = (f_{i_1}(Y_n), \cdots, f_{i_{k'}}(Y_n))$ one can define a function H' defined on $R^{k'}$ and as smooth as H such that $H'(\bar{\tilde{Z}}) = H(\bar{Z})$ where $\bar{\tilde{Z}} = (1/n) \sum_{i=1}^n \tilde{Z}_i$. In view of the positivity of σ^2, $k' \geqq 1$.

Throughout the letters c, d will denote constants (i.e., nonrandom numbers not depending on n, x, z, u, or v).

Let $\chi_j(t)$ denote the jth *cumulant of* $\langle t, Z_1 - \mu\rangle = \sum_{r=1}^k t^{(r)}(Z_1 - \mu)^{(r)}$, and introduce the *Cramér–Edgeworth polynomials*

$$\tilde{P}_r(it) = \sum_{p=1}^r \left\{ \sum{}^* \frac{\chi_{j_1+2}(it)}{(j_1+2)!} \cdots \frac{\chi_{j_p+2}(it)}{(j_p+2)!} \right\} \tag{2.1}$$

$$\chi_j(it) = i^j \chi_j(t) \qquad t \in R^k;\ r = 1, 2, \cdots,$$

where the sum $\sum^*$ is over all p-tuples of positive integers $(j_1, \cdots, j_p)$ satisfying $\sum_{l=1}^p j_l = r$. Letting D_i denote *differentiation with respect to the* ith *coordinate*, write

$$D = (D_1, \cdots, D_k). \tag{2.2}$$

Then $\tilde{P}_r(-D)$ is a differential operator. Write

$$\phi_V(z) = (2\pi)^{-k/2}(\det V)^{-\frac{1}{2}} \exp\{-\tfrac{1}{2}\langle z, V^{-1}z\rangle\}\,, \tag{2.3}$$
$$\xi_{s,n}(z) = [1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2}\tilde{P}_r(-D)]\phi_V(z) \qquad z \in R^k\,.$$

Define the functions

$$g_n(z) = n^{\frac{1}{2}}[H(\mu + n^{-\frac{1}{2}}z) - H(\mu)]\,, \qquad h_1(z) = \textstyle\sum_{i=1}^{p} l_i z^{(i)}\,,$$
$$h_{s-1}(z) = \textstyle\sum l_i z^{(i)} + \frac{1}{2}n^{-\frac{1}{2}} \sum l_{i,j} z^{(i)}z^{(j)} + \cdots \tag{2.4}$$
$$+ \frac{1}{(s-1)!}\, n^{-(s-2)/2} \textstyle\sum l_{i_1,\dots,i_{s-1}} z^{(i_1)} \cdots z^{(i_{s-1})}$$
$$z = (z^{(1)}, \cdots, z^{(k)}) \in R^k\,.$$

Note that h_{s-1} is a Taylor expansion of g_n and write

$$W_n = g_n(n^{-\frac{1}{2}}(\bar{Z} - \mu))\,, \qquad W_n' = h_{s-1}(n^{-\frac{1}{2}}(\bar{Z} - \mu))\,. \tag{2.5}$$

Define the maps

$$T(z) = (z^{(1)}, \cdots, z^{(k-1)}, g_n(z))\,, \qquad T_p(z) = (z^{(1)}, \cdots, z^{(k-1)}, h_p(z)) \tag{2.6}$$

where $p = 1$ or $s - 1$. *Assume* without loss of generality that $l_k > 0$. For the following discussion n_0 is an integer such that for $n > n_0$ the map $T_{s-1}(T)$ is a $C^\infty(C^s)$ diffeomorphism on the set

$$M_n = \{|z| < ((s-1)\Lambda \log n)^{\frac{1}{2}}\} \tag{2.7}$$

onto its image. Here Λ is the *largest eigenvalue of* V.

LEMMA 2.1. *Assume* $\rho_s = E|Z_1|^s < \infty$ *and that all derivatives of* H *of orders* s *and less are continuous in a neighborhood of* $\mu = EZ_1$, *for some* $s \geq 3$. *Then there exist polynomials* q_r *(in* one variable), *whose coefficients do not depend on* n, *such that uniformly over all Borel subsets* B *of* R^1 *one has*

$$\int_{\{g_n(z)\in B\}} \xi_{s,n}(z)\,dz = \int_B dF_n(u) + o(n^{-(s-2)/2})\,, \tag{2.8}$$

where

$$F_n(u) = \int_{-\infty}^{u} [1 + \textstyle\sum_{r=1}^{s-2} n^{-r/2} q_r(v)]\phi_{\sigma^2}(v)\,dv \qquad u \in R^1\,. \tag{2.9}$$

Also, for all nonnegative integers j

$$\int_{M_n} g_n^j(z)\xi_{s,n}(z)\,dz = \int_{-\infty}^{\infty} u^j\,dF_n(u) + o(n^{-(s-2)/2})\,, \tag{2.10}$$
$$\int_{R^k} h_{s-1}^j(z)\xi_{s,n}(z)\,dz = \int_{-\infty}^{\infty} u^j\,dF_n(u) + o(n^{-(s-2)/2})\,.$$

PROOF. By the change of variables $x = T_1^{-1}T(z)$, the first integral in (2.8), when restricted to the set M_n, becomes

$$\int_{\{h_1(x)\in B\}\cap T_1^{-1}T(M_n)} \xi_{s,n}(T^{-1}T_1(x))[l_k/D_k g_n(T^{-1}T_1(x))]\,dx\,. \tag{2.11}$$

Now the elements of the Jacobian matrix of $T(z)$ and those of the inverse of this matrix, as well as their derivatives of orders $s - 1$ and less, are bounded on M_n by constants independent of n. Hence a Taylor expansion yields

$$(T^{-1}T_1(x))^{(k)} - x^{(k)} = (T^{-1}T_1(x))^{(k)} - (T^{-1}T(x))^{(k)} \tag{2.12}$$
$$= \textstyle\sum_{r=1}^{s-2} n^{-r/2} p_r(x) + R(|x|)\cdot o(n^{-(s-2)/2})\,,$$

where p_r's are polynomials in k variables and R is a polynomial in one variable whose coefficients do not depend on n; and the factor $o(n^{-(s-2)/2})$ does not involve x. Using (2.12) and the fact that $(T^{-1}T_1(x))^{(i)} = x^{(i)}$ for $1 \leqq i \leqq k-1$, one reduces (2.11) to

(2.13) $$\int_{\{h_1(x)\in B\}\cap T_1^{-1}T(M_n)} [1 + \sum_{r=1}^{s-2} n^{-r/2} p_r'(x)]\phi_V(x)\,dx + o(n^{-(s-2)/2}),$$

where p_r''s are polynomials (in k variables) whose coefficients do not depend on n. Since $T_1^{-1}T(M_n) \supset \{|x| < ((s-\frac{3}{2})\Lambda \log n)^{\frac{1}{2}}\}$ if $n > n_0$, (2.13) reduces to

$$\int_{\{h_1(x)\in B\}} [1 + \sum_{r=1}^{s-2} n^{-r/2} p_r'(x)]\phi_V(x)\,dx + o(n^{-(s-2)/2}).$$

Recall that $h_1(x) = \sum l_j x^{(j)} = \langle l, x\rangle$ and write

$$G_n(u) = \int_{\{\langle l,x\rangle \leq u\}} [1 + \sum_{r=1}^{s-2} n^{-r/2} p_r'(x)]\phi_V(x)\,dx \qquad u \in R^1.$$

The Fourier–Stieljes transform of G_n is

$$[1 + \sum_{r=1}^{s-2} n^{-r/2} p_r'(-iD)]\phi_V(tl) = [1 + \sum_{r=1}^{s-2} n^{-r/2} q_r'(it)] \exp\left\{-\frac{\sigma^2 t^2}{2}\right\}$$

where q_r''s are polynomials (in one variable) whose coefficients do not depend on n. Define

$$q_r(v) = \left[q_r'\left(-\frac{d}{dv}\right)\phi_{\sigma^2}(v)\right] \Big/ \phi_{\sigma^2}(v)$$

to complete the proof of (2.8). The first relation in (2.10) is proved in the same manner, while the second follows from the first and the inequalities

(2.14) $$\sup_{z\in M_n} |g_n^j(z) - h_{s-1}^j(z)| \leqq d_1 n^{-(s-1)/2}(\log n)^{s/2},$$
$$\int_{\{z\notin M_n\}} h_{s-1}^j(z)\xi_{s,n}(z)\,dz = o(n^{-(s-2)/2}) \qquad j \geqq 0. \ \square$$

PROOF OF THEOREM 1. Let Q_n denote the *distribution of* $n^{\frac{1}{2}}(\bar{Z} - \mu)$ and let Φ_V be the *k-variate normal distribution with mean zero and dispersion matrix V*. It follows from a recent result of Sweeting (1977), Corollary 3 (also see [4], pages 160–162) that

(2.15) $$|Q_n(A) - \phi_V(A)| \leqq c_1 \lambda^{-\frac{3}{2}} \rho_3 n^{-\frac{1}{2}} + c_2 \phi_V((\partial A)^{\varepsilon_n}),$$
$$\varepsilon_n = c_3 \Lambda^{\frac{1}{2}} \lambda^{-\frac{3}{2}} \rho_3 n^{-\frac{1}{2}} \qquad \rho_3 = E|Z_1|^3.$$

Here λ is the smallest (and Λ the largest) eigenvalue of V. Fix $B \in \mathscr{B}$, where $\mathscr{B}$ satisfies (1.6), and in (2.15) take

(2.16) $$A = \{z \in R^k : g_n(z) \in B\}.$$

Since g_n is continuous,

(2.17) $$\partial A \subset \{z \in R^k : g_n(z) \in \partial B\}.$$

Now if $z \in (\partial A)^\varepsilon$, then there exists z' such that $g_n(z') \in \partial B$ and $|z - z'| < \varepsilon$. If, in addition, $z \in M_n$ (see (2.7)), then $|g_n(z) - g_n(z')| \leqq d'\varepsilon$, where d' is an upper bound of $|\text{grad } g_n|$ on M_n^ε (the ε-neighborhood of M_n). Since the Φ_V-probability of the complement of M_n is $o(n^{-(s-2)/2})$, it follows that

(2.18) $$\Phi_V((\partial A)^\varepsilon) \leqq \Phi_V(\{g_n(z) \in (\partial B)^{d'\varepsilon}\}) + o(n^{-(s-2)/2}) \qquad 0 < \varepsilon \leqq 1.$$

But by Lemma 2.1 (relation (2.8)) one has

$$\begin{aligned}\Phi_V(\{g_n(z) \in (\partial B)^{d'\varepsilon}\}) &= \int_{\{g_n \in (\partial B)^{d'\varepsilon}\}} \xi_{s,n}(z)\, dz + o(n^{-(s-2)/2}) \\ &= \int_{(\partial B)^{d'\varepsilon}} \phi_{\sigma^2}(v)\, dv + o(n^{-(s-2)/2}) \\ &= O(\varepsilon) + o(n^{-(s-2)/2})\end{aligned} \tag{2.19}$$

if $\rho_s = E|Z_1|^s$ is finite. Taking $s = 3$ and using (1.6), (2.18) and (2.19) the right side of (2.15) is estimated as $O(n^{-\frac{1}{2}})$ uniformly over $\mathscr{B}$. Again use Lemma 2.1, this time for B itself, to complete the proof of Theorem 1.

Proof of Theorem 2. We first prove part (b) of Theorem 2. From a general result on asymptotic expansion under Cramér's condition (1.16) (see [4], Corollary 20.2, page 214) and the estimates (2.18), (2.19) it follows that

$$\sup_{B \in \mathscr{B}} |Q_n(A) - \int_A \xi_{s,n}(z)\, dz| = o(n^{-(s-2)/2}) \tag{2.20}$$

where $\mathscr{B}$ satisfies (1.6) and A is defined by (2.16). Now use Lemma 2.1 to estimate the integral. It remains to identify F_n and $\Psi_{s,n}$ (see (1.14)). First assume that Z_1 is *bounded*. Since $W_n' = h_{s-1}(n^{\frac{1}{2}}(\bar{Z} - \mu))$ is a polynomial in $n^{\frac{1}{2}}(\bar{Z} - \mu)$ it follows from the asymptotic expansions of moments of Q_n, i.e., of the derivatives of its characteristic function at zero (see [4], Theorem 9.9, page 77), that

$$EW_n'^j = \int_{R^k} h_{s-1}^j(z)\xi_{s,n}(z)\, dz + o(n^{-(s-2)/2}) \qquad j \geqq 0\,. \tag{2.21}$$

By Lemma 2.1 (second relation in (2.10)) one then has

$$EW_n'^j = \int_{-\infty}^{\infty} u^j\, dF_n(u) + o(n^{-(s-2)/2}) \qquad j \geqq 0\,. \tag{2.22}$$

On the other hand, the expression (1.12) differs from $\hat{\psi}_{s,n}$ by $o(n^{-(s-2)/2})$ uniformly on a compact neighborhood of zero, say $\{|t| \leqq 1\}$. Also, according to a result due to James (1955), (1958), and James and Mayne (1962), the cumulants of W_n' satisfy

$$\kappa_{j,n} = O(n^{-(j-2)/2}) \qquad j \geqq 3\,, \tag{2.23}$$

so that, the "approximate cumulants" $\tilde{\kappa}_{j,n}$ (see (1.11)) satisfy

$$\tilde{\kappa}_{j,n} = \kappa_{j,n} + o(n^{-(s-2)/2}) \qquad j \geqq 1\,, \tag{2.24}$$

taking $\tilde{\kappa}_{j,n} = 0$ for $j > s$. Hence (1.12) differs from the characteristic function of W_n' by $o(n^{-(s-2)/2})$ uniformly on $\{|t| \leqq 1\}$. Therefore,

$$\sup_{|t| \leq 1} |\hat{\psi}_{s,n}(t) - E(\exp\{itW_n'\})| = o(n^{-(s-2)/2})\,. \tag{2.25}$$

By the familiar inequality of Cauchy for derivatives of analytic functions, derivatives of $\hat{\psi}_{s,n}$ at zero differ from those of $E(\exp\{itW_n'\})$ by $o(n^{-(s-2)/2})$, proving

$$EW_n'^j = \int_{-\infty}^{\infty} u^j\, d\Psi_{s,n}(u) + o(n^{-(s-2)/2}) \qquad j \geqq 0\,. \tag{2.26}$$

Together (2.22) and (2.26) imply

$$\int_{-\infty}^{\infty} u^j\, dF_n(u) - \int_{-\infty}^{\infty} u^j\, d\Psi_{s,n}(u) = o(n^{-(s-2)/2}) \qquad j \geqq 0\,. \tag{2.27}$$

Since neither F_n nor $\Psi_{s,n}$ involve terms of order $o(n^{-(s-2)/2})$,

$$\int_{-\infty}^{\infty} u^j\, dF_n(u) = \int_{-\infty}^{\infty} u^j\, d\Psi_{s,n}(u) \qquad j \geqq 0\,. \tag{2.28}$$

Now the Fourier–Stieltjes transforms of F_n and $\Psi_{s,n}$ are (extendable to) entire functions on the complex plane whose values and derivatives of all orders coincide at the origin. Hence $F_n = \Psi_{s,n}$, completing the proof of Theorem 2(b) in case Z_1 is bounded. We now proceed with the general case. Recall the polynomials π_r defined by (1.13) and write

$$\bar{q}_r(v) = \left[\pi_r\left(-\frac{d}{dv}\right)\phi_{\sigma^2}(v)\right]\Big/\phi_{\sigma^2}(v) \tag{2.29}$$

$$= \text{coeff. of} \quad n^{-r/2} \quad \text{in} \quad \psi_{s,n}\,.$$

Both q_r and $\bar{q}_r$ are polynomials in the *cumulants of Z_1 of orders s and less.* Denoting the vector of all these cumulants by γ_s write $q_r(\gamma_s)$, $\bar{q}_r(\gamma_s)$ to denote this functional dependence. For $c > 0$ define the truncated random vector Z_{1c} to be equal to Z_1 if $|Z_1| \leq c$ and zero if $|Z_1| > c$. We can choose c so large that the characteristic function of Z_{1c} satisfies Cramér's condition (1.16). Let $\gamma_{s,c}$ denote the vector of all cumulants of Z_{1c} of orders s and less. Since Z_{1c} is a bounded random vector, $q_r(\gamma_{s,c}) = \bar{q}_r(\gamma_{s,c})$. Since $\gamma_{s,c} \to \gamma_s$ as $c \to \infty$ (and q_r, $\bar{q}_r$ are continuous in γ_s), one gets $q_r(\gamma_s) = \bar{q}_r(\gamma_s)$. Proof of Theorem 2(b) is complete.

In order to prove Theorem 2(a) it is now enough to show that, under the given hypothesis,

$$\text{Prob}\,(n^{\frac{1}{2}}(\bar{Z} - \mu) \in A) = \textstyle\int_A \xi_{s,n}(z)\,dz + o(n^{-(s-2)/2}) \tag{2.30}$$

uniformly over all Borel subsets A of R^k. By a result of Bikjalis (1968) this will follow if we can show that there exists an integer p such that $Z_1 + \cdots + Z_p$ has a nonzero absolutely continuous component with respect to Lebesgue measure on R^k. The following result shows that this is true with $p = k$.

LEMMA 2.2. *Assume that G has a nonzero absolutely continuous component (with respect to Lebesgue measure on R^m) whose density is positive on some open ball B in which the functions f_i $(1 \leq i \leq k)$ are continuously differentiable and in which 1, $f_1, \cdots, f_k$ are linearly independent as elements of the vector space of continuous functions on B. Then Q_1^{*k} has a nonzero absolutely continuous component.*

PROOF. To show that the distribution of $Z_1 + \cdots + Z_k = (\sum_1^k f_1(Y_j), \cdots, \sum_1^k f_k(Y_j))$ has a nonzero absolutely continuous component under the given hypothesis define the map (on R^{mk} into R^k)

$$F(y_1, \cdots, y_k) = (\textstyle\sum_1^k f_1(y_j), \cdots, \sum_1^k f_k(y_j))$$

$$y_j = (y_j^{(1)}, \cdots, y_j^{(m)}) \in R^m,\ 1 \leq j \leq k\,.$$

The Jacobian matrix of this map will be denoted by $J_{k,m}$. This matrix may be displayed as $J_{k,m} = [A_1 A_2 \cdots A_k]$, where A_j is a $k \times m$ matrix whose ith row is $(\text{grad}\, f_i)(y_j)$. Clearly, it is enough to show that $J_{k,m}$ has rank k at some $(y_1, \cdots, y_k)$ with y_j in the open ball B for all j. We shall prove this by induction on k (keeping m fixed). Suppose then, as induction hypothesis, that $J_{k_0-1,m}(a_1, \cdots, a_{k_0-1})$ has rank $k_0 - 1$ for some $k_0 - 1 \geq 1$ and for some $(a_1, \cdots, a_{k_0-1})$ with a_j in B for all j. Note that the submatrix formed by the first $(k_0 - 1)$ rows and

$(k_0 - 1)m$ columns of $J_{k_0,m}(a_1, \cdots, a_{k_0-1}, y)$ is $J_{k_0-1,m}(a_1, \cdots, a_{k_0-1})$, while its last m columns are given by $A_{k_0}(y)$, and the first $(k_0 - 1)m$ elements of its last row are formed by $\operatorname{grad} f_{k_0}(a_1), \cdots, \operatorname{grad} f_{k_0}(a_{k_0-1})$.

Let $E_1, \cdots, E_{k_0-1}$ be $(k_0 - 1)$ linearly independent columns among the first $(k_0 - 1)m$ columns of $J_{k_0,m}$ (which exist by the induction hypothesis). Let $C_1, C_2, \cdots, C_m$ be the $(k_0 \times k_0)$ submatrices of $J_{k_0,m}$ formed by augmenting $E_1, E_2, \cdots, E_{k_0-1}$ by the first, second, $\cdots$, mth columns of $A_{k_0}(y)$, respectively. If rank of $J_{k_0,m}(a_1, \cdots, a_{k_0-1}, y)$ is less than k_0 for all y in B, then the determinants of $C_1, \cdots, C_m$ must vanish for all y in B, i.e.,

$$d_1 \frac{\partial f_1(y)}{\partial y^{(i)}} + \cdots + d_{k_0} \frac{\partial f_{k_0}(y)}{\partial y^{(i)}} = 0 \qquad \text{for} \quad i = 1, \cdots, m\,, \quad \text{and} \quad y \in B\,.$$

Here d_j is $(-1)^j$ times the determinant of the submatrix of $J_{k_0,m}$ comprising the columns $E_1, \cdots, E_{k_0-1}$ minus the jth row. Since $d_{k_0} \neq 0$, by induction hypothesis, the above relations are equivalent to saying that the gradient of (the nonzero linear combination) $\sum_1^{k_0} d_j f_j(y)$ vanishes identically in B. This means that $\sum d_j f_j$ is constant on every line segment contained in B; since B is connected, this means that there exists a number d_0 such that $\sum_1^{k_0} d_j f_j(y) = d_0$ for all y in B contradicting the hypothesis of linear independence of $1, f_1, \cdots, f_{k_0}$ in B. Hence there must exist a_{k_0} in B such that $J_{k_0,m}(a_1, \cdots, a_{k_0-1}, a_{k_0})$ has rank k_0. The proof is now completed by noting that the hypothesis of linear independence of $1, f_1$ in B implies that $\operatorname{grad} f_1$ does not vanish identically in B, so that the induction hypothesis is true for $k_0 - 1 = 1$. □

The above lemma improves Lemma 1.4 in [2]. The main idea behind the proof is contained in Dynkin (1951), Theorem 2.

PROOF OF THEOREM 3. We shall need an estimate of tail probabilities due to von Bahr (1967). Let $\{Z_n\}_{n \geq 1}$ be a sequence of i.i.d. random vectors each with mean μ and dispersion matrix V. Let Λ denote the largest eigenvalue of V. Then, if $E|Z_1|^s < \infty$ for some integer $s \geq 3$,

$$\text{(2.31)} \qquad \operatorname{Prob}(|n^{\frac{1}{2}}(\bar{Z} - \mu)| > ((s-1)\Lambda \log n)^{\frac{1}{2}}) \leq d n^{-(s-2)/2} (\log n)^{-s/2}$$

where $\bar{Z} = n^{-1}(Z_1 + \cdots + Z_n)$, and d is bounded on any bounded set of values of Λ.

Fix $\theta_0 \in \Theta$. In view of (2.31), the assumptions (A_1)—(A_4) and inequality (1.28) imply that there are constants d_1, d_2, d_3 such that

$$P_{\theta_0}\left(\left|\frac{1}{n} D_r L_n(\theta_0)\right| > d_1 n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}}\right) \leq d_2 (\log n)^{-s/2} n^{-(s-2)/2} \qquad 1 \leq r \leq p\,,$$

$$\text{(2.32)} \qquad P_{\theta_0}\left(\left|\frac{1}{n} D^\nu D_r L_n(\theta_0) - E_{\theta_0} D^\nu D_r L_1(\theta_0)\right| > d_1 n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}}\right) \leq d_2 (\log n)^{-s/2} n^{-(s-2)/2} \qquad 1 \leq |\nu| \leq s-1\,,$$

$$P_{\theta_0}(|R_{n,r}(\theta)| > |\theta - \theta_0|^s \{d_3 + d_1 n^{-\frac{1}{2}} (\log n)^{\frac{1}{2}}\}) \leq d_2 (\log n)^{-s/2} n^{-(s-2)/2}\,,$$

Therefore, on a set having P_{θ_0}- probability at least $1 - d_4(\log n)^{-s/2}n^{-(s-2)/2}$ one may rewrite (1.27) as

$$(2.33) \qquad (\theta - \theta_0) = (I(\theta_0) + \eta_n)^{-1}\Big[\delta_n + \sum_{2 \le |\nu| \le s-1} \frac{1}{\nu!}(\theta - \theta_0)^\nu E_{\theta_0} D^\nu D_r L_1(\theta_0) + d_3|\theta - \theta_0|^s \varepsilon_n\Big],$$

where η_n is a random matrix and δ_n is a random vector each having norm less than $d_5 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}$ and ε_n is a random vector of norm less than one. Note that there exists a sufficiently large positive constant d_6 and a (nonrandom) integer n_0 such that if $n > n_0$ and $|\theta - \theta_0| \leqq d_6 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}$, the right side of (2.33) is less than $d_6 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}$. It then follows from the Brouwer fixed point theorem (see Milnor (1965), page 14) applied to the expression on the right side of (2.33) (regarded as a function of $\theta - \theta_0$) that there exists a statistic $\hat{\theta}_n$ such that

$$(2.34) \qquad P_{\theta_0}(|\hat{\theta}_n - \theta_0| < d_6 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}, \hat{\theta}_n \text{ solves (1.27)}) \geqq 1 - d_4(\log n)^{-s/2}n^{-(s-2)/2}.$$

To obtain an asymptotic expansion of the distribution of $\hat{\theta}_n$, first define

$$(2.35) \qquad f_\nu(y) = D^\nu \log f(y; \theta_0), \qquad Z_n^{(\nu)} = f_\nu(Y_n) \qquad 1 \leqq |\nu| \leqq s.$$

Consider the random vectors $Z_n = (Z_n^{(\nu)})_{1 \le |\nu| \le s}$ whose coordinates are indexed by ν's. The dimension of Z_n is $k = \sum_{r=1}^{s} \binom{p+r-1}{r}$. From the definition of $\hat{\theta}_n$ one has, outside a set of probability at most $o(n^{-(s-2)/2})$,

$$(2.36) \qquad 0 = \frac{1}{n} D_r L_n(\hat{\theta}_n) = \bar{Z}^{(e_r)} + \sum_{|\nu|=1}^{s-1} \frac{1}{\nu!} \bar{Z}^{(e_r+\nu)}(\hat{\theta}_n - \theta_0)^\nu + R_{n,r}(\hat{\theta}_n) \qquad 1 \leqq r \leqq p,$$

where the rth coordinate of e_r is one and other coordinates zero. Now consider the p equations

$$(2.37) \qquad 0 = z^{(e_r)} + \sum_{|\nu|=1}^{s-1} \frac{1}{\nu!} z^{(e_r+\nu)}(\theta - \theta_0)^\nu \equiv P(\theta, z; r) \qquad 1 \leqq r \leqq p,$$

in the $p + k$ variables θ, z. These equations have a solution at $\theta = \theta_0$, $z = \mu$, where $\mu = EZ_1$, i.e.,

$$(2.38) \qquad \begin{aligned} \mu^{(e_r)} &= 0 & 1 \leqq r \leqq p, \\ \mu^{(\nu)} &= E_{\theta_0} D^\nu \log f(Y_1; \theta_0) & 2 \leqq |\nu| \leqq s. \end{aligned}$$

Also, since $I(\theta_0)$ is nonsingular, the p vectors $(D_1 P(\theta_0, \mu; r)), \cdots, (D_p P(\theta_0, \mu; r))$, $1 \leqq r \leqq p$, are linearly independent. Therefore, by the implicit function theorem, there is a neighborhood N of μ and p uniquely defined real-valued infinitely differentiable functions H_i $(1 \leqq i \leqq p)$ on N such that $\theta = H(z) = (H_1(z), \cdots, H_p(z))$ satisfies (2.37) for $z \in N$, and $\theta_0 = H(\mu)$. By (2.32), $|\bar{Z}^{(e_r)} + R_{n,r}(\hat{\theta}_n)| < d_7 n^{-\frac{1}{2}}(\log n)^{\frac{1}{2}}$ with P_{θ_0}- probability $1 - o(n^{-(s-2)/2})$. Therefore, by (2.36) and the uniqueness part of the implicit function theorem, with P_{θ_0}- probability $1 - o(n^{-(s-2)/2})$ one has

$$\hat{\theta}_n = H(\bar{Z}') \quad \text{with} \quad \bar{Z}'^{(\nu)} = \bar{Z}^{(\nu)} \quad \text{for} \quad 2 \leqq |\nu| \leqq s\,, \tag{2.39}$$
$$= \bar{Z}^{(e_r)} + R_{n,r}(\hat{\theta}_n) \quad \text{for} \quad \nu = e_r \quad 1 \leqq r \leqq p\,.$$

Therefore, by (2.32) and (2.34), there are constants d_8, d_9 such that

$$P_{\theta_0}(|n^{\frac{1}{2}}[H(\bar{Z}) - H(\mu)] - n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0)| \leqq d_8(\log n)^{s/2} n^{-(s-1)/2}) \tag{2.40}$$
$$= P_{\theta_0}(|H(\bar{Z}') - H(\bar{Z})| = |R_{n,r}(\hat{\theta}_n)| \leqq d_8(\log n)^{s/2} n^{-s/2})$$
$$\geqq 1 - d_9(\log n)^{-s/2} n^{-(s-2)/2}\,.$$

In view of (A_6) (and Remark 1.2) Lemma 2.2 applies, so that Theorem 2 yields, for vector H (see Remark 1.1),

$$P_{\theta_0}(n^{\frac{1}{2}}[H(\bar{Z}) - H(\mu)] \in B) = \textstyle\int_B \psi_{s,n}(x)\, dx + o(n^{-(s-2)/2}) \tag{2.41}$$

uniformly over all Borel sets B. Here $\psi_{s,n}$ is given by (1.18) with $M = I^{-1}(\theta_0)D(\theta_0)I^{-1}(\theta_0)$, where $I(\theta_0)$ and $D(\theta_0)$ are defined by (1.25). This evaluation of M follows from (2.33), (2.36), or, alternatively, from a computation of grad $H_r(\mu)$, $1 \leqq r \leqq p$, obtained from inverting the Jacobian matrix (at (θ_0, μ)) of the transformation whose first p coordinate functions are given by the right side of (2.37) and the remaining coordinate functions by $z^{(\nu)}$, $1 \leqq |\nu| \leqq s$. Finally, if $\mathscr{B}$ satisfies (1.31), then it is simple to check that

$$\sup_{B \in \mathscr{B}} \textstyle\int_{(\partial B)^\varepsilon} |\psi_{s,n}(x)|\, dx \leqq d_{10}\varepsilon + o(n^{-(s-2)/2}) \qquad 0 \leqq \varepsilon \leqq 1\,. \tag{2.42}$$

Relations (2.40)—(2.42), with $\varepsilon = d_8(\log n)^{s/2} n^{-(s-1)/2}$, now complete the proof excepting for the uniformity over compacts. By assumptions (A_1)—(A_4), the constants d_8, d_9, d_{10} are bounded on compact K (since so are d_1—d_7). The term $o(n^{-(s-2)/2})$ in (2.41) is uniform on compact K for $B \in \mathscr{B}$ due to the uniformity of the error of approximation of the distribution Q_n of $n^{\frac{1}{2}}(\bar{Z} - \mu)$ by its Edgeworth expansion, assuming, without loss of generality (see Remark 1.2), that the dispersion matrix of Z_1 is nonsingular. Note that we have only made use of (2.41) uniformly over $\mathscr{B}$. For this it is sufficient (see Theorem 2(b)) that Z_1 satisfies Cramér's condition (1.16). Assumptions (A_2) and (A_5) now imply that this condition holds uniformly on compacts K in an appropriate sense (see the first observation in [2] following (1.50), page 11). □

There appears to have grown in recent times a considerable amount of applied work, especially in econometrics, on the formal Edgeworth expansion. See, for example, Chambers (1967), Phillips (1977), Sargan (1976), and references contained in these articles. It may be noted that the conditions imposed by Chambers (1967) (Section 2.2) on the characteristic function of the statistic are not sufficient to insure the existence of a valid asymptotic expansion. Besides, such conditions imposed directly on the statistic are extremely hard to verify, at least in the context of the present article.

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Part II
Large Time Asymptotics for Markov Processes I: Diffusion

Chapter 5
Martingale Methods for the Central Limit Theorem

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5.1 Introduction

As the name suggests, central limit theorem or CLT does play a central role in probability theory. Early masters like De Moivre, Laplace, Gauss, Lindeberg, Lévy, Kolmogorov, Lyapunov, and Bernstein studied the case of sums of independent random variables. Their results were then extended to sums of dependent random variables by various authors. For sums of the form $\sum_i V(X_i)$ where X_i is a stationary Markov chain, the CLT was proved by Markov himself. The proof consisted of leaving large gaps to create enough independence but not large enough to make a difference in the sum. It is a bit delicate to balance the two and requires assumptions on the mixing properties of the stationary process. If the summands form a stationary sequence and the partial sums is a martingale relative to the natural filtration, it was observed by Paul Lévy that the CLT was valid under virtually no additional conditions. An early version of this result can be found in Doob's book [5] on Stochastic Processes and a more modern version in Billingsley [3].

5.2 Methods for Proving the CLT

Since the central limit theorem for martingales is easy, it is natural to ask if the sum $S_n = X_1 + \cdots + X_n$ can be written as $M_n + A_n$, where M_n is a martingale and A_n is negligible. If this can be accomplished the proof for the CLT would be greatly simplified.

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Let us consider Brownian motion $x(t)$ on the circle $S = [0,1]$ with end points identified. Let $V(x)$ be continuous function on S satisfying $\int_0^1 V(x)dx = 0$. We are interested in proving a central limit theorem for

$$y(t) = \int_0^t V(x(s))ds$$

or in functional form, the convergence of the process

$$y_\lambda(t) = \frac{1}{\sqrt{\lambda}}\int_0^{\lambda t} V(x(s))ds$$

to a Brownian motion on $R = (-\infty,\infty)$ with variance $\sigma^2 t$ as $\lambda \to \infty$ and determine σ^2 in terms of V. Because Brownian motion on the circle is exponentially mixing it is not difficult to adapt the earlier method of rewriting the integral as the sum of integrals over disjoint intervals separated by gaps and prove the central limit theorem in this manner. The limiting variance will be

$$\sigma^2 = 2\int_0^\infty E^P[V(x(0))V(x(t))]dt$$

where P is the stationary version of the Brownian motion on S with Lebesgue measure as the invariant measure.

We will now explore two other methods that look different from each other but are closely related.

The martingale method proceeds as follows. Since $V(x)$ has mean zero there is a function $W(x)$ with mean 0 such that

$$\frac{1}{2}W''(x) = -V(x)$$

By Itô's formula

$$W(x(t)) - W(x(0)) = -\int_0^t V(x(s))ds + \int_0^t W'(x(s))dx(s) = -y(t) + M(t)$$

In particular,

$$|y(t) - M(t))| \le 2\sup_x |W(x)|$$

Since W is bounded, the central limit theorem for $y(t)$ reduces to proving it for $M(t) = \int_0^t W'(x(s))dx(s)$, which is a continuous martingale. It can therefore be time changed to a Brownian motion with the clock

$$D(t) = \int_0^t [W'(x(s))]^2 ds$$

and the distribution of $\frac{M(t)}{\sqrt{t}}$ is the same as that of $Y(\frac{D(t)}{t})$ for some other Brownian motion $Y(t)$. But, by the ergodic theorem, $\frac{D(t)}{t} \to \int |W'(x)|^2 dx$ and we have convergence to a Gaussian with mean 0 and variance $D = \int |W'(x)|^2 dx$. Or better still,

$$\frac{1}{\lambda}[M(\lambda t)]^2 - \frac{1}{\lambda} D(\lambda t)$$

is a martingale. It is not hard to establish tightness for the family P_λ of distributions of the processes $\frac{1}{\sqrt{\lambda}} y(\lambda t)$ in $C[0, T]$ and with respect to any limiting measure Q on $C[0, T]$, the evaluation maps $x(t)$ is a martingale as is

$$x^2(t) - ct$$

with

$$c = \int_0^1 |W'(x)|^2 dx = 2 \int_0^\infty E^P[V(x(0))V(x(t))dt]$$

This determines the limiting measure Q as Brownian motion with variance ct and requires only the law of large numbers for $D(t)$, i.e., the ergodic theorem for P.

There is another way of looking at this as a problem of singular perturbation in PDE. The pair $x(t)$ and $y(t) = \int_0^t V(x(s))ds$ can be viewed as a degenerate two-dimensional diffusion on $S \times R$, with generator

$$L = \frac{1}{2} D_x^2 + V(x) D_y$$

Considering instead $x(\frac{t}{\epsilon^2})$ and $\epsilon y(\frac{t}{\epsilon^2})$ leads to

$$L_\epsilon = \frac{1}{2\epsilon^2} D_x^2 + \frac{1}{\epsilon} V(x) D_y$$

We are interested in the behavior of the solution $u_\epsilon = u_\epsilon(t, x, y)$ of the equation

$$\frac{\partial u_\epsilon}{\partial t} + L_\epsilon u_\epsilon = 0$$

with the initial condition $u(T, x, y) = f(y)$. We try a solution of the form

$$u_\epsilon(t, x, y) = u_0(t, x, y) + \epsilon u_1(t, x, y) + \epsilon^2 u_2(t, x, y) + \cdots$$

substitute it in the equation and equate like powers of ϵ. We obtain the equations

$$\frac{1}{2} D_x^2 u_0(t, x, y) = 0$$

$$\frac{1}{2} D_x^2 u_1(t, x, y) + V(x) D_y u_0(t, x, y) = 0$$

$$D_t u_0(t, x, y) + \frac{1}{2} D_x^2 u_2(t, x, y) + V(x) D_y u_1(t, x, y) = 0$$

for u_0, u_1, u_2 that are periodic in x. Solving them yields the following. u_0 cannot depend on x. Therefore $u_0(t,x,y)$ can only be a function $v_0(t,y)$ of t and y. Then $\frac{1}{2}D_x^2 u_1$ has to equal the product $-V(x)D_y v_0(t,y)$. Since V has mean 0 on S this is possible by solving $\frac{1}{2}W'' = -V$ and taking $u_1(t,x,y) = W(x)v_0(t,y)$. For the last equation to be solvable with $u_0(0,y) = f(y)$ we need for each (t,y)

$$D_t v_0(t,y) - [\int_0^1 V(x)W(x)dx] D_y^2 v_0(t,y) = 0$$

or

$$D_t v_0(t,y) + \frac{\sigma^2}{2} D_y^2 v_0(t,y) = 0; \quad v_0(T,y) = f(y)$$

and

$$\sigma^2 = -\frac{1}{2}\int W(x)W''(x)dx = \frac{1}{2}\int [W'(x)]^2 dx$$

With

$$F_\epsilon(t,x) = v_0(t,y) + \epsilon u_1(t,x,y) + \epsilon^2 u_2(t,x,y)$$

it is an easy computation to show that many terms cancel out and we get

$$D_t F_\epsilon + L_\epsilon F_\epsilon = O(\epsilon)$$

We can now apply the maximum principle to conclude that the solution u_ϵ of

$$D_t u_\epsilon + L_\epsilon u_\epsilon = 0; \quad u(T,y) = f(y)$$

satisfies $|u_\epsilon - F_\epsilon| \le C\epsilon$ and therefore $u_\epsilon \to v_0$ which is the CLT. This is really the PDE version of the martingale approximation.

5.3 A Bit of History

Martingale approximations in the proof of the central limit theorem have emerged in many places often independently. In the late seventies Bensoussan, Lions, and Papanicolaou [1] used singular perturbation techniques to prove results on homogenization, which in certain situations can be interpreted as a central limit theorem. This was explored further in an article by Papanicolaou, Stroock, and Varadhan [11]. In Soviet Union, Sergei Kozlov [10] published a fair body of material on homogenization. Gordin and Lifšic in [6] provide a central limit theorem for functions of Markov chains using explicitly the martingale approximation. This was extended to continuous time Markov processes by Rabi Bhattacharya in [2]. Kipnis and Varadhan [9] provide a general result for reversible Markov processes and the martingale methods are now used regularly in different situations, for instance in Kifer-Varadhan [8]. A point to note is that CLT for functions of a Markov process is proved when the process has the stationary distribution. The methods actually show that the invariant measure of the set of starting points for which the Gaussian approximation has an error at least ϵ goes to 0 as $t \to \infty$. The validity of the CLT for every starting point can be proved under additional Doeblin type assumptions. The question of validity of the CLT for almost all starting points under the stationary measure has been considered by several authors. References can be found in Derriennic and Lin [4].

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Chapter 6
Ergodicity and Central Limit Theorems for Markov Processes

Thomas G. Kurtz

Keywords Ergodicity, Invariant measures,Markov processes, Generators, Diffusions, Harris recurrence, Martingale central limit theorem, Functional central limit theorem

6.1 Introduction

There are several contexts in the theory of Markov processes in which the term *ergodicity* is used, but in all of these, assertions of the form

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} h(X_k) = \int h d\pi, \tag{6.1}$$

or in continuous time,

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t h(X(s))ds = \int h d\pi, \tag{6.2}$$

for some probability measure, π, appear. Limits of this form are essentially laws of large numbers, and given such a limit, it is natural to ask about rates of convergence or fluctuations, in particular, to explore the behavior of the rescaled deviations,

$$\sqrt{n}\left(\frac{1}{n}\sum_{k=1}^{n} h(X_k) - \int h d\pi\right) \text{ or } \sqrt{t}\left(\frac{1}{t}\int_0^t h(X(s))ds - \int h d\pi\right).$$

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Many times during his career, Rabi has studied problems of this form. The goal of these brief comments is to review some of his results and provide some of the background needed to read his papers.

All processes we consider will take values in a complete separable metric space (E, r). They will be temporally homogeneous and Markov in discrete or continuous time. In discrete time, the *transition function* will be denoted by $P(x, \Gamma)$, that is, there is a filtration $\{\mathcal{F}_k\}$ such that the process of interest $X = \{X_k, k = 0, 1, \ldots\}$ satisfies

$$P\{X_{k+1} \in \Gamma | \mathcal{F}_k\} = P(X_k, \Gamma), \quad k = 0, 1, \ldots, \Gamma \in \mathcal{B}(E), \tag{6.3}$$

where $\mathcal{B}(E)$ denotes the Borel subsets of E. The filtration may be larger than the filtration generated by $\{X_k\}$. When X and $\{\mathcal{F}_k\}$ satisfy (6.3), we will say that X is $\{\mathcal{F}_k\}$-*Markov* with transition function P.

In continuous time, the transition function will be denoted by $P(t, x, \Gamma)$ and there will be a filtration $\{\mathcal{F}_t\}$ such that the process $\{X(t), t \geq 0\}$ satisfies

$$P\{X(s+t) \in \Gamma | \mathcal{F}_s\} = P(t, X(s), \Gamma), \quad s, t \geq 0, \Gamma \in \mathcal{B}(E). \tag{6.4}$$

Setting

$$T(t)f(x) = \int_E f(y)P(t, x, dy), \quad f \in B(E),$$

where $B(E)$ is the space of bounded, Borel measurable functions on E, the Markov property implies $\{T(t)\}$ is a *semigroup*, that is

$$T(s)T(t)f = T(s+t)f.$$

The semigroup can (and will be) defined for larger classes of functions as is convenient.

The notion of an operator A being a *generator* for a Markov process can be defined in a variety of ways, but essentially always implies

$$T(t)f = f + \int_0^t T(s)Af\,ds,$$

which in turn implies

$$f(X(t)) - f(X(0)) - \int_0^t Af(X(s))ds \tag{6.5}$$

is a martingale for any filtration satisfying (6.4).

The analog in discrete time to the continuous-time semigroup is obtained by defining the linear operator

$$Pf(x) = \int_E f(y)P(x, dy)$$

and observing that

$$E[f(X_{k+n})|\mathcal{F}_k] = P^n f(X_k),$$

and that

$$M_n = f(X_n) - f(X_0) - \sum_{k=0}^{n-1}(Pf(X_k) - f(X_k)) \tag{6.6}$$

is a martingale for every $f \in B(E)$. Consequently,

$$A = P - I$$

in discrete time plays the role of the generator in continuous time. The martingale properties (6.5) and (6.6) are central to the study of Markov processes and are the basis for the central limit theorems that Rabi and others have given.

By the *initial distribution* of a Markov process, we mean the distribution of X_0 in the discrete case and of $X(0)$ in the continuous-time case. The finite dimensional distributions of a Markov process are determined by its initial distribution and its transition function. If we want to emphasize the initial distribution μ of the process, we will write $\{X_k^\mu\}$ or $\{X^\mu(t)\}$.

The following lemma will prove useful in studying discrete time Markov processes.

Lemma 1. *Let $P(x,\Gamma)$ be a transition function on E. There exists a measurable space $(U,\mathcal{U})$, a measurable mapping $\alpha : U \times E \to E$, and a probability distribution ν on $(U,\mathcal{U})$ such that if ξ has distribution ν, then $\alpha(\xi,x)$ has distribution $P(x,\cdot)$.*

Consequently, if X_0 has distribution $\mu \in \mathcal{P}(E)$ and $\xi_1,\xi_2,\ldots$ is a sequence of independent, ν-distributed, U-valued random variables that is independent of X_0, then for $\mathcal{F}_k = \sigma(X_0,\xi_1,\ldots,\xi_k)$, $\{X_k\}$ defined recursively by

$$X_{k+1} = \alpha(\xi_{k+1}, X_k), \quad k = 0,1,\ldots,$$

is a $\{\mathcal{F}_k\}$-Markov process with initial distribution μ and transition function $P(x,\Gamma)$.

Proof. The construction in [8] gives α for ξ uniformly distributed on $[0,1]\times[0,1]$. A slight modification allows ξ to be uniform on $[0,1]$.

Remark 1. If the mapping $x \in E \to P(x,\cdot) \in \mathcal{P}(E)$ is continuous taking the weak topology on $\mathcal{P}(E)$, then α given by the Blackwell and Dubins construction has the property that for each $x_0 \in E$, the mapping $x \in E \to \alpha(x,\xi)$ is almost surely continuous at x_0.

The next section reviews ideas of ergodicity of Markov processes and gives some of the basic results. The final section considers central limit theorems exploiting the martingale properties mentioned above. We assume that all continuous-time Markov processes considered are cadlag.

6.2 Ergodicity for Markov Processes

Ideas of ergodicity for Markov processes all relate to the existence of stationary distributions for the processes. In discrete time, $\pi \in \mathcal{P}(E)$ is a stationary distribution if

$$\int_E P(x,\Gamma)\pi(dx) = \pi(\Gamma), \quad \Gamma \in \mathcal{B}(E),$$

and in continuous time, if

$$\int_E T(t)f(x)\pi(dx) = \int_E f(x)\pi(dx), \quad f \in B(E), t \geq 0,$$

which is equivalent to requiring

$$\int_E Af(x)\pi(dx) = 0$$

for a sufficiently large class of f.

If π is a stationary distribution and we take π to be the initial distribution for the process, then $\{X_k^\pi\}$ (or $\{X^\pi(t)\}$) will be a stationary process. If $\{X_k^\pi\}$ is ergodic as defined generally for stationary processes, that is, the tail σ-field

$$\mathcal{T} = \cap_n \sigma(X_k^\pi, k \geq n)$$

only contains events of probability zero or one, we will say that π is an *ergodic stationary distribution*. If there is only one stationary distribution, it must be ergodic. If π is an ergodic stationary distribution, then taking $X = X^\pi$, (6.1) or (6.2) hold for all $h \in B(E)$, or more generally, for all $h \in L^1(\pi)$.

The questions of existence and uniqueness of stationary distributions are among the fundamental questions in the study of Markov processes. If, as is typically the case,

$$P : C_b(E) \to C_b(E), \tag{6.1}$$

or

$$T(t) : C_b(E) \to C_b(E), \quad t \geq 0, \tag{6.2}$$

where $C_b(E)$is the space of bounded continuous functions on E, proof of existence of a stationary distribution can be reduced to the proof of relative compactness of a sequence of probability measures.

Theorem 1. *Assume that* $\{T(t)\}$ *satisfies* (6.2) *and for a corresponding Markov process* $\{X^\mu(t)\}$*, define a family of probability measures* $\{\nu_t\}$ *by*

$$\begin{aligned} \nu_t f = E[\frac{1}{t}\int_0^t f(X(s))ds] &= \frac{1}{t}\int_0^t E[f(X(s))]ds \\ &= \frac{1}{t}\int_0^t \int_E T(s)f d\mu ds, \quad f \in B(E). \end{aligned} \tag{6.3}$$

Then as $t \to \infty$*, any weak limit point of* $\{\nu_t\}$ *is a stationary distribution for* $\{T(t)\}$.

Similarly, in the discrete-time case, if P satisfies (6.1), any weak limit point of $\{\nu_n\}$ defined by

$$\nu_n f = \frac{1}{n}\sum_{k=0}^{n-1} E[f(X_k)] \tag{6.4}$$

is a stationary distribution for P.

Proof. Suppose $t_n \to \infty$ and $\{\nu_{t_n}\}$ converges weakly to π. Observe that for each $f \in C_b(E)$ and $t > 0$,

$$\frac{1}{t_n}\int_t^{t+t_n} E[f(X(s))]ds = \nu_{t_n} T(t) f$$

has the same limit as $\nu_{t_n} f$. Consequently, $\pi f = \pi T(t) f$, and π is a stationary distribution.

The proof in the discrete case is essentially the same.

The natural approach to proving the existence of the sequence $\{\nu_{t_n}\}$ is to prove relative compactness for $\{\nu_t\}$. Since relative compactness in $\mathcal{P}(E)$ is equivalent to tightness, we have the following.

Corollary 1. *Let E be compact. If $\{T(t)\}$ satisfies (6.2), then there exists at least one stationary distribution for $\{T(t)\}$. Similarly, if P satisfies (6.1), then there exists at least one stationary distribution for P.*

More generally, relative compactness is usually proved by obtaining a Lyapunov function for the process. In particular, we want to find a function $\psi : E \to [0, \infty)$ such that for each $a \ge 0$, the level set

$$\Gamma_a = \{x \in E : \psi(x) \le a\}$$

is compact and for some initial distribution μ,

$$K \equiv \sup_{t \ge 0} E[\psi(X^\mu(t))] < \infty.$$

It follows that

$$P\{X^\mu(t) \notin \Gamma_a\} = P[\psi(X^\mu(t)) > a\} \le \frac{K}{a}$$

and that

$$\nu_t(\Gamma_a^c) \le \frac{\nu_t \psi}{a} \le \frac{K}{a},$$

so $\{\nu_t\}$ is tight and hence relatively compact.

The notion of a *stochastic Lyapunov functions* was developed in [14] and reflects ideas dating back to [10] and [13]. There is a large literature on constructing such functions. In discrete time, we have the following simple condition.

Lemma 2. *Let $\psi : E \to [0, \infty)$. Suppose that there exist $a \ge 0$ and $0 \le b < 1$ such that*

$$P\psi(x) \le a + b\psi(x). \tag{6.5}$$

Then for each n

$$P^n\psi(x) \le a\frac{1-b^{n-1}}{1-b} + b^n\psi(x),$$

and hence for $\mu \in \mathcal{P}(E)$ *satisfying* $\int_E \psi d\mu < \infty$,

$$\sup_n E[\psi(X_n^\mu)] \le \frac{a}{1-b} + \int_E \psi d\mu < \infty.$$

Consequently, if ψ *has compact level sets and* P *satisfies (6.1), then there exists at least one stationary distribution for* P.

The analogous result in the continuous-time case is somewhat more delicate. Rewriting (6.5) as

$$(P-I)\psi(x) \le a - (1-b)\psi(x)$$

and recalling that $P - I$ plays a role analogous to the generator A suggests looking for ψ satisfying

$$A\psi(x) \le a - \epsilon\psi(x),$$

for some positive a and ϵ. To this point, we have only considered A to be defined so that f and Af are in $B(E)$. For many Markov processes, for example, diffusions, the extension of the generator to a large class of unbounded ψ is clear, but even in the diffusion setting with smooth ψ, in general we can only claim that

$$\psi(X(t)) - \psi(X(0)) - \int_0^t A\psi(X(s))ds$$

is a local martingale, not a martingale. Note, however, that if ψ is bounded below and $A\psi$ is bounded above, this local martingale will also be a supermartingale. With that observation in mind, the following lemma provides the desired extension.

The following is essentially a consequence of Fatou's lemma.

Lemma 3. *For* $n = 1, 2, \ldots$, *let* $f_n, Af_n \in B(E)$, *and*

$$f_n(X(t)) - f_n(X(0)) - \int_0^t Af_n(X(s))ds$$

be a martingale. Suppose $f_n \ge 0$, $\sup_{n,x} Af_n(x) < \infty$, *and for each* $x \in E$, $\{f_n(x)\}$ *and* $\{Af_n(x)\}$ *converge. Denote the limits* ψ *and* $A\psi$. *Then*

$$\psi(X(t)) - \psi(X(0)) - \int_0^t A\psi(X(s))ds \tag{6.6}$$

is a supermartingale.

The supermartingale property is exactly what is needed to give the continuous-time analog of Lemma 2.

Lemma 4. *Let measurable functions* $\psi, A\psi : E \to \mathbb{R}$ *satisfy* $\psi \geq 0$ *and* $\sup_{x \in E} A\psi(x) < \infty$. *For* $\mu \in \mathcal{P}(E)$ *satisfying* $\int_E \psi d\mu < \infty$, *assume that (6.6) with* X *replaced by* X^μ *is a supermartingale. Suppose*

$$A\psi(x) \leq a - \epsilon\psi(x)$$

Then

$$E[\psi(X^\mu(t))] \leq \frac{a}{\epsilon} \vee \int_E \psi d\mu. \tag{6.7}$$

Consequently, if ψ *has compact level sets and* $\{T(t)\}$ *satisfies (6.2), then there exists at least one stationary distribution for* $\{T(t)\}$.

Proof. Let Z^μ denote the supermartingale. Then

$$\begin{aligned}
e^{\epsilon t}\psi(X^\mu(t)) &= \psi(X^\mu(0)) + \int_0^t e^{\epsilon s} d\psi(X^\mu(s)) + \int_0^t \epsilon e^{\epsilon s}\psi(X^\mu(s))ds \\
&= \psi(X^\mu(0)) + \int_0^t e^{\epsilon s} dZ^\mu(s) + \int_0^t e^{\epsilon s}(\epsilon\psi(X^\mu(s)) + A\psi(X^\mu(s)))ds \\
&\leq \psi(X^\mu(0)) + \int_0^t e^{\epsilon s} dZ^\mu(s) + \int_0^t e^{\epsilon s} a ds.
\end{aligned}$$

Since $E[\int_0^t e^{\epsilon s} dZ^\mu(s)] \leq 0$,

$$E[\psi(X^\mu(t))] \leq e^{-\epsilon t}\int_E \psi d\mu + \frac{a}{\epsilon}(1 - e^{-\epsilon t}),$$

and the lemma follows.

We can relax the conditions of Lemma 4 and still obtain relative compactness of $\{\nu_t\}$ but without the moment estimate (6.7).

Lemma 5. *Let measurable functions* $\psi, A\psi : E \to \mathbb{R}$ *satisfy* $\psi \geq 0$ *and* $K = \sup_{x \in E} A\psi(x) < \infty$. *For* $\mu \in \mathcal{P}(E)$ *satisfying* $\int_E \psi d\mu < \infty$, *assume that (6.6) with* X *replaced by* X^μ *is a supermartingale. Suppose that for each* $a > 0$

$$\Gamma_a = \{x : A\psi(x) \geq -a\}$$

is compact. Then $\{\nu_t\}$ *defined by (6.3) is relatively compact, and if* $\{T(t)\}$ *satisfies (6.2), there exists at least one stationary distribution for* $\{T(t)\}$.

If E *is locally compact and* $\{T(t)\}$ *satisfies (6.2), then existence of a stationary distribution holds as long as* Γ_a *is compact for some* $a > 0$.

Remark 2. The assumption that Γ_a is compact only for some $a > 0$ is, in general, not enough to ensure relative compactness of $\{\nu_t\}$. If, however, the process is Harris recurrent (see Section 6.2.2), then existence of a stationary distribution implies convergence of $\{\nu_t\}$.

Proof. The supermartingale property implies

$$-\int_E A\psi d\nu_t = -\frac{1}{t}E[\int_0^t A\psi(X(s))ds] \leq \frac{1}{t}\int_E \psi d\mu - \frac{1}{t}E[\psi(X(t))]] \leq \frac{1}{t}\int_E \psi d\mu,$$

and for $a > 0$,

$$a\nu_t(\Gamma_a^c) \leq K + \frac{1}{t}\int_E \psi d\mu,$$

giving tightness and hence relative compactness for $\{\nu_t\}$.

The second part of the lemma follows by the observation that $\{\nu_t\}$ is relatively compact as a probability measure on the one-point compactification of E and the compactness of Γ_a for some $a > 0$ implies that any limit point ν_∞ satisfies $\nu_\infty(\Gamma_a) > 0$ and hence $\nu_\infty(E) > 0$. Normalizing the restriction of ν_∞ to E to be a probability measure gives a stationary distribution for $\{T(t)\}$. See Theorem 4.9.9 of [9].

The following lemma gives conditions which coupled with some kind of irreducibility imply recurrence, but not necessarily positive recurrence.

Lemma 6. *Let measurable functions $\psi, A\psi : E \to \mathbb{R}$ satisfy $\psi \geq 0$ and $K = \sup_{x\in E} A\psi(x) < \infty$. For $\mu \in \mathcal{P}(E)$ satisfying $\int_E \psi d\mu < \infty$, assume that (6.6) with X replaced by X^μ is a supermartingale. Suppose that for each $a > 0$,*

$$\Gamma_a = \{x : \psi(x) \leq a\}$$

is compact and that there exists a_0 such that

$$\sup_{x\in\Gamma_{a_0}^c} A\psi \leq 0.$$

Let $\tau_0 = \inf\{t \geq 0 : X^\mu(t) \in \Gamma_{a_0}$ and $\gamma_a = \inf\{t \geq 0 : X^\mu(t) \notin \Gamma_a\}$. Then

$$\lim_{a\to\infty} P\{\gamma_a \leq \tau_0\} = 0. \tag{6.8}$$

Proof. It is at least not immediately obvious that $\gamma_a < \infty$ implies $\psi(X^\mu(\gamma_a)) \geq a$, so some randomization may be necessary for a complete proof, but assuming this inequality holds, the supermartingale property implies

$$aP\{\gamma_a \leq \tau_0\} \leq E[\psi(X^\mu(\gamma_a \wedge \tau_0))] \leq \int_E \psi d\mu,$$

and (6.8) follows.

Example 1. In [3], Rabi gives a class of ψ of the form $\psi(x) = F(|x - z|)$ for nondegenerate diffusion processes which satisfy the conditions of Lemma 6. (Actually, in Rabi's notation, we need to set $\psi(x) = -F(|x - z|)$.) The non-degeneracy assumption then ensures Harris recurrence (see below). He also formulates similar conditions that imply transience and gives a construction of an F such that $\psi(x) = -F(|x - z|)$ satisfies the conditions of the second part of Lemma 5.

A central idea in the study of uniqueness of stationary distributions is the notion of *Harris recurrence*.

6.2.1 Harris Recurrence

Harris irreducibility requires the existence of a measure φ on $\mathcal{B}(E)$ such that $\varphi(B) > 0$ implies that the Markov process visits B with positive probability, regardless of the initial distribution. If the process visits such B infinitely often with probability one, or in the continuous time case, the process visits B for arbitrarily large times, that is, $\tau_n = \inf\{t > n : X(t) \in B\}$ is finite almost surely for each n, the process is *Harris recurrent*. As long as φ is σ-finite, without loss of generality, we can and will assume φ is a probability measure. In discrete time, the classical conditions for Harris recurrence can be formulated under the assumption that there exists a function $\varepsilon : E \to [0, 1]$ such that the transition function satisfies

$$P(x, B) \geq \varepsilon(x)\varphi(B) \tag{6.9}$$

and that for each initial condition μ, the Markov process satisfies

$$P\{\sum_{k=1}^{\infty} \varepsilon(X_k^\mu) = \infty\} = 1. \tag{6.10}$$

The following lemma illustrates the significance of these conditions.

Lemma 7. *Let $\mu \in \mathcal{P}(E)$, and suppose that (6.9) and (6.10) hold. Then there exists a probability space with a process X^μ, a filtration $\{\mathcal{F}_k^\mu\}$, and a $\{\mathcal{F}_k^\mu\}$-stopping time τ^μ such that X^μ is $\{\mathcal{F}_k^\mu\}$-Markov with initial distribution μ and transition function $P(x, \Gamma)$ and the distribution of $X_{\tau^\mu}^\mu$ is φ.*

Proof. We enlarge the state space to be $E \times \{-1, 1\}$ and define the new transition function by

$$Q(x, \theta, \Gamma \times \{\theta\}) = P(x, \Gamma) - \varepsilon(x)\varphi(\Gamma)$$

and

$$Q(x, \theta, \Gamma \times \{-\theta\}) = \varepsilon(x)\varphi(\Gamma).$$

If (X^μ, Θ) is a Markov process with this transition function such that X_0^μ has distribution μ, then X^μ is a Markov process with transition function $P(x,\Gamma)$ and initial distribution μ, and the desired stopping time is $\tau^\mu = \min\{k : \theta_k \neq \theta_{k-1}\}$. Note that

$$P\{\tau^\mu > n\} = E[\prod_{k=0}^{n-1}(1 - \varepsilon(X_k^\mu))]$$

and (6.10) implies $P\{\tau^\mu < \infty\} = 1$.

Much of the work on Harris recurrence is done under weaker conditions of the form

$$\sum_{n=1}^{\infty} a_n P^n(x,\Gamma) \geq \varepsilon(x)\varphi(\Gamma),$$

where $a_n(x) \geq 0$, $\sum_{n=1}^{\infty} a_n(x) = 1$, or in continuous time,

$$\int_0^\infty P(t,x,\Gamma)a_x(dt) \geq \varepsilon(x)\varphi(\Gamma),$$

where a_x is a probability distribution on $(0,\infty)$, and typically, $\varepsilon(x)$ has the form $\varepsilon \mathbf{1}_C(x)$ for some constant $\varepsilon > 0$ and $C \in \mathcal{B}(E)$. The analog of Lemma 7 holds under these conditions, at least if (6.10) is replaced by

$$P\{\sum_{k=1}^{\infty} \varepsilon(X_k^\mu)^2 = \infty\} = 1 \text{ or } P\{\int_0^\infty \varepsilon(X^\mu(s))^2 ds = \infty\} = 1.$$

The existence of these stopping times implies the desired uniqueness of the stationary distribution and convergence in total variation of ν_n and ν_t.

Lemma 8. *Let $\varphi \in \mathcal{P}(E)$. Suppose that for each $\mu \in \mathcal{P}(E)$, on some probability space, there exists a process X^μ a filtration $\{\mathcal{F}_k^\mu\}$, and a $\{\mathcal{F}_k^\mu\}$-stopping time τ^μ such that X^μ is $\{\mathcal{F}_k^\mu\}$-Markov with initial distribution μ and transition function P and $X_{\tau^\mu}^\mu$ has distribution φ. Then there is at most one stationary distribution for P.*

If there is a stationary distribution π, then for each initial distribution $\mu \in \mathcal{P}(E)$, $\{\nu_n\}$ defined by (6.4) converges in total variation to π.

The analogous result holds in continuous time.

Proof. Suppose π_1 and π_2 are stationary distributions for P. Let X^{π_1} and X^{π_2} satisfy the hypotheses of the lemma. By the ergodic theorem, for each $h \in B(E)$, we can define

$$H_{\pi_i}^h = \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} h(X_k^{\pi_i}) = \lim_{n\to\infty} \frac{1}{n}\sum_{k=\tau^{\pi_i}}^{\tau^{\pi_i}+n-1} h(X_k^{\pi_i}) = \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} h(X_{\tau^{\pi_i}+k}^{\pi_i}).$$

By the strong Markov property, $H_{\pi_1}^h$ and $H_{\pi_2}^h$ must have the same distribution. Since $\pi_i h = E[H_{\pi_i}^h]$, $\pi_1 = \pi_2$.

Under the hypotheses of the lemma, for $h \in B(E)$ and $\mu \in \mathcal{P}(E)$,

$$|E[\frac{1}{n}\sum_{k=0}^{n-1} h(X_k^\mu)] - E[\frac{1}{n}\sum_{k=0}^{n-1} h(X_k^\varphi)]|] \leq \|h\|(P\{\tau^\mu > k\} + \frac{2k}{n}),$$

and hence

$$|E[\frac{1}{n}\sum_{k=0}^{n-1} h(X_k^\mu)] - \pi h| \leq \|h\|(P\{\tau^\mu > k\} + P\{\tau^\pi > k\} + \frac{4k}{n}), \tag{6.11}$$

and taking the sup over $h \in B(E)$ with $\|h\| \leq 1$ gives the convergence in total variation.

If τ^φ satisfies $0 < E[\tau^\varphi] < \infty$, then $\tau_1 = 0$ and $\tau_2 = \tau^\varphi$ provide an example of τ_1 and τ_2 in the following lemma.

Lemma 9. *Let X be $\{\mathcal{F}_k\}$-Markov with transition function P, and let τ_1 and τ_2 be stopping times satisfying $\tau_1 \leq \tau_2$ and $0 < E[\tau_2 - \tau_1] < \infty$ such that X_{τ_1} and X_{τ_2} have the same distribution. Then π defined by*

$$\pi h = \frac{E[\sum_{k=\tau_1+1}^{\tau_2} h(X_k)]}{E[\tau_2 - \tau_1]}$$

is a stationary distribution for P.

In continuous time,

$$\pi h = \frac{E[\int_{\tau_1}^{\tau_2} h(X(s))ds]}{E[\tau_2 - \tau_1]}.$$

Remark 3. In the case $0 < E[\tau^\varphi] < \infty$, this observation is essentially the renewal argument of [1] and [16].

Proof. Since

$$M_n = h(X_n) - h(X_0) - \sum_{k=0}^{n-1}(Ph(X_k) - h(X_k))$$

is a martingale,

$$0 = E[h(X_{\tau_2}) - h(X_{\tau_1})] = E[\sum_{k=\tau_1}^{\tau_2 - 1}(Ph(X_k) - h(X_k)),$$

and hence,

$$\pi P h = \pi h,$$

so π is a stationary distribution for P.

Example 2. In [6], Rabi and Mukul Majumdar consider processes in $E = (0,1)$ of the form

$$X_{n+1} = \xi_{n+1} X_n (1 - X_n),$$

where the $\{\xi_k\}$ are iid with values in $(0,4)$. Clearly, this process satisfies (6.1). Under the assumption that the distribution of ξ has an absolutely continuous part with a density that is strictly positive on some interval, they give conditions for Harris recurrence.

Example 3. The inequality in (6.11) and the analogous inequality in continuous time,

$$|E[\frac{1}{t}\int_0^t h(X^\mu(s))ds] - \pi h| \le \|h\|(P\{\tau^\mu > r\} + P\{\tau^\pi > r\} + \frac{4r}{t}), \tag{6.12}$$

actually give rates of convergence. Under aperiodicity assumptions, one can replace the average by $E[h(X^\mu(t))]$ and eliminate the $O(t^{-1})$ term. In [7], Rabi and Aramian Wasielak give conditions under which this can be done for a class of diffusion processes.

6.2.2 Conditions without Harris Recurrence

Harris recurrence is very useful when it holds, or perhaps more to the point, when it can be shown that it holds. In general, it does not hold, even in relatively simple settings. Perhaps the best known example is the "Markov process" in $[0,1)$ given by the recursion

$$X_{n+1} = X_n + z \bmod 1,$$

for some irrational z.

For an example with more interesting probabilistic structure, let $E = \{-1,1\}^\infty$, and consider a generator of the form

$$Af(x) = \sum_{k=1}^{\infty} \lambda_k (f(\eta_k x) - f(x)), \tag{6.13}$$

where $\lambda_k > 0$, $\sum_k \lambda_k < \infty$, and $\eta_k x$ is obtained by replacing x_k by $-x_k$. If $x, y \in E$ differ on infinitely many components, then $P(t,x,\cdot)$ and $P(t,y,\cdot)$ are mutually singular for all t, but for all $x \in E$, $P(t,x,\cdot)$ converges weakly to the distribution under which the components are independent symmetric Bernoulli.

In general, infinite dimensional processes provide a source of examples that are not Harris recurrent even if ergodic. We will not address any more examples of this type, but see [11] for recent work in this direction.

There is a need for techniques for studying ergodicity for processes that are not Harris recurrent. One approach that appears frequently in Rabi's work involves the notion of *splitting* and is discussed in the paper by Ed Waymire in this volume. A second approach considered by Rabi and Gopal Basak in [2] is by verifying *asymptotical flatness*, that is, by showing that X^x and X^y can be coupled in such a way that for each compact $K \subset E$ and $\varepsilon > 0$,

$$\lim_{t\to\infty} \sup_{x,y\in K} P\{|X^x(t) - X^y(t)| > \varepsilon\} = 0.$$

For example, if one rewrites the generator in (6.13) as

$$Af(x) = \sum_{k=1}^{\infty} 2\lambda_k(\frac{1}{2}f(\eta_k^1 x) + \frac{1}{2}f(\eta_k^{-1}x) - f(x)), \tag{6.14}$$

where $\eta_k^1 x$ is obtained from x by replacing x_k by 1 and $\eta_k^{-1}x$ is obtained by replacing x_k by -1, then the coupling can be obtained using independent Poisson processes $\{N_k\}$, N_k with intensity $2\lambda_k$, and at the lth jump of N_k replacing x_k by ξ_{kl}, where the $\{\xi_{kl}\}$ are independent symmetric Bernoulli.

Example 4. In [2], Rabi and Gopal Basak consider diffusions of the form

$$X^x(t) = x + \int_0^t BX^x(s)ds + \int_0^t \sigma(X^x(s))dW(s).$$

One has a natural coupling simply by using the same Brownian motion W for both X^x and X^y. Lyapunov-type arguments are again employed but with analytic estimates rather than simply compactness arguments. In particular, the arguments employ ψ (v in the notation of the paper) of the form

$$\psi(x) = (x \cdot Cx)^{1-\varepsilon},$$

for appropriately chosen positive definite C and $\varepsilon \in [0, 1)$. Different choices of C are applied to $\psi(X^x(t))$ to ensure the existence of a stationary distribution and to $\psi(X^x(t)-X^y(t))$ to give the asymptotic flatness.

6.3 Central Limit Theorems

There are many version of the martingale central limit theorem. See, for example, [15, 17, 12]. The following version is from Theorem 7.1.4 of [9].

Theorem 2. *Let $\{M_n\}$ be a sequence of cadlag, $\mathbb{R}^d$-valued martingales, with $M_n(0) = 0$, and let $A_n = [M_n]$ be the matrix of covariations, that is,*

$$A_n^{ij}(t) = [M_n^i, M_n^j]_t.$$

Suppose that for each $t \geq 0$,

$$\lim_{n\to\infty} E[\sup_{s\leq t} |M_n(s) - M_n(s-)|] = 0$$

and

$$\lim_{n\to\infty} A_n(t) = A(t),$$

where A is deterministic and continuous. Then $\{M_n\}$ converges in distribution to a Gaussian process M such that M has independent increments, $E[M(t)] = 0$, and $[M^i, M^j]_t = E[M^i(t)M^j(t)] = A^{ij}(t)$.

If

$$A(t) = \int_0^t \sigma(s)\sigma(s)^T ds,$$

for some $d \times m$-matrix-valued function σ, then we can write

$$M(t) = \int_0^t \sigma(s) dW(s),$$

where W is an $\mathbb{R}^m$-valued standard Brownian motion.

Example 5. Let π be an ergodic stationary distribution for a Markov semigroup $\{T(t)\}$. Then $\{T(t)\}$ extends to $L^2(\pi)$ and is strongly continuous on $L^2(\pi)$. Let A be the Hille-Yosida generator for the semigroup on $L^2(\pi)$. Then for each $f \in \mathcal{D}(A)$, the domain of A,

$$M^f(t) = f(X^\pi(t)) - f(X^\pi(0)) - \int_0^t Af(X^\pi(s))ds$$

is a square integrable martingale.

Then, for $h \in L^2(\pi)$, ergodicity implies

$$\lim_{n\to\infty} \frac{1}{n} \int_0^{nt} h(X^\pi(s))ds = \pi h t,$$

and Theorem 2.1 of [4] gives the functional central limit theorem for the scaled deviations,

$$Z_n^h(t) = \frac{1}{\sqrt{n}} \int_0^{nt} (h(X^\pi(s)) - \pi h)ds.$$

The key assumption is that there exists $f \in \mathcal{D}(A)$ such that $Af = h - \pi h$. Then

$$Z_n^h(t) = \frac{1}{\sqrt{n}}(f(X^\pi(nt)) - f(X^\pi(0))) - \frac{1}{\sqrt{n}} M^f(nt).$$

Consequently, we have the functional central limit theorem for $\{Z_n^h\}$ provided we can prove the functional central limit theorem for $\{\frac{1}{\sqrt{n}} M^f(n\cdot)\}$. Observe that the quadratic variation of $\frac{1}{\sqrt{n}} M^f(n\cdot)$ is the same as the quadratic variation for $U_n(t) = \frac{1}{\sqrt{n}} f(X^\pi(n\cdot))$ and that by Itô's formula,

$$\begin{aligned}[U_n]_t &= U_n(t)^2 - \frac{1}{n}\int_0^t 2f(X^\pi(ns-))df(X^\pi(ns)) \\ &= U_n(t)^2 - \frac{1}{n}\int_0^t 2f(X^\pi(ns-))dM^f(ns) - \int_0^t 2f(X^\pi(ns))Af(X^\pi(ns))ds \\ &\to -t\int_E 2f(x)Af(x)\pi(dx).\end{aligned} \tag{6.1}$$

By Theorem 2, the convergence of Z_n^h follows. Of course, under the assumptions of Lemma 8, the same result will hold for X^μ for all $\mu \in \mathcal{P}(E)$.

If f is smooth and X^π is an $\mathbb{R}^d$-valued diffusion,

$$X^\pi(t) = X^\pi(0) + \int_0^t \sigma(X(s))dW(s) + \int_0^t b(X(s))ds,$$

then

$$f(X^\pi(t)) = f(X^\pi(0)) + \int_0^t \nabla f(X^\pi(s))^T\sigma(X^\pi(s))dW(s) + R(t),$$

where R is continuous with finite variation, so we can also write

$$\begin{aligned}[U_n]_t &= \frac{1}{n}\int_0^{nt} \nabla f(X^\pi(s))^T\sigma(X^\pi(s))\sigma(X^\pi(s))\nabla f(X^\pi(s))ds \\ &\to \int_{\mathbb{R}^d} \nabla f(x)^T\sigma(x)\sigma(x)^T\nabla f(x)\pi(dx).\end{aligned} \tag{6.2}$$

Example 6. In [5], Rabi considers diffusions in $\mathbb{R}^d$ of the form

$$X(t) = X(0) + \int_0^t u_0 b(X(s))ds + \int_0^t \sigma(X(s))dW(s),$$

under the assumption that σ is the square root of a positive definite matrix and σ and b are periodic in the sense that

$$\sigma(x+z) = \sigma(x) \text{ and } b(x+z) = b(x) \quad z \in \mathbb{Z}^d.$$

At least under additional regularity assumptions on σ and b, $Y(t) = X(t) \bmod \mathbf{1}$, $\mathbf{1} \in \mathbb{Z}^d$, the vector with each component 1, is a Markov process in $[0,1)^d$ which has a unique, ergodic stationary distribution π. Then

$$\lim_{n\to\infty} \frac{1}{n}X(nt) = \lim_{t\to\infty}\frac{1}{n}\int_0^{nt} u_0 b(X(s))ds = \lim_{n\to\infty}\frac{1}{n}\int_0^{nt} u_0 b(Y(s))ds = u_0\bar{b}t,$$

where $\bar{b} = \pi b$. Rabi gives the corresponding central limit theorem showing the convergence of

$$V_n(t) = \frac{1}{\sqrt{n}}(X(nt) - nu_0\bar{b}t).$$

For simplicity, assume $X(0) = 0$. Setting

$$M_1^n(t) = \frac{1}{\sqrt{n}}(X(nt) - \int_0^{nt} u_0 b(Y(s))ds) = \frac{1}{\sqrt{n}} \int_0^{nt} \sigma(Y(s))dW(s),$$

the convergence of M_1^n follows from Theorem 2 and the ergodicity of Y.

Note that $V_n = M_1^n + Z^n$, where

$$Z^n(t) = \frac{1}{\sqrt{n}} u_0 \int_0^{nt} (b(Y(s)) - \bar{b})ds.$$

Then Z^n is of the form treated in [4], Example 5. Let $\hat{A}$ denote the generator for Y, which will satisfy $\hat{A}f(x \bmod \mathbf{1}) = Af(x)$, if f extends periodically to an element in the domain of A. Rabi shows the existence of a twice continuously differentiable g satisfying

$$\hat{A}g(y) = b(y) - \bar{b},$$

and setting

$$M_2^n(t) = \frac{u_0}{\sqrt{n}}(g(Y(nt)) - g(0) - \int_0^{nt} (b(Y(s)) - \bar{b})ds),$$

we have

$$V_n(t) = M_1^n(t) - M_2^n(t) + \frac{u_0}{\sqrt{n}}(g(Y(nt)) - g(0)).$$

Since

$$M_2^n(t) = \frac{u_0}{\sqrt{n}} \int_0^{nt} \nabla g(X(s))^T \sigma(X(s))dW(s) + R_n(t),$$

where R_n is continuous with finite variation,

$$[M_1^n - M_2^n]_t = \frac{1}{n} \int_0^{nt} (I - u_0 \nabla g(X(s))^T)\sigma(X(s))\sigma(X(s))^T (I - u_0 \nabla g(X(s)))ds.$$

Setting $a = \sigma\sigma^T$,

$$D = \int_{[0,1)^d} (I - u_0 \nabla g(y)^T) a(y)(I - u_0 \nabla g(y))\pi(dy),$$

and V_n converges in distribution to a mean zero Brownian motion with covariance matrix D. The form of D derived here differs from the form in [5], but compare (6.1) and (6.2).

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Chapter 7
Reprints: Part II

R.N. Bhattacharya and Coauthors

Criteria for recurrence and existence of invariant measures for multidimensional diffusions. The Annals of Probability. 6 (1978), 541–553. © 1978 Institute of Mathematical Statistics.

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7.1 "Criteria for recurrence and existence of invariant measures for multidimensional diffusions"

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CRITERIA FOR RECURRENCE AND EXISTENCE OF INVARIANT MEASURES FOR MULTIDIMENSIONAL DIFFUSIONS[1]

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Let $L = \frac{1}{2} \sum_{i,j=1}^{k} a_{ij}(x)(\partial^2/\partial x_i \partial x_j) + \sum_{i=1}^{k} b_i(x)(\partial/\partial x_i)$ be an elliptic operator such that $a_{ij}(\cdot)$ are continuous and $b_i(\cdot)$ are measurable and bounded on compacts. Criteria for transience, null recurrence, and positive recurrence of diffusions on R^k governed by L are derived in terms of the coefficients of L.

1. Introduction. The main objective of this article is to obtain criteria for transience, positive recurrence, and null recurrence of diffusions on R^k governed by elliptic operators $L = \frac{1}{2} \sum_{i,j=1}^{k} a_{ij}(x)(\partial^2/\partial x_i \partial x_j) + \sum_{i=1}^{k} b_i(x)(\partial/\partial x_i)$ in terms of the coefficients of L. The matrix $((a_{ij}(x)))$ is assumed to be nonsingular for each x; the functions $a_{ij}(\cdot)$ are continuous, and the functions $b_i(\cdot)$ are Borel measurable and bounded on compacts. For the case $k = 1$ complete characterizations are known (see, e.g., Mandl (1968)). For $k > 1$ important criteria were announced without proof by Khas'minskii (1960) in a supplement to his paper [3], under the hypothesis that the coefficients of L are thrice continuously differentiable. The first derivation of criteria for recurrence and transience analogous to Khas'minskii's is due to Friedman (1973), who assumed the coefficients to be Lipschitzian on compacts and to satisfy certain growth conditions at infinity. As far as we know there has not appeared in the literature any proof of Khas'minskii's criteria (or analogous ones) for positive and null recurrence. Since positive recurrence is essentially equivalent to the existence of a (unique) invariant probability measure determining the ergodic behavior of the diffusion (see, e.g., Khas'minskii (1960), Maruyama and Tanaka (1959)), such criteria are of importance. Theorem 3.5 provides a criterion for positive recurrence which implies the corresponding criterion of Khas'minskii (1960) (Theorem III of his Supplement). It also provides a criterion for null recurrence which is comparable to Khas'minskii's (when specialized to Khas'minskii's assumptions), although neither implies the other. We are unable to verify Khas'minskii's criterion for null recurrence. Theorem 3.3 is an improvement upon Friedman's criteria for transience and recurrence. The criteria derived in this article are exact if L is radial near infinity. Among other results we mention Theorem 3.2 establishing a dichotomy (into transience and recurrence) in the class of all diffusions considered here.

Throughout this article we assume $k \geqq 2$.

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2. Notation and preliminaries. This section is devoted to background material. Proofs are given only when results are not readily available in the desired form.

Let $L = \frac{1}{2}\sum_{i,j=1}^{k} a_{ij}(x)(\partial^2/\partial x_i\,\partial x_j) + \sum_{i=1}^{k} b_i(x)(\partial/\partial x_i)$ be an elliptic operator on R^k. More precisely, we assume

(A) The matrix $((a_{ij}(x)))$ is real symmetric and positive definite for each x in R^k, the functions $a_{ij}(\cdot)$ are continuous. The functions $b_i(\cdot)$ are real valued, Borel measurable and bounded on compacts.

For $N = 1, 2, \cdots, 1 \leqq i, j \leqq k$, define

$$\begin{aligned} a_{ij,N}(x) &= a_{ij}(x) \\ b_{i,N}(x) &= b_i(x) \qquad \text{if } |x| \leqq N, \end{aligned}$$

$$\begin{aligned} a_{ij,N}(x) &= a_{ij}(x_0) \\ b_{i,N}(x) &= b_i(x_0) \qquad \text{if } |x| = cx_0 \text{ for some } x_0,\ |x_0| = N, \\ &\qquad\qquad\quad \text{and some } c > 1. \end{aligned}$$

Let $L_N = \frac{1}{2}\sum_{i,j=1}^{k} a_{ij,N}(x)(\partial^2/\partial x_i\,\partial x_j) + \sum_{i=1}^{k} b_{i,N}(x)(\partial/\partial x_i)$.

For $A \subset R^k$, $\bar{A}$ denotes the *closure* of A and A^c denotes the *complement of* A. Also, ∂A denotes the *boundary of* A. The symbol $|x|$ stands for the *Euclidean norm of* x.

Denote the space $C([0, \infty): R^k)$ of all continuous functions on $[0, \infty)$ into R^k by Ω'. Endow Ω' with the topology of uniform convergence on compact subsets of $[0, \infty)$. Let $\mathscr{M}'$ denote the Borel sigma field of Ω'. Let $X(t) = X(t, \cdot)$ be the tth coordinate map: $X(t, \omega) = \omega(t)$ for $\omega \in \Omega'$. The sigma field generated by $\{X(s): 0 \leqq s \leqq t\}$ is denoted by $\mathscr{M}_t'$ $(0 \leqq t < \infty)$. A function τ on Ω' into $[0, \infty]$ is a *stopping time* if $\{\tau \leqq t\} \in \mathscr{M}_t'$ for all $t \geqq 0$. If τ is a stopping time then the map X_τ^- on Ω' into Ω' defined by

$$X_\tau^-(t) = X(\tau \wedge t) \qquad t \geqq 0$$

is measurable and is called the *process stopped at* τ. The *pre-τ sigma field* $\mathscr{M}_\tau'$ is generated by $\{X(\tau \cap t): t \geqq 0\}$. Also measurable on the restriction of $(\Omega', \mathscr{M}')$ to $\{\tau < \infty\}$ is the map X_τ^+ defined by

$$X_\tau^+(t) = X(\tau + t) \qquad t \geqq 0.$$

Let $\{P_x: x \in R^k\}$ be a family of probability measures on $(\Omega', \mathscr{M}')$ such that for every a.s. (P_x) finite stopping time τ a regular conditional distribution of X_τ^+ given $\mathscr{M}_\tau'$ is $P_{X(\tau)}$. We then say that X is a *strong Markov process* under P_x. Such a process is said to be *strong Feller* if for every bounded real measurable function f on R^k the function: $x \to E_x f(X(t))$ is continuous on R^k for each $t > 0$. Here E_x denotes *expectation under* P_x. The following result due to Stroock and Varadhan ([7]—[9]) will be frequently used in this article.

THEOREM 2.1. *If, in addition to the hypothesis* (A), $a_{ij}(\cdot)$ *and* $b_i(\cdot)$ *are bounded on* R^k, *then for each* x *in* R^k *there exists a unique probability measure* P_x *on* $(\Omega', \mathscr{M}')$

such that (i) $P_x(X(0) = x) = 1$, (ii) *for every bounded real f on R^k having bounded and continuous first and second order derivatives, the process*

$$f(X(t)) - \int_0^t Lf(X(s))\,ds \qquad t \geqq 0$$

is a martingale under P_x. Further, (a) *X is strong Markov and strong Feller, and* (b) *support of P_x* is $\Omega_x' = \{\omega \in \Omega' : \omega(0) = x\}$.

Let $P_{x,N}$ denote the probability measure in Theorem 2.1 with $L = L_N$.

The following simple result will also be needed. For any set A, χ_A is the *indicator function* of A.

LEMMA 2.2. *Let U be a nonempty bounded open subset of R^k. Let*

$$\tau_U = \inf\{t \geqq 0 : X(t) \notin U\}\,. \tag{2.1}$$

Under the hypothesis of Theorem 2.1, *for every bounded real Borel measurable function f on U, the function $E_x(\chi_{\{\tau_U > t\}} f(X(t)))$ is continuous on U. If ϕ is a real valued bounded measurable function on ∂U, then the function $E_x(\phi(X(\tau_U)))$ is continuous on U.*

PROOF. The first assertion is proved in Dynkin (1965) (Volume II, page 30, relation (13.4)). It is of course necessary to check Dynkin's hypothesis that

$$\lim_{t\downarrow 0} \sup_{x \in D} P_x(|X(t) - x| > \varepsilon) = 0 \tag{2.2}$$

for every compact subset D of U.

But (2.1) follows from the inequality (see Stroock and Varadhan (1969), page 355)

$$\sup_{x \in R^k} P_x(|X(t) - x| > \varepsilon) \leqq 2k \exp\{-(\varepsilon - \beta t)^2/2\alpha t\} \qquad \varepsilon > 0,\ t > 0 \tag{2.3}$$

where β^2 is an upper bound of $\sum b_i^2(x)$ for all x, and α is an upper bound for the largest eigenvalue of $((a_{ij}(x)))$, $x \in R^k$. To prove the second assertion define $\tilde{\phi}$ on $\bar{U}$ by letting $\tilde{\phi} = \phi$ on ∂U and $\tilde{\phi} = c$ on U where $c \leqq \phi(x)$ for all x in ∂U. Then, according to Dynkin (1965) (Volume II, page 30, relation (13.5)), the function $h_t(x) \equiv E_x\tilde{\phi}(X(\tau_U \wedge t))$ is continuous on U for every $t > 0$. Letting $t \uparrow \infty$, one has $h_t(x) \uparrow \phi(x)$. Hence ϕ is lower semicontinuous. Similarly, $-\phi$ is lower semicontinuous. □

To construct probability measures P_x under the hypothesis (A) replace the "state space" R^k by its *one point compactification* $R^k \cup \{\infty\}$. Let $\Omega = C([0, \infty) : R^k \cup \{\infty\})$ be the set of all continuous functions on $[0, \infty)$ into $R^k \cup \{\infty\}$ and endow Ω with the topology of uniform convergence (relative to some metric metrizing $R^k \cup \{\infty\}$) on compact subsets of $[0, \infty)$. Let $\mathscr{M}$ be the Borel sigma field of Ω. We continue to denote by $X(t)$ the tth *coordinate map* (this time on Ω into $R^k \cup \{\infty\}$). Also, $\mathscr{M}_t$ will denote the sigma field generated by $\{X(s) : 0 \leqq s \leqq t\}$, and $\mathscr{M}_\tau$ will denote the *pre-τ sigma field* for any stopping time τ (relative to $\mathscr{M}_t$, $t \geqq 0$) on Ω. Denote by P_∞ the *probability measure degenerate at ω_∞* where $\omega_\infty(t) = \infty$ for all $t \geqq 0$. For $x \neq \infty$, one way to construct P_x is to introduce the product probability space $(E, \mathscr{E}, \mu)$, where E is the Cartesian product $\times_{x,N} \Omega'_{x,N}$ (each $\Omega'_{x,N}$ being a copy of Ω'), $\mathscr{E}$ is the product sigma field, and μ is the product probability $\times_{x,N} P_{x,N}$. If x_0, N_0 are such that $|x_0| < N_0$, define a map Y on E into Ω by requiring that $Y(t) = X_{x_0,N_0}(t)$ (here $X_{x,N}(t)$ is the tth coordinate map on $\Omega'_{x,N}$) for $t \leqq \eta_1 \equiv \inf\{s \geqq 0 : |X_{x_0,N_0}(s)| = N_0\}$, $Y(t) = X_{X(\eta_i),N_0+i}(t)$ for $\eta_i < t \leqq \eta_{i+1}$, where $\eta_{i+1} - \eta_i = \inf\{s \geqq 0 : X_{X(\eta_i),N_0+i}(s)| = N_0 + i\}$; let $\eta_\infty = \lim_{i\uparrow\infty} \eta_i$ and define $Y(t) = \infty$ for $\eta_\infty \leqq t < \infty$. We denote by P_{x_0} the probability measure on $(\Omega, \mathscr{M})$ induced by Y, i.e., $P_{x_0} = \mu \circ Y^{-1}$. It is simple to check from this construction that the *coordinate process* $X = \{X(t) : 0 \leqq t < \infty\}$ on Ω *is a strong Markov process under* P_x, $x \in R^k \cup \{\infty\}$.

On Ω define the stopping times τ_U for open subsets U of R^k as in (2.1), and define the *explosion time* ζ by

$$\zeta = \lim_{N\uparrow\infty} \tau_{B(0:N)} \tag{2.4}$$

where $B(0 : N) = \{x \in R^k : |x| < N\}$. The probability measure P_x $(x \in R^k)$ is said to be *conservative* if $P_x(\zeta = \infty) = 1$. A Borel measurable real valued function f on R^k will be said to be *L-harmonic* on an open subset G of R^k if it is bounded on compacts, and for all x in G

$$f(x) = E_x f(X(\tau_U)) \tag{2.5}$$

for every neighborhood U of x having compact closure $\bar{U}$ in G. It may be remarked at this stage that the notation P_x, E_x used here is consistent with that used earlier. For it follows immediately from the construction that under the hypothesis of Theorem 2.1 the present P_x has support Ω_x' and coincides with the corresponding P_x in Theorem 2.1 on Ω_x'. Also, if (A) holds, then for $|x| < N$ the present measure P_x agrees with the earlier $P_{x,N}$ on $\mathscr{M}_{\tau_{B(0:N)}}$ (i.e., on the trace of this sigma field on Ω_x'). From now on we regard all measures P_x, $P_{x,N}$ to be defined on $(\Omega, \mathscr{M})$, and E_x, $E_{x,N}$ are corresponding expectations.

Part (a) of the following lemma may also be obtained from Dynkin (1965), Volume II, Theorem 13.2, page 31.

LEMMA 2.3. *Assume* (A) *holds.* (a) *Every L-harmonic function on an open subset G of R^k is continuous in G.* (b) *(Maximum principle.) Let f be a nonnegative L-harmonic function on a connected open subset G of R^k. Then f is either strictly positive or identically zero.*

PROOF. (a) If f is L-harmonic in G, $x \in G$, and U is a neighborhood of x such that the closure $\bar{U}$ of U is compact in G, then

$$f(x) = E_x f(X(\tau_U)) = E_{x,N} f(X(\tau_U)) , \tag{2.6}$$

provided $U \subset B(0 : N)$. By Lemma 2.2 the last expression in (2.6) is continuous in U.

(b) Suppose $f(x_0) = 0$. Let $B = B(x_0 : \varepsilon)$ be the open ball with center x_0 and radius ε such that $\bar{B} \subset G$. Then

$$0 = f(x_0) = E_{x_0} f(X(\tau_B)) = \int_{\partial B} f(y) \Pi(x_0, dy) ,$$

where $\Pi(x_0, dy)$ is the distribution of $X(\tau_B)$ under P_{x_0} and, hence, under $P_{x_0,N}$ if $N > |x_0| + \varepsilon$. By Theorem 2.1 the support of $\Pi(x_0, dy)$ is ∂B. Since $f \geqq 0$ and continuous it follows that $f \equiv 0$ on ∂B. Therefore, $f \equiv 0$ on G. □

LEMMA 2.4. *Assume* (A) *holds.* (a) *If U is a nonempty open subset of R^k, $U \neq R^k$, then $x \to P_x(\tau_U < \infty)$ is positive and continuous on U.* (b) *If U_1, U_2 are two nonempty open subsets of R^k such that $\bar{U}_1 \cap \bar{U}_2 = \phi$, $\bar{U}_2{}^c = R^k \backslash \bar{U}_2$ is connected, then $x \to P_x(\tau_{\bar{U}_1^c} < \tau_{\bar{U}_2^c})$ is positive and continuous on $\bar{U}_1{}^c \cap \bar{U}_2{}^c$.*

PROOF. It follows from the strong Markov property that both the functions in question are L-harmonic and, therefore, continuous. To prove positivity in (b) (which implies positivity in (a)) let $x \in \bar{U}_1{}^c \cap \bar{U}_2{}^c$. Take an open ball $B \subset U_1$ and let B_1 be a bounded open set such that $x \in B_1$, $B \subset B_1 \subset \{|x| < N\}$, $B_1 \cap \bar{U}_2 = \phi$. Then $P_x(\tau_{\bar{U}_1^c} < \tau_{\bar{U}_2^c}) \geqq P_x(\tau_{\bar{B}^c} < \tau_{\bar{B}_1^c}) = P_{x,N}(\tau_{\bar{B}^c} < \tau_{\bar{B}_1^c})$. The last expression is positive, since the support of $P_{x,N}$ is Ω_x'. □

LEMMA 2.5. *Assume* (A) *holds. If P_{x_0} is conservative for some $x_0 \in R^k$, then P_x is conservative for all $x \in R^k$ and the process $\{X(t): t \geqq 0\}$ has the strong Feller property.*

PROOF. Since $x \to P_x(\zeta < \infty)$ is harmonic, the first assertion follows. To prove the second let f be a real valued bounded Borel measurable function on R^k. Assume P_x is conservative for all $x \in R^k$. Fix x_0 in R^k. One has

$$\begin{aligned}(2.7)\qquad |E_x f(X(t)) - E_{x,N} f(X(t))| &= |\textstyle\int \chi_{\{\tau_{B(0:N)} \leqq t\}} f(X(t))[P_x(d\omega) - P_{x,N}(d\omega)]| \\ &\leqq 2\|f\|[1 - P_{x,N}(\tau_{B(0:N)} > t)] \qquad t > 0\,,\end{aligned}$$

where $\|f\| = \sup |f(x)|$. Choose $\varepsilon > 0$ and fix N such that the last expression in (2.7) is less than $\varepsilon/3$ if $x = x_0$. Since $x \to P_{x,N}(\tau_{B(0:N)} > t)$ is continuous on R^k (by Lemma 2.2), and $x \to E_{x,N} f(X(t))$ is continuous (since X is strongly Feller under $P_{x,N}$, $x \in R^k$), there exists $\delta > 0$ such that if $|x - x_0| < \delta$, then

$$\begin{aligned}|E_x f(X(t)) - E_{x_0} f(X(t))| &\leqq 2\|f\|[1 - P_{x,N}(\tau_{B(0:N)} > t) + 1 - P_{x_0,N}(\tau_{B(0:N)} > t)] \\ &\quad + |E_{x,N} f(X(t)) - E_{x_0,N} f(X(t))| < \varepsilon\,. \qquad \square\end{aligned}$$

LEMMA 2.6. *Assume* (A) *holds, U is a bounded open subset of R^k. Then $\sup_{x \in U} E_x(\tau_U) < \infty$.*

PROOF. Let N be such that $B(0: N) \supset \bar{U}$. Then $E_x \tau_U = E_{x,N} \tau_U$ for $x \in U$. Fix $t_0 > 0$. Since $\Omega_x' = \{\omega \in \Omega' : \omega(0) = x\}$ is the support of $P_{x,N}$, $P_{x,N}(\tau_U > t_0) \leqq P_{x,N}(|X(t_0)| < N) < 1$ for all $x \in \bar{U}$. Since $x \to P_{x,N}(|X(t_0)| < N)$ is continuous, $\sup_{x \in \bar{U}} P_{x,N}(\tau_U > t_0) < 1$. Now use the inequality (see, e.g., Dynkin (1965), Volume I, Lemma 4.3, page 111)

$$E_{x,N} \tau_U \leqq \frac{t_0}{1 - \sup_{x \in U} P_{x,N}(\tau_u > t_0)}\,. \qquad \square$$

Finally, a nonzero measure m on the Borel sigma-field $\mathscr{B}^k$ of R^k is said to be *invariant* for the Markov process P_x, $x \in R^k$, if for all $B \in \mathscr{B}^k$ and all $t > 0$,

$$(2.10)\qquad m(B) = \textstyle\int_{R^k} P_x(\{X(t) \in B\}) m(dx)\,.$$

We shall henceforth refer to P_x, $x \in R^k$, or to the coordinate process under P_x, $x \in R^k$, *as the diffusion with generator L.*

3. Criteria for recurrence and transience. Assume (A) holds, and consider the diffusion X (under P_x, $x \in R^k$) with generator L. *A point x in R^k is said to be recurrent* for this diffusion if given any $\varepsilon > 0$

$$P_x(X(t) \in B(x:\varepsilon) \text{ for a sequence of } t\text{'s increasing to infinity}) = 1 , \tag{3.1}$$

where $B(x:\varepsilon) = \{y: |y - x| < \varepsilon\}$. It follows that x is a recurrent point if and only if for every $\varepsilon > 0$ and every a.s. (P_x) finite random variable τ

$$P_x(X(t) \in B(x:\varepsilon) \text{ for some } t > \tau) = 1 . \tag{3.2}$$

A point x is transient if

$$P_x(|X(t)| \to \infty \text{ as } t \to \infty) = 1 . \tag{3.3}$$

If all points of a diffusion are recurrent, the *diffusion itself is called recurrent.* If all points of a diffusion are transient, the *diffusion is called transient.* It will be presently shown (see Theorem 3.2) that if (A) holds every diffusion is either recurrent or transient. Since different authors often use different definitions of recurrence and transience (see, e.g., Maruyama and Tanaka (1959), Khas'minskii (1960), and Friedman (1973)), it is useful to show that these definitons are equivalent.

PROPOSITION 3.1. *Assume that* (A) *holds. The following statements are equivalent.*

(a) *The diffusion is recurrent.*

(b) $P_x(X(t) \in U$ *for some* $t \geqq 0) = 1$ *for all* $x \in R^k$ *and all nonempty open* U.

(c) *There exists a compact set* K *of* R^k *such that* $P_x(X(t) \in K$ *for some* $t \geqq 0) = 1$ *for all* $x \in R^k$.

(d) $P_x(X(t) \in U$ *for a sequence of t's increasing to infinity*$) = 1$ *for all* $x \in R^k$ *and all nonempty open* U.

(e) *There exist a point z in* R^k, *a pair of numbers* r_0, r_1, $0 < r_0 < r_1$, *and a point* $y \in \partial B(z:r_1) = \{y': |y' - z| = r_1\}$ *such that* $P_y(\tau_{\bar{B}^c(z:r_0)} < \infty) = 1$.

PROOF. The implications (b) $\Rightarrow$ (c), (b) $\Rightarrow$ (e), (d) $\Rightarrow$ (a), are obvious. We prove (a) $\Rightarrow$ (b), (b) $\Rightarrow$ (d), (c) $\Rightarrow$ (b), (e) $\Rightarrow$ (c).

(a) $\Rightarrow$ (b). Assume (a), $x \in R^k$, U nonempty open, $x \notin U$. Let B be an open ball such that $\bar{B} \subset U$. Choose $\varepsilon > 0$ such that $\overline{B(x:\varepsilon)} \cap \bar{B} = \phi$. Let U_1 be a bounded open set containing $\overline{B(x:\varepsilon)} \cup \bar{B}$. Define $\eta_1 = \tau_{U_1}$, $\eta_{2i} = \inf\{t > \eta_{2i-1}: X(t) \in \partial B(x:\varepsilon)\}$, $\eta_{2i+1} = \inf\{t > \eta_{2i}: X(t) \in \partial U_1\}$ $(i = 1, 2, \cdots)$. By Lemma 2.6 and recurrence of x, η_i's are a.s. (P_x) finite stopping times. Consider the events $A_0 = \{X(t) \in \bar{B} \text{ for some } t \in [0, \eta_1)\}$, $A_i = \{X(t) \in \bar{B} \text{ for some } t \in [\eta_{2i-1}, \eta_{2i})\}$ $(i = 1, 2, \cdots)$. Since $y \to P_y(\tau_{\bar{B}^c} < \tau_{\overline{B(x:\varepsilon)}^c})$ is positive and continuous on $\bar{B}^c \cap \overline{B(x:\varepsilon)}^c$ (Lemma 2.4(b)).

$$\delta \equiv \inf\nolimits_{y \in \partial U_1} P_y(\tau_{\bar{B}^c} < \tau_{\overline{B(x:\varepsilon)}^c}) > 0 . \tag{3.4}$$

Using the strong Markov property and induction on n one obtains $P_x(\bigcap_{i=0}^n A_i^c) \leqq (1-\delta)^n$. Thus

$$(3.5)\qquad P_x(X(t) \in U \text{ for no } t \geqq 0) \leqq P_x(X(t) \in \bar{B} \text{ for no } t \geqq 0) \leqq \lim_{n\to\infty} P_x(\textstyle\bigcap_{i=0}^n A_i^c) = 0 .$$

(b) $\Rightarrow$ (d). Let $x \in R^k$, U nonempty open, B an open ball and $\varepsilon > 0$ such that $\bar{B} \cap \overline{B(x:\varepsilon)} = \phi$ and $\bar{B} \subset U$. Define $\theta_1 = \inf\{t \geqq 0 : X(t) \in \partial B(x:\varepsilon)\}$, $\theta_{2i} = \inf\{t > \theta_{2i-1} : X(t) \in \partial B\}$, $\theta_{2i+1} = \inf\{t > \theta_{2i} : X(t) \in \partial B(x:\varepsilon)\}$ $(i = 1, 2, \cdots)$. By (b) and the strong Markov property, θ_i's are a.s. (P_x) finite. Also, $\theta_i \uparrow \infty$ a.s. (P_x) as $i \uparrow \infty$; otherwise, with positive P_x probability the sequences $\{X(\theta_{2i-1}) : i = 1, 2, \cdots\}$ and $\{X(\theta_{2i}) : i = 1, 2, \cdots\}$ converge to a common limit, which is impossible since $\partial B(x:\varepsilon)$ and ∂B are disjoint.

(c) $\Rightarrow$ (b). Let K be as in (c), B an arbitrary open ball, $x \in R^k$. Let U be an open ball containing $\bar{B} \cup K$. Define $\eta_1' = \tau_{K^c}$, $\eta_{2i}' = \inf\{t > \eta_{2i-1}' : X(t) \in \partial U\}$, $\eta_{2i+1}' = \inf\{t > \eta_{2i}' : X(t) \in K\}$ $(i = 1, 2, \cdots)$. By (c), the strong Markov property and Lemma 2.6, the η_i''s are a.s. (P_x) finite. Now proceed as in the proof of (a) $\Rightarrow$ (b), i.e., define A_i's with η_i''s in place of η_i's, and define $\delta = \inf_{y\in K} P_y(A_1)$; by Lemma 2.4 (b), $\delta > 0$; and $P_x(X(t) \in \bar{B} \text{ for no } t \geqq 0) \leqq P_x(\bigcap_{i=1}^n A_i^c) \leqq (1-\delta)^n$ for all n.

(e) $\Rightarrow$ (c). Follows from Lemma 2.4 (a) and the maximum principle (Lemma 2.3 (b)), if one takes $K = \overline{B(z:r_0)}$. □

The next result establishes a dichotomy in the class of all diffusions for which (A) holds.

THEOREM 3.2. *Assume* (A) *holds.* (a) *If there exists a recurrent point, then the diffusion is recurrent.* (b) *If there exists no recurrent point, then the diffusion is transient.*

PROOF. (a) Suppose y is a recurrent point. Choose r_0, r_1 $(0 < r_0 < r_1)$, z such that $|y - z| = r_1$. It has been shown in the course of the proof of Proposition 3.1 ((a) $\Rightarrow$ (b), (3.5)) that $P_y(X(t) \in \partial B(z:r_0) \text{ for some } t \geqq 0) = P_y(X(t) \in \overline{B(z:r_0)} \text{ for some } t \geqq 0) = 1$. By Proposition 3.1 (e), the diffusion is recurrent.

(b) Suppose no point in R^k is recurrent. Fix $x \in R^k$. Let r be an arbitrary positive number such that $r > |x|$. By Proposition 3.1 (e) and the maximum principle (Lemma 2.3 (b)), for each $r_1 > r$ one has

$$\delta_{r_1} \equiv \sup_{|y|=r_1} P_y(\tau_{\overline{B(0:r)}^c} < \infty) < 1 .$$

Define $\eta_1 = \inf\{t \geqq 0 : X(t) \in \partial B(0:r_1)\}$, $\eta_{2i} = \inf\{t > \eta_{2i-1} : X(t) \in \overline{B(0:r)}\}$, $\eta_{2i+1} = \inf\{t > \eta_{2i} : X(t) \in \partial B(0:r_1)\}$ $(i = 1, 2, \cdots)$. By Lemma 2.6 and the strong Markov property, for all $i \geqq 1$

$$(3.6)\qquad \begin{aligned} &P_x(X(t) \in \overline{B(0:r)} \text{ for some sequence of } t\text{'s increasing to infinity}) \\ &\leqq P_x(\eta_{2i+1} < \infty) = E_x(\chi_{\{\eta_{2i-1}<\infty\}} P_{X(\eta_{2i-1})}(\tau_{\overline{B(0:r)}^c} < \infty)) \\ &\leqq \delta_{r_1} P_x(\eta_{2i-1} < \infty) \leqq \cdots \leqq \delta_{r_1}^i . \end{aligned}$$

Hence the left side of (3.6) is zero and

$$P_x(\liminf_{t\to\infty} |X(t)| > r) = 1 .$$

Since this holds for all $r > 0$, the proof is complete. □

The next theorem improves and extends a result of Friedman (1973). The criteria for recurrence and transience derived in Theorem 3.3 were announced without proof earlier by Khas'minskii (1960) (Theorem II of his Supplement) under the additional assumption that the coefficients of L are thrice continuously differentiable. To prove it we introduce some notation.

Let F be a real-valued twice continuously differentiable function on $(0, \infty)$. Let $z \in R^k$. Consider the function

$$f(x) = F(|x - z|) \qquad x \in R^k , \quad |x - z| > 0 . \tag{3.7}$$

A straightforward differentiation yields

$$\begin{aligned} \frac{\partial f(x)}{\partial x_i} &= \frac{(x_i - z_i)}{|x - z|} F'(|x - z|) , \\ \frac{\partial^2 f(x)}{\partial x_i^2} &= \frac{(x_i - z_i)^2}{|x - z|^2} F''(|x - z|) - \frac{(x_i - z_i)^2}{|x - z|^3} F'(|x - z|) + \frac{F'(|x - z|)}{|x - z|} , \\ \frac{\partial^2 f(x)}{\partial x_i \partial x_j} &= \frac{(x_i - z_i)(x_j - z_j)}{|x - z|^2} F''(|x - z|) - \frac{(x_i - z_i)(x_j - z_j)}{|x - z|^3} F'(|x - z|) \\ & \qquad i \neq j,\ |x - z| > 0 . \end{aligned} \tag{3.8}$$

Now fix $r_0 > 0$ and write $x' = x - z$ and

$$\begin{aligned} &A_z(x) = \textstyle\sum_{i,j=1}^k a_{ij}(x' + z) x_i' x_j' / |x'|^2 , \qquad B(x) = \textstyle\sum_{i=1}^k a_{ii}(x' + z) , \\ &C_z(x) = 2 \textstyle\sum_{i=1}^k x_i' b_i(x' + z) , \qquad \bar{\beta}_z(r) = \sup_{|x'|=r} \frac{B(x) - A_z(x) + C_z(x)}{A_z(x)} , \\ &\underline{\beta}_z(r) = \inf_{|x'|=r} \frac{B(x) - A_z(x) + C_z(x)}{A_z(x)} , \qquad \bar{\alpha}_z(r) = \sup_{|x'|=r} A_z(x) , \\ &\underline{\alpha}_z(r) = \inf_{|x'|=r} A_z(x) , \qquad \bar{I}_z(r) = \int_{r_0}^r \frac{\bar{\beta}_z(u)}{u} du , \qquad \underline{I}_z(r) = \int_{r_0}^r \frac{\underline{\beta}_z(u)}{u} du . \end{aligned} \tag{3.9}$$

It is easy to check that

$$2Lf(x) = A_z(x) F''(|x - z|) + \frac{F'(|x - z|)}{|x - z|} [B(x) - A_z(x) + C_z(x)] . \tag{3.10}$$

THEOREM 3.3. *Assume* (A) *holds.* (a) *If for some* $r_0 > 0$ *and* z

$$\int_{r_0}^\infty \exp\{-\bar{I}_z(r)\}\, dr = \infty , \tag{3.11}$$

then the diffusion with generator L is recurrent. (b) *If for some* $r_0 > 0$ *and* z

$$\int_{r_0}^\infty \exp\{-\underline{I}_z(r)\}\, dr < \infty , \tag{3.12}$$

then the diffusion with generator L is transient.

PROOF. (a) Assume (3.11) holds. Define

$$(3.13)\qquad F(r) = -\int_{r_0}^{r} \exp\{-\bar{I}_z(u)\}\, du\,, \qquad f(x) = F(|x-z|) \qquad |x-z| \geqq r_0\,.$$

Let x be such that $r \equiv |x-z| > r_0$. Define stopping times

$$(3.14)\qquad \eta = \inf\{t \geqq 0: X(t) \in \partial B(z: r_0)\}\,, \qquad \eta_N = \eta \wedge \tau_{B(z:N)}\,.$$

By Theorem 2.1, and optional sampling (see Nevue (1965), page 142), $f(X(t \wedge \eta_N)) - \int_0^{t\wedge\eta_N} Lf(X(s))\, ds$ $(t \geqq 0)$ is a P_x-martingale, provided $|x-z| < N$. Hence, for $r \equiv |x-z| > r_0$,

$$(3.15)\qquad \begin{aligned} &2E_x F(|X(t \wedge \eta_N) - z|) - 2F(r) \\ &= E_x \int_0^{t\wedge\eta_N} 2Lf(X(s))\, ds \\ &\geqq E_x \int_0^{t\wedge\eta_N} A_z(X(s)) \left[F''(|X(s)-z|) + \frac{F'(|X(s)-z|)}{|X(s)-z|}\bar{\beta}_z(|X(s)-z|)\right] ds \\ &= 0\,, \end{aligned}$$

by the relations

$$(3.16)\qquad F'(u) \leqq 0\,, \qquad F''(u) + \frac{1}{u}F'(u)\bar{\beta}_z(u) = 0 \qquad u \geqq r_0\,.$$

Letting $t \uparrow \infty$ in (3.15) and remembering that $\eta_N < \infty$ a.s. (P_x), one obtains

$$(3.17)\qquad -E_x F(|X(\eta_N) - z|) \leqq -F(r) = \int_{r_0}^{r} \exp\{-\bar{I}_z(u)\}\, du\,.$$

On evaluating the left side of (3.17) one has

$$(3.18)\qquad P_x(\eta > \tau_{B(z:N)}) \int_{r_0}^{N} \exp\{-\bar{I}_z(u)\}\, du \leqq \int_{r_0}^{r} \exp\{-\bar{I}_z(u)\}\, du\,.$$

Letting $N \uparrow \infty$ one gets

$$(3.19)\qquad P_x(\eta = \infty) \leqq \lim_{N\uparrow\infty} \frac{\int_{r_0}^{r} \exp\{-\bar{I}_z(u)\}\, du}{\int_{r_0}^{N} \exp\{-\bar{I}_z(u)\}\, du} = 0\,.$$

Hence $P_x(\eta < \infty) = 1$ and the diffusion is recurrent by Proposition 3.1 (e).

(b) Assume (3.12) holds. Define

$$G(r) = \int_{r_0}^{r} \exp\{-\underline{I}_z(u)\}\, du\,, \qquad g(x) = G(|x-z|) \qquad |x-z| \geqq r_0\,.$$

Since $G'(u) \geqq 0$ and $G''(u) + (1/u)G'(u)\underline{\beta}_z(u) = 0$ for $u \geqq r_0$, one obtains, as above,

$$(3.20)\qquad E_x G(|X(\eta_N) - z|) - G(|x-z|) \geqq 0$$

or,

$$(3.21)\qquad P_x(\eta > \tau_{B(z:N)}) \int_{r_0}^{N} \exp\{-\underline{I}_z(u)\}\, du \geqq \int_{r_0}^{|x-z|} \exp\{-\underline{I}_z(u)\}\, du\,.$$

Hence, letting $N \uparrow \infty$,

$$(3.22)\qquad P_x(\eta = \infty) \geqq \int_{r_0}^{|x-z|} \exp\{-\underline{I}_z(u)\}\, du \Big/ \int_{r_0}^{\infty} \exp\{-\underline{I}_z(u)\}\, du > 0\,.$$

Hence the diffusion is not recurrent (by Proposition 3.1) and therefore, it is transient (by Theorem 3.2). □

A recurrent diffusion admits a unique (up to a constant multiple) sigma finite invariant measure. This fact was proved by Maruyama and Tanaka (1959) in a more abstract setting and by Khas'minskii (1960). Khas'minskii's proof applies immediately to the present context. The following fact, which is easily deduced from Theorem 3.3 of Khas'minskii (1960) in conjunction with Lemma 2.6 and Proposition 3.1, will be needed.

LEMMA 3.4. *Assume* (A) *holds.* (a) *The diffusion is recurrent and admits a finite invariant measure if there exists* z *in* R^k *such that*

$$\sup_{y\in\partial B(z:r_1)} E_y(\tau_{\overline{B(z:r_0)}^c}) < \infty \tag{3.23}$$

for some r_0, r_1 *satisfying* $0 < r_0 < r_1$. (b) *If there exist some* z *in* R^k *and positive numbers* r_0, r_1 $(0 < r_0 < r_1)$ *satisfying*

$$E_y(\tau_{\overline{B(z:r_0)}^c}) = \infty \tag{3.24}$$

for all $y \in \partial B(z: r_1)$, *then there does not exist a finite invariant measure.*

Our final result is

THEOREM 3.5. *Assume* (A) *holds.* (a) *The diffusion with generator* L *is recurrent and admits a finite invariant measure* (*unique up to a constant multiple*) *if there exists* z *in* R^k *and* $r_0 > 0$ *such that*

$$\int_{r_0}^{\infty} \exp\{-\bar{I}_z(u)\}\,du = \infty\,, \tag{3.25}$$

$$\int_{r_0}^{\infty} \frac{1}{\underline{\alpha}_z(u)} \exp\{\bar{I}_z(u)\}\,du < \infty\,. \tag{3.26}$$

(b) *If there exist* z *in* R^k *and* $r_0 > 0$ *such that* (3.25) *holds and*

$$\lim_{N\to\infty} \frac{\int_{r_0}^{N} \exp\{-\bar{I}_z(s)\}(\int_{r_0}^{s} [\exp\{\bar{I}_z(u)\}/\bar{\alpha}_z(u)]\,du)\,ds}{\int_{r_0}^{N} \exp\{-\underline{I}_z(u)\}\,du} = \infty\,, \tag{3.27}$$

then the recurrent diffusion does not admit a finite invariant measure.

PROOF. (a) Assume (3.25), (3.26). Define

$$F(r) = -\int_{r_0}^{r} \exp\{-\bar{I}_z(s)\} \left(\int_s^{\infty} \frac{1}{\underline{\alpha}_z(u)} \exp\{\bar{I}_z(u)\}\,du\right) ds \qquad r > r_0\,. \tag{3.28}$$

Then

$$F'(r) = -\exp\{-\bar{I}_z(r)\} \int_r^{\infty} \frac{1}{\underline{\alpha}_z(u)} \exp\{\bar{I}_z(u)\}\,du < 0\,, \tag{3.29}$$

$$F''(r) = -\frac{\bar{\beta}_z(r)}{r} F'(r) + \frac{1}{\underline{\alpha}_z(r)} \qquad r \geqq r_0\,.$$

Let

$$f(x) = F(|x - z|) \qquad |x - z| \geqq r_0\,.$$

Then, using (3.29),

$$2Lf(x) \geqq A_z(x)/\underline{\alpha}_z(|x - z|) \geqq 1 \qquad |x - z| \geqq r_0\,. \tag{3.30}$$

If η, η_N are as in (3.14) then, as in the proof of Theorem 3.3,

$$\begin{aligned}2E_x f(|X(t \wedge \eta_N) - z|) - 2F(|x - z|) \\ \geq E_x \int_0^{t\wedge\eta_N} 2Lf(X(s))\, ds \\ \geq E_x(t \wedge \eta_N) \qquad r_0 \leq |x - z| \leq N .\end{aligned} \tag{3.31}$$

First letting $t \uparrow \infty$ in (3.31) and then letting $N \uparrow \infty$, one has

$$E_x(\tau_{\overline{B(z:r_0)}^c}) = E_x \eta \leq -2F(|x - z|) , \tag{3.32}$$

since $\eta_N \uparrow \eta$ a.s. (P_x) as $N \uparrow \infty$ (due to recurrence). Now apply Lemma 3.4(a).

(b) Assume (3.25), (3.27) hold. Define

$$\begin{aligned}G(r) &= \int_{r_0}^{r} \exp\{-\bar{I}_z(s)\} \left(\int_{r_0}^{s} \frac{1}{\bar{\alpha}_z(u)} \exp\{\bar{I}_z(u)\}\, du\right) ds , \\ g(x) &= G(|x - z|) \qquad |x - z| \geq r_0 .\end{aligned} \tag{3.33}$$

Since $G'(r) \geq 0$ and $G''(r) = -(1/r)\bar{\beta}_z(r)G'(r) + 1/\bar{\alpha}_z(r)$, $2Lg(x) \leq 1$. Therefore, one has

$$E_x(t \wedge \eta_N) \geq 2E_x G(|X(t \wedge \eta_N) - z|) - 2G(|x - z|) . \tag{3.34}$$

Letting $t \uparrow \infty$ in (3.34) one gets

$$\begin{aligned}E_x(\eta_N) &\geq 2E_x G(|X(\eta_N) - z|) - 2G(|x - z|) \\ &= 2P_x(\tau_{B(z:N)} < \eta)G(N) - 2G(|x - z|) .\end{aligned} \tag{3.35}$$

Let $N \uparrow \infty$ to obtain, using (3.21),

$$E_x(\eta) \geq 2 \lim_{N\to\infty} \frac{\int_{r_0}^{|x-z|} \exp\{-\underline{I}_z(u)\}\, du}{\int_{r_0}^{N} \exp\{-\underline{I}(u)\}\, du} \cdot G(N) - 2G(|x - z|) = \infty .$$

The proof is now complete by Lemma 3.4(b). □

Following the terminology used for Markov chains one may call a point x in R^k *positive recurrent* for the diffusion with generator L if for every r_0, r_1 $(0 < r_0 < r_1)$ one has $E_x(\theta(x; r_0, r_1)) < \infty$, where

$$\theta(x; r_0, r_1) = \inf\{t > \tau_{B(x:r_1)} : |X(t) - x| = r_0\} .$$

If x is recurrent but not positive recurrent then x is called *null recurrent*. If all points in R^k are positive (null) recurrent, the *diffusion is called positive* (respectively, *null*) *recurrent*. In this terminology, Theorem 3.5 provides criteria for positive and null recurrence. The criterion for positive recurrence extends a criterion announced by Khas'minskii (1960; Theorem III of his Supplement) to more general coefficients. The criterion for null recurrence given here is comparable in strength to Khas'minskii's (1960; Theorem III of Supplement), when specialized to Khas'minskii's hypothesis; however, neither implies the other.

An indication of the sensitivity of the criteria provided by Theorems 3.3, 3.5 are afforded by the fact that if for some z the functions $A_z(x)$, $B(x) + C_z(z)$, defined by (3.10), are functions of $|x'|$ for sufficiently large $|x'|$, then the criteria are exact.

For in this case one may delete the "bars" and assert: (i) the diffusion is recurrent if and only if $\int_{r_0}^{\infty} \exp\{-I_z(u)\}\, du = \infty$ for some $r_0 > 0$; (ii) a recurrent diffusion is positive or null according as $\int_{r_0}^{\infty} [\exp\{I_z(u)\}/\alpha_z(u)]\, du$ is finite or infinite.

4. Some remarks. This section is devoted to some miscellaneous comments on the material in the preceding sections.

First, the definition of transience used in this article leaves open the possibility that a transient diffusion may be nonconservative. In order to restrict oneself to conservative diffusions one may use the following criterion for explosion essentially proved by McKean (1969), pages 102–104, and earlier stated by Khas'minskii (1960) (Theorem I of his Supplement), extending a one-dimensional result of Feller: *Assume that, in addition to* (A), *the coefficients* a_{ij}, b_i *are Lipschitzian on compacts.* (a) *If, for some* $z \in R^k$ *and some* $r > 0$,

$$\int_r^{\infty} \exp\{-\underline{I}_z(s)\} \left(\int_r^s \frac{1}{\bar{\alpha}_z(u)} \exp\{\bar{I}_z(u)\}\, du\right) ds = \infty\,, \tag{4.1}$$

then the diffusion is conservative. (b) *If, for some* $z \in R^k$ *and some* $r > 0$,

$$\int_r^{\infty} \exp\{-\underline{I}_z(s)\} \left(\int_r^s \frac{1}{\underline{\alpha}_z(u)} \exp\{\underline{I}_z(u)\}\, du\right) ds < \infty\,, \tag{4.2}$$

then the diffusion is almost surely explosive, i.e., $P_x(\zeta < \infty) = 1$ *for all* $x \in R^k$.

Secondly, the problem of studying diffusions (in our sense) on those open subsets of R^k which are C^2-diffeomorphic to R^k is easily reduced to the investigation on R^k in view of Itô's lemma (see McKean (1969)) which enables one to compute "drift" and "diffusion" coefficients of the transformed process, at least when the corresponding process on R^k has coefficients which are Lipschitzian on compacts.

Finally, suppose that the coefficients of L satisfy (A) and are Hölder continuous on compacts. Using standard results from the theory of elliptic partial differential equations one can show that if z is a positive recurrent point then the function $u(y) = E_y(\tau_{\overline{B(z:r_0)}^c})$ is continuous on $\overline{B(z:r_0)}^c$ for every $r_0 > 0$ (indeed, it is twice differentiable and satisfies $Lu = -1$). From the uniqueness (up to a constant multiple) of the invariant measure and Lemma 3.4 it then follows that all points in R^k are positive recurrent. There is then a complete classification of diffusions into transient, null recurrent, and positive recurrent ones.

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7.2 "On the functional central limit theorem and the law of the iterated logarithm for Markov processes"

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On the Functional Central Limit Theorem and the Law of the Iterated Logarithm for Markov Processes

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Summary. Let $\{X_t: t \geqq 0\}$ be an ergodic stationary Markov process on a state space S. If $\hat{A}$ is its infinitesimal generator on $L^2(S, dm)$, where m is the invariant probability measure, then it is shown that for all f in the range of $\hat{A}$, $n^{-1/2} \int_0^{nt} f(X_s)\, ds$ $(t \geqq 0)$ converges in distribution to the Wiener measure with zero drift and variance parameter $\sigma^2 = -2\langle f, g\rangle = -2\langle \hat{A} g, g\rangle$ where g is some element in the domain of $\hat{A}$ such that $\hat{A} g = f$ (Theorem 2.1). Positivity of σ^2 is proved for nonconstant f under fairly general conditions, and the range of $\hat{A}$ is shown to be dense in $1^{\perp}$. A functional law of the iterated logarithm is proved when the $(2+\delta)$th moment of f in the range of $\hat{A}$ is finite for some $\delta > 0$ (Theorem 2.7(a)). Under the additional condition of convergence in norm of the transition probability $p(t, x, dy)$ to $m(dy)$ as $t \to \infty$, for each x, the above results hold when the process starts away from equilibrium (Theorems 2.6, 2.7(b)). Applications to diffusions are discussed in some detail.

1. Introduction and Summary

Let $\{X_t: t \geqq 0\}$ be a continuous parameter Markov process on a *state space* S having a transition probability function $p(t, x, dy)$. Assume that there exists an *invariant probability measure* m for p and that the process starting with (initial) distribution m is *ergodic* (i.e., the shift invariant sigma-field is trivial). Assume also, for purposes of measurability, that the process is progressively measurable. The *functional central limit theorem* (FCLT) is said to hold for some m-integrable f on S if the sequence of stochastic processes

$$\left\{ n^{-1/2} \int_0^{nt} \left(f(X_s) - \int f\, dm\right) ds \quad (t \geqq 0): n = 1, 2, \ldots \right\}$$

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converges in distribution to a Wiener measure W_{σ^2} with zero drift and variance parameter $\sigma^2 \geqq 0$. Without loss of generality assume $\int f dm = 0$. Unlike discrete parameter Markov chains (which are specified by a one-step transition probability function), a Markov process in continuous time is generally specified by infinitesimal conditions (e.g., rates of transitions from one state to another for pure jump processes, drift and diffusion coefficients for diffusions). Theorem 2.1 says that, under the initial distribution m, the FCLT holds for all f belonging to *the range* $\mathscr{R}_{\hat{A}}$ *of the infinitesimal generator* $\hat{A}$ (on $L^2(S, dm)$), and that the variance parameter of the limiting Wiener measure is

$$\sigma^2 = -2\langle f, g\rangle = -2\langle \hat{A}g, g\rangle, \tag{1.1}$$

where g is some element in the *domain* $\mathbb{D}_{\hat{A}}$ of $\hat{A}$ satisfying $\hat{A}g = f$. It is also shown (Proposition 2.4) that $\sigma^2 > 0$ for all nonconstant (a.s. dm) bounded f in $\mathscr{R}_{\hat{A}}$, provided for some $t > 0$ and all x the transition probability $p(t, x, dy)$ and the invariant measure $m(dy)$ are mutually absolutely continuous; if, however, $\hat{A}$ is selfadjoint, then $\sigma^2 > 0$ for all nonzero $f \in \mathscr{R}_{\hat{A}}$, without the additional assumptions of boundedness and mutual absolute continuity (Remark 2.4.1). The linear space $\mathscr{R}_{\hat{A}}$ is also shown to be dense in the set of all square untegrable functions with mean zero if $\mathbb{D}_{\hat{A}}$ is dense in L^2, or, equivalently, if the transition semigroup is *strongly continuous* on L^2, which is a very mild restriction (Proposition 2.3).

One may say that Theorem 2.1 deals with the case when the process is already in equilibrium. When the process starts away from equilibrium (i.e., the initial distribution is not m), the FCLT holds for all $f \in \mathscr{R}_{\hat{A}}$, if the tail sigmafield is trivial under all initial distributions μ, or, equivalently, if $p(t, x, dy)$ converges to $m(dy)$ in norm for all x, as $t \to \infty$ (Theorem 2.6). A Strassen-type *functional law of the iterated logarithm* (FLIL) is proved in Theorem 2.7.

The above strengthen and generalize earlier results proved in an elegant paper by Baxter and Brosamler (1976) for the special case of diffusions on compact manifolds. Since Doeblin's well known condition holds in this case, $p(t, x, dy)$ converges to $m(dy)$ in norm exponentially fast uniformly in x as $t \to \infty$. This is generally not true for noncompact state spaces, and for the most part, the special methods used by Baxter and Brosamler (1976) do not extend to the general case under consideration. Their computation of the variance for this special case is easily shown to agree with (1.1).

A result analogous to Theorem 2.1 (although not in a functional form) has been proved for discrete parameter Markov chains by Gordin and Lifšic (1978). The continuous parameter case treated here is more delicate and is based on semigroup theory. One of the common features of both proofs is a theorem proved independently by Billingsley (1961) and Ibragimov (1963) which asserts that the CLT holds for a square integrable martingale sequence whose successive differences form an ergodic stationary process. This theorem is ideally suited for our purposes.

Since the results of this article mentioned above are fairly general, one expects to do some extra work in specific classes of applications. This includes finding criteria (in terms of the infinitisimal conditions)

(1) for the existence of an invariant probability measure and its ergodicity,
(2) for f to belong to $\mathscr{R}_{\hat{A}}$,
(3) for $p(t, x, dy)$ to converge in norm to $m(dy)$ as $t \to \infty$, etc.

The well known Proposition 2.1 (which is stated here for the sake of completeness) says that ergodicity is equivalent to zero being a simple eigenvalue of $\hat{A}$. A sufficient condition for (3) is m-recurrence (see Remark 2.6.2). Examples in the last section illustrate how (1), (2), (3) may be verified for some important classes of Markov processes, and provide comparisons with results obtained earlier by the renewal method by Mandl (1968) for one dimensional diffusions and recently by Bhattacharya and Ramasubramanian (1982) for multidimensional diffusions.

2. Main Results

Let S be a nonempty set, and $\mathscr{B}(S)$ a sigmafield of subsets of S. Let $p(t, x, dy)$ be a *transition probability function* on S, i.e.,

(i) $p(t, x, dy)$ is a probability measure on $\mathscr{B}(S)$ for each pair (t, x): $t > 0$, $x \in S$;

(ii) for each $\mathscr{B} \in \mathscr{B}(S)$, the function $(t, x) \to p(t, x, B)$ is Borel measurable on $(0, \infty) \times S$;

(iii) the *Chapman-Kolmogorov relation* $p(t+s, x, B) = \int_S p(s, z, B)\, p(t, x, dz)$ holds for all $B \in \mathscr{B}(S)$ and all $t > 0$, $s > 0$.

Let $\mathbb{B}$ denote the Banach space of all real bounded measurable functions f on $(S, \mathscr{B}(S))$ into $(\mathbb{R}^1, \mathscr{B}^1)$ ($\mathscr{B}^1$ is the Borel sigmafield of $\mathbb{R}^1$) endowed with the 'sup norm' $\|f\| = \sup\{|f(x)|: x \in S\}$. In view of the Chapman-Kolmogorov relation (iii), the *transition operators* T_t: $t > 0$, defined by

$$(T_t f)(x) = \int_S f(y)\, p(t, x, dy) \qquad t > 0,\ x \in S, \tag{2.1}$$

form a semigroup of positive contractions on $\mathbb{B}$. Let $\mathbb{B}_0$ be the *center* of this semigroup, i.e.,

$$\mathbb{B}_0 = \{f \in \mathbb{B}: \|T_t f - f\| \to 0 \text{ as } t \to 0\}. \tag{2.2}$$

The *infinitesimal generator* A of $\{T_t: t > 0\}$ is defined on the domain $\mathbb{D}_A = \{f \in \mathbb{B}_0: \|(T_t f - f)/t - g\| \to 0$ for some $g \in \mathbb{B}_0$, as $t \downarrow 0\}$, by

$$Af = \lim_{t \downarrow 0} \frac{T_t f - f}{t}, \tag{2.3}$$

the limit being in sup norm.

Suppose now that $p(t, x, dy)$ admits an *invariant probability measure* m (on $(S, \mathscr{B}(S))$):

$$\int p(t, x, B)\, m(dx) = m(B) \qquad \text{for all } B \in \mathscr{B}(S). \tag{2.4}$$

Then $\{T_t: t > 0\}$ is a contraction semigroup on $L^2(S, dm)$:

$$\begin{aligned} \|T_t f\|_2^2 &= \int (T_t f(x))^2\, m(dx) \leq \int (T_t f^2)(x)\, m(dx) \\ &= \int f^2(x)\, m(dx) = \|f\|_2^2. \end{aligned} \tag{2.5}$$

Let $\hat{B}_0$ denote the center of this semigroup (on $L^2(S, dm)$ with respect to the norm $\|\cdot\|_2$) and $\hat{A}$ its infinitesimal generator on the domain $\mathbb{D}_{\hat{A}}$. Since $\|\cdot\|_2$ is weaker than $\|\cdot\|$, $\hat{\mathbb{B}}_0 \supset \mathbb{B}_0$, $\mathbb{D}_{\hat{A}} \supset \mathbb{D}_A$, and $\hat{A}$ is an extension of A on $L^2(S, dm)$.

Let $\{X_t: t \geqq 0\}$ be a stationary Markov process having transition probability $p(t, x, dy)$ and initial distribution m, defined on some probability space $(\Omega, \mathscr{A}, Q)$ on which an increasing family of sigmafields $\{\mathscr{F}_t: t \geqq 0\}$ ($\mathscr{F} \subset \mathscr{A}$ for all t) is given such that

(i) X_t is $\mathscr{F}_t$-measurable, and
(ii) $E(f(X_{t+s})/\mathscr{F}_s) = (T_t f)(X_s)$ a.s. (dQ) for all m-integrable f.

It will be assumed throughout that for each $t > 0$ the function $(t', \omega) \to X_{t'}(\omega)$ on $[0, t] \times \Omega$ is measurable with respect to the sigmafield $\mathscr{B}[0, t] \times \mathscr{F}_t$, where $\mathscr{B}[0, t]$ is the Borel sigmafield on $[0, t]$. In the usual Markov process jargon X_t is thus *progressively measurable*. Note that this is a rather mild restriction and is met whenever S is a metric space ($\mathscr{B}(S)$ is then the Borel sigmafield on S) and $t \to X_t(\omega)$ is right continuous (see Blumenthal and Getoor (1968), p. 34). For every set $F \in \sigma\{X_t: t \geqq 0\}$ there exist a countable set $\{t_1, t_2, \ldots\} \subset [0, \infty)$ and a measurable set G of the product space $(S^{\{t_1, t_2, \ldots\}}, \bigotimes_i \mathscr{B}(S^{\{t_i\}}))$ such that $F = \{\omega \in \Omega: (X_{t_1}(\omega), X_{t_2}(\omega), \ldots) \in G\}$ (see Doob (1953), p. 604). Such *a set F is* said to be *shift-invariant* if for all $t > 0$, $F = F \circ \theta_t = \{\omega \in \Omega: (X_{t_1+t}(\omega), X_{t_2-t}(\omega), \ldots) \in G\}$. The *shift-invariant sigmafield* $\mathscr{I}$ is the collection of all such shift-invariant sets. The stationary Markov process $\{X_t: t \geqq 0\}$ is said to be *ergodic* if $\mathscr{I}$ is trivial, i.e., if its sets have probabilities zero or one.

For each $T > 0$, and each $f \in L^1(S, dm)$, the map $\omega \to T^{-1/2} \int_0^{Tt} f(X_s(\omega))\, ds$ induces a probability measure on the (Borel sigmafield of the) space $C[0, \infty)$ of all real continuous functions on $[0, \infty)$ endowed with the topology of uniform convergence on compact subsets of $[0, \infty)$. Weak convergence of probability measures on $C[0, \infty)$ has its usual meaning (see Billingsley (1968), p. 7).

Below $\mathscr{R}_{\hat{A}}$ ($\mathscr{R}_A$) denotes the *range of* $\hat{A}$ (A): $\mathscr{R}_{\hat{A}} = \{\hat{A}g: g \in \mathbb{D}_{\hat{A}}\}$. Note that if $g \in \mathbb{D}_{\hat{A}}$, then

$$\int \hat{A}g(x)\, m(dx) = \left(\frac{d}{dt} \int T_t g(x)\, m(dx)\right)_{t=0} = \frac{d}{dt} \left(\int g(x)\, m(dx)\right)_{t=0} = 0. \tag{2.6}$$

Theorem 2.1. *Let $\{X_t: t \geqq 0\}$ be a progressively measurable stationary ergodic Markov process having transition probability function $p(t, x, dy)$ and invariant initial distribution m.* (a) *If $f \in \mathscr{R}_{\hat{A}}$ then, as $n \to \infty$, the distribution of the stochastic process $\left\{n^{-1/2} \int_0^{nt} f(X_s)\, ds: t \geqq 0\right\}$ converges weakly to the Wiener measure with zero drift and variance parameter*

$$\sigma^2 = -2\langle f, g \rangle = -2 \int f(x)\, g(x)\, m(dx), \tag{2.7}$$

where g is any element of $\mathbb{D}_{\hat{A}}$ satisfying

$$\hat{A}g = f. \tag{2.8}$$

Proof. Let (2.8) hold. Using the identity (see Dynkin (1965), p. 23, relation (1.5))

$$T_t g(x) - g(x) = \int_0^t T_s \hat{A} g(x)\, ds \qquad \text{(a.e. } dm), \tag{2.9}$$

it is simple to check that

$$Y_n(g) = g(X_n) - \int_0^n \hat{A} g(X_s)\, ds \qquad (n = 1, 2, \ldots) \tag{2.10}$$

is a square integrable martingale, whose differences

$$\Delta_n(g) = g(X_{n+1}) - g(X_n) - \int_n^{n+1} \hat{A} g(X_s)\, ds \qquad (n = 0, 1, 2, \ldots)$$

form a stationary ergodic sequence. By a result of Billingsley (1961) and Ibragimov (1963) (the functional form used here is due to Billingsley (1968), Theorem 23.1, pp. 205–208), the distribution of

$$Z_n(t) = n^{-1/2}(Y_{[nt]}(g) + (nt - [nt])\, \Delta_{[nt]}(g)) \qquad (t \geq 0), \tag{2.11}$$

converges weakly to the Wiener measure with zero drift and variance parameter

$$\sigma^2 = E(\Delta_0(g))^2 = E\left[g(X_1) - g(X_0) - \int_0^1 \hat{A} g(X_s)\, ds\right]^2. \tag{2.12}$$

Here we have made use of (2.6), which implies that $E\Delta_n(g) = 0$. Now

$$\begin{aligned} \left| Z_n(t) + n^{-1/2} \int_0^{nt} \hat{A} g(X_s)\, ds \right| &\leq n^{-1/2} \left(|g(X_{[nt]})| + |\Delta_{[nt]}(g)| + \int_{[nt]}^{[nt]+1} |\hat{A} g(X_s)|\, ds \right) \\ &= n^{-1/2}(I_1([nt]) + I_2([nt]) + I_3([nt])), \end{aligned} \tag{2.13}$$

say. But, given any $\varepsilon > 0$,

$$\begin{aligned} \sum_{n=1}^{\infty} Q(I_j(n) > \varepsilon \sqrt{n}) &= \sum_{n=1}^{\infty} Q(I_j(1) > \varepsilon \sqrt{n}) \leq \int_0^{\infty} Q(I_j(1) > \varepsilon \sqrt{v})\, dv \\ &= \frac{2}{\varepsilon^2} \int_0^{\infty} Q(I_j(1) > u)\, u\, du = \varepsilon^{-2} E(I_j(1))^2 < \infty \qquad (j = 1, 2, 3), \end{aligned} \tag{2.14}$$

so that $n^{-1/2} I_j(n) \to 0$ (a.s. dm) as $n \to \infty$, implying that

$$\sup \{n^{-1/2}(I_1([nt] + I_2[nt] + I_3[nt]) : 0 \leq t \leq t_0\} \to 0 \qquad \text{a.s. as } n \to \infty,$$

for every $t_0 > 0$. It remains to show (2.7). For each positive integer n one has, since martingale differences are orthogonal,

$$\sigma^2 = nE\left[g(X_{1/n}) - g(X_0) - \int_0^{1/n} \hat{A} g(X_s)\, ds\right]^2. \tag{2.15}$$

On the other hand,

$$E\left[g(X_{1/n})-g(X_0)-\int_0^{1/n}\hat{A}g(X_s)\,ds\right]^2=E(g(X_{1/n})-g(X_0))^2$$
$$+E\left(\int_0^{1/n}\hat{A}g(X_s)\,ds\right)^2-2E\left[(g(x_{1/n})-g(X_0))\int_0^{1/n}\hat{A}g(X_s)\,ds\right]$$
$$=2\int g^2(x)\,m(dx)-2E(g(X_0)\,E(g(X_{1/n})/\mathscr{F}_0))+E\left(\int_0^{1/n}\hat{A}g(X_s)\,ds\right)^2$$
$$-2E\left[(g(X_{1/n})-g(X_0))\int_0^{1/n}\hat{A}g(X_s)\,ds\right]$$
$$=2\int g^2(x)\,m(dx)-2\int g(x)\,T_{1/n}\,g(x)\,m(dx)+o(n^{-1})$$
$$=2\int g^2(x)\,m(dx)-2\int g(x)([g(x)+n^{-1}\hat{A}g(x)]+o(n^{-1}))\,m(dx)+o(n^{-1})$$
$$=-\frac{2}{n}\int g(x)\,\hat{A}g(x)\,m(dx)+o\left(\frac{1}{n}\right), \tag{2.16}$$

where we have used the elementary inequalities

$$E\left(\int_0^{1/n}\hat{A}g(X_s)\,ds\right)^2\leqq E\left(\frac{1}{n}\int_0^{1/n}(\hat{A}g(X_s))^2\,ds\right)=\frac{1}{n^2}\int(\hat{A}g(x))^2\,m(dx),$$
$$E\left|(g(X_{1/n})-g(X_0))\cdot\int_0^{1/n}\hat{A}g(X_s)\,ds\right|$$
$$\leqq(E(g(X_{1/n})-g(X_0))^2)^{1/2}\left(E\left(\int_0^{1/n}\hat{A}g(X_s)\,ds\right)^2\right)^{1/2}$$
$$=\left(-\frac{2}{n}\int g(x)\,\hat{A}g(x)\,m(dx)+o(n^{-1})\right)^{1/2}\cdot\frac{1}{n}\left(\int(\hat{A}g(x))^2\,m(dx\right)^{1/2}$$
$$=O(n^{-3/2}). \tag{2.17}$$

Using (2.16) in (2.15) one gets

$$\sigma^2=-2\langle g,\hat{A}g\rangle+o(1). \tag{2.18}$$

The term $o(1)$ must vanish, since the left side of (2.18) is independent of n. □

Remark 2.1.1. Suppose f_i $(i=1,2,\ldots,k)\in\mathscr{R}_{\hat{A}}$, then $\sum_1^k\alpha_i f_i\in\mathscr{R}_{\hat{A}}$ for every k-tuple of reals $(\alpha_1,\ldots,\alpha_k)$. Hence applying the conclusion of Theorem 2.1 to $\sum_1^k\alpha_i f_i$ for every k-tuple of reals, one proves that the distribution of $\left(n^{-1/2}\int_0^{nt}f_i(X_s)\,ds\ (i=1,2,\ldots,k)\right)$ converges weakly to a k-dimensional Wiener measure with drift vector $\mathbf{0}=(0,\ldots,0)$ and dispersion matrix $((a_{ij}=-\langle\hat{A}g_i,g_j\rangle-\langle g_i,\hat{A}g_j\rangle))$, $1\leqq i$, $j\leqq k$.

Remark 2.1.2. Suppose m is an invariant probability measure for a transition probability function $p(t, x, dy)$. Since $\hat{A}$ is a closed operator, its *null space* $N_{\hat{A}} = \{h \in \mathbb{D}_{\hat{A}}: \hat{A}h = 0\}$ is a closed subset of $L^2(S, dm)$. Therefore, given $f \in \mathscr{R}_{\hat{A}}$ there exists a unique $g \in \mathbb{D}_{\hat{A}} \cap N_{\hat{A}}^{\perp}$ such that $\hat{A}g = f$. One may take this g in (2.7).

Now suppose $h \in N_{\hat{A}}$. Then $\hat{A}h = 0$ and $T_t h = h$ for all t. This implies, by the martingale convergence theorem applied to the square integrable martingale $\{h(X_t): t \geqq 0\}$, that $h(X_t) = E(Z/\sigma\{X_s: s \leqq t\})$ for a shift-invariant square integrable random variable $Z = \lim h(X_t)$. Since $Z = Z \circ \theta_t$, and the distribution of $(Z \circ \theta_t, X_t)$ is the same as that of (Z, X_0), one has $h(X_0) = E(Z/\sigma\{X_0\}) = E(Z \circ \theta_t/\sigma\{X_t\}) = E(Z \circ \theta_t/\sigma\{X_s: s \leqq t\}) = h(X_t)$ a.s. Hence $Z = h(X_0)$ a.s. This implies that *the ergodicity of* $\{X_t: t \geqq 0\}$ *is equivalent to* $N_{\hat{A}}$ *being the one dimensional subspace of* $L^2(S, dm)$ *spanned by constants.* Another way of stating this is

Proposition 2.2. *Let m be an invariant probability measure for $p(t, x, dy)$. Then the following statements are equivalent:*

(a) *The Markov process having transition probability p and initial distribution m is ergodic.*

(b) *0 is a simple eigenvalue of $\hat{A}$.*

The next result assures us that $\mathscr{R}_{\hat{A}}$ is fairly large.

Proposition 2.3. *Let $p(t, x, dy)$ be a transition probability function having an invariant probability measure m. Suppose that $\mathbb{D}_{\hat{A}}$ is dense in $L^2(S, dm)$ (i.e., $\hat{\mathbb{B}}_0 = L^2(S, dm)$). Then*

(a) $N_{\hat{A}} = N_{\hat{A}^*}$, *and*

(b) *$\mathscr{R}_{\hat{A}}$ is dense in $\{1\}^{\perp}$ if and only if $N_{\hat{A}}$ is one dimensional (i.e., the Markov process is ergodic).*

(c) *If for some $\lambda > 0$, the resolvent $(\lambda - \hat{A})^{-1}$ is compact, then $\mathscr{R}_{\hat{A}}$ is closed; and if, in addition, 0 is a simple eigenvalue of $\hat{A}$, then $\mathscr{R}_{\hat{A}}$ is the space of all $f \in L^2(S, dm)$ such that $\int f\,dm = 0$.*

Proof. (a) Suppose $h \in N_{\hat{A}}$ then $h(X_t) = h(X_0)$ a.s. Therefore, for all $g \in \mathbb{D}_{\hat{A}}$ one has

$$\begin{aligned}\langle \hat{A}g, h\rangle &= \lim_{t \downarrow 0} \left\langle \frac{T_t g - g}{t}, h \right\rangle = \lim_{t \downarrow 0} t^{-1}(Eh(X_0)\,g(X_t) - Eh(X_0)\,g(X_0)) \\ &= \lim_{t \downarrow 0} t^{-1}(Eh(X_t)\,g(X_t) - Eh(X_0)\,g(X_0)) = 0.\end{aligned} \tag{2.19}$$

This shows $\mathscr{R}_{\hat{A}} \subset N_{\hat{A}}^{\perp}$. Since $\mathbb{D}_{\hat{A}}$ is dense in L^2, $\hat{A}^*$ is well defined, and $\bar{\mathscr{R}}_{\hat{A}} = N_{\hat{A}^*}^{\perp}$. Hence $N_{\hat{A}^*}^{\perp} \subset N_{\hat{A}}^{\perp}$, so that $\overline{N_{\hat{A}^*}} \supset N_{\hat{A}}$. $\hat{A}^*$ is a closed operator; hence $N_{\hat{A}^*}$ is a closed set, and one has $N_{\hat{A}^*} \supset N_{\hat{A}}$. Conversely, suppose $h \in N_{\hat{A}^*}$. Then for all $g \in \mathbb{D}_{\hat{A}}$ one has

$$\frac{d}{dt}\langle T_t g, h\rangle = \langle \hat{A}T_t g, h\rangle = \langle T_t g, \hat{A}^* h\rangle = 0, \tag{2.20}$$

i.e., $\langle T_t g, h\rangle = \langle g, h\rangle$, or $T_t^* h = h$. Now

$$0 \leqq \|T_t h - h\|_2^2 = \|T_t h\|_2^2 + \|h\|_2^2 - 2\langle T_t h, h\rangle$$
$$\leqq 2\|h\|_2^2 - 2\langle h, T_t^* h\rangle = 2\|h\|_2^2 - 2\|h\|_2^2 = 0, \tag{2.21}$$

implying $T_t h = h$ and, therefore, $\hat{A}h = 0$. Thus $N_{\hat{A}^*} \subset N_{\hat{A}}$.

(b) Since $\mathscr{R}_{\hat{A}} = N_{\hat{A}^*}^{\perp} = N_{\hat{A}}^{\perp}$ (the second equality follows from part (a)), the assertion follows from Proposition 2.2.

(c) Write $\hat{A}_\lambda = \lambda^2(\lambda - \hat{A})^{-1} - \lambda$; then $\hat{A}_\lambda = \lambda\hat{A}(\lambda - \hat{A})^{-1}$ (see, e.g., Dynkin (1965), p. 31). Therefore, $\mathscr{R}_{\hat{A}} = \mathscr{R}_{\hat{A}_\lambda}$. On the other hand, since $V = \lambda^2(\lambda - \hat{A})^{-1}$ is compact, the range of $V - \lambda$ is closed (see Yosida (1965), Lemma, p. 283). □

Remark 2.3.1. It was observed by Gordin and Lifšic (1978), p. 393, that for discrete parameter Markov processes which are ϕ-mixing with $\phi(n) \to 0$, the *maximal correlation* $\rho(n)$ goes to zero exponentially fast and, therefore, the central limit theorem holds for all $f \perp 1$. This extends to the continuous parameter case as follows: Write $\rho(t) = \sup\{\|T_t f\|_2 : f \perp 1, \|f\|_2 = 1\} = \sup\{\langle T_t f, g\rangle : f, g \perp 1, \|f\|_2 = 1, \|g\|_2 = 1\}$. Suppose $\rho(t) \to 0$; then $\rho(t) \to 0$ exponentially fast (see Rosenblatt (1971), Chap. VII). Hence if $f \perp 1$ the function $g = -\int_0^\infty T_t f\,dt$ satisfies

(i) $\|g\|_2 \leqq \left(\int_0^\infty \rho(t)\,dt\right)\|f\|_2$ and

(ii) $\lim_{s \downarrow 0} s^{-1}(T_s g - g) = \lim_{s \downarrow 0} s^{-1}\int_0^s T_t f\,dt = f$, provided $f \in \hat{B}_0$, the center of the semigroup.

Thus if $\mathbb{D}_{\hat{A}}$ is dense in $L^2(S, dm)$ (i.e., if $\{T_t : t > 0\}$ is a strongly continuous semigroup on $L^2(S, dm)$), and $\rho(t) \to 0$, then $\hat{A}^{-1}$ is bounded on $1^{\perp}$, implying $\mathscr{R}_{\hat{A}} = 1^{\perp}$. Since $\rho(t) \leqq 2\phi(t)^{1/2}$ (see Billingsley (1968), p. 170), the last assertion holds if $\rho(t)$ is replaced by the ϕ-mixing coefficient $\phi(t)$.

Our next task is to show that, at least under some reasonable additional conditions, the variance parameter σ^2 in (2.7) is strictly positive unless $f = 0$ (a.s. dm). The idea of the proof is taken from Baxter and Brosamler (1976), Theorem 4.16. The actual proof, however, is simpler and more widely applicable.

Proposition 2.4. *In addition to the hypothesis in Theorem* 2.1 *assume that, for each pair* $(t, x) \in (0, \infty) \times S$, $p(t, x, dy)$ *and* $m(dy)$ *are mutually absolutely continuous. Then if* $f \in \mathscr{R}_{\hat{A}}$ *and* f *is bounded (a.s. dm), then the variance parameter* σ^2 *in* (2.7) *is strictly positive, unless* $f = 0$ *(a.s. dm).*

Proof. Suppose $f \in \mathscr{R}_{\hat{A}}$, f bounded, and $f \neq 0$. Let $g \in \mathbb{D}_{\hat{A}}$ be such that $\hat{A}g = f$. If possible suppose $\sigma^2 = 0$. Since differences of the martingale $Y_t = g(X_t) - \int_0^t f(X_s)\,ds$ over successive nonoverlapping time intervals of equal length form a stationary sequence of martingale differences one must have, choosing a separable version of the martingale if necessary,

$$Q\left(g(x_t) - g(X_0) - \int_0^t f(X_s)\,ds = 0 \text{ for all } t \geqq 0\right) = 1. \tag{2.22}$$

Thus, with probability one, $\int_0^t f(X_s)\,ds = g(X_t) - g(X_0)$ for all t. Using the same argument as given in the last paragraph of the proof of Theorem (4.16) in Baxter and Brosamler (1976), one shows that $g(X_t) - g(X_0) = 0$ (a.s. dQ). Choose and fix $t > 0$. Since g is not an a.s. constant, there exist numbers $a < b$ and sets $A, B \in \mathscr{B}(S)$ such that

(i) $g < a$ on A, $g > b$ on B, and
(ii) $m(A) > 0$, $m(B) > 0$.

Hence, writing $p(t, x, y)$ for a strictly positive version of the density of $p(t, x, dy)$ with respect to $m(dy)$,

$$Q(\{g(X_0) < a, g(X_t) > b\}) = \int_{\{g(y) > b\}} \int_{\{g(x) < a\}} p(t, x, y)\, m(dx)\, m(dy) > 0, \tag{2.23}$$

which contradicts $g(X_t) - g(X_0) = 0$ a.s. □

Remark 2.4.1. Under the hypothesis of Theorem 1 the variance parameter σ^2 can be shown to be strictly positive for all nonzero $f \in \mathscr{R}_{\hat{A}}$, provided $\hat{A}$ is selfadjoint. For in this case an immediate consequence of the spectral theorem is: $\langle \hat{A} g, g \rangle \leqq 0$ for all $g \in \mathbb{D}_{\hat{A}}$, with equality if and only if g belongs to the eigenspace of 0, i.e., g is a constant (a.s. dm). This extends Remark (4.29) in Baxter and Brosamler (1976).

Remark 2.4.2. Let $t \to X_t$ denote a deterministic periodic motion on the unit circle. Let m denote the unique invariant initial distribution. (In case the motion is uniform, m is the usual Haar measure.) This stationary Markov process is ergodic. If f is bounded and $\int f\,dm = 0$, then $\int_0^t f(X_s)\,ds$ is bounded (in t). Hence $\sigma^2 = 0$. This counterexample is due to C.M. Newman.

Let us now consider a progressively measurable Markov process $\{X_t : t \geqq 0\}$ with state space S, initial distribution μ and transition probability p defined on some probability space $(\Omega, \mathscr{A}, Q_\mu)$. As μ varies let the probability space vary. In this notation, $Q = Q_m$. The tail sigmafield is $\mathscr{T} = \bigcap_{t \geqq 0} \{X_s : s \geqq t\}$. The tail sigmafield is *Q_μ-trivial* if $Q_\mu(A) = 0$ or 1 for all $A \in \mathscr{T}$. The following proposition is essentially proved in Orey (1971), Proposition 4.3, pp. 19–20.

Proposition 2.5. *Let p be a transition probability admitting an invariant initial distribution m. Then the following statements are equivalent:*

(a) *The tail sigmafield is Q_μ-trivial for every initial distribution μ.*

(b) $\|p(t, x, dy) - m(dy)\|_v \to 0$ *as* $t \to \infty$, *for every* $x \in S$. *Here* $\|v\|_v$ *denotes the variation norm of a signed measure* v.

Note that if condition (b) (or (a)) of Proposition 2.5 holds, then for every m-integrable f one has

$$Q_\mu\left(\lim_{T \to \infty} T^{-1} \int_0^T f(X_s)\,ds = \int f\,dm\right) = 1, \tag{2.24}$$

whatever be the initial distribution μ. For the event C within parentheses is the same as $C \circ \theta_t = \left\{ \lim_{T\to\infty} T^{-1} \int_t^{T+t} f(X_s)\, ds = \int f dm \right\}$ for every $t>0$. Hence the left side of (2.24) equals $E_\mu d(X_t)$ where $d(x) = Q_{\delta_x}(C)$ and E_μ denotes expectation with respect to μ. Now $E_m d(X_t) = Q_m(C) = 1$, by the ergodic theorem. Therefore,

$$\begin{aligned} |Q_\mu(C)-1| &= |E_\mu d(X_t) - E_m d(X_t)| \\ &= |\iint d(y)(p(t,x,dy)-m(dy))\, \mu(dx)| \\ &\leq \|p(t,x,dy)-m(dy)\|_v \to 0 \quad \text{as } t\to\infty. \end{aligned} \tag{2.25}$$

Hence (2.24) holds. We can now prove the following useful result.

Theorem 2.6. *Let p be a transition probability admitting an invariant initial distribution m. Assume that $\|p(t,x,dy)-m(dy)\| \to 0$ as $t\to\infty$, for all $x\in S$. Suppose $f\in\mathscr{R}_{\hat{A}}$. Then for every μ, the Q_μ-distributions of the random functions $n^{-1/2}\int_0^{nt} f(X_s)\, ds$ $(t\geq 0)$ converge weakly to the Wiener measure with zero drift and variance parameter σ^2 given by (2.7).*

Proof. Fix a probability measure μ on S. Write Z_n for the random function $n^{-1/2}\int_0^{nt} f(X_s)\, ds$ $(t\geq 0)$. Let ψ be a real valued bounded continuous function on $C[0,\infty)$. For $h>0$ let $Z_{n,h}$ denote the random function $n^{-1/2}\int_h^{nt+h} f(X_s)\, ds$ $(t\geq 0)$. Then $E_\mu \psi(Z_{n,h}) = E_{\mu_h}\psi(Z_n)$, where μ_h is the Q_μ-distribution of X_h. Note that $|E_{\mu_h}\psi(Z_n) - E_m\psi(Z_n)| \leq \|\psi\|_\infty \int \|p(h,x,dy)-m(dy)\|_v\, \mu(dx) \to 0$ as $h\to\infty$, uniformly for all n. Choose $h(n)\to\infty$, $h(n)=o(n^{-1/2})$. Then by Theorem 1, $E_m\psi(Z_n)\to\int\psi\, dW_{\sigma^2}$ (where W_{σ^2} is the limiting Wiener measure), and one has $\lim E_\mu \psi(Z_{n,h(n)}) \to \int \psi\, dW_{\sigma^2}$ as $n\to\infty$. By the ergodic theorem and (2.24),

$$\sup\left\{ \left| Z_{n,h(n)}(t) - n^{-1/2}\int_0^{h(n)+nt} f(X_s)\, ds \right| : t\geq 0 \right\} \leq n^{-1/2}\int_0^{h(n)} |f(X_s)|\, ds \to 0$$

in Q_μ-probability as $n\to\infty$. Finally, the change of time $\theta_n(t) = (t-h(n)/n)\vee 0$, applied to the process $n^{-1/2}\int_0^{h(n)+nt} f(X_s)\, ds$ shows that $E_\mu\psi(Z_n)\to\int\psi\, dW_{\sigma^2}$ as $n\to\infty$ (see Billingsley (1968), pp. 144–145). □

Remark 2.6.1. Recall that a transition probability p is said to satisfy *Doeblin's condition* if there exist

(i) a probability measure ν on $(S, \mathscr{B}(S))$,
(ii) $t_0 > 0$, and
(iii) $\varepsilon\in(0,1)$,

such that $p(t_0, x, B) \leq 1-\varepsilon$ whenever $\nu(B)\leq\varepsilon$, for all x. It is well known (see Doob (1953), Theorem 2.1, p. 256) that under this condition there exists a unique invariant probability measure m and that $\|p(t,x,dy)-m(dy)\|_v \to 0$ exponentially fast as $t\to\infty$, uniformly for $x\in S$. In particular, the ϕ-mixing coefficient $\phi(t)$ goes to zero exponentially fast as $t\to\infty$. Thus by Theorem 2.6 and Remark 2.3.1 it follows that for all $f\perp 1$, the conclusion of Theorem 2.6 holds, provided $\{T_t: t>0\}$ *is strongly continuous on* $L^2(S, dm)$.

Although the requirement of strong continuity on $L^2(S, dm)$ (i.e., $\hat{\mathbb{B}}_0 = L^2(S, dm)$) is quite mild, a functional CLT holds even without this restriction for all $f\perp 1$ in the present case (see Billingsley (1968), Theorem 20.1, p. 174).

Remark 2.6.2. We shall say that a transition probability function p has the *m-recurrence property* for some probability measure m if there exists a $t_0>0$ such that, for each $x\in S$, the Markov chain $X_0=x, X_{t_0}, \ldots, X_{nt_0}, \ldots$, having transition probability $p(t_0)$ has the property: $\operatorname{Prob}(X_{nt_0}\in B$ for some $n)=1$ for all $B\in\mathscr{B}(S)$ such that $m(B)>0$. It follows from the Corollary on p. 25 in Orey (1971) that if p admits an invariant probability measure m with respect to which it is m-recurrent, then $\|p(t, x, dy)-m(dy)\|_v\to 0$ as $t\to\infty$. For ergodic diffusions on R^k this was checked in Bhattacharya and Ramasubramanian (1982), Theorem 2.7 and Lemma 2.8.

The next result is a Strassen-type law of the iterated logarithm, which generalizes Theorem 7.1 of Baxter and Brosamler (1976).

Theorem 2.7. (a) *In addition to the hypothesis in Theorem* 2.1 *assume that* $\int |f|^{2+\delta}\, dm<\infty$ *for some* $\delta>0$. *Then with* Q_m*-probability one, the sequence of random functions*

$$\left\{(2n\log\log n)^{-1/2}\int_0^{nt} f(X_s)\, ds:\ 0\leqq t\leqq 1\right\},\qquad n=2, 3, \ldots,$$

is relatively compact in $C[0, 1]$ *and the set of limit points is the set of all absolutely continuous functions* θ *on* $[0, 1]$ *satisfying*

$$\int_0^1 \theta'(t)^2\, dt\leqq\sigma^2,\qquad \theta(0)=0. \tag{2.26}$$

(b) *If, in addition to the above hypothesis, one has* $\|p(t, s, dy)-m(dy)\|_v\to 0$ *as* $t\to\infty$, *for all* x, *then the above conclusion holds a.s.* Q_μ, *for every initial distribution* μ.

Proof. (a) Applying Corollary 4.2 in Hall and Heyde (1980), p. 118, to the sequence of differences $\Delta_n g$ of the martingale $Y_n(g)$ defined by relation (2.10), and using the estimates (2.13), (2.14), one gets the desired result. Note that for the case $\sigma^2=0$ the result is trivially true, again in view of (2.14) and the fact that $\int_0^n f(X_s)\, ds=g(X_n)-g(X_0)$ for all n (a.s. dQ_m).

(b) Since the event, whose probability is to be shown to equal one, belongs to the shift invariant sigmafiled, the relations (2.25) hold for this event (in palce of C). □

There are important classes of Markov processes for which the norm convergence of $p(t, x, dy)$ to $m(dy)$ is either false or has not been proven, although the existence of an invariant probability measure and ergodicity can often be checked (diffusions with jumps is one example). On the other hand, for physical applications it is often unrealistic to assume that the Markov process starts off in equilibrium. The following result salvages the situation somewhat. The notation is the same as introduced before the statement of Proposition 2.5.

Theorem 2.8. *Let $p(t, x, dy)$ admit an invariant probability measure m, and let $\{X_t: t \geqq 0\}$ be ergodic under Q_m.* (a) *Fix $f \in \mathscr{R}_A$. Then the FCLT and the FLIL hold for f under Q_{δ_x} for almost all x outside an m-null set.* (b) *If μ is absolutely continuous with respect to m, then the FCLT and the FLIL hold for all $f \in \mathscr{R}_A$ under Q_μ.*

Proof. (a) Let $Ag = f$ for some $g \in \mathbb{D}_A$. Then $\Delta_n(g)$ (see the proof of Theorem 2.1) is a uniformly bounded sequence of martingale differences. Also, writing $\phi(x) = E_x \Delta_0^2(g)$, one has

$$Q_m(C) = 1, \tag{2.27}$$

where $C = \left\{\omega: N^{-1} \sum_{n=0}^{N-1} \phi(X_n) \to E_m(\Delta_0^2(g)) = -2\langle f, g\rangle\right\}$. Hence $Q_{\delta_x}(C) = 1$ for all x outside an m-null set M. For x not in M one may now apply Theorem 4.1 (for FCLT) and Corollary 4.1 (for FLIL) of Hall and Heyde (1980).

(b) $Q_m(C) = 1$ implies $Q_\mu(C) = 1$. Hence proceed as in (a). □

3. Miscellaneous Examples

Example 1. (Diffusions on compact manifolds.) For diffusions generated by smooth strictly elliptic operators $L = \frac{1}{2}\sum a_{ij}(x)\,\partial^2/\partial x_i\,\partial x_j + \sum b_i(x)\,\partial/\partial x_i$ (in local coordinates) on a compact connected C^∞-manifold, the transition probability density $p(t, x, y)$ (with respect to the volume element $(\det a^{-1/2}(x))\,dx$) is smooth and positive for $t > 0$. Therefore, Doeblin's condition holds and Theorems 2.6 and 2.7(b) apply. Also $\mathscr{R}_{\tilde{A}} = 1^\perp$, since B_0 is easily seen to contain $C^\infty(M)$, which is dense in $L^2(M, dm)$. The same results apply to diffusions on a compact connected manifold with boundary which are generated by smooth strictly elliptic operators subject to Neumann type boundary conditions. See Mckean (1969), Chap. 4, for basic properties.

Example 2. (Feller's one dimensional diffusions.) Here $S = (-\infty, \infty)$ or $(-\infty, r_1]$, or $[r_0, \infty)$, or $[r_0, r_1]$ $(r_0 < r_1)$, a finite measure $\bar{m}$ is given on S such that every nonempty open subinterval of S has positive $\bar{m}$-measure. The operator A is given by $\frac{d}{d\bar{m}}\frac{d}{dx}$ with boundary condition (for g) $(-1)^i g'(r_i) - \sigma_i f(r_i) = 0$ $(i = 0, 1)$ applied to the boundary r_i (when S has such a boundary). Here $f = \frac{d}{d\bar{m}}\frac{d}{dx} g$, and $\sigma_i \geqq 0$. These processes have continuous trajectories. Details may be found in Itô and Mckean (1965) or Mandl (1968). Since such diffusions are *point recurrent* (i.e., the process starting from some point reaches every other point with probability one), and since the expected time to reach any given point is finite (this is known as the property of *positive recurrence*), if follows from standard Markov process theory that there exists a unique invariant probability measure m. Also since point recurrence obviously implies m-recurrence, $\|p(t,x,dy)-m(dy)\|_v \to 0$ as $t\to\infty$ (see Remark 2.6.2). Here $\mathbb{B}_0$ is the set of all real continuous functions on S, having finite limits at infinite end points. Hence $\bar{\mathscr{R}}_A = 1^{\perp}$ (Proposition 2.3(b)) and Theorems 2.6 and 2.7(b) apply. One may actually compute $\mathscr{R}_{\hat{A}}$. Let us consider the case $S=(-\infty,\infty)$. By solving the second order ordinary differential equation $\hat{A}g=f$, one can show that $f\in\mathscr{R}_{\hat{A}}$ iff $x\to\int_0^x \int_{(-\infty,y]} f(z)\,\bar{m}(dz)\,dy$ is in L^2. Also it is not difficult to check that

$$\sigma^2 = -2\langle f,g\rangle = 2(\bar{m}(S))^{-1}\int_{(-\infty,\infty)} f(x)\left[\int_x^0 dy \int_{(-\infty,y]} f(z)\,\bar{m}(dz)\right]\bar{m}(dx). \quad (3.1)$$

This last expression makes sense iff

$$\int_{(-\infty,\infty)}\left| f(x)\left[\int_x^0 dy \int_{(-\infty,y]} f(z)\,\bar{m}(dz)\right]\right| \bar{m}(dx) < \infty. \quad (3.2)$$

One needs to assume that

(i) $f\in L^2$, $f\perp 1$, and

(ii) $x\to\int_0^x \int_{(-\infty,y]} f(z)\,\bar{m}(dz)\,dy\in L^2$,

in order to apply Theorem 2.6 (or Theorem 2.1). On the other hand, the method of renewal (i.e., dividing up the integral $\int_0^t f(X_s)\,ds$ into contributions over successive cycles – each cycle comprising a return to the starting point a subsequent to the first visit to another point b) yields a somewhat better result: *the conclusions of Theorem* 2.6 *and Theorem* 2.7(b) *hold for all f such that* $\int f\,dm = 0$ *and* (3.2) *is finite* (see Theorem 9, p. 94; Theorem 10, p. 96 in Mandl (1968)). To illustrate this point take $\bar{m}(dz)=(1+z^4)^{-1}dz$, $f(z)=|z|^\delta - \int |z|^\delta\,\bar{m}(dz)/\bar{m}(S)$ for some $\delta\in(2,5/2)$. Then $\int |f(z)|^{3/2}\,m(dz)=\infty$, but (3.2) is finite.

Finally note that (if $\sigma_i=0$ $(i=0,1)$, in presence of boundaries) $\hat{A}$ is self-adjoint, so that $\sigma^2>0$ for $f\in\mathscr{R}_{\hat{A}}$, $f\neq 0$. Verifiable criteria for compactness of the resolvent operator $(\lambda-\hat{A})^{-1}$ is given in Itô and McKean (1965), p. 154. For maximal correlation to go to zero one only requires that 0 be an isolated point of the spectrum of $\hat{A}$.

Example 3. (*Diffusions on* R^k, $k\geq 2$.) Let $L=\frac{1}{2}\sum a_{ij}(x)\,\partial^2/\partial x_i\,\partial x_j + \sum b_i(x)\,\partial/\partial x_i$ be an elliptic operator, with $((a_{ij}(x)))$ positive definite for each x, the functions $a_{ij}(x)$ being continuous and $b_i(x)$ being Borel measurable and bounded on compacts. Sufficient conditions (as well as some necessary ones) for the diffusion generated by L to admit an invariant probability measure m are given in terms of the coefficients a_{ij}, b_i, in Khas'minskii (1960), and Bhattacharya (1978). For $k\geq 2$ diffusions are never point recurrent. It is proved in Bhattacharya and Ramasubramanian (1982), however, that in case an invariant probability measure m (necessarily unique) exists, the diffusion is m-recurrent, so that $\|p(t,x,dy)-m(dy)\|_v \to 0$ as $t\to\infty$. It is also not difficult to show that $\mathbb{D}_A$ contains all C^∞ functions with compact support, so that $\overline{\mathbb{D}_{\hat{A}}} = L^2(R^k, dm)$. Hence $\mathcal{R}_{\hat{A}}$ is dense in $1^\perp$. But, in general, $\mathcal{R}_{\hat{A}}$ is not closed. Hence one needs to find verifiable conditions on f guaranteeing that $f\in\mathcal{R}_{\hat{A}}$. These may be obtained by the methods used in [4]. From the point of view of the renewal method, conditions analogous to (3.2) are given in [4] (Theorem 2.9, relations (2.31), (2.32)). Again these conditions, in general, do not require that $f\in L^2(R^k, dm)$. The positivity of the variance for all nonzero $f\in\mathcal{R}_{\hat{A}}$ may be proved by deriving the following alternate expression for the variance. Let $\hat{A}g=f$. Then

$$\sigma^2 = \langle a \operatorname{grad} g, \operatorname{grad} g\rangle = \int_{R^k} \left(\sum_{i,j=1}^{k} a_{ij}(x) \frac{\partial g}{\partial x_i}\frac{\partial g}{\partial x_j}\right) m(dx). \tag{3.3}$$

To prove this assume that $a_{ij}(x)$ and $b_i(x)$ are Lipschitzian on compacts. Then by Itô's lemma (see McKean (1969), pp. 43–45) one has

$$E_m\left(g(X_t)-g(X_0)-\int_0^t f(X_s)\,ds\right)^2$$
$$= E_m \int_0^t \sum a_{ij}(X_s)\frac{\partial g}{\partial x_i}(X_s)\frac{\partial g}{\partial x_j}(X_s)\,ds = t\int \sum a_{ij}(x)\frac{\partial g}{\partial x_i}\frac{\partial g}{\partial x_j}(x)\,m(dx). \tag{3.4}$$

Example 4. (Diffusions on the the torus.) Let L be as in Example 3, but assume that the coefficients are periodic with period 1 in each coordinate. Let $\{X_t = (X_t^{(1)},\dots,X_t^{(k)})\}$ be the corresponding diffusion starting at some x. Define $Y_t^{(i)} = X_t^{(i)}$ (mod 1), $1\leqq i\leqq k$. Then $\{Y_t: t\geqq 0\}$ is a diffusion on the torus T^k (which may be identified with $[0,1)^k$ as a set). Let m be the invariant probability measure for this diffusion. One may write $b(X_t)=\beta(Y_t)$, $a^{1/2}(X_t)=\gamma(Y_t)$ for some β, γ. Then $Z_n(t)=n^{-1/2}\int_0^{nt}(b(X_s)-\int_{[0,1)^k} b\,dm)\,ds$ is asymptotically (as $n\to\infty$) a Wiener process with zero drift and dispersion matrix $\delta=((\delta_{ij}))$ given by

$$\delta_{ij} = \langle a \operatorname{grad} g_i, \operatorname{grad} g_j\rangle = \int_{[0,1)^k} \sum a_{i'j'}(x)\frac{\partial g_i}{\partial x_{i'}}\frac{\partial g_j}{\partial x_{j'}}\, m(dx), \tag{3.5}$$

where g_i is a periodic solution of

$$L g_i = b_i - \bar{b}_i = \tilde{b}_i \qquad (\bar{b}_i = \int b_i\,dm). \tag{3.6}$$

In a beautiful work using stochastic integrals Bensoussan, Lions and Papanicolau (1978), Chap. 3, have shown that $n^{-1/2}(X_{nt}-\bar{b}nt)$ converges in distribution to the Wiener process with zero drift and dispersion matrix D given by

$$D = \int_{[0,1)^k} \left(\frac{dg}{dx}-I\right) a(x) \left(\frac{dg}{dx}-I\right)' m(dx)$$
$$= \bar{a}+\delta-\theta, \tag{3.7}$$

where

$$\bar{a} = \int_{[0,1)^k} a(x)\,m(dx), \qquad \theta = \int_{[0,1)^k} \left(\frac{dg}{dx}\,a(x) + a(x)\left(\frac{dg}{dx}\right)'\right) m(dx). \tag{3.8}$$

In the stochastic integral representation,

$$n^{-1/2}(X_{nt}-n\bar{b}t)=n^{-1/2}X_0+Z_n(t)+U_n(t)\simeq Z_n(t)+U_n(t),$$
$$U_n(t)=n^{-1/2}\int_0^{nt} a^{1/2}(X_s)\,dB(s), \tag{3.9}$$

where $B(s)$ is standard Brownian motion. Although Z_n and U_n are asymptotically Gaussian with dispersions δ and $\bar{a}$, respectively, *they are not asymptotically independent.* In fact, for $k=1$ one easily checks that

$$\bar{a}=\frac{2}{\alpha}\int_0^1 \phi(x)\,dx, \qquad \delta=\frac{2}{\alpha}\left(\int_0^1 \phi(x)\,dx-\left(\int_0^1 \phi(x)^{-1}\,dx\right)^{-1}\right),$$
$$\theta=\frac{4}{\alpha}\left(\int_0^1 \phi(x)\,dx-\left(\int_0^1 \phi(x)^{-1}\,dx\right)^{-1}\right), \tag{3.10}$$

where $\phi(x)=\exp\left\{2\int_0^x a(y)^{-1}\tilde{b}(y)\,dy\right\}$, $\alpha=\int_0^1 2a(x)^{-1}\phi(x)\,dx$. Since the arithmatic mean $\int_0^1 \phi(x)\,dx$ is greater than the harmonic mean $\left(\int_0^1 \phi(x)^{-1}\,dx\right)^{-1}$ unless $\phi(x)\equiv 1$, i.e., $\tilde{b}\equiv 0$ (in which case $\delta=\theta=0$), in presence of a nonconstant drift one has $D>\bar{a}+\delta$. Also, no matter what the coefficients may be, $D<4\bar{a}$.

Example 5. (Diffusions with jumps.) Diffusions with jumps on $S=R^k$ are governed by certain linear integro-differential operators, one component of which is an elliptic operator and the other an integral operator governing (pure) jumps. They may be constructed by an extension of Itô's stochastic integration theory (see, e.g., Gihman and Skorohod (1968), Part II, Chaps. 1, 2). As is done in the case of multidimensional diffusions (e.g., in [3, 4, 16]), one may obtain upper and lower bounds to solutions of certain integro-differential equations to derive criteria for tightness and, thereby, of existence of invariant probability measures. For example, specializing Theorem 3, p. 333 of [11] to time independent coefficients and requiring that the elliptic operator be nondegenerate, in addition to the condition for the boundedness of the second moment already imposed, one can prove that the corresponding Markov process admits a unique invariant probability measure m, and that with this as the initial distribution, the process is ergodic. Theorem 2.1 may then be applied to functions f which are shown to belong to $\mathscr{R}_{\hat{A}}$ by a method analogous to that described in Example 3 and in [4]. The details will appear elsewhere. To obtain a central limit theorem when the process starts at an arbitrary initial distribution, one needs to prove the *strong Feller property:* $x\to p(t,x,B)$ is continuous for all Borel sets B and $t>0$. This is, in general, a difficult analytical problem.

We conclude with the remark that those central limit theorems which use mixing type conditions are generally not applicable to diffusions (or other Markov processes) on noncompact spaces. Even in the cases of one dimensional diffusions and birth and death processes it is not difficult to prove, via the so-called *inverse spectral problem* (see Dym and McKean (1976), Chaps.

5, 6), the existence of ergodic Markov processes having selfadjoint generators $\hat{A}$ with discrete spectra clustering near zero in such a manner that Rosenblatt's coefficient of strong mixing goes to zero more slowly than any (negative) power of t, as $t \to \infty$.

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Note Added in Proof. A better result than Proposition 2.3(c) is the following. Proposition 2.3(c′): *Suppose* 0 *is a simple eigenvalue of* $\hat{A}$. *Then* $\mathscr{R}_{\hat{A}}=\{1\}^{-}$ *if and only if* 0 *is an isolated point of the spectrum of* $\hat{A}$. To prove this note that if the simple eigenvalue 0 is an isolated point of the spectrum of $\hat{A}$ then $(\lambda-\hat{A})^{-1}$ has a Laurent series expansion $\lambda^{-1}B_1+\sum_{n=0}^{\infty}\lambda^n A_n$ in $\{0<|\lambda|<\lambda_0\}$ for some positive λ_0; here B_1 is the projection onto the null space of $\hat{A}$ (i.e., the space of constants), and A_n are bounded operators which annihilate constants and satisfy $A_n=(-1)^n A_0^{n+1}$. It follows that on $\{1\}^{\perp}$ one has $(\lambda-\hat{A})^{-1}=\sum_{n=0}^{\infty}\lambda^n A_n$, convergent for $|\lambda|<x_0$. In particular, $-\hat{A}^{-1}=A_0$ is bounded on $\{1\}^{\perp}$. Conversely, suppose $\mathscr{R}_{\hat{A}}=\{1\}^{\perp}$. Then $\hat{A}^{-1}$ is bounded on $\{1\}^{\perp}$; hence 0 is in the resolvent set of $\tilde{A}$ which is the restriction of $\hat{A}$ to $\{1\}^{\perp}$. Since the resolvent set is open, there exists $\lambda_0>0$ such that $(\lambda-\tilde{A})^{-1}$ is bounded for $|\lambda|<\lambda_0$. Since $(\lambda-\hat{A})^{-1}$ is bounded on the span of $\{1\}$ for $\lambda\neq 0$, it follows that $(\lambda-\hat{A})^{-1}$ is bounded for $0<|\lambda|<\lambda_0$.

7.3 "A central limit theorem for diffusions with periodic coefficients"

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A CENTRAL LIMIT THEOREM FOR DIFFUSIONS WITH PERIODIC COEFFICIENTS[1]

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It is proved that if X_t is a diffusion generated by the operator $L = \frac{1}{2} \sum a_{ij}(x)\partial^2/\partial x_i \partial x_j + \sum u_0 b_i(x)\partial/\partial x_i$ having periodic coefficients, then $\lambda^{-1/2}(X_{\lambda t} - \lambda u_0 \bar{b} t)$, $t \geq 0$, converges in distribution to a Brownian motion as $\lambda \to \infty$. Here $\bar{b}$ is the mean of $b(x) = (b_1(x), \cdots, b_k(x))$ with respect to the invariant distribution for the diffusion induced on the torus $T^k = [0, 1)^k$. The dispersion matrix of the limiting Brownian motion is also computed. In case $\bar{b} = 0$ this result was obtained by Bensoussan, Lions and Papanicolaou (1978). (See Theorem 4.3, page 401, as well as the author's remarks on page 529.) The case $\bar{b} \neq 0$ is of interest in understanding how solute dispersion in a porous medium behaves as the liquid velocity increases in magnitude.

1. The limit theorem. Let $L = \frac{1}{2} \sum_{i,j=1}^k a_{ij}(x)\partial^2/\partial x_i \partial x_j + \sum_{i=1}^k u_0 b_i(x)\partial/\partial x_i$ be a differential operator ($k \geq 1$), whose coefficients satisfy the following assumptions.

Assumptions. (1) *For each* x *the* $(k \times k)$ *matrix* $((a_{ij}(x)))$ *is symmetric and positive definite*; (2) *the functions* $a_{ij}(x)$, $b_i(x)$ *are real valued and periodic, i.e.,* $a_{ij}(x + \nu) = a_{ij}(x)$, $b_i(x + \nu) = b_i(x)$ *for all* x *and all vectors* ν *with integers as coordinates* $(1 \leq i, j \leq k)$; (3) *the functions* $a_{ij}(x)$ *have bounded second order derivatives, and* $b_i(x)$ *have continuous first order derivatives*; (4) u_0 *is a real parameter.*

Let $(\Omega, \mathscr{A}, P^{\pi'})$ be a probability space on which are defined (1) a random vector X_0 with values in $\mathbb{R}^k$ and distribution π', and (2) a standard k-dimensional *Brownian motion* $\{B_t = (B_t^{(1)}, \cdots, B_t^{(k)}): t \geq 0\}$ which is independent of X_0. In case $\pi'(\{x\}) = 1$, $P^{\pi'}$ will also be denoted by P^x. $E^{\pi'}$ denotes *expectation* under $P^{\pi'}$.

Let $\{X_t: t \geq 0\}$ be the solution (continuous, nonanticipative) to Itô's stochastic integral equation

$$(1.1) \quad X_t = X_0 + \int_0^t u_0 b(X_s)\, ds + \int_0^t \sigma(X_s)\, dB_s, \quad (X_t = (X_t^{(1)}, \cdots, X_t^{(k)})),$$

where $\sigma(x)$ is the positive square root of $((a_{ij}(x)))$. The $P^{\pi'}$*-distribution* of $\{X_t: t \geq 0\}$ is a probability measure on (the Borel sigmafield of) the space $C([0, \cdots): \mathbb{R}^k)$ of continuous functions on $[0, \infty)$ into $\mathbb{R}^k$, endowed with the topology of uniform convergence on compact subsets of $[0, \infty)$. Note that

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$\{X_t: t \geq 0\}$ is a Markov process. Let $p(t, x, y)$ be the transition probability density (with respect to Lebesgue measure on $\mathbb{R}^k$) of this Markov process. Because of periodicity of the coefficients one has

$$(1.2) \qquad p(t; x, y) = p(t; x + \nu, y + \nu)$$

for every vector ν with integral coordinates.

We shall write

$$(1.3) \qquad \dot{x} = (x^{(1)}(\text{mod } 1), \cdots, x^{(k)}(\text{mod } 1)) \quad (x = (x^{(1)}, \cdots, x^{(k)}) \in \mathbb{R}^k),$$

$$(1.4) \qquad \dot{X}_t = X_t(\text{mod } 1) = (X_t^{(1)}(\text{mod } 1), \cdots, X_t^{(k)}(\text{mod } 1))$$

In view of (1.2), $\dot{X}_t$ is a Markov process on the state space $T^k = [0, 1)^k$ having the transition probability density function (with respect to Lebesgue measure on $[0, 1)^k$)

$$(1.5) \qquad \dot{p}(t; x, y) = \sum_{\nu \in \mathbb{Z}^k} p(t; x, y + \nu), \quad (x, y \in [0, 1)^k).$$

Assumptions (1)–(3) imply, by the maximum principle (Friedman, 1975, Chapter 6),

$$(1.6) \qquad \inf_{x,y \in [0,1]^k} p(t; x, y) > 0, \quad (t > 0).$$

Therefore,

$$(1.7) \qquad \inf_{x,y \in [0,1)^k} \dot{p}(t; x, y) > 0, \quad (t > 0).$$

This implies Döblin's condition and irreducibility (Doob, 1953, Theorem 2.1, page 256; Bensoussan, Lions and Papanicolaou, 1978, Theorem 3.2, page 373), and the existence of a probability density $\pi(x)$ on $[0, 1)^k$ and positive constants c, β such that

$$(1.8) \qquad \int_{[0,1)^k} \dot{p}(t; x, y)\pi(x)\, dx = \pi(y) \quad \text{a.e.} \quad (dy) \quad \text{on} \quad [0, 1)^k$$

and

$$(1.9) \qquad \sup_{x \in [0,1)^k} \int_{[0,1)^k} |\dot{p}(t; x, y) - \pi(y)|\, dy \leq ce^{-\beta t} \quad (t > 0)$$

The following proposition is easy to prove.

PROPOSITION 1. *The P^x-distribution of $\{X_t - x: t \geq 0\}$ is the same as the $P^{\dot{x}}$-distribution of $\{X_t - \dot{x}: t \geq 0\}$.*

Next consider the discrete parameter stochastic process

$$(1.10) \qquad Y_m \doteq X_m - X_{m-1} \qquad (m = 1, 2, \cdots).$$

Denote by $\mathscr{F}_t$ the sigmafield generated by $\{X_s: 0 \leq s \leq t\}$. By the Markov property and Proposition 1, the conditional distribution of the stochastic process $\{X_{m+n-1} - X_{n-1}: m = 1, 2, \cdots\}$ given $\mathscr{F}_{n-1}$ is the same as the $P^{\dot{x}}$-distribution of $\{X_m - \dot{x}: m = 1, 2, \cdots\}$ with $x = X_{n-1}$. But $\{\dot{X}_m: m = 0, 1, 2, \cdots\}$ is a *stationary* *sequence* under P^π. Hence the (unconditional) P^π-distribution of $\{X_{m+n-1} - X_{n-1}: m = 1, 2, \cdots\}$ equals the P^π-distribution of $\{X_m - \dot{X}_0: m = 1, 2, \cdots\}$. In particular, the P^π-distribution of $\{Y_{m+n-1} = (X_{m+n-1} - X_{n-1}) - (X_{m-1+n-1} - X_{n-1}): m = 1, 2, \cdots\}$ is the same as the P^π-distribution of $\{Y_m = (X_m - \dot{X}_0) - (X_{m-1} - \dot{X}_0): m = 1, 2, \cdots\}$. This proves that $\{Y_m: m = 1, 2, \cdots\}$ is a *stationary sequence* under P^π.

Now let B be a Borel subset of $(\mathbb{R}^k)^{\mathbb{Z}^+}$, where $\mathbb{Z}^+ = \{1, 2, \cdots\}$. Then

$$\begin{aligned} &P^\pi(\{Y_{m+n+j}: j = 1, 2, \cdots\} \in B)/\mathcal{F}_m \\ &\quad = E^\pi(P^{\dot{X}_{m+n}}(\{Y_j: j = 1, 2, \cdots\} \in B)/\mathcal{F}_m) \\ &\quad = E^\pi(f(\dot{X}_{m+n})/\mathcal{F}_m) = E^\pi(f(\dot{X}_{m+n})/\dot{X}_m), \end{aligned} \tag{1.11}$$

where $f(x) = P^x(\{Y_j: j = 1, 2, \cdots\} \in B)$. By (1.8), (1.9)

$$\begin{aligned} &|E(f(\dot{X}_{m+n})/\dot{X}_m) - E^\pi f(\dot{X}_{m+n})| \\ &\quad = \left| \int_{[0,1)^k} f(y)\dot{p}(n; \dot{X}_m, y)\, dy - \int_{[0,1)^k} f(y)\pi(y)\, dy \right| \\ &\quad \le c\, \|f\|_\infty e^{-\beta n} \le ce^{-\beta n}. \end{aligned} \tag{1.12}$$

Combining (1.11), (1.12) and recalling the definition of ϕ-mixing (Billingsley, 1968, page 166) one arrives at the following result.

PROPOSITION 2. *Under P^π the sequence $\{Y_m: m = 1, 2, \cdots\}$ defined by* (1.10) *is stationary and ϕ-mixing, with a ϕ-mixing coefficient which decays to zero exponentially fast.*

Consider the real Hilbert space $L^2([0, 1)^k, \pi)$ with inner product and norm

$$\langle f, g\rangle = \int_{[0,1)^k} f(y)g(y)\pi(y)\, dy, \quad \|f\| = (\langle f, f\rangle)^{1/2}. \tag{1.13}$$

Let $\{\dot{T}_t: t > 0\}$ be the strongly continuous semigroup of contractions on this space defined by

$$(\dot{T}_t f)(x) = \int_{[0,1)^k} \dot{p}(t; x, y,)f(y)\, dy, \quad (x \in [0, 1)^k). \tag{1.14}$$

Let $\hat{A}$ be the infinitesimal generator of this semigroup on the domain $\mathcal{D}_{\hat{A}}$. Let $\mathcal{R}_{\hat{A}}$ be the range of $\hat{A}$. Then $\mathcal{R}_{\hat{A}} = 1^\perp$, the set of all functions f in $L^2([0, 1)^R, \pi)$ such that $\langle f, 1\rangle = 0$, and given any $f \in 1^\perp$ there exists a unique element g in $\mathcal{D}_{\hat{A}} \cap 1^\perp$ such that (Bhattacharya, 1982, Theorem 2.1 and Remark 2.3.1)

$$\hat{A}_g = f, \quad g(x) = -\int_0^\infty (\dot{T}_t f)(x)\, dt. \tag{1.15}$$

We will denote this element by $\hat{A}_{1^\perp}^{-1} f$:

$$g = \hat{A}_{1^\perp}^{-1} f. \tag{1.16}$$

Now write

$$\bar{b}_i = \langle b_i, 1\rangle, \quad \bar{b} = (\bar{b}_1, \cdots, \bar{b}_k),$$
$$(1.17) \qquad \bar{a}_{ij} = \langle a_{ij}, 1\rangle, \quad \bar{a} = ((\bar{a}_{ij})),$$
$$g_i = \hat{A}_1^{-1}(b_i - \bar{b}_i), \quad (1 \le i \le k).$$

Under Assumptions (1)–(4), g_i is (equivalent to) a twice continuously differentiable function, when extended to $\mathbb{R}^k$ periodically, and $\pi(y)$ is a continuously differentiable periodic function (Bensoussan et al., 1978, 386–401).

The main result of this article may be stated as follows.

THEOREM 3. *Under Assumptions* (1)–(4), *no matter what the initial distribution* π' *is, the stochastic process*

$$(1.18) \qquad \{Z_{t,\lambda} \doteq \lambda^{-1/2}(X_{\lambda t} - \lambda u_0 t\bar{b}) : t \ge 0\}$$

converges weakly, as $\lambda \to \infty$, *to a Brownian motion with zero drift and dispersion matrix* $D = ((D_{ij}))$ *given by*

$$D_{ij} = -u_0^2\langle b_i, g_j\rangle - u_0^2\langle b_j, g_i\rangle + \bar{a}_{ij}$$
$$(1.19) \qquad + \int_{[0,1)^k} u_0\left\{g_i(y) \sum_{r=1}^k \frac{\partial}{\partial y_r}(a_{rj}(y)\pi(y)) + g_j(y) \sum_{r=1}^k \frac{\partial}{\partial y_r}(a_{ri}(y)\pi(y))\right\} dy.$$

PROOF. First let the initial distributions be $\pi(x)\,dx$. Write

$$S_n = Y_1 + \cdots + Y_n - nu_0\bar{b} = \sum_{m=1}^n (Y_m - u_0\bar{b}) = X_n - X_0 - nu_0\bar{b},$$
$$(1.20) \qquad W_{t,n} = \frac{S[nt]}{\sqrt{n}} + \frac{(t - ([nt]/n))Y_{[nt]+1}}{\sqrt{n}},$$

where $[nt]$ is the integer part of nt. Then, in view of Proposition 2, $\{W_{t,n} : t \ge 0\}$ converges in distribution to a Brownian motion with zero drift, as $n \to \infty$. (See Billingsley, 1968, Theorem 20.1, page 174, where the result is stated for $W'_{t,n} = S_{[nt]}/\sqrt{n}$. It is easy to check that $\max\{|W_{t,n} - W'_{t,n}| : 0 \le t \le T\} \to 0$ in probability for every $T > 0$.)

Now, fix a $T > 0$ arbitrarily and note that

$$\max_{0 \le t < T} |W_{t,n} - Z_{t,n}|$$
$$(1.21) \qquad \le \frac{|X_0| + |u_0\bar{b}|}{\sqrt{n}} + \frac{1}{\sqrt{n}} \max_{1 \le m \le [nT]} \max_{0 \le t' \le 1} |X_{m+t'} - X_m - t'u_0\bar{b}|.$$

The sequence $\max\{|X_{m+t'} - X_m - t'u_0\bar{b}| : 0 \le t' \le 1\}$ is stationary. Also, the exponential martingale inequality (Friedman, 1975, page 93) may be used to prove that the common distribution of this sequence has finite moments of all orders. Chebyshev's inequality may be used now to show that the last summand on the right side of (1.21) converges to zero in probability, as $n \to \infty$. Hence $\{Z_{t,n}: t \geq 0\}$ converges in distribution to a Brownian motion.

Now let the initial distribution be π', different from π. In view of (1.12) one has

$$\text{(1.22)}\qquad \lim_{m\to\infty}\sup_B |P^{\pi'}(\{Y_{m+j}: j = 1, 2, \cdots\} \in B) - P^{\pi}(\{Y_{m+j}: j = 1, 2, \cdots\} \in B)| = 0,$$

where the supremum is taken over all Borel subsets B of $(\mathbb{R}^k)^{\mathbb{Z}^+}$.

Define

$$\text{(1.23)}\qquad \begin{aligned} S_{m,n} &= Y_{m+1} + \cdots + Y_{m+n} - nu_0\bar{b}, \\ W_{t,m,n} &= \frac{S_{m,[nt]}}{\sqrt{n}} + \frac{(t - ([nt]/n))Y_{m+[nt]+1}}{\sqrt{n}}. \end{aligned}$$

It follows from (1.22) that the (variation) norm distance between the measures induced by $W_{t,n}$ under P^{π} and $W_{t,m,n}$ under $P^{\pi'}$ (on $C([0, \infty): \mathbb{R}^k)$) goes to zero as $m \to \infty$, *uniformly for all* n. Also for every positive integer m and every $T > 0$, whatever the initial distribution π',

$$\text{(1.24)}\qquad \begin{aligned} &\max_{0\le t\le T} |W_{t,m,n} - W_{t,n}| \\ &\le \frac{1}{\sqrt{n}} \max_{1\le r\le[nT]} |Y_r + Y_{r+1} + \cdots + Y_{r+m-1}| \\ &\quad + \frac{m|\bar{b}|u_0}{\sqrt{n}} \to 0 \quad \text{in probability as} \quad n \to \infty, \end{aligned}$$

by the same type of moment estimates as used for (1.21). If ψ is a real bounded continuous function on $C([0, \infty): \mathbb{R}^k)$, then by (1.24),

$$\text{(1.25)}\qquad \begin{aligned} &\limsup_{n\to\infty} |E^{\pi'}\psi(W_{t,n}) - E^{\pi}\psi(W_{t,n})| \\ &\le \limsup_{n\to\infty} |E^{\pi'}\psi(W_{t,n}) - E^{\pi'}\psi(W_{t,m,n})| \\ &\quad + \limsup_{n\to\infty} |E^{\pi'}\psi(W_{t,m,n}) - E^{\pi}\psi(W_{t,n})| \\ &= \limsup_{n\to\infty} |E^{\pi'}\psi(W_{t,m,n}) - E^{\pi}\psi(W_{t,n})|. \end{aligned}$$

But the last expression in (1.25) goes to zero as $m \to \infty$. The proof of convergence to a Brownian motion is completed by observing that $\max\{|Z_{t,\lambda} - Z_{t,[\lambda]}|: 0 \le t \le T\}$ goes to zero for every sample point, as $\lambda \to \infty$.

It remains to compute D_{ij}. Let us first show that $\{|Z_{1,\lambda}|^2: \lambda \ge 1\}$ is uniformly integrable with respect to P^{π}. One has

$$\text{(1.26)}\qquad \begin{aligned} E^{\pi}|Z_{1,\lambda}^{(i)}|^4 &= \lambda^{-2}E^{\pi}\left(u_0 \int_0^{\lambda} b_i(X_s)\,ds + \int_0^{\lambda} \textstyle\sum_{r=1}^k \sigma_{ir}(X_s)\,dB_s^{(r)} + X_0^{(i)} - u_0\lambda\bar{b}_i\right)^4 \\ &\le \lambda^{-2}3^3\left\{E^{\pi}(X_0^{(i)})^4 + u_0^4E^{\pi}\left(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\,ds\right)^4 \right. \\ &\qquad \left. + E^{\pi}\left(\int_0^{\lambda} \textstyle\sum_{r=1}^k \sigma_{ir}(X_s)\,dB_s^{(r)}\right)^4\right\}. \end{aligned}$$

It is known that (McKean, 1969, page 40)

$$E^{\pi}\left(\int_0^{\lambda} \sum_{r=1}^{k} \sigma_{ir}(X_s)\, dB_s^{(r)}\right)^4 \leq c_1\lambda^2 \tag{1.27}$$

for some c_1 which does not depend on λ. Also, writing $f(x) = b_i(x) - \bar{b}_i$, one has

$$\begin{aligned} E^{\pi}\left(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\, ds\right)^4 &= E^{\pi}\left(\int_0^{\lambda} f(X_s)\, ds\right)^4 \\ &= 24 \int_0^{\lambda}\int_{s_1}^{\lambda}\int_{s_2}^{\lambda}\int_{s_3}^{\lambda} E^{\pi} f(\dot{X}_{s_1}) f(\dot{X}_{s_2}) f(\dot{X}_{s_3}) f(\dot{X}_{s_4})\, ds_4\, ds_3\, ds_2\, ds_1 \\ &= 24 \int_0^{\lambda}\int_{s_1}^{\lambda}\int_{s_2}^{\lambda}\int_{s_3}^{\lambda} \langle f, \dot{T}_{s_2-s_1} f(\dot{T}_{s_3-s_2}(f(\dot{T}_{s_4-s_3} f)))\rangle\, ds_4\, ds_3\, ds_2\, ds_4 \\ &\leq 24 \int_0^{\lambda}\int_{s_1}^{\lambda}\int_{s_2}^{\lambda}\int_{s_3}^{\lambda} 2c^2 \|f\| \cdot \|f\|_{\infty}^3 e^{-\beta(s_2-s_1)} e^{-\beta(s_4-s_3)}\, ds_4\, ds_3\, ds_2\, ds_1. \end{aligned} \tag{1.28}$$

The last inequality follows from (1.12) (with n replaced by s):

$$\begin{aligned} \|\dot{T}_s f\|_{\infty} &= \sup_x |\dot{T}_s f(x)| \leq c\|f\|_{\infty} e^{-\beta s}, \\ |\langle f, \dot{T}_s g\rangle| &= |\langle f, \dot{T}_s(g - E^{\pi}g)\rangle| \leq \|f\|\ \|\dot{T}_s(g - E^{\pi}g)\| \\ &\leq c\|f\| \cdot 2\|g\|_{\infty} e^{-\beta s}, \end{aligned} \tag{1.29}$$

applied first to $g = f(\dot{T}_{s_3-s_2}(f(\dot{T}_{s_4-s_3})))$ and $s = s_2 - s_1$, and then to $g = f$ and $s = s_4 - s_3$. A straightforward evaluation of the last multiple integral in (1.28) yields

$$E^{\pi}\left(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\, ds\right)^4 \leq c_2\lambda^2, \tag{1.30}$$

where c_2 does not depend on λ. Using (1.27), (1.30) in (1.26) one gets the desired uniform integrability. It now follows that

$$\begin{aligned} D_{ij} &= \lim_{\lambda\to\infty} E^{\pi} Z_{1,\lambda}^{(i)} Z_{1,\lambda}^{(j)} \\ &= \lim_{\lambda\to\infty} \frac{1}{\lambda}\Bigg[u_0^2 E^{\pi}\left(\int_0^{\lambda} (b_i(\dot{X}_s) - \bar{b}_i)\, ds \cdot \int_0^{\lambda} (b_j(\dot{X}_s) - \bar{b}_j)\, ds\right) \\ &\quad + u_0 E^{\pi}\left(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\, ds \cdot \int_0^{\lambda} \sum_{r=1}^{k} \sigma_{jr}(X_s)\, dB_s^{(r)}\right) \\ &\quad + u_0 E^{\pi}\left(\int_0^{\lambda} (b_j(X_s) - \bar{b}_j)\, ds \cdot \int_0^{\lambda} \sum_{r=1}^{k} \sigma_{ir}(X_s)\, dB_s^{(r)}\right) \\ &\quad + E^{\pi}\left(\int_0^{\lambda} \sum_{r=1}^{k} \sigma_{ir}(X_s)\, dB_s^{(r)} \cdot \int_0^{\lambda} \sum_{r=1}^{k} \sigma_{jr}(X_s)\, dB_s^{(r)}\right)\Bigg] \end{aligned} \tag{1.31}$$

By Theorem 2.1 and Remark 2.3.1 in Bhattacharya (1982) and relation (1.30) one has

$$(1.32)\quad \begin{aligned} &\lim_{\lambda\to\infty} \frac{u_0^2}{\lambda} E^{\pi}\left(\int_0^{\lambda} (b_i(\dot{X}_s) - \bar{b})\, ds \cdot \int_0^{\lambda} (b_j(\dot{X}_s) - \bar{b}_j)\, ds\right) \\ &\quad = u_0^2(\langle -b_i - \bar{b}_i, g_j\rangle + \langle -b_j - \bar{b}_j, g_i\rangle) = -u_0^2(\langle b_i, g_j\rangle + \langle b_j, g_i\rangle). \end{aligned}$$

Also, from a standard result in stochastic integrals (Friedman, 1975, Chapter 4),

$$(1.33)\quad \begin{aligned} &E^{\pi}\left(\int_0^{\lambda} \textstyle\sum_{r=1}^k \sigma_{ir}(X_s)\, dB_s^{(r)} \cdot \int_0^{\lambda} \sum_{r=1}^k \sigma_{jr}(X_s)\, dB_s^{(r)}\right) \\ &\quad = \int_0^{\lambda} E^{\pi}(\textstyle\sum_{r=1}^k \sigma_{ir}(\dot{X}_s)\sigma_{jr}(\dot{X}_s))\, ds = \int_0^{\lambda} \bar{a}_{ij}\, ds = \lambda \bar{a}_{ij}. \end{aligned}$$

It remains to estimate the second and third terms in (1.31). For this estimation we make use of the definition of stochastic integrals as limits (at least in L^2 w.r.t. the product measure $P^{\pi} \times ds$ on $\Omega \times [0, \lambda]$). One has

$$(1.34)\quad \begin{aligned} &\textstyle\sum_{r=1}^k E^{\pi}\left(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\, ds \cdot \int_0^{\lambda} \sigma_{jr}(X_s)\, dB_s^{(r)}\right) \\ &\quad = \textstyle\sum_{r=1}^k E^{\pi}\left(\int_0^{\lambda} \left((b_i(X_t) - \bar{b}_i) \int_0^{t} \sigma_{jr}(X_s)\, dB_s^{(r)}\right) dt\right), \end{aligned}$$

using the orthogonality of $b_i(X_t) - \bar{b}_i$ and the stochastic integral over $[t, \lambda]$. Fix $\varepsilon > 0$, sufficiently small. Then

$$(1.35)\quad \begin{aligned} &E^{\pi}\left(\int_0^{\lambda} \left((b_i(X_t) - \bar{b}_t)\left(\int_{(t-\varepsilon)\vee 0}^{t} \sigma_{jr}(X_s)\, dB_s^{(r)}\right) dt\right)\right)^2 \\ &\quad \le E^{\pi}\left(2 \sup\{|b_i(x)| : x \in \mathbb{R}^k\} \cdot \left(\int_0^{\lambda} \left| \int_{(t-\varepsilon)\vee 0}^{t} \sigma_{jr}(X_s)\, dB_s^{(r)} \right| dt\right)\right)^2 \\ &\quad \le c_3 E^{\pi}\left(\int_0^{\lambda} \left| \int_{(t-\varepsilon)\vee 0}^{t} \sigma_{jr}(X_s)\, dB_s^{(r)} \right| dt\right)^2 \\ &\quad \le c_3 \lambda E^{\pi}\left(\int_0^{\lambda} \left(\int_{(t-\varepsilon)\vee 0}^{t} \sigma_{jr}(X_s)\, dB_s^{(r)}\right)^2 dt\right) \\ &\quad = c_3 \lambda \int_0^{\lambda} \left(\int_{(t-\varepsilon)\vee 0}^{t} (E^{\pi}\sigma_{jk}^2(X_s))\, ds\right) dt \le c_4 \lambda^2 \varepsilon \end{aligned}$$

for appropriate positive constants c_2, c_4. It is, therefore, enough to evaluate the last expression in (1.34) with t replaced by $t - \varepsilon$. Now, writing $E^x f(X_t) = T_t f(x)$,

one has

$$\sum_{r=1}^{k} E^{\pi}\left(\int_0^{\lambda}\left((b_i(X_t)-\bar{b}_i)\int_0^{t-\varepsilon}\sigma_{jr}(X_s)\,dB_s^{(r)}\right)dt\right)$$

$$= \sum_{r=1}^{k}\lim_{h\downarrow 0}E^{\pi}\left(\int_0^{\lambda}(b_i(X_t)-\bar{b}_i)\{\textstyle\sum_{m=0}^{[(t-\varepsilon)/h]}\sigma_{jr}(X_{mh})\right.$$

$$(1.36)\qquad \left.(B_{(m+1)h}^{(r)}-B_{mh}^{(r)})\}\,dt\right)$$

$$= \sum_{r=1}^{k}\lim_{h\downarrow 0}E^{\pi}\left(\int_0^{\lambda}\{\textstyle\sum_{m=0}^{[(t-\varepsilon)/h]}T_{t-(m+1)h}(b_i-\bar{b}_i)(X_{(m+1)h})\right.$$

$$\left.\cdot\,\sigma_{jr}(X_{mh})(B_{(m+1)h}^{(r)}-B_{mh}^{(r)})\}\,dt\right).$$

By Itô's lemma (Friedman, 1975, page 90) one has

$$T_{t(m+1)h}(b_i-\bar{b}_i)(X_{(m+1)h})$$

$$= T_{t-(m+1)h}(b_i-\bar{b}_i)(X_{mh})$$

$$(1.37)\qquad +\int_{mh}^{(m+1)h}LT_{t-(m+1)h}(b_i-\bar{b}_i)(X_s)\,ds$$

$$+\int_{mh}^{(m+1)h}\operatorname{grad}T_{t-(m+1)h}(b_i-\bar{b}_i)(X_s)\sigma(X_s)\,dB_s.$$

Now $(t', x)\to LT_{t'}(b_i-\bar{b}_i)(x)$ is bounded on $[\varepsilon/2, \lambda]\times\mathbb{R}^k$, since this function is continuous on $[\varepsilon/2, \lambda]\times\mathbb{R}^k$ (Friedman, 1975, Chapter 6) and periodic in x. Hence, for $h<\varepsilon/2$, the first integral in (1.37) is bounded above by c_5h. Also,

$$x\to\operatorname{grad}T_{t'}(b_i-\bar{b}_i)(x)$$

is differentiable with a derivative which is continuous on $[\varepsilon/2, \lambda]\times\mathbb{R}^k$. Since this derivative is also periodic, the second integrand in (1.37) differs from

$$\operatorname{grad}T_{t-(m+1)h}(b_i-\bar{b}_i)(X_{mh})\sigma(X_{mh})$$

by a quantity smaller than c_6h. Therefore, the second integral differs from

$$\operatorname{grad}T_{t-(m+1)h}(b_i-\bar{b}_i)(X_{mh})\sigma(X_{mh})(B_{(m+1)h}-B_{mh})$$

by a quantity whose square has expectation less than c_7h^2. In view of this it is easy to check that (1.36) equals

$$\lim_{h\downarrow 0} \sum_{r=1}^{k} \int_0^{\lambda} E^{\pi}\Big\{\sum_{m=0}^{[(t-\varepsilon)/h]} \Big[\sum_{r'=1}^{k} \Big(\frac{\partial}{\partial x_{r'}} T_{t-(m+1)h}(b_i - \bar{b}_i)\Big)(X_{mh})$$

$$\times \Big(\sum_{r''=1}^{k} \sigma_{r'r''}(X_{mh})(B^{(r'')}_{(m+1)h} - B^{(r'')}_{mh})\Big)\Big]\sigma_{jr}(X_{mh})(B^{(r)}_{(m+1)h} - B^{(r)}_{mh})\Big\}\, dt$$

$$= \lim_{h\downarrow 0} \sum_{r=1}^{k} \int_0^{\lambda} E^{\pi}\Big\{\sum_{m=0}^{[(t-\varepsilon)/h]} \Big[\sum_{r'=1}^{k} \Big(\frac{\partial}{\partial x_{r'}} T_{t-(m+1)h}(b_i - \bar{b}_i)\Big)(X_{mh})$$

$$\times \sigma_{r'r}(X_{mh})\sigma_{jr}(X_{mh})(B^{(r)}_{(m+1)h} - B^{(r)}_{mh})^2\Big]\Big\}\, dt$$

(1.38)
$$= \int_0^{\lambda} \int_0^{t-\varepsilon} \Big(\sum_{r'=1}^{k} E^{\pi}\Big\{\Big(\frac{\partial}{\partial x_{r'}} T_{t-s}(b_i - \bar{b})\Big)(X_s) a_{jr'}(X_s)\Big\}\Big)\, ds\, dt$$

$$= \int_0^{\lambda} \int_0^{t-\varepsilon} \Big[\sum_{r'=1}^{k} \int_{[0,1)^k} \Big(\frac{\partial}{\partial x_{r'}} T_{t-s}(b_i - \bar{b}_i)\Big)(x) a_{jr'}(x)\pi(x)\, dx\Big]\, ds\, dt$$

$$= -\int_0^{\lambda} \int_0^{t-\varepsilon} \Big[\sum_{r'=1}^{k} \int_{[0,1)^k} T_{t-s}(b_i - \bar{b}_i)(x) \frac{\partial}{\partial x_{r'}} (a_{jr'}(x)\pi(x))\, dx\Big]\, ds\, dt$$

$$= -\int_0^{\lambda} \Big\{\int_{[0,1)^k} \Big(\int_0^{t-\varepsilon} T_{t-s}(b_i - \bar{b}_i)(x)\, ds\Big)\Big(\sum_{r'=1}^{k} \frac{\partial}{\partial x_{r'}} (a_{jr'}(x)\pi(x))\Big)\, dx\Big\}\, dt.$$

Since

$$\int_0^{t-\varepsilon} T_{t-s}(b_i - \bar{b}_i)(x)\, ds$$

(1.39)
$$= \int_{\varepsilon}^{t} T_s(b_i - \bar{b}_i)(x)\, ds$$

$$= \int_{\varepsilon}^{t} \dot{T}_s(b_i - \bar{b}_i)(x)\, ds \to -g_i(x) - \int_0^{\varepsilon} \dot{T}_s(b_i - \bar{b}_i)(x)\, ds,$$

uniformly in $x \in [0, 1)^k$ as $t \to \infty$, (1.38), (1.35), (1.34) yield

(1.40)
$$\lim_{\lambda\to\infty} \frac{1}{\lambda} \sum_{r=1}^{k} E^{\pi}\Big(\int_0^{\lambda} (b_i(X_s) - \bar{b}_i)\, ds \cdot \int_0^{\lambda} \sigma_{jr}(X_s)\, dB_s^{(r)}\Big)$$

$$= \int_{[0,1)^k} g_i(x)\Big(\sum_{r'=1}^{k} \frac{\partial}{\partial x_{r'}} (a_{jr'}(x)\pi(x))\Big)\, dx.$$

Using (1.32), (1.33), and (1.40) in (1.31) one obtains the desired result (1.19). Q.E.D.

Extensions. I. The functional central limit theorem proved above holds if Assumption (3) is replaced by (3′): $a_{ij}(x)$ *are continuous and* $b_i(x)$ *are Borel* *measurable and bounded.* The proof of convergence to a Brownian motion may be carried out as above. An alternative proof in this case may also be given by the renewal method (see Bhattacharya and Ramasubramanian, 1982). In computing D_{ij} all the steps can be justified, except (1.40). This is the main reason why the smoothness assumption (3) was made.

II. Let B_ν be an open ball of radius r with center at the (lattice) point ν, where $0 < r < ½$. Let $B = UB_\nu$, the union being over all ν in $\mathbb{Z}^k$. Consider the diffusion on $\mathbb{R}^k\backslash B$ whose transition probability density function $p(t; x, y)$ satisfies the equation $\partial p/\partial t = Lp$ in the interior and a Neumann boundary condition on ∂B (e.g., vanishing of the conormal derivative $\sum_{i,j=1}^{k} (x_i - \nu_i)a_{ij}(x)\partial p/\partial x_j$ on ∂B). If $\{X_t: t \geq 0\}$ is this diffusion, then $\{\dot{X}_t: t \geq 0\}$ is a diffusion on $T^k\backslash\dot{B}$, where $\dot{B}$ is the image of B under the map $x \to \dot{x}$. The diffusion on the torus is ergodic and its transition probability density $p(t; x, y)$ is bounded away from zero (for each $t > 0$). Therefore, Propositions 1, 2 carry over to this case, and as a consequence so does the first part of the proof of Theorem 3. Hence $\{\lambda^{-1/2}(X_{\lambda t} - \lambda u_0 t\bar{b}): t \geq 0\}$ converges to a Brownian motion with zero drift, as $\lambda \to \infty$. Here $\bar{b}_i = \int_{T^k\backslash\dot{B}} b_i(x)\pi(x)dx$, $\pi(x)\,dx$ being the invariant probability for $\dot{p}$.

2. Concluding remarks. Suppose the diffusion matrix is αI, where α is a positive constant and I is the $k \times k$ identity matrix. Suppose also that $\text{div}\, b(x) = 0$ for all x. In this case $\pi(x) \equiv 1$, i.e., the invariant distribution is the uniform distribution on the torus. In various examples of this type numerical computation of the diagonal elements D_{ii} of the dispersion matrix D, using (1.19), shows that D_{ii} increase with u_0; at first approximately quadratically, and then at higher values possibly at a linear rate. These computations as well as their significance in modelling solute transport in porous media will appear in Bhattacharya and Gupta (1984). However, D can be explicitly computed for the case $k = 1$ for general periodic functions $b(x)$ and $a(x) > 0$; this computation shows that D *goes to zero* as $u_0 \to \infty$. This is not really a great surprise. For, in the one dimensional case, as u_0 increases $\dot{X}_t$ winds around the same path (the circle) faster; the fluctuations become less important and $\dot{X}_\lambda - u_0\lambda\bar{b}$ is close to zero for large λ. In two or higher dimensions this does not happen unless the coordinates are separated. Detailed computations will appear in the article mentioned above.

Note also that in case $((a_{ij}(x))) = \alpha I$, and $\text{div}\, b(x) = 0$ for all x, the last two terms in (1.19) vanish. In particular, one has

$$D_{ii} = -2u_0^2\langle b_i, g_i\rangle + \alpha. \tag{2.1}$$

In problems of interest in solute dispersion the first term dominates (and goes to infinity as u_0 goes to infinity).

Check also that in this model the first term in (2.1) remains the same if the period is taken to be u_0, while the factor u_0 in the drift is taken to be 1. Thus asymptotic steady increase in dispersion with respect to the magnitude of the mean (liquid) velocity is equivalent to its asymptotic steady increase with respect to the spatial scale of heterogeneity. This is the so-called *scale effect* which has also been observed repeatedly in hydrological experiments (Molinary et al., 1977).

Of course, in the context of solute dispersion in porous media, the assumption of a periodic liquid velocity field is much too idealized. Unfortunately, this seems to be the only broad class of drift functions with nonzero mean (or large scale average of some sort) for which the central limit theorem has been proved. There is a novel central limit theorem type result due to Papanicolaou and Varadhan (1979) for the case of an L in divergence form:

$$L = \tfrac{1}{2} \textstyle\sum_{i=1}^{k} (\partial/\partial x_i)(\sum_{j=1}^{k} a_{ij}(x)\partial/\partial x_j),$$

with the functions $a_{ij}(x)$ *almost periodic* in the sense of Bohr. But the divergence theorem shows that in this case the large scale volume average of the drift is zero, which (in the context of solute transport) says that the higher scale velocity of the liquid is zero. This makes the result inapplicable to the present context. An appropriate extension of the result together with a perturbation expansion of the dispersion coefficients in a parameter like u_0 would be of much interest.

An entirely different type of model has been considered by Gelhar and Axness (1983) and independently by Winter, Newman and Neuman (1983). The results of Winter et al. (1983) are somewhat more general. In their model they take $((a_{ij}(x))) = I$, and the drift as $\mu + \varepsilon U(x)$, where μ is a constant (mean) vector, ε is a small parameter and $U(x)$ is a *mean zero stationary ergodic random field* (indexed by the spatial parameter x). Assuming that the central limit theorem does hold, Winter et al. (1983) obtain a perturbation expansion of the dispersion matrix of the limiting Gaussian distribution (or Brownian motion). It would be important to prove such a central limit theorem. For the case $\mu = 0$, div $b = 0$, Papanicolaou and Pironeau (1981) have proved that $\{\varepsilon X_{t/\varepsilon^2} : t \geq 0\}$ converges to a Brownian motion as $\varepsilon \downarrow 0$, and have computed the dispersion matrix of the limiting Brownian motion. The case of nonzero mean velocity, however, is the one of importance for solute dispersion in porous media, and this case remains open.

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7.4 "Refinements of the multidimensional central limit theorem and applications"

On the central limit theorems for diffusions with almost periodic coefficients. Sankhyā. The Indian Journal of Statistics. Series A 50 (1988), 9–25 (with S. Ramasubramanian).

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ON THE CENTRAL LIMIT THEOREM FOR DIFFUSIONS WITH ALMOST PERIODIC COEFFICIENTS

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SUMMARY. We consider a class of n-dimensional elliptic generators having almost periodic coefficients depending on finitely many rationally independent frequencies in each coordinate. A strong law of large numbers and a functional central limit theorem are proved for such diffusions.

1. Introduction

In this article we study asymptotic behaviour of diffusions on $\boldsymbol{R}^n$ whose drift and diffusion coefficients are *almost periodic* depending on M_j rationally independent frequencies $\omega_r^{(j)}$, $1 \leqslant r \leqslant M_j$, in the jth coordinate ($1 \leqslant j \leqslant n$).

In the case of a diffusion whose generator is in the self-adjoint divergence form and whose coefficients come from a random field, a novel functional central limit theorem was obtained by Papanicolaou and Varadhan (1979) under the general condition that the random field is stationary and ergodic. Kozlov (1979), (1980) contain similar results ; but the regularity arguments in Kozlov (1979) appear to have a gap. However Kozlov (1979) contains some significant ideas which we have made use of. While Kozlov's approach is purely analytical, ours is primarily probabilistic. We also mention the work of Papanicolaou and Pironeau (1981), in which the diffusion matrix is the identity and the drift vector is a mean-zero divergence free stationary ergodic random field. In all these articles the large scale mean is zero. The point of departure in the present article is the consideration of drift velocities whose *large scale mean need not be zero*. Part of the motivation for looking at this comes from the problem of modeling solute dispersion in an aquifer (Bhattacharya *et al.*, 1987 ; Gelhar and Axness, 1983 ; Winter *et al.*, 1984) and analyzing the limiting dispersion as a function of the large scale velocity.

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A 1–2

It may be noted that for arbitrary strictly elliptic generators with *periodic* coefficients the pathwise central limit theorem holds (see Bensoussan, Lions and Papanicolaou (1978), Bhattacharya (1985), and the remark on p. 846 in Papanicolaou and Varadhan (1979)).

2. Preliminaries and the law of large numbers

It will be assumed throughout that $b_k(.)$, $a_{kk'}(.)$ are real-valued functions on $\boldsymbol{R}^n$ of the form

$$b_k(x) = \sum_{m} b_k^{(m)} \exp\left\{i \sum_{j=1}^{n} x_j \sum_{r=1}^{M_j} m_r^{(j)} \omega_r^{(j)}\right\} \ (1 \leqslant k \leqslant n),$$

$$a_{kk'}(x) = \sum_{m} a_{kk'}^{(m)} \exp\left\{i \sum_{j=1}^{n} x_j \sum_{r=1}^{M_j} m_r^{(j)} \omega_r^{(j)}\right\} \quad (1 \leqslant k, k' \leqslant n). \quad \ldots \quad (2.1)$$

Here $M_1, M_2, \ldots, M_n$ are fixed positive integers ; for each $j(1 \leqslant j \leqslant n)$ one has a given set of M_j *rationally independent* (i.e., independent over the field of rationals) positive numbers $\omega_r^{(j)}$, $1 \leqslant r \leqslant M_j$; the sums in (2.1) are over a *finite* set of integer vectors $m = (m_r^{(j)} : 1 \leqslant r \leqslant M_j,\ 1 \leqslant j \leqslant n) \in \boldsymbol{Z}^M$ where

$$M = M_1 + M_2 + \ldots + M_n. \quad \ldots \quad (2.2)$$

The coefficients $b_k^{(m)}$, $a_{kk'}^{(m)}$ are complex constants. For each $x \in \boldsymbol{R}^n$ the $n \times n$ matrix $a(x) \doteq ((a_{kk'}(x)))$ is symmetric and positive definite and

$$\lambda_0 \doteq \inf_{x \in \boldsymbol{R}^n} \text{(smallest eigenvalue of } a(x)) > 0. \quad \ldots \quad (2.3)$$

In order to avoid ending up with the periodic case it will be assumed that $M > n$.

For each $c = (c_r^{(j)} : 2 \leqslant r \leqslant M_j,\ 1 \leqslant j \leqslant n) \in \boldsymbol{R}^{M-n}$ denote by H_c the n-dimensional hyperplane in $\boldsymbol{R}^M$ given by

$$H_c = \{y = (y_r^{(j)} : 1 \leqslant r \leqslant M_j,\ 1 \leqslant j \leqslant n) : y_r^{(j)} = y_1^{(j)} + c_r^{(j)},\ \ 2 \leqslant r \leqslant M_j\}. \quad \ldots \quad (2.4)$$

We shall adopt the following convention throughout : if $M_j = 1$, then terms involving subscripts $r \geqslant 2$ and superscripts j will be omitted.

Let Q denote the following discrete subgroup of $\boldsymbol{R}^{M-n}$:

$$Q = \{m_r^{(j)}(2\pi/\omega_r^{(j)}) + m_1^{(j)}(2\pi/\omega_1^{(j)}) :\ 2 \leqslant r \leqslant M_j,\ 1 \leqslant j \leqslant n) : m \in \boldsymbol{Z}^M\}). \quad \ldots \quad (2.5)$$

Write $f \in Trig\ (\boldsymbol{\omega})$ if f is a finite sum of the form

$$f(x) = \sum_{m} f^{(m)} \exp\left\{ i \sum_{j=1}^{n} x_j \sum_{r=1}^{M_j} m_r^{(j)} \omega_r^{(j)} \right\}, \quad \ldots \quad (2.6)$$

where $f^{(m)}$ are complex numbers.

A complex-valued function $h(y)$ on $\boldsymbol{R}^M$ will be said to be *periodic* $(2\pi/\boldsymbol{\omega})$ if it is periodic with period $2\pi/\omega_r^{(j)}$ in the coordinate $y_r^{(j)}(1 \leqslant r \leqslant M_j, 1 \leqslant j \leqslant n)$.

If $f \epsilon$ *Trig* $(\boldsymbol{\omega})$ is given by (2.6) define

$$\hat{f}(y) = \sum_m f^{(m)} \exp \left\{ i \sum_{j=1}^{n} \sum_{r=1}^{M_j} m_r^{(j)} \omega_r^{(j)} y_r^{(j)} \right\}. \quad \ldots \quad (2.7)$$

Then $\hat{f}$ is periodic $(2\pi/\boldsymbol{\omega})$, and f may be identified with the restriction of $\hat{f}$ to the hyperplane H_0.

Lemma 2.1 : *Q is dense in $\boldsymbol{R}^{M-n}$.*

Proof : It is sufficient to prove that if $\omega_1, \omega_2, \ldots, \omega_k$ are rationally independent positive numbers then $\{(q_1\omega_1^{-1}+q_2\omega_2^{-1}, q_1\omega_1^{-1}+q_3 w_3^{-1}, \ldots, q_1\omega_1^{-1}+q_k\omega_k^{-1}) : q_1, q_2, \ldots, q_k \epsilon \boldsymbol{Z})$ is dense in $\boldsymbol{R}^{k-1}$. Take $\omega_1 = 1$ without essential loss of generality. It is clear that

$$q_1 \,(\text{mod } \omega_j^{-1}) = \omega_j^{-1}\,(q_1\omega_j \,(\text{mod } 1)), j = 2, \ldots, k. \quad \ldots \quad (2.8)$$

Now, by Kronecker's theorem (Hardy and Wright (1959), p. 382), $\{(q_1\omega_2 \,(\text{mod } 1), q_1\omega_3 \,(\text{mod } 1), \ldots, q_1\omega_k \,(\text{mod } 1)) : q_1 \epsilon \boldsymbol{Z}\}$ is dense in $[0, 1]^{k-1}$. Therefore, by (2.8), $\{(q_1 \,(\text{mod } \omega_2^{-1}), q_1 \,(\text{mod } \omega_3^{-1}), \ldots, q_1 \,(\text{mod } \omega_k^{-1})) : q_1 \epsilon \boldsymbol{Z})$ is dense in $[0, \omega_2^{-1}]\times\ldots\times[0, \omega_k^{-1}]$. Consequently, $D \doteq \{q_1+q_2\omega_2^{-1}, q_1+q_3\omega_3^{-1}, \ldots, q_1+q_k \omega_k^{-1}) : q_1, q_2, \ldots, q_k \epsilon \boldsymbol{Z}\}$ is dense in $[0, \omega_2^{-1}]\times\ldots\times]0, \omega_k^{-1}]+(q_2'\omega_2^{-1}, \ldots, q_k' \omega_k^{-1})$ for every choice of integers $q_2', \ldots, q_k'$. Hence D is dense in $\boldsymbol{R}^{k-1}$.

Henceforth $\mathcal{J}$ will denote the M-dimensional *torus* $\prod_{j=1}^{n} \prod_{r=1}^{M_j} [0, 2\pi/\omega_r^{(j)})$ $\{\dot{y} = y \epsilon \boldsymbol{R}^M\}$ where

$$\dot{y} \equiv \zeta(y)) \doteq (y_r^{(j)} \,(\text{mod } 2\pi/\omega_r^{(j)}) : 1 \leqslant r \leqslant M_j, 1 \leqslant j \leqslant n). \quad \ldots \quad (2.9)$$

Let $\hat{a}_{kk'}(.)$, $\hat{b}_k(\cdot)$ be defined on $\boldsymbol{R}^M$ by (2.7). Since $a_{kk'}(.)$ may be viewed as the restriction of $\hat{a}_{kk'}(.)$ on H_0 and since $\zeta(H_0)$ is dense in $\mathcal{J}$ (Hardy and Wright, 1959, Theorem 444, p. 382), it follows by the periodicity and continuity of $\hat{a}_{kk'}(.)$ on $\boldsymbol{R}^M$ and by (2.3) that the smallest eigenvalue of $\hat{a}(y)$ $\doteq ((\hat{a}_{kk'}(y)))$ is bounded away from zero :

$$\inf_{y \epsilon \boldsymbol{R}^M} (\text{smallest eigenvalue of } \hat{a}(y)) = \lambda_0 > 0. \quad \ldots \quad (2.10)$$

Let $\hat{\sigma}(y) \doteq ((\hat{\sigma}_{kk'}(y)))$ denote the $n\times n$ symmetric positive definite square root of $\hat{a}(y)$.

Let $(\Omega, \mathcal{F}, p)$ be a probability space on which is defined an n-dimensional standard Brownian motion $B(t) = (B_1(t), B_2(t), \ldots, B_n(t))$, $t \geqslant 0$, which is adapted to a right continuous increasing family of P-complete sigmafields $\mathcal{I}_t$, $t \geqslant 0$.

Let $Y(t) = (Y_r^{(k)}(t) : 1 \leqslant r \leqslant M_k, 1 \leqslant k \leqslant n)$, $t \geqslant 0$, be the continuous nonaticipative solution to Itô's stochastic differential equations

$$dY_r^{(k)}(t) = \hat{b}_k(Y(t))dt + \sum_{k'=1}^{n} \hat{\sigma}_{kk'}(Y(t))dB_{k'}(t),$$
$$(1 \leqslant r \leqslant M_k, 1 \leqslant k \leqslant n), \qquad \ldots (2.11)$$

subject to some initial condition $Y(0) = Z$, where Z is an M dimensional random vector independent of $B(t)$, $t \geqslant 0$.

For all $c = (c_r^{(j)} : 2 \leqslant r \leqslant M_j, 1 \leqslant j \leqslant n)$ define the functions (on $\mathbf{R}^n$)

$$b_{k,c}(x) = \sum_m b_{k,c}^{(m)} \exp\left\{ i \sum_{j=1}^{n} x_j \sum_{j=1}^{M_j} m_r^{(j)} \omega_r^{(j)} \right\},$$

$$a_{kk',c}(x) = \sum_m a_{kk',c}^{(m)} \exp\left\{ i \sum_{j=1}^{n} x_j \sum_{r=1}^{M_j} m_r^{(j)} \omega_r^{(j)} \right\} \qquad \ldots (2.12)$$

where

$$b_{k,c}^{(m)} = b_k^{(m)} \exp\left\{ i \sum_{j=1}^{n} \sum_{r=2}^{M_j} c_r^{(j)} m_r^{(j)} \omega_r^{(j)} \right\},$$

$$a_{kk',c}^{(m)} = a_{kk'}^{(m)} \exp\left\{ i \sum_{j=1}^{n} \sum_{r=2}^{M_j} c_r^{(j)} m_r^{(j)} \omega_r^{(j)} \right\}. \qquad \ldots (2.13)$$

Note that $dY_r^{(k)}(t) - dY_1^{(k)}(t) = 0$ for $2 \leqslant r \leqslant M_k$. Hence

$$Y_r^{(k)}(t) = Y_1^{(k)}(t) + (Y_r^{(k)}(0) - Y_1^{(k)}(0)),\ t \geqslant 0, \qquad \ldots (2.14)$$

with probability one.

From (2.11)–(2.14) and (2.4) the following lemma is immediate. Write

$$\partial_k = \sum_{r=1}^{M_k} \partial/\partial y_r^{(k)} \ (1 \leqslant k \leqslant n). \qquad \ldots (2.15)$$

Lemma 2.2 : (i) $Y(t)$, $t \geqslant 0$, *is a singular diffusion on* $\mathbf{R}^M$ *generated, in the sense of Itô, by*

$$\tilde{L} \doteq \frac{1}{2} \sum_{k=1}^{n} \partial_k \left[\sum_{k'=1}^{n} \hat{a}_{kk'}(y)\partial_{k'} \right] + \sum_{k=1}^{n} \hat{b}_k^*(y)\partial_k \qquad \ldots (2.16)$$

where $\hat{b}_k^*$ *is defined on* $\mathbf{R}^M$ *by* (2.7) *from the function (on* $\mathbf{R}^n$*)*

$$b_k^*(x) \doteq b_k(x) - \sum_{k'=1}^{n} (\partial/\partial x_{k'})\, a_{kk'}(x),\ (1 \leqslant k \leqslant n). \qquad \ldots (2.17)$$

(ii) *If* $Y(0) \in H_c$ *(with probability one), then* $(Y_1^{(1)}(t), Y_1^{(2)}(t), \ldots, Y_1^{(n)}(t))$, $t \geqslant 0$, *is a nonsingular diffusion on* $\boldsymbol{R}^n$ *with drift coefficients* $b_{k,c}(.)$ *and diffusion coefficients* $a_{kk'}, c(\cdot)$, *and its generator may be expressed as*

$$L_c \doteq \frac{1}{2} \sum_{k=1}^{n} \partial/\partial x_k \left[\sum_{k'=1}^{n} a_{kk',c}(x)\partial/\partial x_{k'} \right]$$

$$+ \sum_{k=1}^{n} b^*_{k,c}(x)\partial/\partial x_k, \qquad \ldots \quad (2.18)$$

where $b^*_{k,c}(x) = b_{k,c}(x) - \sum_{k'=1}^{n} (\partial/\partial x_{k'}) \quad a_{kk',c}(x)$, $b^*_{k,0} = b^*_k$. *In particular, if* $c = 0$ *then this n-dimensional diffusion has drift coefficients* $b_k(.)$ *and diffusion coefficients* $a_{kk'}(.)$ $(1 \leqslant k,\ k' \leqslant n)$.

Note that $\dot{Y}(t) \equiv \zeta(Y(t))$, $t \geqslant 0$, is a *Markov process with state space* $\mathcal{J}$, since $\hat{b}_k(\cdot)$, $\hat{a}_{kk'}(\cdot)$ are periodic $(2\pi/\omega)$.

Lemma 2.3 : *Assume div* $b^*(x) \doteq \sum_{k=1}^{n} (\partial/\partial x_k) b^*_k(x) \equiv 0$. *Then* (i) *the Lebesgue measure on* $\boldsymbol{R}^M$ *is invariant for* $Y(t)$, $t \geqslant 0$, *and* (ii) *the normalized Lebesgue measure* $\pi(dz)$ *on* $\mathcal{J}$ *is an invariant probability for the Markov process* $\dot{Y}(t)$, $t \geqslant 0$.

Proof: (i) In view of the assumption div $b^* = 0$ the formal adjoint L^*_c of L_c (and $\widetilde{L}^*$ of $\widetilde{L}$) annihilates constant functions. One may then check that the n-dimensional Lebesgue measure is invariant for the diffusion with generator L_c. Integrating first along H_c for a fixed c and then over a set of c values the result is proved. The precise change of variables involved is given by (2.21) below.

(ii) Let $p(t\,;y, B)$, $\dot{p}(t\,;y, C)$ denote the *transition probabilities* of the processes $Y(t)$, $t \geqslant 0$, and $\dot{Y}(t)$, $t \geqslant 0$, respectively. For all Borel sets C of $\mathcal{J}$ one has

$$\begin{aligned}
\pi(C) &= \int_{\boldsymbol{R}^M} p(t\,; y, C)\, dy \\
&= \sum_{m \in \boldsymbol{Z}^M} \int_{\mathcal{J} + \left(m_1^{(1)} 2\pi/\omega_1^{(1)}, \ldots, m_{M_n}^{(n)} 2\pi/\omega_{M_n}^{(n)}\right)} p(t; y, C)\, dy \\
&= \sum_{m \in \boldsymbol{Z}^M} \int_{\mathcal{J}} p\left(t\,; y - \left(m_1^{(1)} 2\pi/\omega_1^{(1)}, \ldots, m_{M_n}^{(n)} 2\pi/\omega_{M_n}^{(n)}\right), C\right) dy \\
&= \int_{\mathcal{J}} \sum_{m} p\left(t\,; y, C + \left(m_1^{(1)} 2\pi/\omega_1^{(1)}, \ldots, m_{M_n}^{(n)} 2\pi/\omega_{M_n}^{(n)}\right)\right) dy \\
&= \int_{\mathcal{J}} \dot{p}\,(t\,; \dot{y}, C)\, \pi(dy).
\end{aligned}$$

Let $\Gamma = C([0, \infty) : \mathcal{J})$ be the set of all continuous functions on $[0, \infty)$ into $\mathcal{J}$. Let P^y denote the distribution of $\dot{Y}(t)$, $t \geqslant 0$, (i.e., a probability measure on the Borel sigmafield of Γ) when $Y(0) \equiv y$. Clearly $P^y = P^{\dot{y}}$. Let P^{π} denote the corresponding distribution when $Y(0)$ has distribution π (the normalized Lebesgue measure on $\mathcal{J}$). Then $P^{\pi}(F) = \int_{\mathcal{J}} P^y(F)\pi(dy)$ for all Borel subsets F of Γ.

Lemma 2.4 : *Let B be a Borel subset of $\mathcal{J}$ such that, for some $t > 0$,*

$$1_B(\gamma(0)) = 1_B(\gamma(t)) \textit{ for almost all } (w.r.t.\ P^{\pi})\gamma\epsilon\Gamma, \qquad \ldots \quad (2.19)$$

where $1_B(y)$ is the indicator function of the set B. Then there exists a Borel subset C of $\boldsymbol{R}^{M-n}$ such that $\pi(B\Delta\zeta(\hat{B})) = 0$ where

$$\hat{B} = \bigcup_{c\epsilon C} H_c, \qquad \ldots \quad (2.20)$$

ζ is the map $y \to \dot{y}$ (see (2.9)) and Δ denotes symmetric difference.

Proof : Let φ, ψ be linear maps on $\boldsymbol{R}^M$ (into $\boldsymbol{R}^{M-n}$, $\boldsymbol{R}^n$, respectively) defined by

$$\varphi(y) = (y_r^{(k)} - y_1^{(k)} : 2 \leqslant r \leqslant M_k,\ 1 \leqslant k \leqslant n),$$

$$\psi(y) = (\varphi(y), y_1^{(1)}, y_1^{(2)}, \ldots, y_1^{(n)}). \qquad \ldots \quad (2.21)$$

Then ψ is nonsingular with Jacobian determinant one. Let μ_r denote Lebesgue measure on $\boldsymbol{R}^r$. For $c\epsilon\boldsymbol{R}^{M-n}$, $z\epsilon\boldsymbol{R}^n$, the transition probability $q(t\,;\,(c, z), D) \doteq P^{\pi}(\{\psi(\gamma(t))\,\epsilon\, D\} \,|\, \psi(\gamma(0)) = (c, z))$ may be expressed as

$$q(t\,;\,(c, z), D) = \int_{D_{c,}} f_c(t\,;\,z, z')\,\mu_n(dz'), \qquad \ldots \quad (2.22)$$

where $D_{c\cdot} = \{z'\epsilon\boldsymbol{R}^n : (c, z')\epsilon D\}$, and $f_c(t\,;\,z, z')$ is the strictly positive continuous density (w.r.t μ_n) of the transition probability of the n-dimensional diffusion generated by L_c (see (2.18)). On taking conditional expectation given $\gamma(0)$ in (2.19) one has $1_B(\dot{y}) = \dot{p}(t\,;\,\dot{y}, B)$ a.s. π, i.e.,

$$1_{\zeta^{-1}(B)}(y) = p(t\,;\,y, \zeta^{-1}(B)) \text{ a.e. } \mu_M. \qquad \ldots \quad (2.23)$$

Writing $F = \psi(\zeta^{-1}(B))$ and using (2.22)), one may express (2.23) as

$$1_F((c, z)) = \int_{F_{c\cdot}} f_c(t\,;\,z, z')\,\mu_n(dz') \textit{ a.e. } \mu_M, \qquad \ldots \quad (2.24)$$

i.e., there exists a μ_M-null set J such that (2.24) holds for all $(c, z) \notin J$. Hence

$$\mu_n(\boldsymbol{R}^n \setminus F_{c\cdot}) = 0 \qquad \ldots \quad (2.25)$$

for almost all (w.r.t. μ_{M-n})c in

$$C = \{c \in \boldsymbol{R}^{M-n} \ : \mu_n(F_{c.}) > 0\}. \qquad \ldots \quad (2.26)$$

It follows from (2.25), (2.26) and Fubini's theorem that

$$\mu_M((C \times \boldsymbol{R}^n)\Delta F) = 0. \qquad \ldots \quad (2.27)$$

Let $\hat{B}$ be as in (2.20), with C as in (2.26). Then

$$\hat{B} = \psi^{-1}(C \times \boldsymbol{R}^n), \qquad \ldots \quad (2.28)$$

and (2.27) implies

$$\mu_M(\hat{B}\Delta\zeta^{-1}(B)) = 0,$$

and, therefore,

$$\pi(\zeta(\hat{B})\Delta B) = 0. \qquad \ldots \quad (2.29)$$

The main result of this section is the following.

Theorem 2.5 : *Suppose* div $b^*(x) \equiv 0$. (i) *If* $Y(0)$ *has distribution* π, *then* $\dot{Y}(t)$, $t \geqslant 0$, *is a stationary ergodic Markov process on* $\mathcal{J}$. (ii) *Let* $X(t\,;\,c)$ *denote an n-dimensional diffusion with drift coefficients* $b_{k,c}(\cdot)$ *and diffusion coefficients* $a_{kk',c}(\cdot)$. *Then for all* $c \in \boldsymbol{R}_3^{M-n}$ *outside a set of zero* ($M-n$ *dimensional*) *Lebesgue measure,*

$$\lim_{t \to \infty} \frac{X(t\,;\,c)}{t} = \bar{b} \doteq (b_1^{(0)}, b_2^{(0)}, \ldots, b_n^{(0)}) \text{ a.s.}, \qquad \ldots \quad (2.30)$$

whatever the initial distribution of $X(t\,;\,c)$.

Proof : (i) Suppose $Y(0)$ has distribution π. Then $\dot{Y}(t)$, $t \geqslant 0$, is a stationary process with distribution $\boldsymbol{P}^{\pi}$. Let F be a shift-invariant Borel set of $\Gamma = C([0, \infty) : \mathcal{J})$. There exists a Borel set B of $\mathcal{J}$ such that (Doob, (1953), p. 460)

$$P^{\pi}(F\Delta\{\gamma(t) \in B\}) = 0 \text{ for all } t \geqslant 0. \qquad \ldots \quad (2.31)$$

In particular, $P^{\pi}(\{\gamma(0) \in B\}\Delta\{\gamma(t) \in B\}) = 0$ for all $t > 0$, i.e., (2.19) holds. Hence, by Lemma 2.4, there exists a Borel set $C \subset \boldsymbol{R}^{M-n}$ such that $\pi(B\Delta\zeta(\hat{B}))$ $= 0$ with $\hat{B}$ given by (2.20). Let $G = C+Q = \{c+q : c \in C,\ q \in Q\}$, where Q is the set (2.5). Since $\zeta(H_c) = \zeta(H_{c'})$ if $c-c' \in Q$ one has $\zeta(\hat{B}) = \zeta(U_{c \in G}\ H_c)$ We need to prove $P^{\pi}(F) = 0$ or 1, i.e.,

$$\pi(\zeta(\hat{B})) = 0 \text{ or } 1. \qquad \ldots \quad (2.32)$$

Suppose that (2.32) *is not true,* so that $0 < \pi(\zeta(\hat{B})) < 1$. Then

$$\mu_{M-n}(G) > 0,\ \mu_{M-n}(\boldsymbol{R}^{M-n} \setminus G) > 0. \qquad \ldots \quad (2.33)$$

But G is invariant under translation by elements of Q which is *dense* in $\boldsymbol{R}^{M-n}$ (Lemma 2.1). If (2.33) holds, then one may find two compact sets $K_1 \subset G$, $K_2 \subset \boldsymbol{R}^{M-n}\setminus G$ both with *positive* μ_{M-n}-measure ; but the convolution $1_{K_1} * 1_{K_2}$ vanishes on the dense set Q ; this convolution is continuous (indeed its Fourier transform is integrable), so that $1_{K_1} * 1_{K_2} \equiv 0$, which is false. Hence (2.33) is false, and (2.32) is true.

(ii) Let $Y(0)$ have distribution π. Then, by the ergodic theorem applied to the time integral, and the maximal inquality applied to the stochastic integral in (2.11), one has a.s. (P),

$$\lim_{t\to\infty} \frac{Y_r^{(k)}(t)}{t} = b_k^{(0)} \, (1 \leqslant r \leqslant M_k,\ 1 \leqslant k \leqslant n). \qquad \ldots \quad (2.34)$$

Let $\bar{P}^y$ be the distribution of $(Y_1^{(1)}(t), \ldots, Y_1^{(n)}(t))$, $t \geqslant 0$, (on $C([0, \infty) : \boldsymbol{R}^n)$) when $Y(0) \equiv y$. Note that $\bar{P}^y$ is the distribution of $X(t\,;c)$, $t \geqslant 0$, if $y \in H_c$ and $X(0\,;c) \equiv \bar{y} \doteq (y_1^{(1)}, \ldots, y_1^{(n)})$. Now (2.34) implies that $\mu_M(\boldsymbol{R}^M \setminus B) = 0$, where $B = \{y \in \boldsymbol{R}^M : g(y) = 1\}$, $g(y) \doteq P(\{(2.34)$ holds $\mid Y(0) = y\})$. Since $X(t\,;c)$, $t \geqslant 0$, is a nonsingular n-dimensional diffusion, $g(y)$ is continuous on H_c ; also, by the maximum principle, $g(y) \equiv 1$ on H_c if $B \cap H_c \neq \phi$ (see, e.g., Bhattacharya (1978), Lemma 2.3). It follows that $B = \bigcup_{c \in C} H_c$ with C a Borel subset of $\boldsymbol{R}^{M-n}$ such that $\mu_{M-n}(\boldsymbol{R}^{M-n} \setminus C) = 0$.

3. The central limit theorem

We continue to use the notation of Section 2.

Let $\mathcal{L}^2(\mathcal{T})$ denote the usual Hilbert space of (equivalence classes) of real-valued functions square integrable with respect to the normalized Lebesgue measure π on $\mathcal{T}$. The inner product on $\mathcal{L}^2(\mathcal{T})$ will be denoted by $<, >$, and norm by $\|\cdot\|_0$. Let O_N be the subspace

$$O_N = \left\{ \varphi \in \mathcal{L}^2(\mathcal{T}) : \varphi(y) = \sum_{0 \neq |m| \leqslant N} \varphi^{(m)} \exp\left\{ i \sum_{j=1}^{n} \sum_{r=1}^{M_j} y_r^{(j)}\, m_r^{(j)}\, \omega_r^{(j)} \right\} \right\} \ldots \quad (3.1)$$

where $|m| = \sum_{j,r} |m_r^{(j)}|$. We shall use $\bar{O}_N$ to denote *projection onto* O_N.

Recall the singular differential operator $\tilde{L}$ on $\boldsymbol{R}^M$ defined by (2.16)

Lemma 3.1 : *Suppose div* $b^* = 0$. *Then for each* $N \geqslant 1$, $\bar{O}_N \tilde{L}$ *is a* 1—1 *map on* O_N *onto* O_N.

Proof: Clearly, $\bar{O}_N \tilde{L}\varphi \in O_N$ for each $\varphi \in O_N$. Now div $b^*(x) = 0$ implies $\sum_{k=1}^{n} \partial_k \hat{b}_k^*(y) \equiv 0$, so that for every $\varphi \in O_N$

$$\int_{\mathcal{J}} \left[\sum_{k=1}^{n} \hat{b}_k^*(y)\, \partial_k\, \varphi(y) \right] \varphi(y)\, \pi\,(dy)$$

$$= -\frac{1}{2} \int_{\mathcal{J}} \left[\sum_{k=1}^{n} \partial_k\, \hat{b}_k^*(y) \right] \varphi^2(y)\, \pi(dy) = 0. \qquad \ldots \quad (3.2)$$

By (2.10), (3.2) and the self-adjointness of $\bar{O}_N$, one has for every $\varphi \in O_N$, $\varphi \neq 0$,

$$< \bar{O}_N \tilde{L}\varphi, \varphi > = < \tilde{L}\varphi, \varphi > = -\frac{1}{2} \int_{\mathcal{J}} \left[\sum_{k, k'=1}^{n} \hat{a}_{kk'}\,(y)\, \partial_k\, \varphi(y)\, \partial_{k'}\, \varphi(y) \right] \pi(dy)$$

$$\leqslant -\frac{\lambda_0}{2} \int_{\mathcal{J}} \sum_{k=1}^{n} (\partial_k\, \varphi(y))^2\, \pi(dy) \qquad \ldots \quad (3.3)$$

$$= -\frac{\lambda_0}{2} \sum_{k=1}^{n} \sum_{0 \neq |m| \leqslant N} |\varphi^{(m)}|^2 \left[\sum_{r=1}^{M_k} m_r^{(k)} \omega_r^{(k)} \right]^2 < 0.$$

For $\sum_{r=1}^{M_k} m_r^{(k)}\, \omega_r^{(k)}$ is nonzero for each k and each $m \neq 0$.

Hence $\bar{O}_N\, \tilde{L}$ is $1-1$ on O_N into O_N. Since O_N is finite dimensional, $\bar{O}_N\, \tilde{L}$ is $1-1$ on O_N *onto* O_N.

For infinitely differentiable periodic $(2\pi/\boldsymbol{\omega})$ functions φ on $\boldsymbol{R}^M$ define

$$\|\varphi\|_s = \left[\sum_{|\alpha| \leqslant s} \int_{\mathcal{J}} |\partial_1^{\alpha_1}\, \partial_2^{\alpha_2} \ldots \partial_n^{\alpha_n}\, \varphi(y)\,|^2 \pi\,(dy) \right]^{1/2} (s = 0, 1, 2, \ldots), \quad \ldots \quad (3.4)$$

where $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ is a multi-index and $|\alpha| = \alpha_1 + \ldots + \alpha_n$.

Lemma 3.2: *Suppose div* $b^*(x) \equiv 0$. *Let* $f \in Trig\ (\boldsymbol{\omega})$ *with* $f^{(0)} = 0$. *Let* $\hat{f}$ *be given by* (2.7), *the sum being over* m *satisfying* $|m| \leqslant N_0$. *Then for every* $N \geqslant N_0$ *there exists a unique* $\hat{u}_N \in O_N$ *such that* $\bar{O}_N\, \tilde{L}\hat{u}_N = \hat{f}$, *and for all* $s = 0, 1, 2, \ldots,$ *one has*

$$\sum_{k=1}^{n} \|\partial_k \hat{u}_N\|_s^2 \leqslant c(s), \qquad \ldots \quad (3.5)$$

where $c(s)$ *does not depend on* N.

Proof: Since $\hat{f} \in O_N$ for all $N \geqslant N_0$ one has, by Lemma 3.1, a unique $\hat{u}_N \in O_N$ such that $\bar{O}_N \tilde{L}\hat{u}_N = \hat{f}$ for $N \geqslant N_0$. One then has (as in Kozlov (1979), p. 487)

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$$|<\widetilde{L}\hat{u}_N, \hat{u}_N>| = |<\bar{O}_N\widetilde{L}\hat{u}_N, \hat{u}_N>| = |<\hat{f}, \hat{u}_N>| = |\sum_{m\neq 0} f^{(m)}u_N^{(m)}|$$

$$= \left| \sum_{m\neq 0} \frac{1}{\delta} f^{(m)} \left[\sum_{r=1}^{M_k} m_r^{(k)}\omega_r^{(k)} \right]^{-1} . \delta \left[\sum_{r=1}^{M_k} m_r^{(k)}\omega_r^{(k)} \right] u_N^{(m)} \right|$$

$$\leqslant \frac{1}{2} \sum_{1\leqslant |m| < N_0} \frac{1}{\delta^2} |f^{(m)}|^2 \left| \sum_{r=1}^{M_k} m_r^{(k)}\omega_r^{(k)} \right|^{-2}$$

$$+ \frac{1}{2} \delta^2 \sum_{1\leqslant |m| \leqslant N} |u_N^{(m)}|^2 \left[\sum_{r=1}^{M_k} m_r^{(k)}\omega_r^{(k)} \right]^2$$

$$= c_k(\delta, f) + \frac{1}{2} \delta^2 \|\partial_k \hat{u}_N\|_0^2. \quad \ldots \quad (3.6)$$

Also, from the calculations in (3.3),

$$|<\widetilde{L}\hat{u}_N, \hat{u}_N>| \geqslant \frac{\lambda_0}{2} \sum_{k=1}^{n} \|\partial_k \hat{u}_N\|_0^2. \quad \ldots \quad (3.7)$$

From (3.6), (3.7) one obtains

$$\sum_{k=1}^{n} \|\partial_k \hat{u}_N\|_0^2 \leqslant c(0), \quad \ldots \quad (3.8)$$

proving (3.5) for $s = 0$.

In order to prove (3.5) for $s > 0$, introduce the differential operator

$$\widetilde{D}_s = \left[\sum_{k=1}^{n} \partial_k^2 \right]^s (s = 0, 1, 2, \ldots). \quad \ldots \quad (3.9)$$

On integration by parts one has

$$<\widetilde{D}_s\widetilde{L}\partial_k\hat{u}_N, \partial_k\hat{u}_N> = -\frac{1}{2} \sum_{j=1}^{n} <\widetilde{D}_s \sum_{j'=1}^{n} \hat{a}_{jj'}(.)\partial_{j'}\partial_k\hat{u}_N, \partial_j\partial_k\hat{u}_N>$$

$$+ \sum_{j=1}^{n} <\widetilde{D}_s(\hat{b}_j^*(.)\partial_j\partial_k\hat{u}_N), \partial_k\hat{u}_N>$$

$$= - \sum_{j,j',k_1,\ldots,k_s=1}^{n} (1/2)(-1)^s \times$$

$$\times <\partial_{k_1}\ldots\partial_{k_s}(\hat{a}_{jj'}(.)\partial_{j'}\partial_k\hat{u}_N), \partial_{k_1}\ldots\partial_{k_s}\partial_j\partial_k\hat{u}_N>$$

$$+(-1)^s \sum_{j,k_1,\ldots,k_s=1}^{n} <\partial_{k_1}\ldots\partial_{k_s}(\hat{b}_j^*(.)\partial_j\partial_k\hat{u}_N), \partial_{k_1}\ldots\partial_{k_s}\partial_k\hat{u}_N>.$$

$$\ldots \quad (3.10)$$

Using Leibniz rule for differentiation of products one gets, from (3.10) and and (2.10),

$$| < \widetilde{D}_s \widetilde{L} \partial_k \hat{u}_N, \partial_k u_N > | \geqslant \frac{1}{2} \sum_{k_1,\ldots,k_s=1}^{n} < \sum_{j,j'=1}^{n} \hat{a}_{jj'}(.) \partial_{k_1} \ldots \partial_{k_s} \partial_j, \partial_k \hat{u}_N,$$

$$\partial_{k_1} \ldots \partial_{k_s} \partial_j \partial_k \hat{u}_N > -c_1(s) \|\partial_k \hat{u}_N\|_s^2 - c_2(s) \|\partial_k \hat{u}_N\|_{s+1} \|\partial_k \hat{u}_N\|_s$$

$$\geqslant c_3(s) \|\partial_k \hat{u}_N\|_{s+1}^2 - c_1(s) \|\partial_k \hat{u}_N\|_s^2 - c_2(s) \|\partial_k \hat{u}_N\|_s \|\partial_k \hat{u}_1\|_{s+1}. \quad \ldots \quad (3.11)$$

We shall now prove (3.5) by induction on s. Suppose it holds for $s \leqslant s_0$. Then

$$| < \widetilde{D}_{s_0} \widetilde{L} \partial_k \hat{u}_N, \partial_k \hat{u}_N > | \leqslant | \widetilde{D}_{s_0} \partial_k \widetilde{L} \hat{u}_N, \partial_k \hat{u}_N > |$$

$$+ \frac{1}{2} \left| < \widetilde{D}_{s_0} \sum_{j,j'=1}^{n} \partial_j \{ (\partial_k \hat{a}_{jj'}(.)) \partial_j, \hat{u}_N), \partial_k \hat{u}_N > \right|$$

$$+ \left| < \widetilde{D}_{s_0} \sum_{j=1}^{n} (\partial_k \hat{b}_j^*(.)) \partial_j \hat{u}_N, \partial_k \hat{u}_N > \right|. \quad \ldots \quad (3.12)$$

Since $\partial_k \hat{u}_N = \bar{O}_N \partial_k \hat{u}_N$, and $\widetilde{D}_{s_0} \partial_k$ commutes with $\bar{O}_N$, one has

$$\left| < \widetilde{D}_{s_0} \partial_k \tilde{L} \hat{u}_N, \partial_k \hat{u}_N > \right| = \left| < \widetilde{D}_{s_0} \partial_k \bar{0}_N \tilde{L} \hat{u}_N, \partial_k \hat{u}_N > \right|$$

$$= \left| < \widetilde{D}_{s_0} \partial_k \hat{f}, \partial_k \hat{u}_N > \right| \leqslant c_4(s_0) \|\partial_k \hat{u}_N\|_0 \leqslant c_5(s_0), \quad \ldots \quad (3.13)$$

by (3.8). Also, the differential operator $\widetilde{D}_{s_0}$ is of order $2s_0$ and on expressing it as a sum of products of two differential operators each of order s_0, and integrating by parts one gets

$$\frac{1}{2} \left| < \widetilde{D}_{s_0} \sum_{j,j'=1}^{n} \partial_j \{ (\partial_k \hat{a}_{jj'}(.)) \partial_{j'} \hat{u}_N \}, \partial_k \hat{u}_n > \right|$$

$$\leqslant c_6(s_0) \left[\sum_{j=1}^{n} \|\partial_j \hat{u}_N\|_{s_0+1} \right] \|\partial_k \hat{u}_N\|_{s_0} \leqslant c_7(s_0) \left[\sum_{j=1}^{n} \|\partial_j \hat{u}_N\|_{s_0+1} \right]. \quad \ldots \quad (3.14)$$

One similarly obtains

$$\left| < \widetilde{D}_{s_0} \sum_{j=1}^{n} (\partial_k \hat{b}_j^*(.)) \partial_j \hat{u}_N, \partial_k \hat{u}_N > \right|$$

$$\leqslant c_8(s_0) \left[\sum_{j=1}^{n} \|\partial_j \hat{u}_N\|_{s_0} \right] \|\partial_k \hat{u}_N\|_{s_0} \leqslant c_9(s_0). \quad \ldots \quad (3.15)$$

Using (3.13)-(3.15) in (3.12) one gets

$$\sum_{k=1}^{n} |<\widetilde{D}_{s_0}\widetilde{L}\,\partial_k\,\hat{u}_N,\,\partial_k u_N>|$$

$$\leqslant c_{10}(s_0)+c_{11}(s_0)\left[\sum_{j=1}^{n}\|\partial_j\,\hat{u}_N\|_{s_0+1}\right]. \quad \ldots \quad (3.16)$$

On the other hand, (3.11) and the induction hypothesis yield

$$\sum_{k=1}^{n} |<\widetilde{D}_{s_0}\widetilde{L}\,\partial_k\,\hat{u}_N,\,\partial_k\,\hat{u}_N>| \geqslant c_2(s)\sum_{k=1}^{n}\|\partial_k\,\hat{u}_N\|^2_{s_0+1}$$

$$-c_{12}(s_0)-c_{13}(s_0)\left[\sum_{k=1}^{n}\|\partial_k\,\hat{u}_N\|_{s_0+1}\right]. \quad \ldots \quad (3.17)$$

From (3.16), (3.17) one easily obtains

$$\sum_{j=1}^{n}\|\partial_j\hat{u}_N\|_{s_0+1} \leqslant c_{14}(s_0). \quad \ldots \quad (3.18)$$

In the proof of Theorem 3.4 we apply Lemma 3.2 (as well as Lemma 3.3 below) with $\hat{f} = \hat{b}_k - b_k^{(0)}$, and $N_0 = \Sigma\,\Sigma m_r^{(j)}$ in the representation (2.1).

For the next lemma we shall need the following hypothesis (see Kozlov, 1979, p. 489) concerning $\omega_r^{(k)}$).

Condition (**C**). *There exists a positive integer* s_0 *and a positive number* δ *such that*

$$\left|\sum_{r=1}^{M_k} m_r^{(k)}\omega_r^{(k)}\right| \geqslant \delta\left[\sum_{r=1}^{M_k}\left|m_r^{(k)}\right|\right]^{-s_0} (k = 1, 2, \ldots, n), \quad \ldots \quad (3.19)$$

for all $m = (m_r^{(k)}: 1 \leqslant r \leqslant M_k,\ 1 \leqslant k \leqslant n) \in \mathbf{Z}^M$ $(m \neq 0)$.

It may be noted that outside a set of Lebesgue measure (M-dimensional) zero, all M-tuples $(\omega_r^{(k)}) : 1 \leqslant r \leqslant M_k,\ 1 \leqslant k \leqslant n)$ satisfy (3.19) if $\delta > 0$ and s_0 is sufficiently large. (Sprindzuk, 1979, Theorem 12, p. 33).

It is easy to check (see Kozlov, 1979, p. 492) that condition (*C*) implies

$$\|\hat{u}_N\|^2_{s-s_0} \leqslant c_{15}(s)\sum_{j=1}^{n}\|\partial_j\hat{u}_N\|^2_s \quad (s \geqslant s_0). \quad \ldots \quad (3.20)$$

Now let $\dot{T}_t$, $t \geqslant 0$, denote the *semigroup of* transition operators on $\mathcal{L}^2(\mathcal{J})$ defined by

$$(\dot{T}_t f)(y) = E(f(\dot{Y}(t))\,|\,\dot{Y}(0) = y) = \int_{\mathcal{J}} f(z)\dot{p}(t\,;\,y,\,dz). \quad \ldots \quad (3.21)$$

It is simple to check that this is a contraction semigroup. Let $\mathcal{D}_{\tilde{A}}$ denote the set of all f in $\mathcal{L}^2(\mathcal{T})$ such that the following limit exists in $\mathcal{L}^2$:

$$\tilde{A}f \doteq \lim_{t \downarrow 0} \frac{\dot{T}_t f - f}{t}. \qquad \ldots (3.22)$$

The operator $\tilde{A}$ is the *infinitesimal generator* of the semigroup and $\mathcal{D}_{\tilde{A}}$ its *domain*. Let $\mathcal{R}_{\tilde{A}}$ denote the *range* of $\tilde{A}$.

Lemma 3.3 : *Suppose div* $b^* = 0$ *and condition* (***C***) *holds. Let* $f \in Trig\,(\omega)$ *be such that* $f^{(0)} = 0$, *where* f *is represented as in* (2.6). *Let* $\hat{f}$ *be defined by* (2.7). *Then there exists* $\hat{g} \in \mathcal{D}_{\tilde{A}}$ *such that* $\tilde{A}\hat{g} = \hat{f}$, *and there exist* $\hat{g}_N \in O_N(N = 1, 2, \ldots)$ *such that* $\hat{g}_N \to \hat{g}$ *and* $\tilde{A}\hat{g}_N \to \tilde{A}\hat{g} = \hat{f}$ *in* $\mathcal{L}^2$*-norm, as* $N \to \infty$.

Proof : Let $\hat{u}_N$ be the unique solution of $\bar{O}_N \tilde{L} \hat{u}_N = \hat{f}$, for $N \geqslant N_0$. By Lemma 3.2, and (3.20),

$$\sup_{n \geqslant N_0} \|\hat{u}_N\|_s^2 < \infty \; (s = 1, 2, \ldots). \qquad \ldots (3.23)$$

Now it is easy to check using Ito's lemma and path continuity of $\dot{Y}(s)$ that all infinitely differeniable functions which are periodic $(2\pi/\omega)$, regarded as elements of $\mathcal{L}^2(\mathcal{T})$, belong to $\mathcal{D}_{\tilde{A}}$, and $\tilde{A} = \tilde{L}$ when restricted to this class of functions. Hence $\hat{u}_N \in \mathcal{D}_{\tilde{A}}$, and (3.23) implies that $\hat{u}_N$ and $\tilde{A}\hat{u}_N \equiv \tilde{L}\hat{u}_N$, $N \geqslant N_0$, are norm-bounded. Therefore, there exists a subsequence N' of the integers such that $\hat{u}_{N'}$ converges *weakly* to $\hat{g}$, say, and $\tilde{A}\hat{u}_{N'}$ converges *weakly* to $\hat{h}$, say. Thus $(\hat{g}, \hat{h})$ belongs to the *weak closure* of the graph of $\tilde{A}$ restricted to $0 = \bigcup_{N=1}^{\infty} 0_N$. Since (i) $O \subset \mathcal{D}_{\tilde{A}}$, (ii) the graph of $\tilde{A}$ is closed, and (iii) the weak closure of the graph of $\tilde{A}$ restricted to O equals its *strong closure* (Yoshida, 1966, Theorem 11, p. 125), it follows that $(\hat{g}, \hat{h})$ belongs to the graph of $\tilde{A}$, i.e., $\hat{g} \in \mathcal{D}_{\tilde{A}}$ and $\tilde{A}\hat{g} = \hat{h}$. Also for all $u \in 0$ one has

$$< \hat{h}, u > = \lim_{N' \to \infty} < \tilde{A}\hat{u}_{N'}, u >$$

$$= \lim_{N' \to \infty} < \bar{O}_{N'} \tilde{A}\hat{u}_{N'}, u > = < \hat{f}, u >. \qquad \ldots (3.24)$$

Since O is dense in $1^{\perp}$, $\hat{h} \in 1^{\perp}$ (since $\boldsymbol{R}_{\tilde{A}} \subset 1^{\perp}$; Bhattacharya, (1982, Relation (2.6)) and $\hat{f} \in 1^{\perp}$, it follows that $\hat{h} = \hat{f}$.

Finally, again using the fact that the weak closure of the restriction of the graph of $\tilde{A}$ to O equals its strong closure, the second assertion follows.

Theorem 3.4 : *Suppose div $b^* = 0$ and condition* (**C**) *holds. Define*

$$X_\epsilon(t\,;\,c) = \epsilon(X(t/\epsilon^2\,;\,c)) - \frac{t}{\epsilon}\,\bar{b}, \quad \dots \quad (3.25)$$

where $X(t\,;\,c)$ is the n-dimensional diffusion generated by L_c in (2.18), *starting at an arbitrary initial state in $\boldsymbol{R}^n$. For all $c \in \boldsymbol{R}^{M-n}$ outside a set of $(M-n)$-dimensional Lebesgue measure zero, $X_\epsilon(t\,;\,c)$, $t \geqslant 0$, converges weakly as $\epsilon \downarrow 0$ to a Brownian motion with zero drift and dispersion matix*

$$\int_{\mathcal{J}} (\partial\hat{u}(y) - I)\hat{a}(y)(\partial\hat{u}(y) - I)'\pi(dy), \quad \dots \quad (3.26)$$

where $\hat{u}(y) = (\hat{u}_1(y), \dots, \hat{u}_n(y))$ is the unique solution of $\tilde{A}\hat{u}_k = \hat{b}_k - b_k^{(0)}$ $(1 \leqslant k \leqslant n)$ in $1^{\perp}$, and $\partial\hat{u}$ is the $n \times n$ matrix $((\partial_k \hat{u}_{k'}))$.

Proof : By the second part of Lemma 3.3 there exists, for each $j (1 \leqslant j \leqslant n)$, $\hat{u}_{j,N} \in O_N (N = 1, 2, \dots)$ such that, as $N \to \infty$

$$\|\hat{u}_{j,N} - \hat{u}_j\|_0 \to 0, \; \|\tilde{A}\hat{u}_{j,N} - (\hat{b}_j - b_j^{(0)})\|_0 \to 0. \quad \dots \quad (3.27)$$

Since (see (3.3))

$$\|\partial_k \hat{u}_{j,N} - \partial_k \hat{u}_{j,N'}\|_0^2 \leqslant \frac{2}{\lambda_0} < -\tilde{A}(\hat{u}_{j,N} - \hat{u}_{j,N'}),\, \hat{u}_{j,N} - \hat{u}_{j,N'} >, \quad \dots \quad (3.28)$$

it follows from (3.27) that $\partial_k \hat{u}_j \in \mathcal{L}^2(\mathcal{J})$ and

$$\|\partial_k \hat{u}_{j,N} - \partial_k \hat{u}_j\|_0 \to 0 \text{ as } N \to \infty. \quad \dots \quad (3.29)$$

Now let $Y(t)$, $t \geqslant 0$, be the continuous nonanticipative solution of (2.11) with $Y(0) = y$. Then writing

$$W_k(t) \doteq Y_1^{(k)}(t) - Y_1^{(k)}(0) - tb_k^{(0)},$$

$$W(t) \doteq (W_1(t), \dots, W_n(t))', \quad \dots \quad (3.30)$$

one has

$$W(t) = \int_0^t (\hat{b}(Y(s)) - \bar{b})ds + \int_0^t \hat{\sigma}(Y(s))dB(s). \quad \dots \quad (3.31)$$

By Ito's lemma,

$$\hat{u}_{j,N}(Y(t))-\hat{u}_{j,N}(Y(0))$$
$$= \int_0^t \tilde{A}\hat{u}_{j,N}(Y(s))ds + \int_0^t \partial\hat{u}_{j,N}(Y(s)).\ \hat{\sigma}(y(s))dB(s), \ (1 \leqslant j \leqslant n). \quad \dots \ (3.32)$$

In view of (3.27), (3.29) one has the representation (see Ikeda and Watanabe, 1981, Chapter II)

$$\hat{u}_j(Y(t))-\hat{u}_j(Y(0))$$
$$= \int_0^t (\hat{b}_j(Y(s))-b_j^{(0)})ds + \int_0^t \partial\hat{u}_j(Y(s))\hat{\sigma}(Y(s))dB(s) \quad a.s. \ (t \geqslant 0). \quad \dots \ (3.33)$$

From (3.31), (3.33) one has

$$W(t) = \hat{u}(Y(t))-\hat{u}(Y(0))$$
$$- \int_0^t (\partial\hat{u}(Y(s))-I)\hat{\sigma}(Y(s))dB(s) \ a.s. \ (t \geqslant 0). \quad \dots \ (3.34)$$

The quadratic variation of the martingale $W_\varepsilon(t\,;\,c) \doteq X_\varepsilon(t\,;\,c)-\epsilon\hat{u}(Y(t/\epsilon^2))+\epsilon\hat{u}(Y(0))$ is given by

$$Z_\epsilon(t) = \epsilon \int_0^{t/\epsilon^2} (\partial\hat{u}(Y(s))-I)\hat{a}(Y(s))\,(\partial\hat{u}(Y(s))-I)'ds. \quad \dots \ (3.35)$$

Since each element of the integrand is a stationary ergodic stchastic process (when $Y(0)$ has distribution π) having a finite expection, by the ergodic theorem one has a.s.

$$\lim_{\epsilon \downarrow 0} Z_\epsilon(1) = \int_{\mathcal{J}} (\partial\hat{u}(Y)-I)\hat{a}(y)\,(\partial\hat{a}(y)-I)'\pi(dy). \quad \dots \ (3.36)$$

It follows that (3.36) holds with $Y(0) = y_0$ for all $y_0 \in \mathcal{J}$ outside a set of null π-measure. Let $\varphi(y_0)$ denote the probability that (3.36) holds with $Y(0) = y_0$ Since the event that (3.36) holds is shift-invariant, $\varphi(y_0)$ is $\tilde{L}$-harmonic, and its restriction to H_c is L_c-harmonic (see (2.16), (2.18)). Thus if $\varphi(y_0) = 1$ for some $y_0 \in H_c$, then $\varphi(y) = 1$ for *all* $y \in H_c$, by the maximum principle for strictly elliptic operators. Therefore, for all c outside a set $\mathcal{N}$ of zero $(M-n)$-dimensional Lebesgue measure, if $y_0 \in H_c$ then (3.36) holds with initial state y_0. It now follows from (3.34)-(3.36) that with $y_0 \in H_c \ (c \notin \mathcal{N})$, $W_\varepsilon(t\,;\,c)$ converges weakly to the desired Brownian motion (one may show this, e.g., by expressing $\theta.W_\varepsilon(t\,;\,c)$ as a time changed one-dimensional Brownian motion, for each $\theta \in \mathbf{R}^n$)). Finally, $\epsilon\hat{u}(Y(t/\epsilon^2))-\epsilon\hat{u}(Y(0))$ converges to zero uniformly on compact time intervals, with probability one (See Bhattacharya, 1982, p. 189) when the initial distribution is π. Again this implies that $\epsilon\hat{u}(Y(t/\epsilon^2))-\epsilon\hat{u}(Y(0))$ converges to zero uniformly on compact time intervals, with probability one when the initial state lies on H_c, for c lying outside a set of zero $(M-n)$-dimensional Lebesgue measure.

Remark 1 : One may relax the assumption that the sums in (2.1) be over a *finite* set of integer vectors m. The proof of Theorem 2.5 goes over if one assumes

$$\sum_m |b_k^{(m)}| \left[\sum_{j=1}^{n} \left| \sum_{j=1}^{M_j} m_r^{(j)}\omega_r^{(j)} \right| \right] < \infty \; (1 \leqslant k \leqslant n),$$

$$\sum_m |a_{kk'}^{(m)}| \left[\sum_{j=1}^{n} \left| \sum_{r=1}^{M_j} m_r^{(j)}\omega_r^{(j)} \right| \right] < \infty \; (1 \leqslant k, k' \leqslant n). \qquad \ldots \quad (3.37)$$

Theorem 3.4 goes over if the 'finite sum' assumption is replaced by (3.37) and (see (3.6))

$$\sum_m |b_k^{(m)}|^2 \left[\left| \sum_{r=1}^{M_j} m_r^{(j)}\omega_r^{(j)} \right| \right]^{-2} < \infty \; (1 \leqslant k \leqslant n, \; 1 \leqslant j \leqslant n). \qquad \ldots \quad (3.38)$$

In view of condition ($\boldsymbol{C}$), (3.38) may be replaced by the condition

$$\sum_m |b_k^{(m)}|^2 \left[\sum_{r=1}^{M_j} |m_r^{(j)}| \right]^{2s_0} < \infty \; (1 \leqslant k \leqslant n, \; 1 \leqslant j \leqslant n). \qquad \ldots \quad (3.39)$$

Remark 2. With each $y \in \mathcal{J}$ one may associate the set of drift and diffusion coefficients $b_{k,c}(.+z)$, $a_{kk'c}(.+z)$, where $c = (c_r^{(k)} = \bar{y}_r^{(k)} - \bar{y}_1^{(k)} : 2 \leqslant r \leqslant M_k, \; 1 \leqslant k \leqslant n) \in \boldsymbol{R}^{M-n}$ and $z = (z_k = \bar{y}_1^{(k)} : 1 \leqslant k \leqslant n) \in \boldsymbol{R}^n$. When $\bar{y}$ is chosen at random with distribution π, one obtains a *random* field indexed by $x \in \boldsymbol{R}^n : x \to \{(b_{k,c}(x+z))_{1 \leqslant k \leqslant n}, (a_{kk',c}(x+z))_{1 \leqslant k, k' \leqslant n}\}$. This random field is *stationary* (w.r.t. translation on $\boldsymbol{R}^n$) and *ergodic* (See Papanicolaou and Varadhan, 1979). The proof of Theorem 3.4 shows that when the drift and diffusion coefficients arise in this random manner (i.e., as a raalization of this random field) and the corresponding stochastic differential equation is solved with a Brownian motion $B(t)$ independent of this random field (i.e., independent of $\bar{y} \in \mathcal{J}$), then the solution $X(t)$, say, is asymptotically Gaussian: $\epsilon X(t/\epsilon^2) - \frac{t}{\epsilon}\, \bar{b}$, $t \geqslant 0$, converges in distribution to an n-dimensional Brownian motion with zero drift and dispersion matrix (3.26).

Remark 3 : Kozlov (1979) derives estimates such as (3.5) in the self-adjoint case, and infers the smoothness of solutions. Since these estimates concern differentiation in only n directions in an M-dimensional space, the validity of such an inference is doubtful.

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7.5 "Stability in distribution for a class of singular diffusions"

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STABILITY IN DISTRIBUTION FOR A CLASS OF SINGULAR DIFFUSIONS

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A verifiable criterion is derived for the stability in distribution of singular diffusions, that is, for the weak convergence of the transition probability $p(t; x, dy)$, as $t \to \infty$, to a unique invariant probability. For this we establish the following: (i) tightness of $\{p(t; x, dy)\colon t \geq 0\}$; and (ii) asymptotic flatness of the stochastic flow. When specialized to highly nonradial nonsingular diffusions the results here are often applicable where Has'minskii's well-known criterion fails. When applied to traps, a sufficient condition for stochastic stability of nonlinear diffusions is derived which supplements Has'minskii's result for linear diffusions. We also answer a question raised by L. Stettner (originally posed to him by H. J. Kushner): Is the diffusion stable in distribution if the drift is Bx where B is a stable matrix, and $\sigma(\cdot)$ is Lipschitzian, $\sigma(\underline{0}) \neq 0$? If not, what additional conditions must be imposed?

1. Introduction. Consider a diffusion $\{X^x(t)\colon t \geq 0\}$ on $\Re^k$ satisfying Itô's equation

$$X^x(t) = x + \int_0^t BX^x(s)\, ds + \int_0^t \sigma(X^x(s))\, dW(s), \tag{1.1}$$

where B is a $k \times k$ matrix, $\sigma(\cdot)$ is a Lipschitzian $(k \times l)$-matrix-valued function on $\Re^k$ and $\{W(t)\colon t \geq 0\}$ is a standard l-dimensional Brownian motion. Let $p(t; x, dy)$ denote the transition probability of the diffusion. The following definitions apply to general diffusions, and not only to those of the form (1.1) with linear drifts.

Definition 1.1. A diffusion is *stable in distribution* if its transition probability $p(t; x, dy)$ converges weakly to some probability measure $\pi(dy)$, as $t \to \infty$, for every x.

It is clear that stability in distribution implies the existence of a unique invariant probability. It is simple to check that stability in distribution follows from the following: (i) tightness of $\{p(t; x, dy)\colon 0 \leq t < \infty\}$; and (ii) the following notion of asymptotic flatness.

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DEFINITION 1.2. The stochastic flow $\{X^x(t): t \geq 0, x \in \mathfrak{R}^k\}$ is *asymptotically flat* (in probability) *uniformly on compacts* if

$$\sup_{x, y \in K} P(|X^x(t) - X^y(t)| > \varepsilon) \to 0 \quad \text{as } t \to \infty, \tag{1.2}$$

for every $\varepsilon > 0$ and every compact set K.

We will actually derive a stronger property than (1.2) called *asymptotic flatness of the stochastic flow in the δth mean* ($\delta > 0$), which means that for every compact K,

$$\lim_{t \to \infty} \sup_{x, y \in K} E|X^x(t) - X^y(t)|^\delta = 0. \tag{1.3}$$

In the special case when a *trap* x^* exists, that is, $X^{x^*}(t) = x^*$ for all $t \geq 0$, (1.2) with $y = x^*$ implies stochastic stability defined as follows.

DEFINITION 1.3. Let x^* be a trap. Then $\{X^x(t): t \geq 0, x \in \mathfrak{R}^k\}$ is *stochastically stable* (in probability) if for all $\varepsilon_1 > 0$, $\varepsilon_2 > 0$ there exists $\delta > 0$ such that

$$\sup_{0 \leq t < \infty} \sup_{\{x: |x - x^*| \leq \delta\}} P(|X^x(t) - x^*| > \varepsilon_1) < \varepsilon_2. \tag{1.4}$$

Consider the question: Under what conditions on B and $\sigma(\cdot)$ is the diffusion stable in distribution? If $\sigma(\cdot)\sigma(\cdot)'$ is nonsingular, then the existence of an invariant probability is equivalent to stability in distribution, and Has'minskii's well-known criteria apply (Has'minskii [4]; Bhattacharya [2]). Our main interest lies in the *singular* case: $\sigma(x)\sigma(x)'$ is of rank less than k for some x. In this case the existence of a unique invariant probability does not necessarily imply stability in distribution, as may be shown by examples [e.g., $k = 1$, $B = 1$, $\sigma(x) = x$]. If $\sigma(\cdot) \equiv \sigma$ is a constant matrix, then a well-known necessary and sufficient condition for stability is that all eigenvalues of B have negative real parts (see, e.g., Arnold [1], pages 178–187). If $\sigma(\cdot)$ is linear, that is, every element of $\sigma(\cdot)$ is a linear function, then $x = \underline{0}$ is a *trap* and stability in distribution is equivalent to stochastic stability (in probability), which has been extensively studied by Has'minskii [5], Chapter 6. We are primarily interested in the case $\sigma(\underline{0}) \neq 0$, that is, $\underline{0}$ is not a trap. In this case if the diffusion is stable in distribution, the invariant probability has no discrete component. However, one may also derive criteria for stochastic stability by the method used in this article (see Remark 2.4).

The main distinction between nonsingular diffusions and singular ones in the present context is that for nonsingular diffusions *tightness* of $\{p(t; x, dy): t \geq 0\}$ for some x is equivalent to stability in distribution, while this is far from being true in the singular case. Here is a simple but interesting example.

EXAMPLE 1.1. Let $k = 2$, $B = \text{diag}(-1, -1)$ and

$$\sigma(x) = c\begin{pmatrix} x_2 & 0 \\ -x_1 & 0 \end{pmatrix}.$$

Then $R^2(t) := X_1^2(t) + X_2^2(t)$ satisfies $dR^2(t) = (c^2 - 2)R^2(t)\,dt$, so that $R^2(t) = R^2(0) \times \exp\{(c^2 - 2)t\}$. Consider the case $|c| = \sqrt{2}$. Then $R^2(t) = R^2(0)$ for all t, which in particular implies tightness of $\{p(t; x, dy): t \geq 0\}$ for every x. On the other hand, there is an invariant probability on every circle and the angular motion on the circle is a periodic diffusion. If $|c| \neq \sqrt{2}$, the only invariant probability is the point mass at the origin. If $|c| > \sqrt{2}$ and $X(0) \neq \underline{0}$, then $R^2(t) \to \infty$ a.s. as $t \to \infty$. If $|c| < \sqrt{2}$, then the diffusion is stochastically stable a.s. and, therefore, stable in distribution. One may modify this example by taking $\sigma(\cdot)$ so that $\sigma(\cdot)\sigma(\cdot)'$ is nonsingular on $\{|x| < r\}$ for some $r > 0$, and letting $\sigma(\cdot)$ be as above with $c = \pm\sqrt{2}$ on $\{|x| \geq r\}$. In this case the diffusion starting in $\{|x| \leq r\}$ has the limit cycle property, converging in distribution to the invariant probability on $\{|x| = r\}$, but still has infinitely many invariant probabilities—one on each circle $\{|x| = r'\}$, $r' \geq r$.

The following simple example shows that (1.3) alone is not enough and that tightness is needed along with (1.2) [or (1.3)] to establish stability in distribution.

EXAMPLE 1.2. Let $k = 1$, $b(x) = e^{-x}$, $\sigma(x) \equiv 0$. Then $X^x(t) = \ln(t + e^x) \to \infty$ as $t \to \infty$, but $X^x(t) - X^y(t) = \ln((t + e^x)/(t + e^y)) \to 0$ as $t \to \infty$, uniformly for x, y in a compact set K.

Finally, stable singular diffusions are not in general Harris recurrent, nor strongly mixing. To derive central limit theorems and laws of the iterated logarithm for processes such as $\int_0^t f(X(s))\,ds$, a convenient method in this case is to show that f belongs to the range of the infinitesimal generator on $L^2(\Re^k, \pi)$ (Bhattacharya [3]). Estimates of asymptotic flatness such as (2.17) enable one to identify a broad subset of the range.

Some qualitative aspects of asymptotics of singular diffusions have been studied by Kliemann [7].

2. The main result. Assume that, for some $\lambda_0 \geq 0$,

$$\|\sigma(x) - \sigma(y)\| \leq \lambda_0 |x - y|, \quad \text{for all } x, y. \tag{2.1}$$

Throughout $\cdot$ (dot) and $|\ |$ denote euclidean inner product and norm, while $\|\ \|$ denotes matrix norm with respect to $|\ |$. Write

$$\begin{aligned} a(x) &= \sigma(x)\sigma(x)', \\ a(x,y) &= (\sigma(x) - \sigma(y))(\sigma(x) - \sigma(y))'. \end{aligned} \tag{2.2}$$

Write tr(A) for the *trace* of the matrix A. Our main result is:

THEOREM 2.1. *Suppose $\sigma(\cdot)$ is Lipschitzian.*

(a) *If there exist a symmetric positive definite matrix C and a positive constant γ such that*

$$2C(x-y)\cdot B(x-y) - \frac{2C(x-y)\cdot a(x,y)C(x-y)}{(x-y)\cdot C(x-y)} \tag{2.3}$$
$$+ \operatorname{tr}(a(x,y)C) \le -\gamma|x-y|^2, \qquad x \neq y,$$

then the diffusion (1.1) *is stable in distribution.*

(b) *If there exist a symmetric positive definite matrix C and a constant $\beta > 0$ such that*

$$2Cx\cdot Bx - \frac{2Cx\cdot a(x)Cx}{x\cdot Cx} + \operatorname{tr}(a(x)C) \le -\beta|x|^2 \tag{2.4}$$

for all sufficiently large $|x|$,

then there exists an invariant probability.

The inequalities (2.3) and (2.4) arise from the use of the Liapounov function $v(x) := (x\cdot Cx)^{1-\varepsilon}$ [for a suitable $\varepsilon \in [0,1)$] applied, respectively, to the stochastic processes $Z^{x,y}(t) := X^x(t) - X^y(t)$ and $X^x(t)$.

As a corollary we have

COROLLARY 2.2. *Assume $\sigma(\cdot)$ is Lipschitzian and all eigenvalues of B have negative real parts. Assume in addition that*

$$(k-1)\lambda_0^2 < \frac{1}{\Lambda_P}, \tag{2.5}$$

where λ_0 is as in (2.1) *and Λ_P is the largest eigenvalue of*

$$P := \int_0^\infty \exp\{sB'\}\exp\{sB\}\,ds. \tag{2.6}$$

Then the diffusion (1.1) *is stable in distribution.*

PROOF. In order to deduce Corollary 2.2 from Theorem 2.1, let $C = P$. It is not difficult to check that

$$B'P + PB = -I, \tag{2.7}$$

where I is the $k\times k$ identity matrix. Using this, we get $2Px\cdot Bx = x\cdot(PB + B'P)x = -|x|^2$. Also,

$$\operatorname{tr}(a(x,y)P) = \operatorname{tr}(\sqrt{P}\,a(x,y)\sqrt{P})$$

and

$$\frac{2P(x-y)\cdot a(x,y)P(x-y)}{(x-y)\cdot P(x-y)} = \frac{2\sqrt{P}(x-y)\cdot\sqrt{P}a(x,y)\sqrt{P}\sqrt{P}(x-y)}{\sqrt{P}(x-y)\cdot\sqrt{P}(x-y)}$$

$$\geq 2\big(\text{smallest eigenvalue of } \sqrt{P}a(x,y)\sqrt{P}\big).$$

Therefore,

$$\begin{aligned} (2.8)\qquad & -\frac{2P(x-y)\cdot a(x,y)P(x-y)}{(x-y)\cdot P(x-y)} + \operatorname{tr}(a(x,y)P) \\ & \leq \sum_{i=2}^{k} \lambda_i(x,y) - \lambda_1(x,y), \end{aligned}$$

where $\lambda_1(x,y) \leq \lambda_2(x,y) \leq \cdots \leq \lambda_k(x,y)$ are the eigenvalues of $\sqrt{P}a(x,y)\sqrt{P}$. The right side of (2.8) is clearly no larger than

$$(k-1)\|\sqrt{P}a(x,y)\sqrt{P}\| \leq (k-1)(\|P\|)(\|a(x,y)\|) \leq (k-1)\Lambda_P\lambda_0^2|x-y|^2.$$

Now let $\gamma = (1-(k-1)\Lambda_P\lambda_0^2)$ to obtain (2.3). □

REMARK 2.1. Before proceeding with the proof of Theorem 2.1, let us note that if $\sigma(\cdot)$ is Lipschitzian, then (2.3) implies (2.4) for every $\beta \in (0,\lambda)$. To see this simply take $y = 0$ in (2.3) and use the estimate

$$\begin{aligned} (2.9)\qquad -\gamma|x|^2 &\geq 2Cx\cdot Bx - \frac{2Cx\cdot a(x,0)Cx}{x\cdot Cx} + \operatorname{tr}(a(x,0)C) \\ &= 2Cx\cdot Bx - \frac{2Cx\cdot a(x)Cx}{x\cdot Cx} + \operatorname{tr}(a(x)C) + O(|x|) \quad \text{as } |x|\to\infty. \end{aligned}$$

As we shall see in the course of the proof of Theorem 2.1, (2.4) implies the *existence* of an invariant probability, but not *uniqueness*. The stronger condition (2.3) also implies the asymptotic flatness (1.3). The existence of an invariant probability and asymptotic flatness together immediately yield uniqueness and stability.

PROOF OF THEOREM 2.1. Consider the (Liapounov) function

$$(2.10)\qquad v(x) = (x\cdot Cx)^{1-\varepsilon}$$

for some $\varepsilon \in [0,1)$ to be chosen later. Define, for a given pair (x,y) with $x \neq y$,

$$\begin{aligned} Z^{x,y}(t) &:= X^x(t) - X^y(t) \\ (2.11)\qquad &= x - y + \int_0^t BZ^{x,y}(s)\,ds + \int_0^t \big(\sigma(X^x(s)) - \sigma(X^y(s))\big)\,dW(s), \\ \tau_0 &:= \inf\{t \geq 0 : Z^{x,y}(t) = 0\}. \end{aligned}$$

By Itô's lemma (see Ikeda and Watanabe [6], pages 66–67)

$$v(Z^{x,y}(t)) - v(x-y) = \int_0^t \tilde{L}(v)(X^x(s), X^y(s))\,ds \tag{2.12}$$
$$+ \int_0^t (\operatorname{grad} v)(Z^{x,y}(s)) \cdot (\sigma(X^x(s)) - \sigma(X^y(s)))\,dW(s), \qquad t < \tau_0,$$

where writing ∂_i for differentiation with respect to the ith coordinate and using (2.3),

$$\begin{aligned}
\tilde{L}(v)(x,y) &:= B(x-y)\cdot(\operatorname{grad} v)(x-y) + \frac{1}{2}\sum_{i,j=1}^{k} a_{ij}(x,y)(\partial_i\partial_j v)(x-y)\\
&= (1-\varepsilon)((x-y)\cdot C(x-y))^{-\varepsilon}\Big[2B(x-y)\cdot C(x-y)\\
&\qquad -2\varepsilon\frac{(x-y)\cdot Ca(x,y)C(x-y)}{(x-y)\cdot C(x-y)} + \operatorname{tr}(a(x,y)C)\Big]\\
&\le (1-\varepsilon)((x-y)\cdot C(x-y))^{-\varepsilon}\Big[-\gamma|x-y|^2\\
&\qquad +2(1-\varepsilon)\frac{(x-y)\cdot Ca(x,y)C(x-y)}{(x-y)\cdot C(x-y)}\Big]\\
&\le (1-\varepsilon)((x-y)\cdot C(x-y))^{-\varepsilon}\\
&\qquad \times\left[-\gamma|x-y|^2 + 2(1-\varepsilon)\lambda_0^2\Lambda_C|x-y|^2\right].
\end{aligned} \tag{2.13}$$

Here Λ_C is the largest eigenvalue of C. Now choose $\varepsilon \in [0,1)$ such that

$$-\gamma_1 := -\gamma + 2(1-\varepsilon)\lambda_0^2\Lambda_C < 0. \tag{2.14}$$

Then we have

$$\tilde{L}(v)(x,y) \le -\alpha v(x-y), \tag{2.15}$$

with $\alpha := (\gamma_1(1-\varepsilon))/\Lambda_C$. Consider the process $Y(t) := \exp\{\alpha t\}v(Z^{x,y}(t))$. It follows from (2.12) and (2.15) that $\{Y(t\wedge\tau_0): t \ge 0\}$ is a positive supermartingale. In particular,

$$EY(t\wedge\tau_0) \le EY(0) = v(x-y). \tag{2.16}$$

Since $Z^{x,y}(t) = 0$ a.s. for all $t \ge \tau_0$, so that $Y(t) = 0$ for all $t \ge \tau_0$, (2.16) implies $EY(t) \le v(x-y)$. That is,

$$E(Z^{x,y}(t)\cdot CZ^{x,y}(t))^{1-\varepsilon} \le \exp\{-\alpha t\}((x-y)\cdot C(x-y))^{1-\varepsilon} \qquad t \ge 0. \tag{2.17}$$

This establishes the asymptotic flatness of the stochastic flow [in the $2(1-\varepsilon)$th mean].

In view of Remark 2.1, to complete the proof of Theorem 2.1 we need to show that (2.4) implies the existence of an invariant probability. But (2.4) implies $Lv(x) \to -\infty$ as $|x| \to \infty$, and the existence of an invariant probability follows from Has'minskii [5], Theorem 5.1, page 90. Note that v may be modified near the origin to make it twice continuously differentiable on all of $\mathfrak{R}^k$. □

REMARK 2.2 (Almost sure asymptotic flatness). The proof of Theorem 2.1 may be slightly modified to show that if (2.3) holds, then the stochastic flow is asymptotically flat *almost surely*, that is, there exists a finite random variable $V^{x,y}$ such that

$$v(Z^{x,y}(t)) \le V^{x,y}\exp\{-\alpha t\} \quad \text{a.s., } t \ge 0. \tag{2.18}$$

REMARK 2.3 (Nonlinear drift). If instead of a linear drift one has an arbitrary Lipschitzian drift $b(\cdot)$, then Theorem 2.1 holds with $B(x-y)$ [in (2.3)] and Bx [in (2.4)] replaced by $b(x)-b(y)$ and $b(x)$, respectively. There is no essential change in the proof.

REMARK 2.4 (Stochastic stability). If the origin $\underline{0}$ is a *trap*, that is, $\sigma(\underline{0}) = 0$, then $\{p(t; 0, dy)\colon t \ge 0\}$ is trivially tight. In this case the proof of Theorem 2.1 shows that it is enough to check (2.3) with $y = 0$ (for all x). In view of (2.18), the diffusion is then stochastically stable a.s. and in the δth mean, for some $\delta > 0$. More generally, if the drift is $b(\cdot)$ [$b(\cdot)$ and $\sigma(\cdot)$ are assumed to be Lipschitzian] and if x^* is a *trap*, that is, $b(x^*) = 0$, $\sigma(x^*) = 0$, then a sufficient condition that $X_t^x \to x^*$ a.s. and in the δth mean exponentially fast for every x as $t \to \infty$, is

$$\begin{aligned} 2C(x-x^*)\cdot b(x) - \frac{2C(x-x^*)\cdot a(x)C(x-x^*)}{(x-x^*)\cdot C(x-x^*)} + \operatorname{tr}(a(x,x^*)C) \\ \le -\gamma|x-x^*|^2 \quad \text{for all } x \ne x^*, \end{aligned} \tag{2.19}$$

for some positive definite matrix C and some $\gamma > 0$. In the case $b(\cdot)$ and $\sigma(\cdot)$ are both linear, this result may also be derived by the method of Has'minskii [5]. Note that $a(x, x^*) = a(x)$ if $\sigma(x^*) = 0$.

REMARK 2.5. Suppose the left side in (2.3) is *greater than or equal* to $\gamma|x-y|^2$ for some $\gamma > 0$ and all $x \ne y$. Then one may show (by the method of proof for asymptotic flatness) that $|X^x(t) - X^y(t)| \to \infty$ a.s. (and in the δth mean) exponentially fast as $t \to \infty$. This is true for the general nonlinear case, if $B(x-y)$ is replaced by $b(x)-b(y)$. Similarly, if the left side of (2.4) is greater than or equal to $\beta|x|^2$ for all x, then $|X^y(t)| \to \infty$ a.s. as $t \to \infty$ for every y that is not a trap.

REMARK 2.6 (Criterion for stability in distribution for nonsingular diffusions). Since (2.4) ensures tightness, a nonsingular diffusion with drift $b(\cdot)$ is stable in distribution if (2.4) holds [with Bx replaced by $b(x)$]. Although for nonsingular diffusions Has'minskii's useful criterion of positive recurrence is available, it is not very suitable if the infinitesimal generator is far from being radial. We give a simple example where Has'minskii's criterion is not satisfied, but (2.4) holds.

EXAMPLE 2.1. Let $k = 2$, $B = \text{diag}(-1, -1)$, $a(x) = (\delta_1 + \delta_2(x_2)^2)I$, where $\delta_1 > 0$, $\delta_2 \geq 0$ are constants. To apply Has'minskii's criterion we compute (see Bhattacharya [2])

$$\underline{\alpha}(r) := \inf_{|x|=r} \frac{x \cdot a(x)x}{|x|^2} = \delta_1,$$

$$\bar{\beta}(r) := \sup_{|x|=r} \frac{2x \cdot Bx + \text{tr}(a(x))}{(x \cdot a(x)x)/|x|^2} - 1 = \left(1 - \frac{2}{\delta_2}\right) + \frac{2\delta_1/\delta_2}{\delta_1 + \delta_2 r^2}, \tag{2.20}$$

$$\bar{I}(r) := \int_1^r \frac{\bar{\beta}(u)}{u}\, du = \left(1 - \frac{2}{\delta_2}\right)\ln r + O(1).$$

According to Has'minskii's criterion (see [2] and [4]) a sufficient condition for stability in distribution is

$$\begin{aligned} &\int_1^\infty \exp\{-\bar{I}(r)\}\, dr = \infty, \\ &\int_1^\infty \frac{\exp\{\bar{I}(r)\}}{\underline{\alpha}(r)}\, dr < \infty. \end{aligned} \tag{2.21}$$

In the present example,

$$\begin{aligned} &\int_1^\infty \exp\{-\bar{I}(r)\}\, dr = \infty \quad \text{for all } \delta_2 \geq 0, \\ &\int_1^\infty \frac{\exp\{\bar{I}(r)\}}{\underline{\alpha}(r)}\, dr < \infty \quad \text{iff } \delta_2 < 1. \end{aligned} \tag{2.22}$$

Thus, according to Has'minskii's test, the diffusion is stable in distribution if $\delta_2 \in [0, 1)$. On the other hand, taking $C = I$, the left side of (2.4) is $-2|x|^2$. Thus the criterion (2.4) is satisfied and the diffusion is stable in distribution no matter what the value of the nonnegative constant δ_2 is.

REMARK 2.7. A specific question raised by L. Stettner to one of us during a visit to the IMA in 1986 at the University of Minnesota was: Is the diffusion (1.1) stable in distribution if $\sigma(\cdot)$ is Lipschitzian, $\sigma(\underline{0}) \neq 0$, and all eigenvalues of B have negative real parts? It is obvious from (2.5) that the answer is yes for $k = 1$. A counterexample is contained in Example 1.1 for the case $k = 2$ [with $\sigma(\cdot)$ modified near the origin], which can be extended to $k > 2$. The two examples below show that even when restricted to nonsingular diffusions, the answer is "yes" for $k = 1$ and "no" for $k > 1$.

EXAMPLE 2.2 ($k > 2$). Let $B = -\delta I$ ($\delta > 0$), $a(x) = dr^2 I$ ($d > 0$) for $r \equiv |x| \geq 1$; then $a(\cdot)$ is nonsingular and Lipschitzian on $\Re^k$. In this case Has'minskii's criterion (2.21) is *necessary* as well as sufficient. But $\bar{I}(r) = (k - 1 - (2\delta/d))\ln r$ ($r \geq 1$). If $\delta/d < (k-2)/2$, then the first integral in (2.21) converges, implying that the diffusion is *transient*. If $\delta/d = (k-2)/2$, then the first integral in (2.21) diverges, as does the second integral, and the diffusion is *null recurrent*. If $\delta/d > (k-2)/2$, then (2.21) holds so that the diffusion is *positive recurrent* and, therefore, stable in distribution.

EXAMPLE 2.3 ($k = 2$). Let $B = -\delta I$,

$$a(x) = \begin{pmatrix} \lambda_1 x_2^2 + \varepsilon & -\lambda_1 x_1 x_2 \\ -\lambda_1 x_1 x_2 & \lambda_1 x_1^2 + \varepsilon \end{pmatrix},$$

where δ, λ_1 and ε are positive constants. Note that the positive definite square root of $a(x)$ is Lipschitzian in this case. Then

$$\begin{aligned} \bar{\beta}(r) &= \underline{\beta}(r) := \inf_{|x|=r} \frac{(\lambda_1 - 2\delta)|x|^2 + \varepsilon}{\varepsilon} = 1 + \frac{\lambda_1 - 2\delta}{\varepsilon} r^2, \\ \bar{I}(r) &= \underline{I}(r) := \int_1^r \frac{\underline{\beta}(u)}{u}\, du. \end{aligned} \tag{2.23}$$

Has'minskii's criterion for recurrence (or transience) is necessary as well as sufficient here. If $\lambda_1 = 2\delta$, then $\underline{\beta}(r) = 1$ and both the integrals in (2.21) diverge, which implies the diffusion is null recurrent. If $\lambda_1 > 2\delta$, then $\int_1^\infty \exp\{-\underline{I}(r)\}\, dr < \infty$, so that the diffusion is transient and no invariant probability exists.

Acknowledgments. We would like to thank Ananda Weersinghe for bringing his recent manuscript "Almost sure stability of diffusions" to our attention. In this, the author derives asymptotic flatness for a class of stochastic flows assuming certain conditions on the drift and diffusion coefficients. These assumptions are different from ours. For example, when specialized to linear drift and affine linear functions $\sigma_{ij}(x)$, the criterion in that manuscript is similar to (2.3) but omits the middle term on the left. We also wish to thank the referee for helpful suggestions.

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7.6 "Speed of convergence to equilibrium and to normality for diffusions with multiple periodic scales"

Speed of convergence to equilibrium and to normality for diffusions with multiple periodic scales, Stochastic Processes and their Applications. 80, pages 55–86 (with M. Denker & A. Goswami).

Speed of convergence to equilibrium and to normality for diffusions with multiple periodic scales

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Abstract

The present article analyses the large-time behavior of a class of time-homogeneous diffusion processes whose spatially periodic dynamics, although time independent, involve a large spatial parameter 'a'. This leads to phase changes in the behavior of the process as time increases through different time zones. At least four different temporal regimes can be identified: an initial non-Gaussian phase for times which are not large followed by a first Gaussian phase, which breaks down over a subsequent region of time, and a final Gaussian phase different from the earlier phases. The first Gaussian phase occurs for times $1 \ll t \ll a^{2/3}$. Depending on the specifics of the dynamics, the final phase may show up reasonably fast, namely, for $t \gg a^2 \log a$; or, it may take an enormous amount of time $t \gg \exp\{ca\}$ for some $c>0$. An estimation of the speed of convergence to equilibrium of diffusions on a circle of circumference 'a' is provided for the above analysis. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Diffusions; Periodic coefficients; Spectral gaps; Gaussian approximation

1. Introduction and summary

Consider a diffusion $X(\cdot)$ governed by Itô's stochastic integral equation of the form

$$X(t) = x_0 + \int_0^t \{b(X(s)) + \beta(X(s)/a)\}\,\mathrm{d}s + \int_0^t \sigma(X(s))\,\mathrm{d}B(s), \tag{1.1}$$

where $b(x)$ may be thought of as the *local* drift velocity, and $\beta(x/a)$ the *large-scale* drift velocity of $X(\cdot)$. The spatial scale parameter 'a' is large and, therefore, $\beta(x/a)$ changes slowly. As a consequence, one may expect $X(\cdot)$ to be well approximated, during an initial period of time, by $X_1(\cdot)$ satisfying

$$X_1(t) = x_0 + \int_0^t \{b(X_1(s)) + \beta(x_0/a)\}\,\mathrm{d}s + \int_0^t \sigma(X_1(s))\,\mathrm{d}B(s). \tag{1.2}$$

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Notice that the large-scale drift is replaced by a constant $\beta(x_0/a)$. By changing the origin, one may take $x_0=0$ in Eqs. (1.1) and (1.2), so that the dynamics of $X_1(\cdot)$ are completely unaffected by large-scale fluctuations embodied in $\beta(x/a)$. In the case of k-dimensional diffusions it was shown in Bhattacharya and Götze (1995) that $X_1(s)$, $0\leqslant s\leqslant t$, well approximates $X(s)$, $0\leqslant s\leqslant t$, if $t=o(a^{2/3})$, provided $b(\cdot),\beta(\cdot)$ are Lipschitzian and $\sigma(\cdot)$ is a constant nonsingular matrix. Now if $b(\cdot)$ is periodic then $X_1(\cdot)$ is asymptotically a Brownian motion whose parameters can be computed by solving certain elliptic equations (Bensoussan et al., 1978; Bhattacharya, 1985). It follows that for $1\ll t\ll a^{2/3}$, $X(\cdot)$ has the same Brownian motion approximation. The time scale $t=o(a^{2/3})$ for this approximation cannot in general be expanded.

As t becomes larger, the effects of large-scale fluctuations become significant, and $X(\cdot)$ may go through a number of phase changes with time. This phenomenon was analysed in Bhattacharya and Götze (1995) for k-dimensional diffusions ($k\geqslant 2$) such that $b(\cdot)$ and $\beta(\cdot)$ are periodic, having the same period lattice, 'a' a (large) positive integer, $\sigma(\cdot)$ a constant nonsingular $k\times k$ matrix. In addition, it was assumed that $\operatorname{div} b(x)\equiv 0\equiv \operatorname{div}\beta(x)$. The 'divergence-free' assumption was crucial in this analysis, which showed that for times $t\gg a^2\log a$ the diffusion $X(\cdot)$ is again asymptotically a Brownian motion, whose parameters are quite different from those of the initial approximating Brownian motion. The time scale for this later approximation cannot in general be made smaller than $t\gg a^2$.

Under the 'divergence-free' assumption, the diffusion $\dot{X}(t):=X(t)\bmod a$ ($t\geqslant 0$) on the *big torus* $S^k(a):=\{x\bmod a\colon x\in\mathbb{R}^k\}$ has normalized Lebesgue measure as its invariant distribution. This assumption also allows one to use elegant spectral theoretical methods for the analysis of the dispersion matrix (of the limiting Brownian motion approximation for $t\gg a^2\log a$). In the absence of this assumption one cannot in general analytically compute the invariant density, and cannot take recourse to the spectral expansions for the analysis of dispersion.

The present article provides an insight into the case when $b(\cdot)$ and $\beta(\cdot)$ are not divergence-free by analyzing the one-dimensional case, where the differential equations leading to the invariant density and asymptotic variance can be solved explicitly.

The first phase of the asymptotics here are derived much the same way as in Bhattacharya and Götze (1995). Using the Cameron–Martin–Girsanov Theorem (Karatzas and Shreve, 1991, p. 193) it is shown in Theorem 3.1 that the total variation distance between the distributions of $X(\cdot)$ and $X_1(\cdot)$ on $C[0,t]$ goes to zero if $t=o(a^{2/3})$, i.e., as $t/a^{2/3}\to 0$. This is true without any specific assumption (such as periodicity) on $b(\cdot)$ and $\beta(\cdot)$. Theorem 3.3 says that if $b(\cdot)$ is periodic then $X(t)$ is asymptotically Gaussian, provided $1\ll t\ll a^{2/3}$. The asymptotic distribution here is the same as that of $X_1(t)$, so that the asymptotic variance parameter does not depend on $\beta(\cdot)$.

For the final phase of the asymptotics, $b(\cdot)$, $\beta(\cdot)$ and $\sigma(\cdot)$ are assumed to be periodic with the same period 1, $\sigma^2(\cdot)>0$, 'a' a positive integer. Then $\dot{X}(t):=X(t)\bmod a$ ($t\geqslant 0$) is a diffusion on the *big circle* $S^1(a):=\{x\bmod a\colon x\in\mathbb{R}\}$. First, consider '$a$' *fixed*. Then the diffusion $\dot{X}$ is φ-mixing with an exponentially decaying φ-mixing rate with time. It follows that $X(t)$ is asymptotically Gaussian with mean $t(\bar{b}+\bar{\beta}_a)$ and variance $t\alpha^2$, say. Here $\bar{b}$, $\bar{\beta}_a$ are the averages of $b(\cdot)$ and $\beta(\cdot/a)$ w.r.t. the invariant probability $\tilde{\pi}_a(x)\,\mathrm{d}x$ on $S^1(a)$, and $\tilde{\pi}_a$ and α^2 may be computed by solving a couple of second-order ordinary differential equations. The important problem is to figure out how large t must be for this Gaussian approximation to take hold, when the parameter 'a' is very large. Of course, a precise Berry–Esséen-type bound, displaying the constants involved as explicit functions of 'a', would be ideal. In spite of much recent progress on Berry–Esséen bounds (see e.g., Bhattacharya and Ranga Rao, 1976; Götze and Hipp, 1983; Stein, 1972; Tikhomirov, 1980), such a precise and explicit computation for the present case seems very hard. In addition, such bounds generally do not reveal phase changes over different scales of time. The present approach is to let t and 'a' go to infinity simultaneously, and determine how large t should be in relation to 'a' for an effective Gaussian approximation to be valid in the final phase.

Without loss of generality, we assume $\int_0^1 (b(y)/\sigma^2(y))\,\mathrm{d}y = 0$. This may be achieved by adding a constant to $\beta(\cdot)$. Two cases are considered. In Case 1, $\beta(\cdot)$ is bounded away from zero. In case 2, $\sigma^2(\cdot)$ is taken to be a constant and $\int_0^1 \beta(x)\,\mathrm{d}x = 0$. The first order of business, in either case, is to determine the speed with which the distribution $\dot{p}(t;x_0,y)\,\mathrm{d}y$ of $\dot{X}(t)$ approaches the equilibrium $\tilde{\pi}_a(y)\,\mathrm{d}y$ on the big torus $S^1(a)$. For this we estimate the spectral gap of the generator L of $\dot{X}$ on $L^2(S^1(a), \tilde{\pi}_a)$. Since L is not self-adjoint in Case 1, the spectral gap λ_L of $\frac{1}{2}(L + \tilde{L})$ is estimated, $\tilde{L}$ being the generator of the time-reversed process. With this notation, $\lambda_L = \inf\{\langle -\tilde{L}f, f\rangle : f \in \mathscr{D}_{\tilde{L}} \cap 1^{\perp}\}$, where $\langle\,,\,\rangle$ denotes the inner product on $L^2(S^1(a), \tilde{\pi}_a)$, $\mathscr{D}_{\tilde{L}}$ is the domain of $\tilde{L}$, and $1^{\perp}$ is the set of all $f \in L^2$ which have zero mean. Some general facts relating to this estimation are derived in Section 2 (Lemmas 2.1 and 2.3). Detailed computations in Section 4.1 show that, in Case 1, $\lambda_L \geqslant c_1/a^2$ where c_i's are positive constants independent of 'a'. Although λ_L concerns the rate of L^2-convergence of a square integrable density to equilibrium, a little extra work (using an estimate of Aronson (1967) for the fundamental solution of a parabolic equation, and an inequality of Fill (1991)) shows that the rate of convergence to equilibrium in total variation norm is no more than $c_2 a^{1/2}\exp\{-c_1 t/a^2\}$ (Theorem 4.2), whatever be the initial state. Crucial in this estimation of λ_L is the fact that $\max_x \tilde{\pi}_a(x)/\min_x \tilde{\pi}_a(x)$ is bounded away from zero, as $a \to \infty$. The central limit theorem, Theorem 4.5, is based on this estimate of the spectral gap and on a computation of the asymptotic variance (parameter) θ^2. It says that, for $t \gg a^2 \log a$, $\{X(t) - t(\bar{b} + \bar{\beta}_a)\}/\theta\sqrt{t}$ is asymptotically standard normal, and $\theta \equiv \theta(a)$ is bounded away from zero and infinity.

In Case 2, L is self-adjoint: $L = \tilde{L}$. Also, $\max_x \tilde{\pi}_a(x)/\min_x \tilde{\pi}_a(x)$ goes to infinity exponentially fast as $a \to \infty$. This leads to a spectral gap estimate $\lambda_L \geqslant c_3 a^{-2}\exp\{-c_4 a\}$ and a consequent rate of convergence to equilibrium given by $c_5 a^{1/2}\exp\{c_6 a^{-2}\mathrm{e}^{-c_4 a} t\}$. To have an intuitive feeling about λ_L it is better perhaps to look at the scaled diffusion $\dot{Y}$ on the unit torus $S^1 := \{x \bmod 1 : x \in \mathbb{R}\}$, defined by

$$\dot{Y}(t) := \dot{X}(a^2 t)/a, \quad t \geqslant 0. \tag{1.3}$$

The generators L of $\dot{X}$ and A of $\dot{Y}$ are

$$L = \frac{1}{2}\sigma^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \{b(x) + \beta(x/a)\}\frac{\mathrm{d}}{\mathrm{d}x}, \tag{1.4}$$

$$A = \frac{1}{2}\sigma^2\frac{\mathrm{d}^2}{\mathrm{d}y^2} + [a\{b(ay) + \beta(y)\}]\frac{\mathrm{d}}{\mathrm{d}y}.$$

One may check that $\lambda_L = (1/a^2)\lambda_A$ (Proposition 4.1). The invariant density π_a of $\dot{Y}$ on S^1 is given by $\pi_a(x) = a\tilde{\pi}_a(ax)$. In the present Case 2, as $a \to \infty$, all weak limit points of $\pi_a(x)\,\mathrm{d}x$ are discrete distributions with support contained in the finite set F of those points $x^* \in S^1$ where the potential function $\psi(x) := \int_0^x \beta(y)\,\mathrm{d}y$ attains its maximum value (Proposition 4.10). In the case ψ has a unique maximum at x^*, $\pi_a(x)\,\mathrm{d}x$ converges weakly to the degenerate distribution $\delta_{x^*}(\mathrm{d}x)$ at x^*.

Also, in Case 2, one has $\bar{b} + \bar{\beta}_a = 0$. Using the spectral gap estimate given in the preceding paragraph, one may now show that for $t \gg a^2 \exp\{c_7 a\} \log a$, $X(t)/\alpha\sqrt{t}$ converges to the standard normal $\mathcal{N}(0,1)$ (Theorem 4.13). Here α^2 goes to zero exponentially fast, as $a \to \infty$. This has two significant implications. First, since $\alpha^2 t$ must go to infinity in order for a Gaussian approximation to hold, the requirement that t *must be at least as large as an exponential in 'a'* cannot be avoided. Indeed, even if the process $\dot{X}$ is in equilibrium (i.e., the initial distribution is $\tilde{\pi}_a$), the final Gaussian approximation becomes valid only after times exponentially large in 'a'. Secondly, the exceedingly small value of α^2 indicates that dispersivity, or variance per unit time, is almost negligible in the final phase.

The results here are in sharp contrast to those obtained in Bhattacharya and Götze (1995) for the divergence-free case. First, in the latter case it always suffices to have $t \gg a^2 \log a$ for the final phase of asymptotics to take hold. Second, the asymptotic variances (per unit time) never decay as $a \to \infty$ in the divergence-free case, and indeed often grow quadratically with 'a'. One expects that the present one-dimensional results may be extended to certain multidimensional cases of interest, besides the obvious case of independent coordinates.

The present analysis also serves as a pointer to the inadequacy of the Berry–Esséen type bounds under dependence (Stein, 1972; Tikhomirov, 1980) without a careful estimation of the constant involved. Such a bound, which applies to the final phase of the asymptotics here, indicates that the error of normal approximation of $X(t)$ is no more than $\gamma/\sqrt{t}$ for some constant $\gamma > 0$. The problem in using it, without an explicit estimation of γ, is that γ may be reasonably small, as would be the case under the hypothesis of Theorem 4.5; it may also be enormously large, as in the case of Theorem 4.13. The size of γ does not depend only on the exponential phi-mixing rate of $\dot{X}$, and on the bounds for $b(\cdot)$, $\beta(\cdot)$, and σ^2. It also depends crucially on the rate at which the asymptotic dispersivity, under equilibrium, grows or decays. The latter in turn depends delicately on the nature of the coefficients (in our case β), not just on their lower and upper bounds.

2. Estimation of the spectral gap and the speed of convergence to equilibrium for diffusions on S^1

Let $X(t)$, $t \geqslant 0$, be a Markov process on a state space M endowed with a sigma field $\mathcal{M}$. Suppose its transition probability has a density $r(t;x,y)$ with respect to a sigma finite measure ν and that there exists a unique invariant probability $\pi(\mathrm{d}x) = \pi(x)\nu(\mathrm{d}x)$. Write L^2 for the real Hilbert space $L^2(M,\pi)$. Denote by T_t $(t > 0)$ the semigroup of transition operators on L^2,

$$(T_t f)(x) = \int f(y) r(t; x, y) \nu(dy) \quad (f \in L^2). \tag{2.1}$$

Let A denote the infinitesimal generator of this contraction semigroup. We will assume that the domain $\mathscr{D}_A$ of A is dense in L^2, i.e., the semigroup is strongly continuous. Let $q(t; x, y)\nu(dy)$ denote the transition probability of the *time-reversed Markov process*:

$$q(t; x, y) = r(t; y, x) \frac{\pi(y)}{\pi(x)}. \tag{2.2}$$

Let $\tilde{T}_t$, $t > 0$, denote the semigroup of transition operators of the time-reversed process:

$$(\tilde{T}_t g)(x) = \int g(y) q(t; x, y) \nu(dy) \quad (g \in L^2 \equiv L^2(M, \pi)). \tag{2.3}$$

Then, denoting by $\langle , \rangle$ the inner product on L^2,

$$\begin{aligned} \langle T_t f, g \rangle &= \int (T_t f)(x) g(x) \pi(x) \nu(dx) = \int \left[\int f(y) r(t; x, y) \nu(dy) \right] g(x) \pi(x) \nu(dx) \\ &= \int \left[\int g(x) r(t; x, y) \pi(x) \nu(dx) \right] f(y) \nu(dy) \\ &= \int \left[\int g(x) q(t; y, x) \nu(dx) \right] f(y) \pi(y) \nu(dy) = \langle f, \tilde{T}_t g \rangle \quad (f, g \in L^2). \end{aligned} \tag{2.4}$$

In other words, $\tilde{T}_t$ is the *adjoint* of T_t on L^2. Let $\tilde{A}$ denote the infinitesimal generator of $\tilde{T}_t$, $t > 0$. We will assume that $\mathscr{D}_{\tilde{A}}$ is dense in L^2. Denote by $1^\perp$ the closed subspace of L^2 orthogonal to constants. Then $\mathscr{D}_{\tilde{A}} \cap 1^\perp$ is dense in $1^\perp$. The following is an analog of an inequality of Fill (1991). (Also see Diaconis and Stroock (1991)).

Lemma 2.1. *Assume that $\mathscr{D}_{\tilde{A}}$ is dense in L^2. Let $\| \|$, $\langle \rangle$ denote norm and inner product on $L^2 \equiv L^2(M, \pi)$. Define $\lambda \geqslant 0$ by*

$$\lambda = \inf \{ \langle -\tilde{A} f, f \rangle : f \in 1^\perp \cap \mathscr{D}_{\tilde{A}}, \ \|f\| = 1 \}. \tag{2.5}$$

Then if $X(0)$ has a probability density η w.r.t. ν, one has

$$\int |\eta_t(y) - \pi(y)| \nu(dy) \leqslant e^{-\lambda t} \|\psi_0\|, \tag{2.6}$$

where η_t is the density of $X(t)$ w.r.t. ν, and

$$\psi_0(y) = \frac{\eta(y) - \pi(y)}{\pi(y)}. \tag{2.7}$$

Proof. If $\|\psi_0\| = \infty$, there is nothing to prove. Therefore, we assume $\psi_0 \in 1^\perp$. For $g \in 1^\perp \cap \mathscr{D}_{\tilde{A}}$, $\tilde{T}_t g \in 1^\perp \cap \mathscr{D}_{\tilde{A}} (t > 0)$ and, by (2.5),

$$\frac{d}{dt} \|\tilde{T}_t g\|^2 = \frac{d}{dt} \langle \tilde{T}_t g, \tilde{T}_t g \rangle = 2 \langle \tilde{T}_t g, \tilde{A} \tilde{T}_t g \rangle \leqslant -2\lambda \|\tilde{T}_t g\|^2, \tag{2.8}$$

or

$$\|\tilde{T}_t g\|^2 \leqslant e^{-2\lambda t}\|g\|^2, \quad \|\tilde{T}_t g\| \leqslant e^{-\lambda t}\|g\| \quad (g \in 1^\perp \cap \mathscr{D}_{\tilde{A}}). \tag{2.9}$$

Since $1^\perp \cap \mathscr{D}_{\tilde{A}}$ is dense in $1^\perp$ by assumption, inequalities (2.9) hold $\forall g \in 1^\perp$.

Now

$$\tilde{T}_t(\eta/\pi)(y) = \int \frac{\eta(x)}{\pi(x)} q(t; y, x)\nu(\mathrm{d}x) = \int \frac{\eta(x)}{\pi(x)} r(t; x, y)\frac{\pi(x)}{\pi(y)}\nu(\mathrm{d}x)$$
$$= \frac{1}{\pi(y)}\eta_t(y), \tag{2.10}$$

so that $\tilde{T}_t(\psi_0) = \eta_t/\pi - 1$. By the Cauchy–Schwarz inequality and (2.9) one then has

$$\int |\eta_t(y) - \pi(y)|\nu(\mathrm{d}y) = \int \left|\frac{\eta_t(y) - \pi(y)}{\pi(y)}\right| \pi(y)\nu(\mathrm{d}y)$$
$$= \int |(\tilde{T}_t\psi_0)(y)|\pi(y)\nu(\mathrm{d}y) \leqslant \|\tilde{T}_t\psi_0\| \leqslant e^{-\lambda t}\|\psi_0\|. \quad \Box \tag{2.11}$$

Remark 2.2. Note that $\langle -\tilde{A}f, f\rangle = \langle -f, Af\rangle = \frac{1}{2}\langle -(A+\tilde{A})f, f\rangle$ if $f \in \mathscr{D}_A \cap \mathscr{D}_{\tilde{A}}$. Assuming that $\mathscr{D}_A \cap \mathscr{D}_{\tilde{A}}$ is dense in L^2, one may take $\lambda = \inf\{\langle -Af, f\rangle : f \in 1^\perp \cap \mathscr{D}_A \cap \mathscr{D}_{\tilde{A}}, \|f\| = 1\}$. This assumption is satisfied for diffusions on the circle considered in this article.

Consider now a one-dimensional diffusion with continuously differentiable drift and diffusion coefficients, $\mu(x)$ and $\sigma^2(x)$, both periodic with period 1. Assume $\sigma^2(x) > 0\ \forall x$. Such a diffusion $X(\cdot)$ may be regarded as the solution to the Itô equation

$$\mathrm{d}X(t) = \mu(X(t))\,\mathrm{d}t + \sigma(X(t))\,\mathrm{d}B(t), \quad t \geqslant 0, \tag{2.12}$$

subject to an initial condition $X(0) = X_0$, where X_0 is independent of the standard Brownian motion $B(\cdot)$ appearing in Eq. (2.12). Here $\sigma(x)$ is the positive square root of $\sigma^2(x)$.

Let $\dot{X}(\cdot)$ be the process defined by

$$\dot{X}(t) = X(t) \bmod 1, \quad t \geqslant 0. \tag{2.13}$$

Then $\dot{X}(\cdot)$ is a Markov process on the unit circle $S^1 = \{x \bmod 1\colon x \in \mathbb{R}\}$, called a diffusion on the unit circle S^1 (See, e.g., Bhattacharya and Waymire, 1990, p. 400). Its unique invariant probability π has a density $\pi(x)$ (w.r.t. Lebesgue measure on S^1) satisfying the forward equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{1}{2}\sigma^2(x)\pi(x)\right) - \frac{\mathrm{d}}{\mathrm{d}x}(\mu(x)\pi(x)) = 0. \tag{2.14}$$

On integration this yields

$$\pi(x) = c_2\frac{e^{I(0,x)}}{\sigma^2(x)} + 2c_1\frac{e^{I(0,x)}}{\sigma^2(x)}\int_0^x e^{-I(0,y)}\,\mathrm{d}y, \tag{2.15}$$

where

$$I(0,x)=\int_0^x \frac{2\mu(y)}{\sigma^2(y)}\,\mathrm{d}y. \tag{2.16}$$

The boundary condition $\pi(0)=\pi(1)$ leads to

$$c_1=\frac{c_2(1-e^{I(0,1)})}{2e^{I(0,1)}\int_0^1 e^{-I(0,y)}\,\mathrm{d}y}. \tag{2.17}$$

Two cases arise.
Case 1:

$$I(0,1)=0, \tag{2.18}$$

and
Case 2:

$$I(0,1)\neq 0. \tag{2.19}$$

In Case 1, $c_1=0$ and

$$\pi(x)=ce^{I(0,x)}/\sigma^2(x), \tag{2.20}$$

where c is the normalizing constant

$$c=\left(\int_0^1 \frac{e^{I(0,x)}}{\sigma^2(x)}\,\mathrm{d}x\right)^{-1}.$$

In Case 2, with a different normalizing c,

$$\pi(x)=\frac{ce^{I(0,x)}}{\sigma^2(x)}\left\{\frac{e^{I(0,1)}}{e^{I(0,1)}-1}\int_0^1 e^{-I(0,y)}\,\mathrm{d}y-\int_0^x e^{-I(0,y)}\,\mathrm{d}y\right\}. \tag{2.21}$$

Consider the real Hilbert space $L^2\equiv L^2(S^1,\pi)$. Let T_t $(t>0)$ be the strongly continuous contraction semigroup on L^2 defined by

$$(T_tf)(x)=\int_{S^1} f(y)\dot{p}(t;x,y)\,\mathrm{d}y, \quad f\in L^2, \tag{2.22}$$

where $\dot{p}(t;x,y)$ is the transition probability density (w.r.t. Lebesgue measure) of $\dot{X}(\cdot)$. The infinitesimal generator of this semigroup is A defined by

$$(Af)(x)=\tfrac{1}{2}\sigma^2(x)f''(x)+\mu(x)f'(x) \tag{2.23}$$

for all sufficiently smooth periodic f, and then by extension to $\mathscr{D}_A$ by the closure (in $L^2\times L^2$) of the graph of this restriction.

Lemma 2.3. (a) *The infinitesimal generator A is self-adjoint on $L^2(S^1,\pi)$ if* Eq. (2.18) *holds, and non-self-adjoint under* (2.19). (b) *In both cases* (2.18) *and* (2.19), *one has*

$$\langle -\tilde{A}f,f\rangle=\tfrac{1}{2}\|\sigma f'\|^2 \quad \forall f\in\mathscr{D}_{\tilde{A}}, \tag{2.24}$$

and

$$\langle -\tilde{A}f, f\rangle \geqslant \frac{1}{2M}\|f\|^2 \quad \forall f \in 1^{\perp} \cap \mathscr{D}_{\tilde{A}}, \tag{2.25}$$

where

$$M := \sup\left\{ (\sigma^2(z)\pi(z))^{-1} \int_0^z \pi(x)\,\mathrm{d}x \int_z^1 \pi(y)\,\mathrm{d}y\colon z \in S^1 \right\}. \tag{2.26}$$

Proof. (a) Let $f, g \in C^2(S^1)$, i.e., the lifts of f, g to $\mathbb{R}$ are twice continuously differentiable periodic functions. On integration by parts, and using Eq. (2.14), we get

$$\begin{aligned}\langle Af, g\rangle &= \int_0^1 \left\{\frac{1}{2}\sigma^2(x)f''(x) + \mu(x)f'(x)\right\} g(x)\pi(x)\,\mathrm{d}x \\ &= -\int_0^1 f'(x)\left\{\left(\frac{1}{2}\sigma^2(x)\pi(x)\right)' - \mu(x)\pi(x)\right\} g(x)\,\mathrm{d}x \\ &\quad - \int_0^1 \frac{1}{2}\sigma^2(x)f'(x)g'(x)\pi(x)\,\mathrm{d}x. \end{aligned} \tag{2.27}$$

The expression within curly brackets on the right side equals the constant of integration c_1 appearing in Eq. (2.17), which vanishes in the case (2.18), but is nonzero in the case (2.19).

(b) For $f \in C^2(S^1)$, letting $g = f$ in Eq. (2.27), one gets

$$\begin{aligned}-\langle f, \tilde{A}f\rangle = \langle -Af, f\rangle &= c_1 \int_0^1 f'(x)f(x)\,\mathrm{d}x + \frac{1}{2}\|\sigma f'\|^2 \\ &= \frac{c_1}{2}\int_0^1 (f^2)'(x)\,\mathrm{d}x + \frac{1}{2}\|\sigma f'\|^2 = \frac{1}{2}\|\sigma f'\|^2. \end{aligned} \tag{2.28}$$

This proves Eq. (2.24) for all $f \in C^2(S^1)$, and the assertion $\forall f \in \mathscr{D}_{\tilde{A}}$ follows by closure.

It remains to prove (2.25). Let $f \in \mathscr{D}_{\tilde{A}} \cap 1^{\perp}$, $\|f\| = 1$. Then,

$$\begin{aligned} 1 &= \frac{1}{2}\int_0^1\int_0^1 (f(x) - f(y))^2\pi(x)\pi(y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \iint_{x<y} \left(\int_x^y f'(z)\,\mathrm{d}z\right)^2 \pi(x)\pi(y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_0^1 \left\{\int_0^y \left(\int_x^y f'(z)\,\mathrm{d}z\right)^2 \pi(x)\,\mathrm{d}x\right\}\pi(y)\,\mathrm{d}y \\ &\leqslant \int_0^1 \left\{\int_0^y (y-x)\left[\int_x^y (f'(z))^2\,\mathrm{d}z\right]\pi(x)\,\mathrm{d}x\right\}\pi(y)\,\mathrm{d}y \\ &= \int_0^1 (f'(z))^2 \left[\int_z^1 \left\{\int_0^z (y-x)\pi(x)\,\mathrm{d}x\right\}\pi(y)\,\mathrm{d}y\right]\mathrm{d}z \end{aligned}$$

$$\leqslant \int_0^1 (f'(z))^2\sigma^2(z)\pi(z)(\sigma^2(z)\pi(z))^{-1}\left[\int_0^z \pi(x)\,\mathrm{d}x \int_z^1 \pi(y)\,\mathrm{d}y\right]\mathrm{d}z$$

$$\leqslant \|\sigma f'\|^2 \sup_z \left\{(\sigma^2(z)\pi(z))^{-1}\int_0^z \pi(x)\,\mathrm{d}x \int_z^1 \pi(y)\,\mathrm{d}y\right\} \leqslant M\|\sigma f'\|^2. \tag{2.29}$$

The proof of (2.25) is completed on using Eq. (2.28) in (2.29). □

Remark 2.4. The fact that $C^2(S^1)$ is dense in $\mathscr{D}_A$ and in $\mathscr{D}_{\tilde{A}}$ may be proved, e.g., by using Itô's Lemma along the lines of Bhattacharya and Waymire (1990, pp. 604, 605).

Remark 2.5. To compute $\tilde{A}$ in the case (2.19), integrate by parts Eq. (2.27) once more to get

$$\langle Af, g\rangle = \int_0^1 f(x)\left[\left\{\frac{c_1 + (\frac{1}{2}\sigma^2(x)\pi(x))'}{\pi(x)}\right\} g'(x) + \frac{1}{2}\sigma^2(x)g''(x)\right]\pi(x)\,\mathrm{d}x$$

$$= \int_0^1 f(x)\left[\left\{\frac{c_1}{\pi(x)} + \mu(x)\right\} g'(x) + \frac{1}{2}\sigma^2(x)g''(x)\right]\pi(x)\,\mathrm{d}x$$

$$= \langle f, \tilde{A}g\rangle,$$

with

$$\tilde{A} = \left(\frac{c_1}{\pi(x)} + \mu(x)\right)\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2}\,\sigma^2(x)\,\frac{\mathrm{d}^2}{\mathrm{d}x^2},$$

on $C^2(S^1)$.

Combining Lemmas 2.1 and 2.2, we arrive at the following result.

Theorem 2.6. *Let $\dot{X}(\cdot)$ be the diffusion on S^1 defined by* Eq. (2.13), *where $X(\cdot)$ is a diffusion on $\mathbb{R}^1$ with continuously differentiable periodic diffusion coefficient $\sigma^2(\cdot) > 0$ and drift $\mu(\cdot)$, both of period one. Then, if $\dot{X}(0)$ has the distribution $\eta_0(y)\,\mathrm{d}y$, the distribution $\eta_t(y)\,\mathrm{d}y$ of $\dot{X}(t)$ satisfies*

$$\int |\eta_t(y) - \pi(y)|\,\mathrm{d}y \leqslant \|(\eta_0/\pi) - 1\| \exp\left\{-\frac{1}{2M}t\right\} \quad (t > 0), \tag{2.30}$$

where M is given by Eq. (2.26).

3. Diffusions with two spatial scales: phase-one asymptotics

Consider a diffusion $X(\cdot)$ on $\mathbb{R}$ governed by the Itô equation

$$\mathrm{d}X(t) = \{b(X(t)) + \beta(X(t)/a)\}\,\mathrm{d}t + \sigma(X(t))\,\mathrm{d}B(t), \quad X(0) = x_0, \tag{3.1}$$

where $b(\cdot), \beta(\cdot), \sigma(\cdot)$ are bounded and Lipschitzian, $\sigma^2(\cdot)$ is bounded away from 0 and ∞, and 'a' is a positive number. As in Bhattacharya and Götze (1995), one may prove the following result using the Cameron–Martin–Girsanov Theorem (Karatzas and Shreve, 1991, p. 193). Let $X_1(\cdot)$ be the solution of the Itô equation

$$dX_1(t) = \{b(X_1(t)) + \beta(x_0/a)\}\,dt + \sigma(X_1(t))\,dB(t), \quad X_1(0) = x_0. \tag{3.2}$$

Let $p(t;x_0,y)$, $p_1(t;x_0,y)$ be the densities (w.r.t. Lebesgue measure) of $X(t)$ and $X_1(t)$, respectively.

Let $P_{0,t}$ and $P^1_{0,t}$ denote the distributions of the processes $\{X(s)\colon 0 \leqslant s \leqslant t\}$ and $\{X_1(s)\colon 0 \leqslant s \leqslant t\}$, respectively, on $C[0,t]$. Let $\|P_{0,t} - P^1_{0,t}\|_{TV}$ denote the total variation distance between $P_{0,t}$ and $P^1_{0,t}$.

Theorem 3.1. *Under the above assumptions, one has*

$$\|P_{0,t} - P^1_{0,t}\|_{TV} \to 0 \quad \text{as } t/a^{2/3} \to 0. \tag{3.3}$$

In particular,

$$\int_{\mathbb{R}} |p(t;x_0,y) - p_1(t;x_0,y)|\,dy \to 0 \quad \text{as } t/a^{2/3} \to 0.$$

Relation (3.3) *holds uniformly for all initial points* x_0.

Proof. Let φ be a real-valued bounded Borel measurable function on $C[0,t]$, and let X^t_0, $X^t_{1,0}$ denote the restrictions of the diffusions $X(\cdot)$ and $X_1(\cdot)$, respectively, on the interval $[0,t]$. By the Cameron–Martin–Girsanov Theorem, one has

$$E\varphi(X^t_0) - E\varphi(X^t_{1,0}) = E(\varphi(X^t_{1,0})[\exp\{Z(t)\} - 1]), \tag{3.4}$$

where $Z(t)$ is given by

$$\begin{aligned} Z(t) &= \int_0^t \frac{\beta(X_1(s)/a) - \beta(x_0/a)}{\sigma(X_1(s))}\,dB(s) - \frac{1}{2}\int_0^t \left[\frac{\beta(X_1(s)/a) - \beta(x_0/a)}{\sigma(X_1(s))}\right]^2 ds \\ &= \int_0^t I(s)\,dB(s) - \frac{1}{2}\int_0^t I^2(s)\,ds, \quad \text{say.} \end{aligned} \tag{3.5}$$

Letting ℓ denote the Lipschitz constant for $\beta(\cdot)$, and writing $d_1 := \min \sigma^2(x)$, $d_2 := \max\sigma^2(x)$, one has

$$EI^2(s) \leqslant \left(\frac{\ell}{d_1}\right)^2 \frac{1}{a^2} E(X_1(s) - x_0)^2, \tag{3.6}$$

$$\begin{aligned} E(X_1(s) - x_0)^2 &= E\left[\int_0^s \{b(X_1(u)) + \beta(x_0/a)\}\,du + \int_0^s \sigma(X_1(u))\,dB(u)\right]^2 \\ &\leqslant 2(\|b\|_\infty + \|\beta\|_\infty)^2 s^2 + 2d_2 s, \\ &\qquad (\|b\|_\infty := \max |b(x)|,\ \|\beta\|_\infty := \max |\beta(x)|). \end{aligned}$$

Hence

$$E\left(\int_0^t I(s)\,\mathrm{d}B(s)\right)^2 = \int_0^t EI^2(s)\,\mathrm{d}s$$
$$\leqslant 2\left(\frac{\ell_1}{d_1}\right)^2 \frac{1}{a^2}\left\{(\|b\|_\infty + \|\beta\|_\infty)^2\frac{t^3}{3} + d_2\frac{t^2}{2}\right\} \to 0$$
$$\text{as } \frac{t}{a^{2/3}} \to 0. \tag{3.7}$$

From this calculation it follows that both terms on the right side of Eq. (3.5) go to zero in probability as $t/a^{2/3} \to 0$. Now use the relations $0 = E(1-\exp\{Z(t)\}) = E(1-\exp\{Z(t)\})^+ - E(1-\exp\{Z(t)\})^-$, to write $E|1-\exp\{Z(t)\}| = 2E(1-\exp\{Z(t)\})^+ \leqslant 2E(|Z(t)| \wedge 1)$. One may now use Lebesgue's Dominated Convergence Theorem. Thus the left side of Eq. (3.4) goes to zero, as $t/a^{2/3} \to 0$, uniformly over all Borel φ on $C[0,t]$ such that $|\varphi|$ is bounded by 1. In particular, the L^1-distance (on $\mathbb{R}^1$ w.r.t. the Lebesgue measure) between the densities of $X(t)$ and $X_1(t)$ goes to zero as $t/a^{2/3} \to 0$. □

Remark 3.2. If we assume $\beta(\cdot)$ is Lipschitzian, but not necessarily bounded, while $\sigma^2(\cdot)$ is bounded away from 0 and infinity, then (3.3) still holds, but only uniformly over compact sets (independent of 'a') of initial states x_0.

For the rest of this section we assume

$$b(\cdot) \text{ and } \sigma(\cdot) \text{ are Lipschitzian and periodic of period one,} \tag{3.8}$$

and

$$0 < d_1 := \min \sigma^2(x) \leqslant \max \sigma^2(x) := d_2. \tag{3.9}$$

Under these assumptions, $\dot{X}_1(\cdot) := X_1(\cdot) \bmod 1$ is a diffusion on the unit circle S^1. Its unique invariant probability π has a density given by Eq. (2.20) or Eq. (2.21), depending on whether Eq. (2.18) or (2.19) holds, with $I(0,x) = 2\int_0^x [\{b(y) + \beta(x_0/a)\}/\sigma^2(y)]\,\mathrm{d}y$. Write $\mu(x) = b(x) + \beta(x_0/a)$,

$$\hat{b} = \int_0^1 b(x)\pi(x)\,\mathrm{d}x, \tag{3.10}$$

and let g be the twice differentiable periodic solution (on $\mathbb{R}$) of

$$\tfrac{1}{2}\sigma^2(x)g''(x) + \mu(x)g'(x) = b(x) - \hat{b}, \tag{3.11}$$

satisfying

$$\bar{g} \equiv \int_0^1 g(x)\pi(x)\,\mathrm{d}x = 0. \tag{3.12}$$

Then it follows from Bensoussan et al. (1978, Chapter 3) or Bhattacharya (1985), that one has the convergence in law

$$\frac{X_1(t) - t\{\hat{b} + \beta(x_0/a)\}}{\sqrt{t}} \xrightarrow[t\to\infty]{\mathscr{L}} N(0,\gamma^2), \tag{3.13}$$

where

$$\gamma^2 = \int_0^1 \sigma^2(x)(g'(x)-1)^2\pi(x)\,\mathrm{d}x$$
$$= \int_0^1 \sigma^2(x)\pi(x)\,\mathrm{d}x + \int_0^1 \sigma^2(x)(g'(x))^2\pi(x)\,\mathrm{d}x - 2\int_0^1 \sigma^2(x)g'(x)\pi(x)\,\mathrm{d}x. \tag{3.14}$$

Note that in all cases $\gamma^2 > 0$. The normal convergence (3.13) and Theorem 3.1 now imply the following result (also, see Remark 3.1.1).

Theorem 3.3. *Assume* (3.8) and (3.9), *and that* $\beta(\cdot)$ *is Lipschitzian, and let* $x_0 = 0$. *Then as* $t \to \infty$, $t/a^{2/3} \to 0$, *one has*

$$\frac{X(t) - t\{\hat{b} + \beta(0)\}}{\sqrt{t}} \xrightarrow{\mathscr{L}} \mathscr{N}(0, \gamma^2), \tag{3.15}$$

the convergence $\xrightarrow{\mathscr{L}}$ *is in law, or distribution.*

Remark 3.4. Note that, in view of the initial condition $x_0 = 0$ in the hypothesis of Theorem 3.3, the process X_1 does not depend on a.

Remark 3.5. The functional central limit theorem holds for the process X_1 (see Bhattacharya (1985)). By Theorem 3.1, it therefore holds for the process X. In other words, the process $W_\lambda := [\lambda^{-1/2}\{X(\lambda t) - \lambda t(\hat{b} + \beta(0))\}\colon t \geqslant 0]$ converges in distribution to a Brownian motion with diffusion coefficient γ^2, as $\lambda \to \infty$, $\lambda/a^{2/3} \to 0$.

4. Periodic diffusions with two spatial scales: the final phase of asymptotics

The constants c_i, d_i in this section, with subscripts, are positive and independent of a. Consider diffusion (3.1) again, with X_0 independent of $B(\cdot)$,

$$\mathrm{d}X(t) = \{b(X(t)) + \beta(X(t)/a)\}\,\mathrm{d}t + \sigma(X(t))\,\mathrm{d}B(t), \quad X(0) = X_0. \tag{4.1}$$

We assume throughout this section that

$$b(\cdot),\ \beta(\cdot),\ \sigma(\cdot) \text{ are continuously differentiable and periodic with period 1, and '}a\text{' is a positive integer.} \tag{4.2}$$

Also assume

$$d_1 := \min \sigma^2(x) > 0. \tag{4.3}$$

Let $\dot{X}(\cdot)$ be defined by

$$\dot{X}(t) = X(t) \bmod a \quad (t \geqslant 0). \tag{4.4}$$

Then $\dot{X}(\cdot)$ is a diffusion on the circle $S^1(a) := \{x \bmod a;\ x \in \mathbb{R}\}$. It will be convenient for us to scale both $X(\cdot)$ and $\dot{X}(\cdot)$ in space and time as follows. Define

$$Y(t) = X(a^2 t)/a \quad (t \geqslant 0). \tag{4.5}$$

Then $Y(t)$ is governed by the Itô equation

$$\mathrm{d}Y(t) = a\{b(aY(t)) + \beta(Y(t))\}\,\mathrm{d}t + \sigma(aY(t))\mathrm{d}\bar{B}(t),$$

where $\bar{B}(t) = B(a^2 t)/a$ $(t \geqslant 0)$ is again a standard Brownian notion. Since the functions $y \to b(ay)$ and $y \to \sigma(ay)$ are periodic with period $1/a$, they are also periodic with period 1. Therefore, the process

$$\dot{Y}(t) := Y(t) \bmod 1 \quad (t \geqslant 0), \tag{4.6}$$

is a diffusion on the unit circle S^1. Let $\tilde{\pi}_a, \pi_a$ denote the invariant probability densities of $\dot{X}$ and $\dot{Y}$, respectively. The infinitesimal generators L of $\dot{X}$ on $L^2(S^1(a), \tilde{\pi}_a)$ and A of $\dot{Y}$ on $L^2(S^1, \pi_a)$ are given by

$$L = \frac{1}{2}\sigma^2(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \{b(x) + \beta(x/a)\}\frac{\mathrm{d}}{\mathrm{d}x},$$

$$A = \frac{1}{2}\sigma^2(ax)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + a\{b(ax) + \beta(x)\}\frac{\mathrm{d}}{\mathrm{d}x}.$$

Let $\tilde{L}$ and $\tilde{A}$ be the adjoints of L and A. The following proposition relates the spectral gaps of $\frac{1}{2}(L + \tilde{L})$ and $\frac{1}{2}(A + \tilde{A})$.

Proposition 4.1. *Suppose that λ_L is the spectral gap of $\frac{1}{2}(L + \tilde{L})$, and λ_A that of $\frac{1}{2}(A + \tilde{A})$. Then*

$$\lambda_L = \frac{1}{a^2}\,\lambda_A.$$

Proof. Let $g \in C^2(S^1) \cap 1^{\perp} \subset L^2(S^1, \pi_a)$. Then $f(x) := g(x/a) \in C^2(S^1(a)) \cap 1^{\perp} \subset L^2(S^1(a), \tilde{\pi}_a)$, and

$$(Lf)(x) = \frac{1}{a^2}(Ag)(x/a).$$

Therefore, by change of variables,

$$\langle -Lf, f\rangle_{\tilde{\pi}_a} = -\frac{1}{a^2}\int_0^a (Ag)(x/a)g(x/a)\tilde{\pi}_a(x)\,\mathrm{d}x$$

$$= \frac{1}{a^2}\int_0^1 (Ag)(y)g(y)\pi_a(y)\,\mathrm{d}y = \frac{1}{a^2}\langle -Ag, g\rangle_{\pi_a}.$$

Conversely, given $f \in C^2(S^1(a)) \cap 1^{\perp}$, $g(x) := f(ax) \in C^2(S^1) \cap 1^{\perp}$, and the same relations are obtained. □

Without any essential loss of generality we will assume, by adding a constant to the function $\beta(\cdot)$ if necessary that

$$\int_0^1 \frac{b(y)}{\sigma^2(y)}\,\mathrm{d}y = 0. \tag{4.7}$$

The analysis in this section is substantially different depending on whether

$$\int_0^1 \frac{\beta(y)}{\sigma^2(y)}\,\mathrm{d}y$$

is zero or not. Therefore, we split the analysis in two subsections.

4.1. The case $\beta(x)>0\ \forall x$, or $\beta(x)<0\ \forall x$

For the diffusion $\dot{Y}$ in this case (see Eq. (2.16)), writing $[u]$ for the integer part of u,

$$I(0,x) = 2\int_0^x a\left\{\frac{b(ay)+\beta(y)}{\sigma^2(ay)}\right\}\mathrm{d}y = 2\int_{[ax]}^{ax}\frac{b(z)\,\mathrm{d}z}{\sigma^2(z)} + 2a\int_0^x \frac{\beta(z)\,\mathrm{d}z}{\sigma^2(az)},$$

$$I(x,z) := I(0,z) - I(0,x), \quad I(0,1) = 2a\int_0^1 \frac{\beta(y)\,\mathrm{d}y}{\sigma^2(ay)}. \tag{4.8}$$

Therefore, by Eq. (2.21), the invariant density of $(\dot{Y})(\cdot)$ is

$$\begin{aligned}
\pi_a(x) &:= \frac{c}{\sigma^2(ax)}\mathrm{e}^{I(0,x)}\left\{\frac{\mathrm{e}^{I(0,1)}}{\mathrm{e}^{I(0,1)}-1}\int_0^1 \mathrm{e}^{-I(0,z)}\,\mathrm{d}z - \int_0^x \mathrm{e}^{-I(0,z)}\,\mathrm{d}z\right\}\\
&= \frac{c}{\sigma^2(ax)}\int_x^1 \mathrm{e}^{-I(x,z)}\,\mathrm{d}z + \frac{c}{\sigma^2(ax)}\frac{\mathrm{e}^{I(0,x)}}{\mathrm{e}^{I(0,1)}-1}\int_0^1 \mathrm{e}^{-I(0,z)}\,\mathrm{d}z\\
&= \frac{c}{\sigma^2(ax)}\int_x^1 \mathrm{e}^{-I(x,z)}\,\mathrm{d}z + \frac{c}{\sigma^2(ax)}\mathrm{e}^{-I(x,1)}\int_0^1 \mathrm{e}^{-I(0,z)}\,\mathrm{d}z\\
&\quad + \frac{c}{\sigma^2(ax)}\mathrm{e}^{I(0,x)}\left\{\frac{1}{\mathrm{e}^{I(0,1)}-1} - \frac{1}{\mathrm{e}^{I(0,1)}}\right\}\int_0^1 \mathrm{e}^{-I(0,z)}\,\mathrm{d}z.
\end{aligned} \tag{4.9}$$

For specificity, assume $\beta(x)>0\ \forall x$. The case $\beta(x)<0\ \forall x$ is entirely analogous. Write

$$\beta_* := \min_y \beta(y), \quad \beta^* := \max_y \beta(y), \quad \delta := \int_0^1 |b(y)|\,\mathrm{d}y, \quad d_2 := \max_y \sigma^2(y), \tag{4.10}$$

and note that we are assuming

$$\beta_* > 0. \tag{4.11}$$

Then, $\forall 0 \leqslant x \leqslant z \leqslant 1$,

$$\frac{2a\beta_*}{d_2}(z-x) - \frac{2\delta}{d_1} \leqslant I(x,z) \leqslant \frac{2a\beta^*}{d_1}(z-x) + \frac{2\delta}{d_1}. \tag{4.12}$$

Using this in Eq. (4.9) one obtains

$$\begin{aligned}\frac{\sigma^2(ax)\pi_a(x)}{c} \leqslant{}& \int_x^1 \exp\left\{\frac{2\delta}{d_1} - \frac{2a\beta_*}{d_2}(z-x)\right\} \mathrm{d}z \\ &+ \exp\left\{\frac{2\delta}{d_1} - \frac{2a\beta_*}{d_2}(1-x)\right\} \int_0^1 \exp\left\{\frac{2\delta}{d_1} - \frac{2a\beta_*}{d_2} z\right\} \mathrm{d}z \\ &\times \left[1 + \left(\exp\left\{\frac{2a\beta_*}{d_2}\right\} - 1\right)^{-1}\right] \\ &- \exp\left(\frac{2\delta}{d_1}\right) \int_0^{1-x} \exp\left\{\frac{2a\beta_*}{d_2} u\right\} \mathrm{d}u \\ &+ \exp\left(\frac{4\delta}{d_1}\right) \exp\left\{-\frac{2a\beta_*}{d_2}(1-x)\right\} \int_0^1 \exp\left\{-\frac{2a\beta_*}{d_2} z\right\} \mathrm{d}z \\ &\times \left[1 + \left(\exp\left\{\frac{2a\beta_*}{d_2}\right\} - 1\right)^{-1}\right]. \end{aligned} \tag{4.13}$$

Now, using the fact that for any $\lambda > 0$, $A > 0$,

$$\int_0^A \mathrm{e}^{-\lambda x}\,\mathrm{d}x \leqslant \lambda^{-1} \quad \text{and} \quad (\mathrm{e}^{\lambda} - 1)^{-1} \leqslant \lambda^{-1} \tag{4.14}$$

we obtain that, if $\beta_* > 0$,

$$\begin{aligned}\frac{\sigma^2(ax)\pi_a(x)}{c} &\leqslant \exp\left(\frac{2\delta}{d_1}\right) \cdot \frac{d_2}{2a\beta_*} + \exp\left(\frac{4\delta}{d_1}\right) \cdot \frac{d_2}{2a\beta_*} \left(1 + \frac{d_2}{2a\beta_*}\right) \\ &= \frac{d_2}{2a\beta_*} \left[\exp\left\{\frac{2\delta}{d_1}\right\} + \exp\left\{\frac{4\delta}{d_1}\right\} \left(1 + \frac{d_2}{2a\beta_*}\right)\right]. \end{aligned} \tag{4.15}$$

Integrating both sides with respect to x, we obtain

$$\frac{1}{c} \leqslant \frac{1}{2a\beta_*} \left(\frac{d_2}{d_1}\right) \left[\exp\left\{\frac{2\delta}{d_1}\right\} + \exp\left\{\frac{4\delta}{d_1}\right\} \left(1 + \frac{d_2}{2a\beta_*}\right)\right]. \tag{4.16}$$

Next, using the second half of inequality (4.12) in Eq. (4.9),

$$\begin{aligned}\frac{\sigma^2(ax)\pi_a(x)}{c} \geqslant{}& \exp\left\{-\frac{2\delta}{d_1}\right\} \int_x^1 \exp\left\{-\frac{2a\beta^*}{d_1}(z-x)\right\} \mathrm{d}z \\ &+ \left[1 - \left(\exp\left\{\frac{2a\beta^*}{d_1}\right\} - 1\right)^{-1}\right] \exp\left\{-\frac{4\delta}{d_1}\right\} \\ &\times \exp\left\{-\frac{2a\beta^*}{d_1}(1-x)\right\} \times \int_0^1 \exp\left\{-\frac{2a\beta^*}{d_1} z\right\} \mathrm{d}z \\ ={}& \exp\left\{-\frac{2\delta}{d_1}\right\} \left(\frac{d_1}{2a\beta^*}\right) \left[1 - \exp\left\{-\frac{2a\beta^*}{d_1}(1-x)\right\}\right] \\ &+ \left[1 - \left(\exp\left\{\frac{2a\beta^*}{d_1}\right\} - 1\right)^{-1}\right] \exp\left\{-\frac{4\delta}{d_1}\right\} \left(\frac{d_1}{2a\beta^*}\right) \end{aligned}$$

$$\times\exp\left\{-\frac{2a\beta^*}{d_1}(1-x)\right\}\left[1-\exp\left\{-\frac{2a\beta^*}{d_1}\right\}\right]$$

$$\geqslant \exp\left\{-\frac{2\delta}{d_1}\right\}\left(\frac{d_1}{2a\beta^*}\right)-\exp\left\{-\frac{2\delta}{d_1}-\frac{2a\beta^*}{d_1}(1-x)\right\}\left(\frac{d_1}{2a\beta^*}\right)$$

$$\times\left[1-\exp\left\{-\frac{2\delta}{d_1}\right\}\left(1-\exp\left\{-\frac{2a\beta^*}{d_1}\right\}\right)\right]. \tag{4.17}$$

The last expression is minimized by setting $x=1$, so that, after cancellation, one has

$$\frac{\sigma^2(ax)\pi_a(x)}{c}\geqslant \exp\left\{-\frac{4\delta}{d_1}\right\}\left(\frac{d_1}{2a\beta^*}\right)\left(1-\exp\left\{-\frac{2a\beta^*}{d_1}\right\}\right). \tag{4.18}$$

From (4.15) and (4.18) we get

$$\sup_{a\geqslant 1}\frac{\max_x\ \pi_a(x)}{\min_x\ \pi_a(x)}\leqslant c_2'<\infty. \tag{4.19}$$

By using this estimate the quantity M in (2.26) is estimated in the present case as

$$M\leqslant\frac{d_2}{2}\frac{\max\{\pi_a(y):\ y\in S^1\}}{\min\{\pi_a(y):\ y\in S^1\}}\leqslant\frac{d_2}{2}c_2'=c_2,\ \ \text{say}. \tag{4.20}$$

Applying Theorem 2.6 to the transition probability density $\ddot{p}(t;x,y)$ of $\dot{Y}(\cdot)$,

$$\int_{S^1}|\ddot{p}(t+s;x,y)-\pi_a(y)|\,\mathrm{d}y\leqslant\left\|\frac{\ddot{p}(s;x,\cdot)}{\pi_a(\cdot)}-1\right\|\exp\left\{-\frac{t}{2c_2}\right\}. \tag{4.21}$$

In order to estimate the L^2-norm on the right, first use an estimate of Aronson (1967) on the transition probability density $p(t;x,y)$ of the diffusion $X(\cdot)$ governed by Eq. (4.1):

$$p(1;x,y)\leqslant c_3\exp\{-c_4|x-y|^2\} \tag{4.22}$$

where c_3,c_4 are constants independent of a. From (4.22) we deduce the inequality

$$\ddot{p}(1/a^2;x,y)-a\sum_{-\infty<n<\infty}p(1;ax,ay+an)\leqslant ac_5. \tag{4.23}$$

From (4.18) and (4.23) it follows that there exist constants c_6,c_6' independent of a such that one has

$$\left\|\frac{\ddot{p}(1/a^2;x,\cdot)}{\pi_a(\cdot)}-1\right\|^2=\int_{S^1}\frac{\ddot{p}(1/a^2;x,y))^2}{\pi_a(y)}\,\mathrm{d}y-1$$

$$\leqslant c_6'\max_{x,y}(\ddot{p}(1/a^2;x,y)\int_{S^1}\ddot{p}(1/a^2;x,y))\,\mathrm{d}y-1\leqslant c_6 a. \tag{4.24}$$

Using this in (4.21), with $1/a^2$ for s and $t-1/a^2$ for t, one gets

$$\int_{S^1}|\ddot{p}(t;x,y)-\pi_a(y)|\,\mathrm{d}y\leqslant c_7a^{1/2}\exp\{-c_8t\}\quad(t>0). \tag{4.25}$$

Although this estimate is derived for $t \geqslant 1/a^2$, note that c_7 may be adjusted so that it holds for $0 < t < 1/a^2$ as well. Thus we arrive at the following result. Note that the diffusions $\dot{X}$ (on $S^1(a)$) and $\dot{Y}$ (on S^1) are related by

$$\dot{Y}(t) = \frac{\dot{X}(a^2 t)}{a}, \quad \dot{X}(t) = a\dot{Y}(t/a^2). \tag{4.26}$$

We denote by $\dot{p}$ the transition probability density of $\dot{X}$.

Theorem 4.2. *Under Assumptions* (4.2), (4.3) *and* (4.11), *one has*

$$\int_{S^1} |\ddot{p}(t;x,y) - \pi_a(y)| \,\mathrm{d}y \leqslant c_7 a^{1/2} \exp\{-c_8 t\} \quad (t>0), \tag{4.27}$$

$\forall x \in S^1$, *and*

$$\int_{S^1(a)} |\dot{p}(t;x,y) - \tilde{\pi}_a(y)| \,\mathrm{d}y \leqslant c_7 a^{1/2} \exp\{-c_8 t/a^2\} \quad (t>0), \tag{4.28}$$

$\forall x \in S^1(a)$, *where* $\tilde{\pi}_a(x) := \pi_a(x/a)/a$ *is the invariant probability density of* $\dot{X}$. *Here* c_7, c_8 *are positive constants depending only on the functions* $\sigma^2(\cdot)$, $b(\cdot), \beta(\cdot)$, *and not on* 'a'.

Remark 4.3. Inequality (4.28) implies that the total variation distance between the equilibrium distribution of $\dot{X}$ and the distribution of $\dot{X}$ starting at an arbitrary initial state x goes to zero if $t \gg a^2 \log a$, uniformly for all x.

A word of caution on notation: Let $\dot{X}(t)$ have the equilibrium distribution $\tilde{\pi}_a$. For periodic functions f of period a we will write $\bar{f}$ for $Ef(\dot{X}(t))$, while for periodic f with period one $\bar{f}_a$ denotes $Ef(\dot{X}(t)/a)$. When the $\dot{X}$ process is in equilibrium (namely, when $\dot{X}(0)$ has the invariant distribution $\tilde{\pi}_a$ on $S^1(a)$), then the process $\dot{Y}$ is also in equilibrium with $\dot{Y}(t)$ having distribution π_a on the unit circle S^1: $\pi_a(y) = a\tilde{\pi}_a(ay)$. Hence for functions f of period one, $\bar{f}_a = Ef(\dot{Y}(t))$. Since functions f of period one are also of period a (a integral), one has $\bar{f} = Ef(a\dot{Y}(t))$. In general $\bar{f} \neq \bar{f}_a$ for periodic functions of period one, unless the invariant distribution is uniform. Note that the invariant distribution (of $\dot{X}(t)$ or $\dot{Y}(t)$) is uniform if $b(\cdot)$, $\beta(\cdot)$ are constants, a case of little interest to us. Finally, we will denote by $\dot{T}_t$ ($t \geqslant 0$) the transition operators of $\dot{X}$. Thus

$$\begin{aligned}
&(\dot{T}_t f)(y) := E[f(\dot{X}(t)) | \dot{X}(0) = y], \\
&\bar{f} := \int_{S^1(a)} f(x)\tilde{\pi}_a(x)\,\mathrm{d}x = \int_{S^1} f(ay)\pi_a(y)\,\mathrm{d}y, \\
&\bar{f}_a := \int_{S^1(a)} f(x/a)\tilde{\pi}_a(x)\,\mathrm{d}x = \int_{S^1} f(y)\pi_a(y)\,\mathrm{d}y.
\end{aligned} \tag{4.29}$$

Also, let E_x, cov_x, var_x denote expectation, covariance and variance given $\dot{X}(0) = x$, and let E, cov, var denote the same under the equilibrium initial distribution $\tilde{\pi}_a$.

The following corollary of Theorem 4.2 is derived in exactly the same way as Corollary 4.4 in Bhattacharya and Götze (1995). (See also Correction, ibid, Bhattacharya and Götze, 1996.)

Proposition 4.4. *Assume the hypothesis of Theorem* 4.2. *There exist positive constants* c_9 *and* c_{10} *depending only on* c_7, c_8 *of Theorem* 4.2 *such that the following inequalities hold for all bounded measurable* f,g *on* $S^1(a):=\{x \bmod a\colon x\in\mathbb{R}^1\}$:

$$\|\dot{T}_t f - \bar{f}\|_\infty \leqslant c_9 a^{1/2}\|f\|_\infty \exp\{-c_7 t/a^2\} \quad (t>0); \tag{4.30}$$

$$|\mathrm{cov}_x\{f(\dot{X}(s)), g(\dot{X}(t))\}| \leqslant c_{10}a^{1/2}\|f\|_\infty\|g\|_\infty \exp\{-c_7(t-s)/a^2\} \quad (0\leqslant s\leqslant t). \tag{4.31}$$

Proof. Relation (4.30) is an immediate consequence of (4.28). To derive (4.31), use the Markov property to write

$$\begin{aligned}&\mathrm{cov}_x\{f(\dot{X}(s)), g(\dot{X}(t))\}\\ &\quad = E_x[\{f(\dot{X}(s)) - (\dot{T}_s f)(x)\}\{\dot{T}_{t-s}g(\dot{X}(s)) - (\dot{T}_t g)(x)\}],\end{aligned} \tag{4.32}$$

and apply (4.30) to the second factor on the right, and to $\|\dot{T}_t g - \bar{g}\|_\infty$. □

We will make use of Proposition 4.4 to prove Theorem 4.5 below, which says that for

$$t \gg a^2\log a \quad \left(\text{or, } t\to\infty,\ a\to\infty,\ \frac{t}{a^2\log a}\to\infty\right), \tag{4.33}$$

$X(t)$–$X(0)$ is asymptotically Gaussian with mean $t(\bar{b}+\bar{\beta}_a)$ and variance

$$\sigma^2(t) := t\,\overline{\sigma^2\cdot(h'(\cdot)-1)^2} = t\theta^2, \text{ say.} \tag{4.34}$$

Here h is the unique mean-zero solution in $L^2(S^1(a),\tilde{\pi}_a)$ of

$$\begin{aligned}&Lh(x) = b(x) + \beta(x/a) - \bar{b} - \bar{\beta}_a,\\ &L := \frac{1}{2}\sigma^2(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \{b(x)+\beta(x/a)\}\frac{\mathrm{d}}{\mathrm{d}x}.\end{aligned} \tag{4.35}$$

It is clear that the mean of $X(t)-X(0)$ under the equilibrium initial distribution is $t(\bar{b}+\bar{\beta}_a)$. To see that the corresponding (asymptotic) variance is given by Eq. (4.34), use Itô's lemma (see, e.g., Rogers and Williams (1987), (pp. 60–62), or, Bhattacharya and Waymire (1990), (p. 585)) to write

$$\begin{aligned}h(X(t)) - h(X(0)) &= \int_0^t Lh(X(s))\,\mathrm{d}s + \int_0^t \sigma(X(s))h'(X(s))\,\mathrm{d}B(s)\\ &= \int_0^t \left\{b(X(s)) + \beta(X(s)/a) - \bar{b} - \bar{\beta}_a\right\}\mathrm{d}s\\ &\quad + \int_0^t \sigma(X(s))h'(X(s))\,\mathrm{d}B(s),\end{aligned} \tag{4.36}$$

so that

$$\begin{aligned} X(t) - X(0) - t(\bar{b} + \bar{\beta}_a) &\\ \equiv \int_0^t \{b(X(s)) + \beta(X(s)/a) - \bar{b} - \bar{\beta}_a\}\,\mathrm{d}s + \int_0^t \sigma(X(s))\,\mathrm{d}B(s) &\\ = h(X(t)) - h(X(0)) + \int_0^t \sigma(X(s))\{1 - h'(X(s))\}\,\mathrm{d}B(s). & \qquad (4.37) \end{aligned}$$

The expected squared value of the stochastic integral is given by Eq. (4.34), under equilibrium.

For convenience, instead of solving Eq. (4.35) directly, which is not difficult, let us solve the corresponding equation for the scaled process $Y(\cdot)$. That is, find a function g which is periodic with period 1 such that

$$Ag(x) = b(ax) + \beta(x) - \bar{b} - \bar{\beta}_a, \qquad (4.38)$$

where A is the infinitesimal generator of $\dot{Y}$:

$$A := \frac{1}{2}\sigma^2(ax)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + a\{b(ax) + \beta(x)\}\frac{\mathrm{d}}{\mathrm{d}x}. \qquad (4.39)$$

The solution is unique up to an additive constant (which is determined if $\bar{g} = 0$) and is given by

$$\begin{aligned} g(x) = c' + \frac{2}{\sigma^2}\left(\frac{\mathrm{e}^{-I(0,1)}}{1 - \mathrm{e}^{-I(0,1)}}\int_0^1 \mathrm{e}^{I(0,z)} f(z)\,\mathrm{d}z\right)\int_0^x \mathrm{e}^{-I(0,z)}\,\mathrm{d}z &\\ + \frac{2}{\sigma^2}\int_0^x \mathrm{e}^{-I(0,z)}\left(\int_0^z \mathrm{e}^{I(0,y)} f(y)\,\mathrm{d}y\right)\mathrm{d}z; &\\ f(z) := b(az) + \beta(z) - \bar{b} - \bar{\beta}_a. & \qquad (4.40) \end{aligned}$$

Here c' is an arbitrary constant and $I(0,x)$ is as given in Eq. (4.8). It is simple to check that if g satisfies Eq. (4.38), then

$$h(x) := a^2 g(x/a) \qquad (4.41)$$

satisfies Eq. (4.35).

Theorem 4.5. *Assume* (4.2), (4.3), (4.7), *and* (4.11). *Then, as*

$$a \to \infty, \quad t \to \infty, \quad \frac{t}{a^2 \log a} \to \infty, \qquad (4.42)$$

$[X(t) - X(0) - t(\bar{b} + \bar{\beta}_a)]/(\theta\sqrt{t})$ *converges weakly to the standard normal distribution, whatever the initial distribution. Here* $\theta = \theta(a)$ *is bounded away from zero and infinity.*

Proof. Let $\varphi(a)$ $(a = 1, 2, \ldots)$ be a sequence of integers such that

$$\frac{\varphi(a)}{a^2 \log a} \to \infty \quad \text{as } a \to \infty. \qquad (4.43)$$

First assume $\dot{X}(0)$ has the equilibrium initial distribution $\tilde{\pi}_a$. Note that

$$V_r := \frac{1}{\theta}\int_{r-1}^{r} \sigma(\dot{X}(s))\{1 - h'(\dot{X}(s))\}\,\mathrm{d}B(s) \quad (r = 1,\dots,\varphi(a);\ a = 1,2,\dots) \tag{4.44}$$

is a triangular array of martingale differences, since

$$E(V_r \mid \mathscr{F}_{r'}) = 0 \quad \forall r' < r. \tag{4.45}$$

Here $\mathscr{F}_t := \sigma\{X(s)\colon 0 \leqslant s \leqslant t\}$. Write

$$\begin{aligned} u(\dot{X}(r-1)) &:= E(V_r^2 \mid \mathscr{F}_{r-1}) \\ &= \frac{1}{\theta^2} E\left(\int_{r-1}^{r} \sigma^2(\dot{X}(s))\{1 - h'(\dot{X}(s))\}^2\,\mathrm{d}s \mid \mathscr{F}_{r-1}\right). \end{aligned} \tag{4.46}$$

By direct computation one may show that $\|h'\|_\infty$ is bounded in 'a' and $\theta^2 \equiv \theta^2(a)$ is bounded away from zero (see Lemma 4.6 below). Therefore, the following Lindeberg–type condition holds: $\forall \varepsilon > 0$

$$\frac{1}{\varphi(a)} \sum_{r=1}^{\varphi(a)} E(V_r^2 \cdot 1_{\{|V_r| \geqslant \varepsilon\sqrt{\varphi(a)}\}} | \mathscr{F}_{r-1}) \to 0 \text{ in probability, as } a \to \infty. \tag{4.47}$$

To see this use Schwarz inequality to write

$$\begin{aligned} &E(V_r^2 1_{\{|V_r| \geqslant \varepsilon\sqrt{\varphi(a)}\}} \cdot \mathscr{F}_{r-1}) \\ &\leqslant \{E(V_r^4 | \mathscr{F}_{r-1}) \cdot P(|V_r \geqslant \varepsilon\sqrt{\varphi(a)}\ \mathscr{F}_{r-1})\}^{1/2} \\ &\leqslant \{g_1(\dot{X}(r-1)) E(V_r^2 | \mathscr{F}_{r-1})/(\varepsilon^2 \varphi(a))\}^{1/2} \\ &= \{g_1(\dot{X}(r-1)) u(\dot{X}(r-1))\}^{1/2} \frac{1}{\varepsilon\sqrt{\varphi(a)}}. \end{aligned} \tag{4.48}$$

Here (see Bhattacharya and Waymire, 1990, p. 588),

$$g_1(\dot{X}(r-1)) = \frac{9}{\theta^4} \int_{r-1}^{r} E(\sigma^4(\dot{X}(s))\{1 - h'(\dot{X}(s))\}^4 | \mathscr{F}_{r-1})\,\mathrm{d}s \tag{4.49}$$

is bounded (uniformly in 'a', since $1 - h'$ and $1/\theta$ are). From (4.48) one gets (4.47). Let us now show that

$$\frac{1}{\varphi(a)} \sum_{r=1}^{\varphi(a)} u(\dot{X}(r-1)) \to 1 \quad \text{in probability as } a \to \infty. \tag{4.50}$$

Since the expected value of the left side is 1 (for, $Eu(\dot{X}(r)) = E(V_r^2) = 1$), it is enough to show that its variance goes to zero as $a \to \infty$. Write this variance as

$$\frac{1}{\varphi(a)} \operatorname{var}(u(\dot{X}(0))) + \frac{2}{\varphi^2(a)} \sum_{r=1}^{\varphi(a)} \sum_{r'=1}^{r-1} \operatorname{cov}\{u(\dot{X}(r-1)), u(\dot{X}(r'-1))\}. \tag{4.51}$$

The first term goes to zero as $a \to \infty$, since $\|u\|_\infty$ is bounded in 'a'. For the second term, use the estimate (4.31) to write

$$
\begin{aligned}
&\sum_{r'=1}^{r-1} \operatorname{cov}\{u(\dot{X}(r-1)),\ u(\dot{X}(r'-1))\} \\
&\quad \leqslant \sum_{r'=1}^{r-1} \min\{\|u\|_\infty^2,\ c_{10}\|u\|_\infty^2\} \exp\left\{-c_7\left(r - r' - \frac{a^2\log a}{c_7}\right)\Big/ a^2\right\} \\
&\quad \leqslant \left(\frac{a^2\log a}{c_7} + 1\right)\|u\|_\infty^2 \\
&\qquad + c_{10}\|u\|_\infty^2 \sum_{r' \geqslant \frac{a^2\log a}{c_7}+1} \exp\left\{-c_7\left(r - r' - \frac{a^2\log a}{c_7}\right)\Big/ a^2\right\} \\
&\quad \leqslant \left(\frac{a^2\log a}{c_7} + 1\right)\|u\|_\infty^2 + c'_{10}\|u\|_\infty^2 a^2,
\end{aligned}
\tag{4.52}
$$

where c'_{10} does not depend on 'a'. Now use the fact that $(a^2\log a)/\varphi(a) \to 0$, to see that Eq. (4.51) goes to zero as $a \to \infty$. It now follows from the martingale CLT (see, e.g., Bhattacharya and Waymire, 1990, p. 508) that

$$
\begin{aligned}
&\frac{X(\varphi(a)) - X(0) - \varphi(a)(\bar{b} + \bar{\beta}_a)}{\theta\sqrt{\varphi(a)}} \\
&\quad \equiv \frac{h(X(\varphi(a)) - h(X(0)))}{\theta\sqrt{\varphi(a)}} + \sum_{r=1}^{\varphi(a)} \frac{V_r}{\sqrt{\varphi(a)}} \xrightarrow{\mathscr{L}} \mathscr{N}(0,1)
\end{aligned}
\tag{4.53}
$$

as $a \to \infty$, since by Eqs. (4.40) and (4.41),

$$
\begin{aligned}
&\sup_{x,y} |h(x) - h(y)|/\sqrt{\varphi(a)} \\
&\quad = \sup_{x,y} a^2|g(x) - g(y)|/\sqrt{\varphi(a)} = O(a/\sqrt{\varphi(a)}) \longrightarrow 0
\end{aligned}
\tag{4.54}
$$

as $a \to \infty$.

To prove the desired result when $X(0)$ is arbitrary, it will be convenient to write $X^x(t)$ for the diffusion with initial state x. For $s < t$ one may write

$$
\begin{aligned}
&\frac{X^x(t) - x - t(\bar{b} + \bar{\beta}_a)}{\theta\sqrt{\varphi(a)}} \\
&\quad = \frac{X^x(s) - x - s(\bar{b} + \bar{\beta}_a)}{\theta\sqrt{\varphi(a)}} + \frac{X^x(t) - X^x(s) - (t-s)(\bar{b} + \bar{\beta}_a)}{\theta\sqrt{\varphi(a)}}.
\end{aligned}
\tag{4.55}
$$

We will let $s = \psi(a)$, $t = \varphi(a)$, where

$$
\psi(a) \gg a^2\log a, \quad \frac{\psi(a)}{\varphi(a)} \longrightarrow 0 \text{ as } a \to \infty. \tag{4.56}
$$

For example, take $\psi(a)$ to be the integer part of $(\varphi(a)a^2\log a)^{1/2}$. By Eq. (4.37), and the fact that for bounded nonanticipative functionals f one has $E(\int_0^s f(u)\,\mathrm{d}B(u))^2 = \int_0^s (Ef^2(u))\,\mathrm{d}u$, we have

$$E\left(\frac{X^x(s)-x-s(\bar{b}+\bar{\beta}_a)}{\theta\sqrt{\varphi(a)}}\right)^2 \leqslant \frac{[4\|h\|_\infty^2 + 2(\max_z\sigma^2(z))\max_z(1-h'(z))^2]\psi(a)}{\theta^2\varphi(a)} \longrightarrow 0 \quad \text{as } a\to\infty. \tag{4.57}$$

We have used here the estimates in Lemma 4.6 below. Therefore, it is enough to show that the second term on the right in Eq. (4.55) converges in distribution to $\mathcal{N}(0,1)$, with $s=\psi(a)$ and $t=\varphi(a)$. By the Markov property, the conditional distribution of $X^x(t)-X^x(s)$, given $\mathcal{F}_s$, is the same as the distribution of $X^z(t-s)-z$, with $z=X^x(s)$. But the latter distribution may be expressed as $Q_{\dot{z}}(t-s)$ with $\dot{z}=\dot{X}^x(s)$, since it depends only on $\dot{X}^x(s)$ and $t-s$. By Theorem 4.2 (and Remark 4.3) the variation distance between the equilibrium distribution $\tilde{\pi}_a$ and the distribution of $\dot{X}^x(s)$ goes to zero uniformly in x, as $a\to\infty$ (with $s=\psi(a)$). Therefore, the variation distance between the distribution of the second term on the right of Eq. (4.55) and the distribution of

$$\frac{X(t-s)-X(0)-(t-s)(\bar{b}+\bar{\beta}_a)}{\theta\sqrt{\varphi(a)}}, \tag{4.58}$$

with $\dot{X}(0)$ having distribution $\tilde{\pi}_a$, goes to zero as $a\to\infty$. Thus it is enough to show that (4.58) converges in law to $\mathcal{N}(0,1)$. However, we have shown that

$$\frac{X(t-s)-X(0)-(t-s)(\bar{b}+\bar{\beta}_a)}{\theta\sqrt{t-s}} \xrightarrow{\mathcal{L}} \mathcal{N}(0,1). \tag{4.59}$$

Now note that since (4.58) differs from the left side of (4.59) by the factor $\sqrt{(t-s)/\varphi(a)} = \sqrt{(\varphi(a)-\psi(a))/\varphi(a)}$ which goes to 1 as $a\to\infty$, the proof is complete. □

It remains to prove Lemma 4.6 below. Using Eq. (4.41) one obtains

$$h'(x) = ag'(x/a). \tag{4.60}$$

Also (see Eq. (4.34))

$$\theta^2 \equiv \overline{\sigma^2(\cdot)(h'(\cdot)-1)^2} = \int_0^1 \sigma^2(ax)(ag'(x)-1)^2\pi_a(x)\,\mathrm{d}x. \tag{4.61}$$

Lemma 4.6. *Under the hypothesis of Theorem* 4.5, *one has*

$$\sup_{a\geqslant 1,x} |\sigma(x)(1-h'(x)| < \infty, \quad 0 < \liminf_{a\to\infty}\theta^2 \leqslant \limsup_{a\to\infty}\theta^2 < \infty, \tag{4.62}$$

where θ^2 is the variance parameter defined in Eqs. (4.34) *and* (4.61).

Proof. First, it follows from the first relation in (4.8) that

$$\bar{b}+\bar{\beta}_a \equiv \int_0^1 (b(ax)+\beta(x))\pi_a(x)\,\mathrm{d}x$$

$$=\frac{c}{2a}\left\{(1-\mathrm{e}^{-I(0,1)})^{-1}\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y\right\}\int_0^1 \frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{I(0,x)}\,\mathrm{d}x$$

$$-c\int_0^1\left\{\frac{b(ax)+\beta(x)}{\sigma^2(ax)}\,\mathrm{e}^{I(0,x)}\int_0^x \mathrm{e}^{-I(0,y)}\,\mathrm{d}y\right\}\mathrm{d}x$$

$$=\frac{c}{2a}\,\mathrm{e}^{I(0,1)}\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y-\frac{c}{2a}\int_0^1\left(\frac{d}{\mathrm{d}x}\,\mathrm{e}^{I(0,x)}\right)\left(\int_0^x \mathrm{e}^{-I(0,y)}\,\mathrm{d}y\right)\mathrm{d}x$$

$$=\frac{c}{2a}\mathrm{e}^{I(0,1)}\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y$$

$$-\frac{c}{2a}\left[\mathrm{e}^{I(0,1)}\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y-\int_0^1 \mathrm{e}^{I(0,x)}\mathrm{e}^{-I(0,x)}\,\mathrm{d}y\right]$$

$$=\frac{c}{2a}. \tag{4.63}$$

Now (see Eqs. (4.38) and (4.40)) g is a solution of

$$\frac{\sigma^2(ax)}{2}g''(x)+a(b(ax)+\beta(x))g'(x)=b(ax)-\beta(x)-(\bar{b}+\bar{\beta}_a)$$

$$=b(ax)-\beta(x)-\frac{c}{2a}. \tag{4.64}$$

Therefore,

$$ag''(x)+(ag'(x)-1)\left\{\frac{2a}{\sigma^2(x)}(b(ax)+\beta(x))\right\}=-\frac{c}{\sigma^2(ax)}, \tag{4.65}$$

which may be expressed as

$$[(ag'(x)-1)\mathrm{e}^{I(0,x)}]'=-\frac{c}{\sigma^2(ax)}\,\mathrm{e}^{I(0,x)}, \tag{4.66}$$

so that

$$(ag'(x)-1)\mathrm{e}^{I(0,x)}=(ag'(0)-1)-c\int_0^x \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y. \tag{4.67}$$

Using the periodic boundary condition $g'(0)=g'(1)$ one gets, taking $x=1$ in Eq. (4.67),

$$(ag'(0)-1)\mathrm{e}^{I(0,1)}=(ag'(0)-1)-c\int_0^1 \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y, \tag{4.68}$$

or,

$$ag'(0)-1=-c(\mathrm{e}^{I(0,1)}-1)^{-1}\int_0^1 \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y.$$

Therefore,

$$ag'(x)-1=-c\mathrm{e}^{-I(0,x)}\left\{(\mathrm{e}^{I(0,1)}-1)^{-1}\int_0^1 \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y+\int_0^x \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y\right\}. \tag{4.69}$$

It follows from (4.16) and (4.18) that there exist positive constants d_3, d_4 which do not depend on 'a' such that

$$d_3 a \leqslant c \leqslant d_4 a. \tag{4.70}$$

Using this and (4.12) it is straightforward to show (as in estimates (4.13)–(4.19)) that

$$\sup_{x,a\geqslant 1} |\sigma(x)(1-h'(x))| = \sup_{a\geqslant 1,x} |\sigma(ax)||ag'(x)-1| \equiv d_5 < \infty. \tag{4.71}$$

Similarly one may show, using Eq. (4.68) and the fact that $\pi_a(x)$ is bounded away from zero and infinity uniformly in x and 'a' (see (4.19)), that

$$\begin{aligned}&\int_0^1 |\sigma(ax)(ag'(x)-1)|\pi_a(x)\,\mathrm{d}x\\&\quad = |c|\int_0^1 |\sigma(ax)|\mathrm{e}^{-I(0,x)}\left(\int_0^x \frac{\mathrm{e}^{I(0,y)}}{\sigma^2(ay)}\,\mathrm{d}y\right)\pi_a(x)\,\mathrm{d}x + O\left(\frac{1}{a}\right).\end{aligned} \tag{4.72}$$

Now use (4.70), the fact that $|\sigma(\cdot)|$ is bounded away from zero, and that π_a is bounded away from zero, to derive from Eq. (4.72) the inequality

$$\liminf_{a\to\infty} \int_0^1 |\sigma(ax)(ag'(x)-1)|\pi_a(x)\,\mathrm{d}x > 0, \tag{4.73}$$

which implies

$$\liminf_{a\to\infty} \int_0^1 \sigma^2(ax)(ag'(x)-1)^2\pi_a(x)\,\mathrm{d}x > 0, \tag{4.74}$$

yielding $\liminf \theta^2 > 0$. From (4.71) one gets $\limsup \theta^2 < \infty$. □

Remark 4.7. One may show that the functional version of the CLT holds in Theorem 4.5. That is, the process $X_\lambda := \{\theta\sqrt{\lambda t}(X(\lambda t) - \lambda t(\bar{b}+\bar{\beta}_a)):\ t\geqslant 0\}$ converges in distribution to a standard Brownian motion as $a\to\infty$, $\lambda/(a^2\log a)\to\infty$. For tightness, one may use Doob's maximal inequality and the fourth moment estimates used in (4.48)–(4.50). A similar remark applies to Theorem 4.13 coming up later.

4.2. *The case* $\int_0^1 \beta(x)\,\mathrm{d}x = 0$

In this subsection we will assume $\sigma^2(x)$ is a positive constant,

$$\sigma^2(x) \equiv \sigma^2 > 0. \tag{4.75}$$

Then the innocuous assumption (4.7) becomes

$$\int_0^1 b(y)\,\mathrm{d}y = 0. \tag{4.76}$$

The main assumption here is

$$\int_0^1 \beta(x)\,\mathrm{d}x = 0. \tag{4.77}$$

It follows from Lemma 2.3 that the diffusion $\dot{X}$ and its scaled version $\dot{Y}$ are time reversible, that is, the generator A of $\dot{Y}$ is self-adjoint,

$$A := \frac{1}{2}\sigma^2 \frac{d^2}{dx^2} + a\{b(ax) + \beta(x)\}\frac{d}{dx}. \tag{4.78}$$

In this case the invariant density of the process $\dot{Y}(\cdot)$ is given by (see Eqs. (2.20) and (4.8))

$$\pi_a(x) = c\exp\{I(0,x)\}, \quad I(0,x) := \frac{2a}{\sigma^2}\int_0^x \{b(ay) + \beta(y)\}\, dy. \tag{4.79}$$

Since $(2a/\sigma^2)\int_0^x b(ay)\,dy = (2/\sigma^2)\int_0^{ax} b(z)\,dz = (2/\sigma^2)\int_{[ax]}^{ax} b(z)\,dz$, which is bounded by $(2/\sigma^2)\int_0^1 |b(z)|\,dz = (2/\sigma^2)\delta$, it follows that

$$\frac{e^{-2\delta/\sigma^2}}{c}\pi_a(x) \leqslant \exp\left\{(2a/\sigma^2)\int_0^x \beta(y)\,dy\right\} \leqslant \frac{e^{2\delta/\sigma^2}}{c}\pi_a(x). \tag{4.80}$$

Let θ_*, θ^* be the minimum and maximum values, respectively, of $x \to \int_0^x \beta(y)\,dy$. Then

$$\frac{e^{-2\delta/\sigma^2}}{c}\pi_a(x) \leqslant \exp\{2a\theta^*/\sigma^2\}, \quad e^{2a\theta_*/\sigma^2} \leqslant \frac{e^{2\delta/\sigma^2}}{c}\pi_a(x). \tag{4.81}$$

so that

$$\max_{x,y}\frac{\pi_a(x)}{\pi_a(y)} \leqslant (e^{4\delta/\sigma^2})e^{2a(\theta^*-\theta_*)/\sigma^2}. \tag{4.82}$$

Thus, by Lemma 2.3, an estimate of the spectral gap λ_A of $\frac{1}{2}(A+\tilde{A})$ on $L^2(S^1,\pi_a)$ is given by

$$\begin{aligned} \lambda_A &\geqslant 2\sigma^2 \min_x \pi_a(x) \geqslant 2\sigma^2 \Big/ \frac{\max_x \pi_a(x)}{\min_x \pi_a(x)} \geqslant c_1' \, e^{-c_2' a}, \\ c_1' &:= 2\sigma^2 e^{-4\delta/\sigma^2}, \qquad c_2' := e^{2(\theta^*-\theta_*)/\sigma^2}. \end{aligned} \tag{4.83}$$

Therefore, by Proposition 4.1, the spectral gap λ_L of $\frac{1}{2}(L+\tilde{L})$ on $L^2(S^1(a),\tilde{\pi}_a)$ is estimated by

$$\lambda_L \geqslant \frac{1}{a^2}c_1' \, e^{-c_2' a}, \tag{4.84}$$

with c_1', c_2' as given in (4.83). The proof of the theorem below is entirely analogous to that of Theorem 4.2.

Theorem 4.13. *Assume* (4.2) *and* (4.75)–(4.77). *Then the transition probability densities* $\dot{p}$ *of* $\dot{X}$ *and* $\ddot{p}$ *of* $\dot{Y}$ *satisfy the inequalities*

$$\begin{aligned} \int_{S^1} |\ddot{p}(t;x,y) - \pi_a(y)|\,dy &\leqslant c_3' a^{1/2} e^{-\lambda_A t} \\ &\leqslant c_3' a^{1/2}\exp\{-c_1' e^{-c_2' a} t\} \quad (t>0), \end{aligned} \tag{4.85}$$

for all $x \in S^1$, *and*

$$\int_{S^1(a)} |\tilde{p}(t;x,y) - \tilde{\pi}_a(y)|\,\mathrm{d}y \leqslant c_3' a^{1/2} \mathrm{e}^{-\lambda_A t}$$

$$\leqslant c_3' a^{1/2} \exp\left\{-\frac{c_1'}{a^2}\,\mathrm{e}^{-c_2' a} t\right\} \quad (t>0), \tag{4.86}$$

for all $x \in S^1(a)$, *where* c_i' $(i=1,2,3)$ *do not depend on 'a'*.

Remark 4.9. We have not attempted to derive the precise exponential constant $-c_2'$ in the spectral gap estimate in (4.83). Using the first inequality for λ_A in (4.83), along with (4.81), one gets $\lambda_A \geqslant (2\sigma^2 \mathrm{e}^{-2\delta/\sigma^2}) c \exp\{2a\theta_*/\sigma^2\} = c' \exp\{2a\theta_*/\sigma^2\} / \int_0^1 \mathrm{e}^{I(0,x)}\,\mathrm{d}x$, where c' is independent of a. For a method of precise estimation of the exponential constant see Holley et al. (1989), where it is shown that the spectral gap can be exponentially small, i.e., $O(\mathrm{e}^{-\alpha a})$ for some $\alpha > 0$.

A significant difference between the present case and the case in the preceding subsection is brought out by the following result. Recall that θ^* denotes the maximum value, and θ_* the minimum value, of the *potential function* $\psi(x) := \int_0^x \beta(y)\,\mathrm{d}y$.

Proposition 4.10. *Assume the hypothesis of Theorem* 4.8. *Assume also that* $\beta(\cdot)$ *has a finite number of zeros.* (a) *If* $\psi(x)$ *has a unique maximum at* x^*, *then* $\pi_a(x)\,\mathrm{d}x$ *converges weakly to the point mass* $\delta_{x^*}(\mathrm{d}x)$ *at* x^* *as* $a \to \infty$. (b) *In general,* $\{\pi_a(x)\,\mathrm{d}x\colon a \geqslant 1\}$ *is a tight family and all its weak limit points have support contained in the finite set of points in* S^1 *where the maximum value* θ^* *of* ψ *is attained.*

Proof. (a) In this case, for all $x \neq x^*$ in S^1,

$$\frac{\pi_a(x)}{\pi_a(x^*)} = \mathrm{e}^{I(0,x) - I(0,x^*)}$$

$$= \exp\left\{\frac{2a}{\sigma^2}\left(\int_0^x b(ay)\,\mathrm{d}y - \int_0^{x^*} b(ay)\,\mathrm{d}y\right) + \frac{2a}{\sigma^2}(\psi(x) - \psi(x^*))\right\}$$

$$\leqslant \mathrm{e}^{2\delta/\sigma^2} \exp\left\{\frac{2a}{\sigma^2}(\psi(x) - \psi(x^*))\right\} \to 0 \quad \text{as } a \to \infty. \tag{4.87}$$

For inequality (4.87), use the fact that for all $u < v$,

$$\left|\frac{2a}{\sigma^2}\int_u^v b(ay)\,\mathrm{d}y\right| = \frac{2}{\sigma^2}\left|\int_{au}^{av} b(y)\,\mathrm{d}y\right| \leqslant \frac{2}{\sigma^2}\int_0^1 |b(y)|\,\mathrm{d}y = \frac{2\delta}{\sigma^2},$$

since

$$\int_z^{z-1} b(y)\,\mathrm{d}y = 0 \quad \text{for all } z.$$

(b) The proof here is virtually the same, if one chooses x outside the finite set of x^* values where ψ attains its maximum θ^*. □

Example 4.11. Let $b(\cdot)$ be arbitrary (satisfying $\int_0^1 b(y)\,dy = 0$), and $\beta(x) = 4\pi\cos 4\pi x$. Then $\psi(x) \equiv \sin 4\pi x$ has its maximum value $\theta^* = 1$ attained at $x = \frac{1}{8}$ and $x = \frac{5}{8}$. In this case $\pi_a(x)\,dx$ converges weakly to the two-point distribution assigning probabilities $\frac{1}{2}$ and $\frac{1}{2}$ to $x = \frac{1}{8}$ and $x = \frac{5}{8}$. Note also that these two points are the *stable*, or attractive, *fixed points* for the motion $dx(t)/dt = \beta(x(t))$, while $x = \frac{3}{8}$ and $x = \frac{7}{8}$ are *unstable*, or repelling, *fixed points*. It may be shown in this case, using results of Holley et al. (1989), that the spectral gap is $O(e^{-\alpha a})$ for some positive constant α independent of a.

Remark 4.12. In contrast to Example 4.11 one may also construct a potential function $\psi(x)$ with a unique maximum, representing a stable fixed point, together with a single unstable fixed point. For example, take $\psi(x) = \sin 2\pi x$, i.e., $\beta(x) = 2\pi\cos 2\pi x$. In this case the approach to equilibrium should be fast. In an unpublished recent work one of the authors has shown that in a class of examples, including this one, the spectral gap is $O(1/a^2)$ for the $\dot{X}$ process (i.e., for its generator). Our estimates (4.78) and (4.79) of the spectral gap, and of the speed of convergence to equilibrium (See (4.80) and (4.81)), contend against the 'worst case' scenario.

The next result is an analog of Theorem 4.5 again with distinctive differences. In particular, part (b) of the result shows that the variance parameter of the limiting distribution of $X(t)$, i.e., the asymptotic variance of $X(t)$ per unit time, goes to zero exponentially fast as $a \to \infty$.

Theorem 4.13. *Assume the hypothesis of Theorem 4.8. Also assume $\beta(\cdot)$ is not identically zero. Then*

$$\frac{X(t) - X(0)}{\sigma a\theta\sqrt{t}} \xrightarrow{\mathscr{L}} \mathscr{N}(0,1), \tag{4.88}$$

whatever be the initial state $X(0)$, as

$$t \to \infty, \ a \to \infty, \quad t \gg a^2 \exp\left\{\frac{18a}{\sigma^2}(\theta^* - \theta_*)\right\}. \tag{4.89}$$

Here θ^* and θ_* are the maximum and minimum values, respectively, of $\psi(x) = \int_0^x \beta(y)\,dy$, and

$$\theta^2 = \left(\int_0^1 e^{I(0,x)}\,dx \cdot \int_0^1 e^{-I(0,x)}dx\right)^{-1}. \tag{4.90}$$

The variance parameter $\sigma^2 a^2 \theta^2$ goes to zero exponentially fast in 'a' as $a \to \infty$.

Proof. Writing

$$\mu(x) := a\{b(ax) + \beta(x)\}, \tag{4.91}$$

one has

$$\int_0^x \mu(y)\pi_a(y)\,\mathrm{d}y = \frac{\sigma^2}{2}\int_0^x \left(\frac{\mathrm{d}}{\mathrm{d}y}\,\mathrm{e}^{I(0,y)}\right)\mathrm{d}y \Big/ \int_0^1 \mathrm{e}^{I(0,y)}\,\mathrm{d}y$$
$$= \frac{\sigma^2}{2}\left(\mathrm{e}^{I(0,x)} - 1\right) \Big/ \int_0^1 \mathrm{e}^{I(0,y)}\,\mathrm{d}y. \tag{4.92}$$

In particular,

$$\bar{\mu} \equiv \int_0^1 \mu(x)\pi_a(x)\,\mathrm{d}x = 0,$$

that is,

$$\bar{b} + \bar{\beta}_a = 0. \tag{4.93}$$

Now consider the equation

$$Ag_2(x) = \mu(x) \equiv a\{b(ax) + \beta(x)\}. \tag{4.94}$$

On integration one gets

$$g_2'(x) = c_1\mathrm{e}^{-I(0,x)} + 1,$$
$$g_2(x) - c_2 + c_1\int_0^x \mathrm{e}^{-I(0,y)}\,\mathrm{d}y + x. \tag{4.95}$$

The boundary condition $g_2(0) = g_2(1)$ implies

$$c_1 = -\frac{1}{\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y}, \tag{4.96}$$

so that

$$g_2'(x) = 1 - \frac{\mathrm{e}^{-I(0,x)}}{\int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y},$$
$$g_2(x) = c_2 + x - \int_0^x \mathrm{e}^{-I(0,y)}\,\mathrm{d}y \Big/ \int_0^1 \mathrm{e}^{-I(0,y)}\,\mathrm{d}y, \tag{4.97}$$

where c_2 is arbitrary. One may now write

$$\frac{Y(t) - Y(0)}{\sigma\theta\sqrt{t}} = \frac{1}{\sigma\theta\sqrt{t}}\left\{g_2(\dot{Y}(t)) - g_2(\dot{Y}(0)) - \sigma\int_0^t \{g_2'(\dot{Y}(s)) - 1\}\,\mathrm{d}\bar{B}(s)\right\}. \tag{4.98}$$

Since, by Eq. (4.97), $|g_2(x) - g_2(y)|$ is bounded by 2 for $x, y \in [0,1]$, and since it is easily shown that $\theta^2 \geqslant c_1' \exp\{-(2a/\sigma^2)(\theta^* - \theta_*)\}$ (See (4.107) below)

$$\theta\sqrt{t} \geqslant c'\,\mathrm{e}^{-(a/\sigma^2)}(\theta^* - \theta_*)\cdot\sqrt{t} \to \infty \tag{4.99}$$

if (4.89) holds,

$$\frac{g_2(\dot{Y}(t)) - g_2(\dot{Y}(0))}{\theta\sqrt{t}} \to 0 \quad \text{in probability}. \tag{4.100}$$

Using this in Eq. (4.98), one now needs to prove

$$\frac{1}{\theta\sqrt{t}}\int_0^t \{g_2'(\dot{Y}(s))-1\}\,\mathrm{d}\bar{B}(s) \xrightarrow{\mathscr{L}} \mathscr{N}(0,1). \tag{4.101}$$

Now, writing E_{π_a} for the expectation under the equilibrium distribution π_a of $\dot{Y}(s)$, one has

$$\begin{aligned} E_{\pi_a}(g_2'(\dot{Y}(t))-1)^2 &= \frac{\int_0^1 \mathrm{e}^{-2I(0,x)}\pi_a(x)\,\mathrm{d}x}{(\int_0^1 \mathrm{e}^{-I(0,x)}\,\mathrm{d}x)^2} = \frac{\int_0^1 \mathrm{e}^{-I(0,x)}\,\mathrm{d}x}{\int_0^1 \mathrm{e}^{I(0,x)}\,\mathrm{d}x\cdot(\int_0^1 \mathrm{e}^{-I(0,x)}\,\mathrm{d}x)^2} \\ &= \frac{1}{\int_0^1 \mathrm{e}^{I(0,x)}\,\mathrm{d}x\cdot\int_0^1 \mathrm{e}^{-I(0,x)}\,\mathrm{d}x} \\ &= \theta^2. \end{aligned} \tag{4.102}$$

The proof of (4.101) is now structured along the lines of that of Theorem 4.5. However, the estimates, as functions of 'a' are quite different in the present case, and care is needed to check the conditions for the martingale CLT to hold. First assume $\dot{Y}(0)$ has the equilibrium distribution π_a. Let $\mathscr{F}_s := \sigma\{Y(u):\ 0\leqslant u\leqslant s\}$, and consider the triangular array of martingale differences

$$V_r := \frac{1}{\theta}\int_{r-1}^{r}\{1-g_2'(\dot{Y}(s))\}\,\mathrm{d}\bar{B}(s) \quad (r=1,2,\ldots,\varphi(a):\ a=1,2,\ldots), \tag{4.103}$$

where $\varphi(a)$ is a sequence of positive integers satisfying

$$\frac{\varphi(a)}{\exp\{\frac{18a}{\sigma^2}(\theta^*-\theta_*)\}} \to \infty \quad \text{as } a\to\infty. \tag{4.104}$$

Write

$$u(\dot{Y}(r-1)) := E(V_r^2\mid\mathscr{F}_{r-1}) = \frac{1}{\theta^2}E\left(\int_{r-1}^{r}\{1-g_2'(\dot{Y}(s))\}^2\,\mathrm{d}s\mid\mathscr{F}_{r-1}\right). \tag{4.105}$$

Since $I(0,x)=(2/\sigma^2)\int_{[ax]}^{ax} b(y)\,\mathrm{d}y-(2a/\sigma^2)\psi(x)$, where $\psi(x)=\int_0^x \beta(y)\,\mathrm{d}y$, one has

$$-\frac{2\delta}{\sigma^2}+\frac{2a\theta_*}{\sigma^2}\leqslant I(0,x)\leqslant\frac{2\delta}{\sigma^2}+\frac{2a\theta^*}{\sigma^2} \quad (0\leqslant x\leqslant 1), \tag{4.106}$$

where θ^* and θ_* are the maximum and minimum values of $\psi(x)$, respectively. Therefore, by Eqs. (4.97) and (4.102),

$$\begin{aligned} |1-g_2'(x)| &\leqslant \frac{\exp\{\frac{2\delta}{\sigma^2}-\frac{2a\theta_*}{\sigma^2}\}}{\exp\{-\frac{2\delta}{\sigma^2}-\frac{2a\theta^*}{\sigma^2}\}} = \exp\{\frac{4\delta}{\sigma^2}+\frac{2a}{\sigma^2}(\theta^*-\theta_*)\}, \\ \theta^2 &\geqslant \exp\left\{-\frac{4\delta}{\sigma^2}-\frac{2a}{\sigma^2}(\theta^*-\theta_*)\right\}. \end{aligned} \tag{4.107}$$

To find an upper bound for θ^2, assume first that $\theta^*>0$, and let $\psi(x^*)=\theta^*$. Since $\psi'(x)=\beta(x)$, it follows that $\psi(x)\geqslant\theta^*(1-\sigma^2/2a)$ on an interval in $[0,1]$ of length at least $2\theta^*(\sigma^2/2a)/\|\beta\|_\infty = \theta^*\sigma^2/(\|\beta\|_\infty a)$, if the latter is less than one. Therefore,

$$\int_0^1 e^{I(0,x)}\,dx \geqslant \frac{\theta^*\sigma^2}{\|\beta\|_\infty a}\exp\left\{-\frac{2\delta}{\sigma^2}+\frac{2a}{\sigma^2}\theta^*\left(1-\frac{\sigma^2}{2a}\right)\right\}$$
$$= \frac{\theta^*\sigma^2}{\|\beta\|_\infty a}\exp\left\{-\frac{2\delta}{\sigma^2}-\theta^*\right\}\exp\left\{\frac{2a\theta^*}{\sigma^2}\right\} \quad (\theta^*>0). \tag{4.108}$$

Also, since $\psi(0)=0$, $\psi(x)\leqslant\|\beta\|_\infty x$,

$$\int_0^1 e^{-I(0,x)}\,dx \geqslant e^{-2\delta/\sigma^2}\int_0^1 \exp\left\{-\frac{2a\|\beta\|_\infty}{\sigma^2}x\right\}dx$$
$$\geqslant \frac{\sigma^2}{2a\|\beta\|_\infty}\,e^{-2\delta/\sigma^2}. \tag{4.109}$$

If $\theta^*=0$, then $\theta_*<0$ and one has, in the same manner as in the derivation of (4.108) and (4.109),

$$\int_0^1 e^{-I(0,x)}\,dx \geqslant \frac{|\theta_*|\sigma^2}{\|\beta\|_\infty a}\exp\left\{-\frac{2\delta}{\sigma^2}+\theta_*\right\}\exp\left\{\frac{2a\theta_*}{\sigma^2}\right\} \quad (\theta_*<0), \tag{4.110}$$

and

$$\int_0^1 e^{I(0,x)}\,dx \geqslant \frac{\sigma^2}{2a\|\beta\|_\infty}\,e^{-2\delta/\sigma^2}. \tag{4.111}$$

From (4.108)–(4.111) it follows that

$$\int_0^1 e^{I(0,x)}\,dx\cdot\int_0^1 e^{-I(0,x)}\,dx$$
$$\geqslant \exp\left\{-\frac{4\delta}{\sigma^2}-(\theta^*-\theta_*)\right\}\frac{\sigma^4\max\{|\theta^*|,|\theta_*|\}}{2\|\beta\|_\infty a^2}\exp\left\{\frac{2a}{\sigma^2}(\theta^*-\theta_*)\right\}, \tag{4.112}$$

so that

$$\theta^2 \leqslant \exp\left\{\frac{4\delta}{\sigma^2}+(\theta^*-\theta_*)\right\}\frac{2\|\beta\|_\infty}{\sigma^4\max\{|\theta^*|,|\theta_*|\}}a^2\exp\left\{-\frac{2a}{\sigma^2}(\theta^*-\theta_*)\right\}. \tag{4.113}$$

To prove the conditional Lindeberg condition use inequality (4.107), and an estimate of the fourth moment of the stochastic integral (Bhattacharya and Waymire, 1990, p. 588) to get

$$E\left(V_r^2 1_{\{|V_r|\geqslant\varepsilon\sqrt{\varphi(a)}\}}\mid\mathscr{F}_{r-1}\right)$$
$$\leqslant\{E(V_r^4\mid\mathscr{F}_{r-1})\cdot P(|V_r|\geqslant\varepsilon\sqrt{\varphi(a)}\mid\mathscr{F}_{r-1})\}^{1/2}$$
$$\leqslant\frac{3}{\theta^2}\left(\int_{r-1}^r E[\{1-g_2'(\dot Y(s))\}^4\mid\mathscr{F}_{r-1}]\,ds\right)^{1/2}\cdot u^{1/2}(\dot Y(r-1))\frac{1}{\varepsilon\sqrt{\varphi(a)}}$$
$$\leqslant\frac{3}{\theta^3}\exp\left\{\frac{12\delta}{\sigma^2}+\frac{6a}{\sigma^2}(\theta^*-\theta_*)\right\}\frac{1}{\varepsilon\sqrt{\varphi(a)}}$$
$$\leqslant 3\exp\left\{\frac{18\delta}{\sigma^2}-\frac{9a}{\sigma^2}+\frac{9a}{\sigma^2}(\theta^*-\theta_*)\right\}\frac{1}{\varepsilon\sqrt{\varphi(a)}}. \tag{4.114}$$

Then

$$\frac{1}{\varphi(a)}\sum_{r=1}^{\varphi(a)} E(V_r^2 \cdot 1_{\{|V_r|\geqslant \varepsilon\sqrt{\varphi(a)}\}} \mid \mathscr{F}_{r-1})$$
$$\leqslant 3\exp\left\{\frac{18\delta}{\sigma^2}+\frac{9a}{\sigma^2}+\frac{9a}{\sigma^2}(\theta^*-\theta_*)\right\}\frac{1}{\varepsilon\sqrt{\varphi(a)}}\to 0 \quad \text{as } a\to\infty, \tag{4.115}$$

by the hypothesis (4.104). It remains to check that

$$\frac{1}{\varphi(a)}\sum_{r=1}^{\varphi(a)} u(\dot{Y}(r-1))\to 1 \quad \text{in probability as } a\to\infty. \tag{4.116}$$

Since the expected value of the left side is 1, it is enough to show that its variance goes to zero. This variance may be estimated by (see (4.51), (4.52), and (4.85))

$$\frac{1}{\varphi(a)}\operatorname{var}(u(\dot{Y}(0)))+\frac{2}{\varphi(a)}c'_{11}\|u\|_\infty^2\frac{1}{c'_1}\,\mathrm{e}^{c'_2 a}\log a \tag{4.117}$$

where c_i''s are independent of 'a', $c_2'=2(\theta^*-\theta_*)/\sigma^2$. Using (4.117) and

$$\|u\|_\infty\leqslant\frac{1}{\theta^2}\exp\left\{\frac{8\delta}{\sigma^2}+\frac{4a}{\sigma^2}(\theta^*-\theta_*)\right\}\leqslant\exp\left\{\frac{12\delta}{\sigma^2}+\frac{6a}{\sigma^2}(\theta^*-\theta_*)\right\}, \tag{4.118}$$

one obtains, from Eq. (4.118),

$$\operatorname{var}\left(\frac{1}{\varphi(a)}\sum_{r=1}^{\varphi(a)} u(\dot{Y}(r-1))\right)\to 0 \quad \text{as } a\to\infty. \tag{4.119}$$

This completes the proof of (4.88) for times t satisfying (4.89), when $\dot{Y}(0)$ (or, $\dot{X}(0)$) has the equilibrium distribution. When the initial distribution is arbitrary, then one uses (4.85), and proceeds as in the last part of the proof of Theorem 4.8, with $Y(t)$ instead of $X(t)$, using estimates (4.107).

Finally it follows from (4.113) that

$$\sigma^2 a^2\theta^2 \ll \exp\left\{-\frac{2a}{\sigma^2(1+\varepsilon)}(\theta^*-\theta_*)\right\}$$

for every $\varepsilon>0$. □

Remark 4.14. The proof shows that the convergence (4.88) is uniform (e.g., in the Kolmogorov distance for distribution functions) with respect to all initial $X(0)$.

Remark 4.15. Theorems 4.5 and 4.13 imply corresponding asymptotics of the solution $c(t;y)$ of the Fokker–Planck equation

$$\frac{\partial c}{\partial t}=\frac{1}{2}-\frac{\partial}{\partial y}\{(b(y)+\beta(y/a))c\} \quad (t>0,\ y\in\mathbb{R}),$$
$$c(0,y)=\lim_{t\downarrow 0}c(t,y)=c_0(y) \quad (y\in\mathbb{R}). \tag{4.120}$$

The *fundamental solution* of Eq. (4.120) (i.e., $c(t,y)$ under the point initial input $c(0,\mathrm{d}y)=\delta_x(\mathrm{d}y)$) is the transition probability density $p(t;x,y)$ of the diffusion $X(t)$

governed by Eq. (1.1) (See, e.g., Bhattacharya and Waymire, 1990, pp. 377–381). The general solution of Eq. (4.120) may be expressed as

$$c(t,y)=\int_{\mathbb{R}} c_0(x)p(t;x,y)\,\mathrm{d}x \quad (t>0,\, y\in\mathbb{R}). \tag{4.121}$$

If c_0 is localized, e.g., if c_0 has a compact support independent of 'a', then the asymptotics of $c(t,y)$ are the same as those of the distribution of $X(t)$ with an initial distribution $c_0(x)\,\mathrm{d}x$. This correspondence has important implications for the problem of solute transport in porous media (Bhattacharya and Götze, 1995).

Remark 4.16. As a final remark it may be pointed out that the analysis in this article leaves out all those cases where $\beta(x)$ changes sign, but $\int_0^1 \beta(x)\,\mathrm{d}x \neq 0$. For these cases the generator is not self-adjoint, and the invariant density is given by Eq. (2.21).

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Part III
Large Time Asymptotics for Markov Processes II: Dynamical Systems and Iterated Maps

Chapter 8
Dynamical Systems, IID Random Iterations, and Markov Chains

Krishna B. Athreya

Abstract The many areas in mathematical statistics, probability theory, statistics processes, and mathematical analysis to which Professor Rabi Bhattacharya has made important and deep contributions include the topics in the title of this paper. In this paper we shall outline some interesting recent results in these topics.

8.1 Dynamical Systems

Let S be a nonempty set and $T : S \to S$ be a map from S to S. The pair (S, T) is called a *dynamical system*. For each x in S, the sequence $O_x = \{x, T(x), T(T(x)), \cdots, T^{(n)}(x), \cdots\}$, where $T^{(n+1)}(x) = T(T^{(n)}(x))$, $n = 0, 1, 2, \cdots$, with $T^{(0)}(x) \equiv x$ is called the *orbit* of x under the map T. Some topics of interest in the study of dynamical systems are:

(2.1) The existence of a probability distribution π on $(S, \mathcal{S})$ where $\mathcal{S}$ is a σ-algebra of subsets of S, which is *stationary* (also called *invariant*) w.r.t. T, i.e., each A in $\mathcal{S}$, $\pi(A) = \pi(T^{-1}(A))$, assuming, of course, that $T : S \to S$ is $(\mathcal{S}, \mathcal{S})$ measurable.

(2.2) The *convergence* of the empirical distribution of O_x, i.e., if $\mu_n(A|x) \equiv \frac{1}{n}\sum_{j=0}^{n-1} I_A(T^{(j)}(x))$, $A \in \mathcal{S}$ then does $\mu_n(\cdot|x)$ converge in a suitable sense as $n \to \infty$?

(2.3) *Ergodic theorems* of the kind: for $h : S \to \mathbb{R}$, $\mathcal{S}$ measurable the "time average" $\frac{1}{n}\sum_{j=0}^{n-1} h(T^{(j)}(x))$ converges as $n \to \infty$ to the "space average" $\int_S h d\mu$ for some appropriate measure μ on $(S, \mathcal{S})$.

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(2.4) Central limit theorem (CLT) of the kind: for $h : S \to \mathbb{R}$ such that $\int |h| d\pi < \infty$ where π is a stationary (w.r.t. T) distribution on $(S, \mathcal{S})$

$$\pi\Big\{x : a \le \sqrt{n}\frac{\left(\frac{1}{n}\sum_{j=0}^{n-1} h(T^{(j)}(x)) - \int h d\pi\right)}{\sigma} \le b\Big\}$$

converges as $n \to \infty$ to $\dfrac{1}{\sqrt{2\pi}} \displaystyle\int_a^b e^{-u^2/2} du$ for some $0 < \sigma < \infty$ and all a, b in $\mathbb{R}$ with $a < b$, under some further conditions on h and π.

The above four topics have been studied for a number of dynamical systems, especially, those arising in probability theory. Consider the following: Let μ be a probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ where $\mathcal{B}(\mathbb{R})$ is the Borel σ-algebra on $\mathbb{R}$, the real line. Let $S \equiv \mathbb{R}^\infty$, the countable infinite product of $\mathbb{R}$ with itself and $\mathcal{S} \equiv \mathcal{B}(\mathbb{R}^\infty)$ and $\pi = \mu \times \mu \times \mu \times \cdots$, the infinite product measure on $(S, \mathcal{S})$. Let $T : S \to S$ be the map $T(x_1, x_2, x_3, \cdots) = (x_2, x_3, \cdots)$, called the *unilateral shift to the right*. This dynamical system (S, T) has π as a stationary distribution and so (2.1) holds. Next, by the Birkhoff ergodic theorem the empirical distribution converges to $\pi(\cdot)$ in variation norm as it can be shown that T is measure preserving (i.e., π preserving) and ergodic (see Athreya and Lahiri [3]). So (2.2) holds. By the same reasoning (2.3) holds as well.

Finally, if $h(x_1, x_2, \cdots) = \tilde{h}(x_1)$ where $\tilde{h} : S \to \mathbb{R}$ and $\mathcal{S}$ measurable and $\int_S (\tilde{h}(x_1))^2 d\mu(x_1) < \infty$ then the CLT, i.e., (2.4) holds with

$$\sigma^2 = \int (\tilde{h}(x))^2 d\mu(x) - \Big(\int \tilde{h}(x) d\mu(x)\Big)^2.$$

It is not difficult to verify that this dynamical system is isomorphic in an appropriate sense to the Baker map on $\tilde{S} \equiv [0, 1]$ defined by $\tilde{T}(x) = 2x \bmod 1$ and the invariant measure being Lebesgue measure on $[0, 1]$. To see this let $S_0 = \{0, 1\}$ and μ be the Bernoulli distribution $\{\frac{1}{2}, \frac{1}{2}\}$ on S_0. Let T be the unilateral shift to the right on S_0^∞. Now map $x = (\delta_1, \delta_2, \cdots)$ where $\delta_i \in \{0, 1\}$ to $\tilde{x} = \displaystyle\sum_{i=1}^\infty \frac{\delta_i}{2^i}$. Then the dynamical system $(\tilde{S}, \tilde{T}, \text{Lebesgue measure})$ is isomorphic to $(S_0^\infty, T, \mu^\infty)$. This is also an example of what is called the *Bernoulli shift*. See Ornstein [14].

Another example from probability theory is that of a countable state space, positive recurrent, irreducible Markov chain. Let μ be the unique stationary distribution of an irreducible, positive recurrent Markov chain $\{X_n\}_{n\ge 0}$ with countable state space S_0. Let $S = S_0^\infty$, the countable product of S_0 and $\mathcal{S}$ be the σ-algebra in S generated by the finite dimensional sets of the form $\{X_0 = a_0, X_1 = a_1, \cdots, X_n = a_n\}$, $n < \infty$, $a_i \in S_0$, $0 \le i \le n$. Let π be the probability distribution of the Markov chain $\{X_n\}_{n\ge 0}$ with X_0 distributed as μ. Let T be the unilateral shift to the right on S defined by, for $x = (a_0, a_1, a_2, \cdots)$, $Tx = (a_1, a_2, a_3, \cdots)$. Then (S, T) is a dynamical system and π is invariant for (S, T).

Now fix b_0 in S_0 and let $X_0 = b_0$ w. p. 1.

Now set $\tau_0 = 0$, $\tau_1 = \inf\{n : n \ge 1, X_n = b\}$, and recursively let $\tau_{k+1} = \inf\{n : n \ge \tau_k + 1, X_n = b\}$, $k = 0, 1, 2, \cdots$.

Then, by the recurrence of $\{X_n\}_{n\geq 0}$ and in particular of the state b, and by the strong Markov property of $\{X_n\}_{n\geq 0}$, $\{\tau_k\}_{k\geq 0}$ is a *renewal sequence*, i.e., $\{\tau_{k+1}-\tau_k\}_{k\geq 0}$ are i.i.d. positive random variables. Further, if $\eta_k \equiv \{X_{\tau_k+j}, 0\leq j<\tau_k-\tau_{k-1}, \tau_k-\tau_{k-1}\}$ for $k = 1,2,\cdots$ then $\{\eta_k\}_{k\geq 1}$ are i.i.d. *excursions* (see Athreya and Lahiri [3]). Further, by positive recurrence of $\{X_n\}_{n\geq 0}$, $E\tau_1<\infty$. These excursions of $\{X_n\}_{n\geq 0}$ will ensure that the results in (2.1) and (2.3) hold. Further, if $h : S_0 \to \mathbb{R}$ is such that $E\Big(\sum_{j=0}^{\tau_1-1} h(X_j)\Big)^2 < \infty$ then (2.4) will also hold.

The above assertions carry over to the case when $\{X_n\}_{n\geq 0}$ is a Harris recurrent Markov chain with a general state space S_0 (not necessarily countable) and with a σ-algebra $\mathcal{S}_0$ that is countably generated and admits an invariant probability measure. This result can be proved using the *atom technique* of Athreya and Ney [4] and the splitting method of Nummelin [13]. See Athreya and Lahiri [3] for more details.

8.2 IID Random Iterations

Let S be a nonempty set and G be a collection of maps from S to S. Let μ be a probability distribution on G. Let $\{f_i\}_{i\geq 1}$ be i.i.d. elements of G with distribution μ. Let X_0 be a S-valued random variable independent of $\{f_i\}_{i\geq 1}$. Assume all these random variables are defined on a probability space $(\Omega, \mathcal{B}, P)$. Define a sequence of S valued random variables $\{X_n\}_{n\geq 0}$ on $(\Omega, \mathcal{B}, P)$ as follows:

$$X_0(\omega), X_1(\omega) \equiv f_1(X_0(\omega),\omega), \cdots, X_{n+1} = f_{n+1}(X_n(\omega),\omega), \qquad n = 0,1,2,\cdots$$

Definition 1 *The sequence $\{X_n(\omega)\}_{n\geq 0}$ is called an iterated function system generated by the iteration of the i.i.d. maps $\{f_i\}_{i\geq 1}$ and initial value $X_0(\omega)$.*

8.2.1 Examples

1. Let $S = [0,1]$ and $G \equiv \{h_1(x) = \frac{x}{2}, h_2(x) = \frac{1+x}{2}\}$. Let μ be a probability distribution on G such that $\mu\{h_1\} = \alpha, \mu\{h_2\} = 1-\alpha, 0<\alpha<1$. Thus, given $X_0, X_1, \cdots, X_n$,

$$X_{n+1} = \begin{cases} \frac{X_n}{2} & \text{with probability } \alpha \\ \frac{1+X_n}{2} & \text{with probability } 1-\alpha \end{cases}$$

2. *Sierpiński triangle*: Let $S \equiv$ the equilateral triangle with vertices $V_1 = (0,0)$, $V_2 = (1,0)$, $V_3 = (\frac{1}{2}, \sqrt{\frac{3}{4}})$. Let $G \equiv \{h_1(x) = \frac{x+V_1}{2}, h_2(x) = \frac{x+V_2}{2}, h_3(x) = \frac{x+V_3}{2}\}$ and μ be the probability distribution $\mu(h_i) = p_i$, $i = 1,2,3$, with $p_i > 0$, $p_1+p_2+p_3 = 1$. The iterated

function system generated by the iteration of i.i.d. maps $\{f_i\}_{i\geq 1}$ from (G, μ) with initial value $X_0(\omega)$ satisfies: given $X_0, X_1, \cdots, X_n$,

$$X_{n+1} = \frac{X_n + V_i}{2} \qquad \text{with probability } p_i, \qquad \text{i=1,2,3.}$$

3. *Random iteration of affine maps in Euclidean spaces*: The following is a generalization of the above two examples.

   Let $G \equiv \{h_i : 1 \leq i \leq k\}$ be a finite collection of affine maps from $\mathbb{R}^d$ to $\mathbb{R}^d$ for some $0 < d < \infty$. That is, each h_i is of the form $h_i(x) = A_i x + b_i$, A_i a $d \times d$ matrix and b_i a $d \times 1$ vector in $\mathbb{R}^d$, $i = 1, 2, \cdots, k$. Let $\mu \equiv \{p_1, p_2, \cdots, p_k\}$ be a probability distribution. Consider the IID Random Iteration Scheme, for $n \geq 0$,

$$X_{n+1} = f_{n+1}(X_n)$$

   where $\{f_n\}_{n\geq 1}$ are i.i.d. random maps from G with distribution μ and X_0 is chosen from $\mathbb{R}^d$ independently of $\{f_n\}_{n\geq 1}$. M. Barnsley [10] used this Markov chain to construct approximation to sets in $\mathbb{R}^d$.
4. *Random logistic maps*: Let $S = [0, 1]$ and $\{C_n\}_{n\geq 1}$ be a sequence of i.i.d. random variables such that $C_n \in [0, 4]$ w.p.1. Consider the sequence of i.i.d maps of S into itself defined by

$$f_n(x) = C_n x(1 - x), \qquad 0 \leq x \leq 1.$$

   Let $\{X_n\}_{n\geq 0}$ be a sequence of random variables such that X_0 is independent of $\{f_n\}_{n\geq 1}$ and satisfy

$$X_{n+1} = f_{n+1}(X_n) = C_n X_n(1 - X_n), \qquad n = 0, 1, 2, \cdots.$$

   This family was studied in Bhattacharya and Rao [11], Athreya and Dai [2], Athreya and Schuh [8], and many others.
5. *IID random Lipschitz maps*: Let (S, d) be a metric space that is complete. Let G be a collection of maps from S to S that are Lipschitz, i.e.,

$$\forall h \in G, \quad \exists \;\; 0 < C(h) < \infty, \quad d(h(x), h(y)) \leq C(h) d(x, y)$$

   for all x, y in S. Let

$$\sup_{x\neq y} \frac{d(h(x)), h(y))}{d(x, y)} \equiv \mathcal{S}(h)$$

   be the Lipschitz bound on h. Let μ be a probability measure on $(G, \mathcal{G})$ where $\mathcal{G}$ is a σ-algebra of subsets of G. Let $\{f_i\}_{i\geq 1}$ be i.i.d. G valued random variables such that, for all i, f_i has distribution μ. Let X_0 be a random variable with values in S and independent of $\{f_i\}_{i\geq 1}$. Set

$$X_{n+1} = f_{n+1}(X_n), \qquad n = 0, 1, 2, \cdots.$$

   It is not difficult to verify that all the previous examples are special cases of this last one, i.e., iteration of IID random Lipschitz maps.

8.2.2 A Basic Convergence Theorem

Theorem 1 *Assume the set up in example 5 above of i.i.d. random Lipschitz maps. Let* $E|\log \mathcal{S}(f_1)| < \infty$ *and* $E \log \mathcal{S}(f_1) < 0$*. Assume, further, that for* $\forall x \in S$, $\sum_n \mu(d(f_1(x), x) > a_n) < \infty$ *for* $\{a_n\}$ *such that* $\sum_1^\infty a_n e^{-rn} < \infty$ *for some* $0 < r < -E \log \mathcal{S}(f_1)$*. Then, for any distribution of* X_0*, the sequence* X_n *converges in distribution as* $n \to \infty$ *to a probability distribution* π *on* S *and* π *is independent of* X_0*.*

Proof. Since $X_{n+1} = f_{n+1}(X_n)$ for $n \geq 0$, it follows that

$$X_n = f_n(f_{n-1}(\cdots f_1(X_0)\cdots)), \quad n \geq 1.$$

By independence of X_0 and $\{f_i\}_{i\geq 1}$ and since $\{f_i\}_{i\geq 1}$ are i.i.d., X_n has the same distribution as

$$\hat{X}_n = f_1(f_2(\cdots f_n(X_0)\cdots)), \qquad n \geq 1.$$

By the Lipschitz property of $\{f_i\}_{i\geq 1}$,

$$\begin{aligned} d(\hat{X}_{n+1}, \hat{X}_n) &\leq \mathcal{S}(f_1)\mathcal{S}(f_2)\cdots\mathcal{S}(f_n) d(f_{n+1}(X_0), X_0) \\ &= d(f_{n+1}(X_0), X_0) e^{\sum_{i=1}^n \log \mathcal{S}(f_i)}. \end{aligned}$$

Now the strong law implies that for any $0 < r < -E \log \mathcal{S}(f_i)$, w.p.1.,

$$\frac{1}{n}\sum_{i=1}^n \log \mathcal{S}(f_i) < -r \qquad \text{for all large } n$$

Also, by Borel-Cantelli, w.p.1.,

$$d(f_{n+1}(X_0), X_0) \leq a_n \qquad \text{for all large } n.$$

This implies that w.p.1. (since $\sum_{n=1}^\infty a_n e^{-rn} < \infty$),

$$\sum_{n=1}^\infty d(\hat{X}_{n+1}, \hat{X}_n) < \infty \text{ w.p.1. for any initial } X_0.$$

Thus, for any initial X_0, by the triangle inequality of d, $\{\hat{X}_n\}_{n\geq 0}$ is Cauchy in (S, d) w.p.1.

By the completeness of (S, d), $\hat{X}_n$ converges w.p.1. to say $\hat{X}$.

Also, the same argument as above shows that for any $x_0 \neq y_0$, w.p.1.

$$d(\hat{X}_n(x_0), \hat{X}_n(y_0)) \to 0 \qquad \text{as } n \to \infty.$$

So for any initial X_0, $\hat{X}_n \to \hat{X}$ w.p.1. and $\hat{X}$ is independent of X_0.

This implies that X_n converges in distribution to $\hat{X}$ (for any initial X_0), and the distribution of $\hat{X}$ does not depend on X_0. The distribution of $\hat{X}$, say π, is therefore unique.

Corollary 1. *Let (A_n, b_n), $n \geq 1$, be i.i.d. such that for each $n \geq 1$, A_n is a $k \times k$ random matrix and b_n is a $k \times 1$ vector. Let $E \log \|A_1\| < 0$ where for any $k \times k$ matrix*

$$\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|}$$

where x is a $k \times 1$vector and $\|x\|$ is the Euclidean norm of x. Let $E(\log \|b_1\|)^+ < \infty$. Then the i.i.d. random iteration sequence, the AR1 sequence, $X_{n+1} = A_{n+1}X_n + b_{n+1}$ converges, for any initial X_0, in distribution to the random variable

$$\hat{X} \equiv b_1 + A_1 b_2 + A_1 A_2 b_3 + \cdots + A_1 A_2 \cdots A_n b_{n+1} + \cdots$$

which is well defined (since $E \log \|A_1\| < 0$ and $E(\log \|b_1\|)^+ < \infty$).

The examples 1–3 in Section 8.2.1 are covered by the above corollary. It is applicable to Example 4 as well but in this case $\hat{X}$ turns to be zero w.p.1. However, under the hypotheses $E \log C_1 > 0$ and $E|\log(4 - C_1)| < \infty$ there does exist a nontrivial stationary distribution for the Markov chain in Example 4. See Bhattacharya and Rao [11], Athreya and Dai [2]. In Example3, if $\{A_n\}_{n\geq 1}$ are i.i.d. with A_n taking only finitely many values $\{B_1, B_2, \cdots, B_k\}$ where each B_i is an affine contraction and a mild condition on the distribution of b_1 holds, then the limit $\hat{X}$ is a proper random variable in $\mathbb{R}^d$. Further, its support is typically a compact set K with intricate self similar geometry. The limit point set of the orbit of the Markov chain $\{X_n\}$ coincides with the support set of K w.p.1. Barnsley [10] and others have worked on the inverse problem. Namely, given a compact set K in some $\mathbb{R}^d$, $d < \infty$, find a finite number of contractions and an i.i.d. iteration scheme of the kind in Example 3 so that the limit point set of the orbit of the Markov chain $\{X_n\}$ will be exactly K. Barnsley has used the idea to generate what he calls fractal objects such as ferns, flowers, coast lines, brain images as well as applications to image processing and data compression. In Example 3, the support of the stationary measure turns out be the so-called Sierpiński gasket K generated by deleting the open equilateral triangle obtained by joining the midpoints of the sides and doing the same to each of the remaining three equilateral triangles and so on.

A result similar to Theorem 1 was established by Wu [15]. In this result, the f_i's do not have to satisfy the Lipschitz condition of Theorem 1.

Theorem 2 *Let $\{f_n\}_{n\geq 1}$ be i.i.d. maps on a Polish space S to itself. Let for some $0 < p_0 < \infty$,*

$$\sup_{x \neq y} E\left(\frac{d(f_1(x), f_1(y))}{d(x, y)}\right)^{p_0} < 1.$$

Let $E(\log d(f_1(x_0), x_0))^+ < \infty$ *for some* $x_0 \in S$*. Let* $\{X_n\}_{n\geq 0}$ *be defined by*

$$X_{n+1} = f_{n+1}(X_n), \qquad n \geq 0.$$

Then, for any initial X_0*,* X_n *converges in distribution as* $n \to \infty$ *which does not depend on* X_0*.*

Wu [15] gives the following example in which the f_i's are not Lipschitz and hence Theorem 1 is not applicable but the hypothesis of Theorem 2 holds with $k = 1$.

Let $\{\theta_i\}_{i\geq 1}$ be i.i.d. uniform $[0, 1]$ random variables. Let $0 < \alpha < 1$ and let $f_i(x) = (\alpha x + \theta) \bmod 1$, $x \in [0, 1]$. Then it can be shown that

$$P(f_1 \text{ is not Lipschitz in } [0,1]) \geq \alpha$$

but

$$\sup_{x\neq y}\left|\frac{f_1(x) - f_1(y)}{x - y}\right| < 1 \quad \text{and} \quad E|\log|f_1(\frac{1}{2}) - \frac{1}{2}||^+ < \infty$$

and by Theorem 2 above, X_n converges in distribution. It is shown by Wu [15] that this limit is uniform distribution on $[0, 1]$.

In Example 1, if $\alpha \neq \frac{1}{2}$, then the limit random variable $\hat{X}$ will be supported by a set in $[0, 1]$ of Lebesgue measure zero. If $\alpha = \frac{1}{2}$, $\hat{X}$ will have uniform distribution on $[0, 1]$.

8.3 Markov Chains

If $(S, \mathcal{S})$ is a measurable space and $\{f_i(x, \omega)\}_{i\geq 1}$ are i.i.d. random maps from S to S, $\mathcal{S}$ measurable, on some probability space $(\Omega, \mathcal{B}, P)$, the sequence defined by

$$X_{n+1}(\omega) = f_{n+1}(X_n(\omega), \omega) \qquad n \geq 0,$$

X_0 independent of $\{f_i(\cdot, \omega)\}_{i\geq 1}$, then $\{X_n\}_{n\geq 0}$ is a S-valued Markov chain with probability transition function $P(x, A) = P(\omega : f_1(x, \omega) \in A)$ for x in S and A in $\mathcal{S}$.

Here we assume that for each x, $f_1(x, \omega) : \Omega \to S$ is $(\mathcal{B}, \mathcal{S})$ measurable. A natural question is that is the converse true? That is, given a probability transition $P(x, A)$, $x \in S$, $A \in \mathcal{S}$, i.e., $P(\cdot, \cdot)$ is such that for each x in S, $P(x, \cdot)$ is a probability measure on $(S, \mathcal{S})$ and for each A in $\mathcal{S}$, $P(\cdot, A)$ is a $\mathcal{S}$ measurable map from S to $[0, 1]$, does there exist a map $f(x, \omega)$ on some space $S \times \Omega \to S$ where $(\Omega, \mathcal{B}, P)$ is a probability space such that

$$P(x, A) = Pr(\omega : f(x, \omega) \in A) \qquad \forall x \in S, A \in \mathcal{S}.$$

The answer turns out to be yes if S is a Polish space, i.e., a complete, separable, metric space. This was proved by Y. Kifer [12]. See also Athreya and Stenflo [9].

When S is countable and the transition function P reduces to a transition probability matrix $P \equiv ((p_{ij}))$, the map $f(x, \omega)$, $x \in S$ can be constructed on the Lebesgue space $([0, 1], \mathcal{B}[0, 1]$, Lebesgue measure) as follows. Let the transition probabilities in the ith row be $p_{i1}, p_{i2}, p_{i3}, \cdots$. For ω in $[0, 1]$ and $i \in S$

$$
\begin{aligned}
f(i,\omega) &= 1 \quad \text{if } 0 < \omega \le p_{i1} \\
&= 2 \quad \text{if } p_{i1} < \omega \le p_{i1} + p_{i2} \\
&= 3 \quad \text{if } p_{i1} + p_{i2} < \omega \le p_{i1} + p_{i2} + p_{i3}
\end{aligned}
$$

and so on.

Let $\{f_n(\cdot,\cdot)\}_{n\ge1}$ be i.id. copies of the above f. Then, the sequence $\{X_n\}_{n\ge0}$ defined by the IID random iteration scheme

$$X_{n+1}(\omega) = f_{n+1}(X_n,\omega) \qquad n = 0,1,2,\cdots$$

where $X_0(\omega)$ is independent of $\{f_n\}_{n\ge1}$ is a Markov chain with state space S and transition matrix $P \equiv ((p_{ij}))$.

Recall that a Markov chain $\{X_n\}_{n\ge0}$ with a countable state space S is said to be *irreducible* if

$$P(X_n = j \text{ for some } n \ge 1 | X_0 = i) > 0 \qquad \text{for all } i, j \in S.$$

If the state space S is not countable a similar notion of irreducibility was introduced by Harris (see Athreya and Lahiri [3]). Let $(S,\mathcal{S})$ be a measurable space and $P : S\times\mathcal{S} \to [0,1]$ be a transition function. Then a Markov chain $\{X_n\}_{n\ge0}$ with S as its state space and P as its probability transition function is said to *Harris irreducible with reference measure* φ on $(S,\mathcal{S})$ if $A \in \mathcal{S}$, $\varphi(A) > 0$ implies

$$P(X_n \in A \text{ for some } n \ge 1 | X_0 = x) > 0 \qquad \text{for all } x \text{ in } S.$$

It is easily verified that if S is countable, a Markov chain $\{X_n\}$ with state space S is irreducible in the sense defined earlier then it is Harris irreducible with reference measure φ that is simply the counting measure on S.

Next, we discuss Harris irreducibility of Markov chains generated by IID iteration of random S-unimodal maps on $[0,1]$.

Definition 2 *A map* $f : [0,1] \to [0,1]$ *is called* S*-unimodal if*

i) *f is three time differentiable*
ii) *f is unimodal on* $[0,1]$ *with a mode at c in* $(0,1)$ *such that* $f''(c) < 0$*,* $f(\cdot)$ *is strictly increasing in* $(0,c)$ *and strictly decreasing in* $(c,1)$*.*
iii) $f(0) = f(1) = 0$
iv) *the Schwartzian derivative of f:*

$$(Sf)(x) \equiv \begin{cases} \dfrac{f'''(x)}{f'(x)} - \dfrac{3}{2}\left(\dfrac{f''(x)}{f'(x)}\right)^2 & \text{if } f'(x) \ne 0 \\ -\infty & \text{if } f'(x) = 0 \end{cases}$$

is negative for all $0 < x < 1$.

Examples of S-unimodal maps are $f(x) = x(1-x)$, $f(x) = x^2 \sin \pi x$.

Theorem 3 *Let* $S = [0,1]$*,* $A = [0,L]$*,* $0 < L < \infty$*. Assume:*

i) for each θ *in* A*, let* $f(x) \equiv \theta h(x)$*,* $x \in [0,1]$*, where h is S-unimodal as in the above definition.*

ii) there exists an α *in* $(0, L)$ *and a* p *in* $(0, 1)$ *and a positive integer* $m \geq 1$ *such that* $f_\alpha^{(m)}(p) = p$ *and* $|f_\alpha^{(m)}(p)| < 1$ *where* $f_\alpha^{(m)}(\cdot)$ *is the mth iterate of* $f_\alpha(x) \equiv \alpha h(x)$, $0 \leq x \leq 1$.

iii) Let μ *be a probability distribution on* $(0, L)$ *such that there is a* $\delta > 0$ *and a function* ψ *on* $J \equiv (\alpha - \delta, \alpha + \delta)$ *to* $\mathbb{R}^+$ *such that* $\psi(x) > 0$ *for all x in J and*

$$\mu(B) \geq \int_B \psi(u) du \qquad \textit{for all Borel sets } B \subset J.$$

iv) Let $\{\theta_i\}_{i \geq 1}$ *be i.i.d. random variables with distribution* μ *satisfying iii) above and* $\{X_n\}_{n \geq 0}$ *be a Markov chain with values in S defined by the IID random iteration scheme* $X_{n+1} = \theta_{n+1} h(X_n)$ *for* $n \geq 0$ *with* X_0 *being independent of* $\{\theta_i\}_{i \geq 1}$.

Then $\{X_n\}_{n \geq 0}$ *is Harris irreducible.*

An example of a Markov chain $\{X_n\}_{n \geq 0}$ of the above kind is one generated by $h(x) = x(1 - x)$, i.e., the logistic map and $\{\theta_i\}_{i \geq 1}$ are i.i.d. random variables with distribution on $[0, 4]$ where μ the distribution of θ_1 satisfies iii) above. For a proof of Theorem 3 see Athreya [1].

We conclude this paper with statements of a law of large numbers, a central limit theorem for null recurrent Markov chains and a Brownian motion, and an application to Monte Carlo methods for estimating integrals with respect to improper measures. For proofs see Athreya and Roy [5, 7], Athreya et al [6].

Theorem 4 *Let* $\{X_n\}_{n \geq 0}$ *be an irreducible Markov chain with a countable state space S and null recurrent. Fix* $i_0 \in S$. *Let* $T_1 \equiv \min\{n : n \geq 1, X_n = i_0\}$, $T_{j+1} = \min\{n : n \geq T_j + 1, X_n = i_0\}$, $j \geq 1$. *Let* $\eta_j \equiv \{X_i : T_j \leq i < T_{j+1}, T_{j+1} - T_j\}$, $j \geq 1$. *Let* $\pi_k \equiv E\Big(\sum_{i=T_1}^{T_2 - 1} I_{(X_i = k)}\Big)$, $k \in S$. *Then*

i) $\{\eta_j\}_{j \geq 1}$ *are i.i.d.*

ii) $\sum_{k \in S} \pi_k = \infty$

iii) If $\{a_k\}_{k \in S}$ *is such that* $\sum_{k \in S} |a_k| \pi_k < \infty$ *then for any initial distribution*

$$\lambda_n \equiv \frac{1}{N_n} \sum_{j=0}^{n} a_{X_j} \qquad \to \qquad \lambda \equiv \sum_{k \in S} a_k \pi_k \quad \textit{w.p.1}$$

as $n \to \infty$ *where* $N_n \equiv \sum_{j=0}^{n} I_{(X_j = i_0)}$.

iv) If $E\Big(\sum_{j=T_1}^{T_2 - 1} a_{X_j}\Big)^2 < \infty$, *then*

$$\sqrt{N_n} \frac{(\lambda_n - \lambda)}{\sigma_n} \quad \stackrel{d}{\to} \quad N(0, 1)$$

where $\sigma_n^2 = \frac{1}{n}\sum_{i=1}^{n} V_i^2 - \lambda_n^2$, *where* $V_i = \sum_{j=T_i}^{T_{i+1}-1} a_{X_j}$, $i \geq 1$.

Theorem 5 *Let* $\{X_n\}_{n\geq 0}$ *be a simple symmetric random walk on the integer with* $X_0 = 0$ *w.p.1. Let* $\{a_k\}_{k\in\mathbb{Z}}$ *be such that* $\sum_{k\in\mathbb{Z}} |a_k| < \infty$. *Then*

i) $\lambda_n \equiv \frac{1}{N_n}\sum_{j=0}^{n} a_{X_j} \quad \to \quad \lambda \equiv \sum_{k\in\mathbb{Z}} a_k$ *w.p.1 as* $n \to \infty$, *where* $N_n = \sum_{j=0}^{n} I_{(X_j=0)}$.

ii) If $\sum_{k\in\mathbb{Z}} |a_k|\sqrt{|k|} < \infty$ *then there exist* $\{\sigma_n\}_{n\geq 1}$ *such that* $\sigma_n \to \sigma$, $0 < \sigma < \infty$ *and* σ_n *is a function of* $\{X_j\}_{j=0}^n$ *and*

$$\sqrt{N_n}\frac{(\lambda_n - \lambda)}{\sigma_n} \quad \xrightarrow{d} \quad N(0,1).$$

Theorem 6 *Let* $f : \mathbb{R} \to \mathbb{R}$ *be integrable with respect to Lebesgue measure. Let* $\{B(t) : t \geq 0\}$ *be standard Brownian motion. Let* $T_0 = 0$, $T_{k+1} = \inf\{t : t > T_k, \exists\, 0 < s < tB(s) = 1, B(t) = 0\}$, $k \geq 0$. *Then*

i) $\lambda(t) \equiv \frac{1}{N(t)}\int_0^t f(B(u))du \quad \to \quad \lambda \equiv \int_{\mathbb{R}} f(x)dx$ *w.p.1 as* $t \to \infty$ *where* $N(t) = \sum_{k=0}^{\infty} I_{(T_k \leq t)}$.

ii) If $\int |f(x)|\sqrt{|x|}dx < \infty$ *then there exists a function* $\sigma(t)$ *depending on* $\{B(u) : 0 \leq u \leq t\}$ *such that* $\sigma(t) \to \sigma$, $0 < \sigma < \infty$ *w.p.1 as* $t \to \infty$ *and*

$$\sqrt{N(t)}\frac{(\lambda(t) - \lambda)}{\sigma(t)} \quad \xrightarrow{d} \quad N(0,1).$$

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Chapter 9
Random Dynamical Systems and Selected Works of Rabi Bhattacharya

Edward C. Waymire

Abstract Thetopic of random dynamical systems is extremely broad. However the focus of Rabi Bhattacharya's work in this area is largely from the perspective of discrete parameter Markov processes on a general state space S, equipped with a suitable sigmafield $\mathcal{S}$ of measurable subsets. Such Markov processes are either prescribed as evolutions defined by i.i.d. iterated random maps from S to S, or by such a representation theorem that holds for any discrete parameter Markov processes having stationary transition probabilities on a Borel subset S of a Polish space, with Borel sigmafield $\mathcal{S}$. A theme of much of Rabi's work is that of existence and uniqueness of invariant probabilities under conditions in which the Markov process may not be irreducible. These and corresponding problems concerning rates of convergence and various asymptotic limit theorems are representative of the research addressed here. Applications, particularly to geosciences and economics, are also a main theme of Rabi's body of work in this area; however, these will be covered in separate essays and not treated here. The co-authored texts [6, 11] include a variety of such applications.

Keywords Splitting, Iterated maps, Markov, Invariant probability, Non-irreducible

9.1 Introduction and Preliminaries

"Limit theorems and asymptotic analysis" provide a central theme for summarizing the bulk of Rabi's work in probability theory and its applications. The progression from the study of the asymptotics of sums of i.i.d. sequences of random variables to the asymptotics of discrete parameter Markov processes was a naturalstep in this context.

To set the mathematical framework in somewhat general terms, the state space $(S, \mathcal{S})$ is minimally a measurable space, but how general is general? For the purposes of this article

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we will assume, unless explicitly stated otherwise, that S is a Borel subset of a complete and separable metric space, i.e., a *standard space,* [24], and $\mathcal{S}$ is its Borel sigmafield of subsets. One advantage is that any reference to conditional distributions can be assumed to be in terms of *regular* conditional distributions without any further loss of generality.

A *discrete parameter time-homogeneous Markov process with state space S* is a sequence of random variables $X_0, X_1, X_2, \ldots,$ defined on a probability space $(\Omega, \mathcal{F}, P)$ with values in S, such that for each $n \geq 0$, the conditional distribution of X_{n+1} given $\sigma(X_0, X_1, \ldots, X_n)$ coincides with the conditional distribution of X_{n+1} given $\sigma(X_n)$, and is the same for any n. The (regular) conditional distribution of X_{n+1} given $\sigma(X_n)$ is given by a probability $B \to p(x, B), B \in \mathcal{S}$, on the event $[X_n = x]$, i.e., $P(X_{n+1} \in B|\sigma(X_n)) = p(X_n, B), B \in \mathcal{S}, n = 0, 1, 2, \ldots$. The *one-step transition probability* $p(x, dy)$ may be specified so that for each $B \in \mathcal{S}$, $x \to p(x, B), x \in S$, is a nonnegative, Borel measurable function, and for each $x \in S$, the assignment $B \to p(x, B), B \in \mathcal{S}$ is a probability measure on $(S, \mathcal{S})$. The *equilibrium/stability theory* of such processes begins with the notion of *invariant probabilities* π, defined as fixed points of the transformation T^* acting on the space $\mathcal{P}(S)$ of probabilities on $(S, \mathcal{S})$ via

$$T^*\mu(B) = \int_S p(x, B)\mu(dx), \quad B \in \mathcal{S}. \tag{9.1}$$

Stability generally refers to convergence to π in some metric for a class of initial distributions $\mu \neq \pi$. More specifically, in its present use, *stability in distribution* means that there is weak convergence to π from any initial distribution.

Given a probability μ on $(S, \mathcal{S})$ and transition probability kernel $p(x, dy)$, Tulcea's theorem provides the canonical representation given by the coordinate projection process $X_n, n \geq 0$, on the product space $\Omega = S^\infty, \mathcal{F} = \mathcal{S}^{\otimes\infty}$, and $P \equiv P_\mu$, where $X_n(\omega) = \omega_n, \omega = (\omega_0, \omega_1, \ldots) \in \Omega$, and

$$P_\mu(C \times S^\infty) = \int_C \mu(dx_0)p(x_0, dx_1)p(x_1, dx_2)\cdots p(x_{m-1}, dx_m), \quad C \in \mathcal{S}^{\otimes(m+1))}. \tag{9.2}$$

Some basic questions at the heart of equilibrium (stability) theory for such stochastic processes may be delineated as:

- Q1 Conditions for existence of a probability π on $(S, \mathcal{S})$ such that choosing $P(X_0 \in B) = \pi(B), B \in \mathcal{S}$ makes $X_0, X_1, X_2, \ldots$ a stationary process.
- Q2 Conditions for *uniqueness* of π.
- Q3 Conditions (and metrics) for *stability*: convergence of the distribution of X_n as $n \to \infty$.
- Q4 Metric *rates of convergence* in distribution of X_n as $n \to \infty$.
- Q5 Asymptotic *fluctuation laws* for the process $X_0, X_1, \ldots$ under conditions of stationarity.

Remarkable progress has been made over the past one-hundred years and has included contributions by some of history's greatest probabilists. Growing numbers of textbook and research monograph treatments exist for diverse more specialized Markovian models, far too numerous to list in this generality. That said, from the perspective of general theories any such list of references would include the influential books

[20, 27, 30, 29, 31, 33, 16, 26, 28] to list a few. Of course the equilibrium theory of discrete parameter Markov processes entails more questions than Q1-Q5. Additional special structure leads to considerations of *fine scale structure of equilibrium distributions, coupling, mixing times, perfect simulations,* and *MCMC*, for example, and are largely outside the scope of this article, but not outside the scope of Rabi's broader interests. The more comprehensive treatment [6] provides ample evidence of this.

The generic answers to Q1-Q5 learned from the study of irreducible Markov processes are that: (i) sufficiently rapid frequencies of returns to a set of locations (renewals) can provide existence; (ii) some form of irreducibility is sufficient for uniqueness; (iii) periodicities may need to be averaged out for convergence; (iv) rates of convergence in suitable metrics can range from algebraic to geometric depending on the degree of recurrence, e.g., as reflected in moments of return time distributions, and (v) fluctuation laws result from ergodicity and strong mixing properties.

Rabi has taken a broad yet focussed approach to expand on refinements and answers to these basic questions. In particular, within the general framework described above, he asks how one might approach these basic questions in the absence of irreducibility. The obstructions to some classic approaches to uniqueness and convergence questions are perhaps the most obvious. In the absence of irreducibility, even ergodic Markov chains can have a nontrivial tail sigmafield, and fail to have good mixing properties.

For the existence, uniqueness, and stability problems Rabi's view has been to consider a representation by iterations of i.i.d. random maps. For fluctuation laws his approach is to exploit this and/or the martingale difference sequences $g(X_{n+1}) - \int_S g(y)p(X_n, dy), n = 0, 1, 2, \ldots, g \in L^2(S, \pi)$. Specific progress in both regards will briefly be described in the ensuing sections.

The representation of the Markov process as iterations of i.i.d. random maps is as follows, [12, 13, 27]:

Theorem 1 (Blumenthal, Corson 1970, Kifer 1986). *Assume that S is a Borel subset of a complete and separable metric space with Borel sigmafield $\mathcal{S}$. Let $p(x, dy)$ be a one-step transition probability on S. Then there is a set Γ of maps $\gamma : S \to S$ and a probability Q defined on a sigmafield Σ of subsets of Γ such that*
1. the map $(\gamma, x) \to \gamma(x)$ is $\Sigma \otimes \mathcal{S}$ measurable,
2. $p(x, C) = Q(\{\gamma \in \Gamma : \gamma(x) \in C\}), \quad x \in S, C \in \mathcal{S}$.

In view of Theorem 1 one may view the Markov process with initial distribution $\mu(dx)$ and transition probabilities $p(x, dy)$ as a sequence of random variables $X_0, X_1, X_2, \ldots$ defined on a probability space $(\Omega, \mathcal{F}, P)$ according to the successive iterations

$$X_n = \alpha_n \circ \alpha_{n-1} \circ \cdots \circ \alpha_1(X_0), n = 1, 2, \ldots, \tag{9.3}$$

where X_0 is a random variable on $(\Omega, \mathcal{F}, P)$ with values in S and distribution $\mu(dx)$, and $\alpha_1, \alpha_2, \ldots,$ is an i.i.d. sequence of random maps, independent of X_0, having respective distributions Q, i.e., each α_n is a Γ-valued random variable on $(\Omega, \mathcal{F}, P)$ with distribution Q.

Remark 1. Alternatively, one may directly define Markov processes via i.i.d. iterated random maps without regard to a topology for $(S, \mathcal{S})$. However, the topological assumptions will remain throughout this article as they are required by most of the theory developed to answer the basic questions above. The essential generality is in the direction of relaxations of irreducibility than with concern for anything beyond standard topologies.

Accordingly, for the purposes of this article, any of the following may serve as the framework in which the Markov process is presented: (a) $(\Omega, \mathcal{F}, P, X = \{X_n : n = 0, 1, 2, \ldots\})$; (b) $(Q, \Gamma, \Sigma, X_0, \{\alpha_n : n \geq 1\})$, where X_0 is independent of $\{\alpha_n : n \geq 1\}$; (c) $(S, \mathcal{S}, \mu(dx), p(x, dy))$.

In the next section a basic splitting theorem of Bhattacharya and Majumdar [5] will be presented. This involves the introduction of a metric $d_{\mathcal{A}}$ on the space $\mathcal{P}(S)$ of probabilities on $(S, \mathcal{S})$ defined by a collection $\mathcal{A}$ of measurable subsets of S, referred to as a *splitting class*. In Section 9.2 it will be shown that the classic theorem of [21] for monotone maps on $S = \mathbb{R}$ is a special case, as are higher dimensional extensions to partially ordered spaces and classic theorems of Doeblin [19], Harris [25], Nummelin [30], and Athreya and Ney [2]. The problem of finding sufficient conditions for metric completeness of $\mathcal{P}(S)$ with respect to $d_{\mathcal{A}}$ naturally presents itself and will also be discussed from the perspective of [15]. Some illustration of the martingale approach to fluctuation laws and functional limit theorems will be taken up in Section 9.4. This article will be concluded with a brief overview of some related alternative methods that have proven to be successful for this general class of problems, especially where splitting fails, in Section 9.5. The latter will be illustrated with a previously unpublished application arising in mathematical biology/ecology. Overall this is a survey article. Further elaborations, including proofs of the statements and results, are either in the cited papers by Rabi and his co-authors, or can be found in the reference books [6, 11].

9.2 A Splitting Theorem

In an important paper [5], coauthored with Mukul Majumdar, a classic result of Lester Dubins and David Freedman, [21] is generalized with the following substantial extension.

Theorem 2 (Bhattacharya and Majumdar 1999). *Let $\mathcal{P}(S)$ denote the set of probabilities on $(S, \mathcal{S})$. For a subcollection $\mathcal{A} \subset \mathcal{S}$ of measurable subsets of S, define $d_{\mathcal{A}} : \mathcal{P}(S) \times \mathcal{P}(S) \to [0, 1]$ by*

$$d_{\mathcal{A}}(\mu, \nu) = \sup_{A \in \mathcal{A}} |\mu(A) - \nu(A)|, \quad \mu, \nu \in \mathcal{P}(S).$$

Assume

1. *$d_{\mathcal{A}}$ defines a complete metric on $\mathcal{P}(S)$.*
2. *There is a positive integer N such that for any $(\gamma_1, \ldots, \gamma_N) \in \Gamma^N$,*

$$d_{\mathcal{A}}(\mu \circ \tilde{\gamma}^{-1}, \mu \circ \tilde{\gamma}^{-1}) \leq d_{\mathcal{A}}(\mu, \nu), \quad \forall \mu, \nu \in \mathcal{P}(S),$$

where $\tilde{\gamma} = \gamma_N \circ \gamma_{N-1} \circ \cdots \circ \gamma_1$,

3. *There is a $\overline{\chi} > 0$ such that for the same value of N and every $A \in \mathcal{A}$, one has*

$$P((\alpha_N \circ \cdots \circ \alpha_1)^{-1}(A) = S \text{ or } \emptyset) \geq \overline{\chi}.$$

Then there is a unique invariant probability π for the Markov process $X_n = \alpha_n \circ \cdots \circ \alpha_1(X_0), n \geq 1$, where X_0 is independent of $\alpha_1, \alpha_2, \ldots$ and has arbitrary distribution $\mu \in \mathcal{P}(S)$. Moreover,

$$d_{\mathcal{A}}(T^n\mu, \pi) \leq (1 - \overline{\chi})^{[\frac{n}{N}]},$$

where $T^n\mu$ is the distribution of X_n, and $[\frac{n}{N}]$ denotes the integer part of $\frac{n}{N}$.

The essential and clever point of Theorem 2 is to render the map $\mu(dy) \to T^*\mu(dy) = \int_S \mu(dx)p(x, dy)$ a contraction on the complete metric space $(\mathcal{P}(S), d_{\mathcal{A}})$, from which fixed point theory can take over.

A couple specific topologies defined by a metric of the form $d_{\mathcal{A}}$ are as follows:

1. [Kolmogorov metric $d_{\mathcal{K}}$:] $S \subset \mathbb{R}$, $\mathcal{A} = \{(-\infty, x] \cap S : x \in \mathbb{R}\}$.
2. [Total variation metric:] $\mathcal{A} = \mathcal{S}$.

Related results and applications relative to the basic questions will be surveyed in sections to follow.

9.3 Related Results and Applications

In the case that $S = [0, 1]$ and Γ is the set of continuous, monotone maps of S into itself, Dubins and Freedman [21] introduced the following notion of *splitting* on $\mathcal{P}(S)$: A probability on a sigmafield Σ of subsets of Γ *splits* if there is an $x_0 \in S$ such that $\{\gamma \in \Gamma : 0 \leq \gamma(x) \leq x_0, \forall x \in S\}$ and $\{\gamma \in \Gamma : x_0 \leq \gamma(x) \leq 1, \forall x \in S\}$ are each measurable and have positive probability. Taking $\mathcal{A}$ to be the subintervals of the form $[0, x] \subseteq [0, 1]$, one sees that this definition of splitting is a special case of that given in the hypothesis of Theorem 2. For this class of sets the metric $d_{\mathcal{A}} \equiv d_{\mathcal{K}}$ is the Kolmogorov metric and implies weak convergence. It is well known that $\mathcal{P}(S)$ is complete for the Prohorov metric of weak convergence (on separable metric spaces). Moreover $\mathcal{P}(S)$ is complete for the Kolmogorov metric whenever S is a nondegenerate subinterval of $\mathbb{R}$ (or even $\mathbb{R}^k$). Thus, if splitting occurs for this class $\mathcal{A}$ of subsets then Theorem 2 applies, and one gets exponential convergence to a unique invariant probability in the (stronger than Prohorov) Kolmogorov metric.

A yet stronger metric d_1, under which completeness could be established for nondegenerate subintervals S of $\mathbb{R}$, was introduced in [8] as

$$d_1(\mu, \nu) = \sup\{|\int_S f d\mu - \int_S f d\nu| : f \in \mathcal{G}_1\}, \mu, \nu \in \mathcal{P}(S), \tag{9.4}$$

where $\mathcal{G}_1$ is the set of nonnegative, nondecreasing Borel measurable functions on S bounded above by one. In addition it was subsequently shown in [15] that completeness of $(\mathcal{P}(S), d_1)$ also holds in the case $S = \mathbb{R}^k, k \geq 1$, with the monotonicity of $\mathbf{f} = (f_1, \ldots, f_k) : \mathbb{R}^k \to [0, 1]^k \subset \mathbb{R}^k$ defined coordinatewise for each f_i $(1 \leq i \leq k)$ with respect to the usual partial order $\preceq$ on $\mathbb{R}^k$; namely, $(x_1, \ldots, x_k) \preceq (y_1, \ldots, y_k)$ if and only if $x_j \leq y_j, 1 \leq j \leq k$. These latter authors refer to d_1 as the *Bhattacharya metric*, and provide a characterization of Borel subsets $S \subseteq \mathbb{R}^1$ for which d_1 defines a complete metric on $\mathcal{P}(S)$. However, such a characterization is delicate and generally open in higher dimensions than one. Nonetheless completeness of $\mathcal{P}(\mathbb{R}^k)$, together with insightful examples of $S \subseteq \mathbb{R}^2$ such that $\mathcal{P}(S)$ is complete, can be found in [15].

Dubins and Freedman [21] had shown that for strictly increasing, continuous maps on an interval in **R** or an arbitrary closed set, their splitting condition is also necessary for the existence of a unique invariant probability. Rabi and his student, Osook Lee, extended this necessity to nondecreasing maps on compact subsets of $\mathbb{R}^k$. Moreover, continuity of the maps is not required for this conclusion, see [8].

The role of splitting in the context of monotone nondecreasing maps is best understood in terms of Furstenberg's [22] *backward iteration*; a powerful idea introduced for i.i.d. products of random matrices, but of independent interest throughout the study of random dynamical systems and including the Propp-Wilson algorithm for perfect simulations [32]. The essential feature of nondecreasing maps on an interval $[a, b]$, say, is that the backward iterations $\alpha_1 \circ \cdots \circ \alpha_n(a), n \geq 1$, and $\alpha_1 \circ \cdots \circ \alpha_n(b), n \geq 1$, are respectively nondecreasing and nonincreasing sequences, therefore having limits and squeezing all other such iterates starting from $x \in [a, b]$. On the other hand, this is not the case for nonincreasing maps, and Rabi and Mukul Majumdar, [5], showed that splitting was not necessary for the existence of unique invariant probability when the maps are assumed nonincreasing. Moreover this has nothing to do with the continuity of the maps, nor connectivity of S.

I can vividly recall Rabi's enthusiasm for splitting that he shared with me on an extended visit to Indiana University over the summer of 2001. The enthusiasm was contagious and we tried to find a still more widely applicable version of splitting. A modest goal was to at least have a broader understanding of the equilibrium theory from a perspective of splitting. In [10] we built on minorization ideas of Doeblin [19], recurrence theory of Harris [25], splitting ideas of Nummelin [30], regenerative ideas of Athreya and Ney [2], and drift conditions of Foster and Tweedie [28]. This resulted in notions of *localized splitting* and *strict splitting* that proved to be useful for analyzing certain quadratic maps. The localization is analogous to the localization of Doeblin's minorization condition in terms of small sets and small measures, e.g., see [30, 31]. The strictness simply refers to the use of half-open intervals (strict inequalities) in defining the splitting class $\mathcal{A}$.

Random iterations of the quadratic maps $\gamma_\theta(x) := \theta x(1-x)$, for $0 \leq \theta \leq 4$, on the unit interval $S = [0, 1]$ according to i.i.d. selections of the parameter $\theta \in [0, 4]$, provides a rich and intriguing class of examples with which to test many aspects of the general theory. Rabi's initial work in collaboration with B.V. Rao in [9] involved applications when the distribution of the parameter θ is supported on two points θ_1, θ_2, say. There it was discovered that there are values of the parameters in the range $1 < \theta_1 < \theta_2 < 2$, each well below the critical value for the transition to chaos for the respective deterministic dynamical system, for which the invariant probability could be a continuous singular distribution supported on a Cantor set; specifically for parameter values in this range and satisfying

$$\frac{1}{\theta_2^2} - \frac{1}{\theta_2^3} < \frac{1}{\theta_1^2} - \frac{1}{\theta_1^3}, \quad 1 < \theta_1 < \theta_2 \leq 2. \tag{9.5}$$

Rabi once remarked to me that overall he and I seemed to be attracted to very different mathematical structures, his generally being toward smooth, and mine toward singular; but there is something here for everyone. The entire Lebesgue spectrum from atomic to continuous singular to absolutely continuous may show up for the invariant measures for this class of random dynamical systems, and the task of sorting this out for iterated quadratic maps continues to be a substantial open problem; see [4] for another interesting example in this vein.

For quadratic maps, even the existence of a unique invariant probability on $(0,1)$ is not fully understood. In an important paper [1], Athreya and Dai produce an example satisfying $1 < \theta_1 < \theta_2 < 4$ for which there is not a unique invariant probability on $(0,1)$. The characterization of pairs (θ_1, θ_2) for which this phenomena occurs remains a challenging open problem.

9.4 Fluctuation Laws and Limit Theorems

The central limit theorem of Gordin and Lifšic [23] for a discrete parameter Markov process provides a fluctuation law for averages $\frac{1}{n}\sum_{j=1}^{n} g(X_j)$ for a large class of functions $g : S \to \mathbb{R}$ of an ergodic Markov process X having a unique invariant probability. It is based on the Billingsley-Ibragimov central limit theorem for martingales and is especially important from the perspectives of both applicability to non-irreducible Markov processes, and the formula for variance. Rabi's paper [7] provides the central limit theorem for continuous parameter Markov processes together with a beautiful formula for the variance parameter in a general functional central limit theorem for (continuous parameter) Markov processes. A functional law of the iterated logarithm is also obtained in [7]. This theory has also found numerous applications outside of random dynamical systems by Rabi and others. Further applications to random dynamical systems with special structure, e.g., monotone maps, were developed in [8]. A simple illustrative theorem in this context may be stated as follows; in fact, a functional clt is proven with weak convergence to Brownian motion.

Theorem 3 (Bhattacharya-Lee 1988). *Assume that Γ consists of monotone nondecreasing maps on a closed set $S \subseteq \mathbb{R}^k, k \geq 1$. Assume the splitting conditions hold for the splitting class $\mathcal{A}$ given by the collection of subsets of S of the form $\{\mathbf{y} \in S : \gamma(\mathbf{y}) \preceq \mathbf{x}\}$, for $\gamma \in \Gamma$ and the usual partial order $\preceq$ on $\mathbb{R}^k$. Let π be the corresponding unique invariant probability. Then, regardless of the initial distribution X_0, assumed independent of $\{\alpha_n : n \geq 1\}$, one has for every function $h : S \to \mathbb{R}$ expressible as the difference $f_1 - f_2$ of two nondecreasing measurable functions $f_1, f_2 \in L^2(\pi)$,*

$$\frac{1}{\sqrt{n}}\sum_{m=0}^{n-1}\left(h(X_m) - \int_S h d\pi\right) \Rightarrow N(0, \sigma^2),$$

where

$$\sigma^2 = \int_S g^2(x)\pi(dx) - \int_S (Tg(x))^2\pi(dx),$$

for $Tg(x) = \mathbb{E}_x g(X_1) = \int_S g(y)p(x, dy)$, *and* g *defined by*

$$(I - T)g = \overline{h} \equiv h - \int_S h d\pi.$$

9.5 Other Approaches, Problems, and Directions

As noted earlier, in certain instances splitting is precisely the right tool, but this is not always the case. Within the framework of random dynamical systems as iterated i.i.d. random maps, special advantage can be obtained from maps that tend to contract on a complete and separable metric space. For example, Dubins and Freedman [21] obtain the existence of a unique invariant probability π for i.i.d. iterations of contractive maps on a compact metric space S whose distribution Q is defined on the Borel sigmafield of the set Γ of contractions on S with the uniform metric, under the assumption that the support of Q contains a strict contraction. Moreover they prove convergence in distribution to π in this setting. A slightly more general variant for complete and separable metric spaces, and for which this follows as a corollary is given in [6, p. 282, Proposition 7.1]; however, the authors explicitly acknowledge that this is an amplification of the proof given in [21]; see [6, p. 284, Remark 7.4]. Indeed it adds clarity with which one can understand the basic nature of such results.

Diaconis and Freedman [18] also relaxed the topological assumptions on S to that of a complete and separable metric space, and introduced the beautiful idea of "contraction on average" to obtain the existence of a unique invariant probability π. The following variant appears in [6, p. 277, Thereom 7.2] with the added virtue of a relaxed condition on the Lipschitz order of the contraction, but without the exponential rate of convergence in the total variation metric given in [18].

Theorem 4 (Diaconis-Freedman 1999; Bhattacharya-Majumdar 2007). *Let* S *be a complete and separable metric space with metric* d. *Define an* $r-$*th order random Lipschitz coefficient by*

$$L^r = \sup_{x,y\in S, x\neq y} \frac{d(\alpha_r \circ \cdots \circ \alpha_1(x), \alpha_r \circ \cdots \circ \alpha_1(y))}{d(x, y)},$$

and assume $-\infty \leq \mathbb{E} \log L^r < 0$ *for some* $r \geq 1$. *Suppose there is an* $x_0 \in S$ *such that*

$$\mathbb{E} \log^+ d(\alpha_r \circ \cdots \circ \alpha_1(x_0), x_0) < \infty.$$

Then the Markov process $X_n(x) = \alpha_n \circ \cdots \alpha_1(x), n \geq 1, X_0(x) = x$, *has a unique invariant probability* π. *Moreover, one has convergence in distribution of* $X_n(x)$ *to* π.

Finally, we note an important result of Brandt [14] regarding the stability of iterations of i.i.d. affine linear maps; see also [6, 11] for a variety of related results in the context of linear autoregressive time series.

Theorem 5 (Brandt 1986). *Suppose that* $(C_n, D_n), n \geq 1$*, is a stationary, ergodic sequence in* $\mathbb{R}^2$ *such that for some* $r \geq 1$

$$\mathbb{E}\log^+|C_1| < \infty, \quad -\infty \leq \mathbb{E}\log|C_1 \cdots C_r| < 0, \quad \mathbb{E}\log^+|D_n| < \infty.$$

Then the Markov process $X_{n+1} = C_{n+1}X_n + D_{n+1}, n \geq 0$*, has a unique invariant probability* π*. Moreover* X_n *converges in distribution to* π*.*

Remark 2. Generalizations to higher dimensions $S = \mathbb{R}^k$ obtained by [14] were also obtained by Berger[3]. A new proof is given in [6, p. 304, Theorem 3.1].

We conclude this section with an illustration of the use of these last two theorems in a play on the topologies of S to resolve the lack of irreducibility in a problem of interest for mathematical biology; see [17].

Proposition 1 (DeLeenheer, Peckham, Waymire 2015). *Consider the Markov process on* $S = [0, \infty)$ *defined by*

$$X_{n+1} = B_{n+1}\frac{X_n}{A_{n+1} + X_n}, n \geq 0,$$

where $(A_1, B_1), (A_2, B_2) \ldots$ *is an i.i.d. sequence of random vectors having a.s. positive components such that* $\mathbb{E}\log^+ A_n < \infty$*, and* $\mathbb{E}\log^+ B_n < \infty$*.*

- *i If* $\mathbb{E}\log\frac{B_1}{A_1} < 0$ *then* $\pi = \delta_0$ *is the unique invariant probability and* X_n *converges to* δ_0 *in distribution as* $n \to \infty$*.*
- *ii If* $\mathbb{E}\log\frac{B_1}{A_1} > 0$ *then there are two mutually singular invariant distributions,* δ_0 *and* $\rho(dx)$*. Moreover, in this case, if* $P(X_0 > 0) = 1$*, then* X_n *converges in distribution to* $\rho(dx)$ *as* $n \to \infty$*.*

Proof. $S = [0, \infty)$ is a complete and separable metric space. Since 0 is a sure fixed point, if there is to be a unique invariant probability then it must be δ_0. Using the mean value theorem from calculus, one may easily check that the contraction on average property (Theorem 4) applies under the asserted condition, making δ_0 unique, and the process stable in distribution. To explore the possible existence of an invariant probability on the non-complete metric space $(0, \infty)$, we consider the homeomorphic image defined by $Y_n = 1/X_n, n \geq 1$, on $[1, \infty)$. The dynamics of this Markov process is precisely that of i.i.d. iterations of affine linear maps of the form

$$Y_{n+1} = C_{n+1}Y_n + D_{n+1}, \quad n = 0, 1, 2, \ldots,$$

where $C_n = \frac{A_n}{B_n}, D_n = \frac{1}{B_n}, n \geq 1$. Thus, it follows from Brandt's theorem that under the stated conditions there is a unique invariant probability for the reciprocal process. The result follows by continuity of $x \to 1/x$ on $(0, \infty)$, and its inverse.

Perhaps the apparent reciprocity between the bounds on the "random Lipschitz coefficient," of Diaconnis and Freedman, and the "random Liapounov growth rate" of the homeomorphic inverse map, implicit in Brandt's theorem, is not an accident but occurs for a more general class of non-irreducible Markov processes. For another relatively recent exploration of ideas of random dynamical systems in the context of random contractions the reader is referred to [1, 34] and references therein.

9.6 Concluding Remarks

The general equilibrium theory for discrete parameter random dynamical systems will clearly remain a rich and vibrant framework for mathematical research for years to come. Both the depth of the foundational theory and the scope of applications continue to rapidly evolve. The contributions by Rabi and by many others too numerous to mention in this brief survey provide a solid foundation on which to continue to build new approaches to equilibrium and stability theories that can accommodate non-irreducible Markov processes. Such developments seem far from complete but, as illustrated by his efforts in this area, Rabi has provided a solid vision for what can be possible in this most intriguing area of probability theory.

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Chapter 10
Reprints: Part III

R.N. Bhattacharya and Coauthors

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10.1 “Asymptotics of a class of Markov processes which are not in general irreducible”

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ASYMPTOTICS OF A CLASS OF MARKOV PROCESSES WHICH ARE NOT IN GENERAL IRREDUCIBLE

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Let α_n be a sequence of i.i.d. nondecreasing random maps on a subset S of $\mathbb{R}^k$ into itself and let X_0 be a random variable with values in S independent of the sequence α_n. Then $X_n \equiv \alpha_n \cdots \alpha_1 X_0$ is a Markov process. Conditions for the existence of unique invariant probabilities are obtained for such Markov processes which are not in general irreducible, extending earlier results of Dubins and Freedman to multidimensional and noncompact state spaces. In addition, a functional central limit theorem is obtained. These yield new results in time series and economic models.

1. Introduction. One way to study discrete parameter Markov processes is the following [Kifer (1986)]. Let $(S, \mathscr{S})$ be a measurable space, Γ a set of measurable maps on S into itself. Endow Γ with a σ-field $\mathscr{C}$ such that the map $(\gamma, x) \to \gamma(x)$ on $\Gamma \times S$ into S is $\mathscr{C} \otimes \mathscr{S}|\mathscr{S}$-measurable. Let P be a probability measure on $(\Gamma, \mathscr{C})$. On some probability space $(\Omega, \mathscr{F}, Q)$ define a sequence of i.i.d. random maps $\alpha_1, \alpha_2, \ldots$ with common distribution P. For a given random variable X_0, independent of the sequence α_n, define $X_1 = \alpha_1 X_0, \ldots, X_n = \alpha_n X_{n-1} = \alpha_n \cdots \alpha_1 X_0 \cdots$. Then X_n is a Markov process with transition probability $p(x, dy)$ given by

$$p(x, B) = P(\{\gamma \in \Gamma\colon \gamma(x) \in B\}), \qquad x \in S,\ B \in \mathscr{S}. \tag{1.1}$$

We shall often write $X_n(x)$ for X_n in case $X_0 = x$. Denote by P^n the joint distribution of $\alpha_1, \ldots, \alpha_n$, i.e., $P^n = P \times P \times \cdots \times P$ on $(\Gamma^n, \mathscr{C}^{\otimes n})$.

Let $\mathbb{B}(S)$ denote the linear space of all real-valued bounded measurable functions on S. The transition operator T on $\mathbb{B}(S)$ is defined by

$$(Tf)(x) = \int f(y) p(x, dy), \qquad f \in \mathbb{B}(S). \tag{1.2}$$

Its adjoint is T^* defined on the space $\mathscr{M}(S)$ of all finite signed measures on $(S, \mathscr{S})$ by

$$(T^*\mu)(B) = \int p(x, B)\mu(dx), \qquad \mu \in \mathscr{M}(S). \tag{1.3}$$

Let $\mathscr{P}(S) \subset \mathscr{M}(S)$ denote the set of all probability measures on $(S, \mathscr{S})$. Recall that a probability measure π on $(S, \mathscr{S})$ is said to be invariant for p if it is a fixed point of T^*: $T^*\pi = \pi$.

We shall write $p^{(n)}(x, dy)$ for the n-step transition probability, with $p^{(1)} = p$. Then $p^{(n)}(x, dy)$ is the distribution of $\alpha_n \cdots \alpha_1 x$.

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The transition probability p may not be φ-irreducible for any nonzero σ-finite measure φ. Recall that p is φ-irreducible if $\varphi(B) > 0$ implies that for each x there exists n such that $p^{(n)}(x, B) > 0$. There is an extensive literature on the asymptotic properties of Markov processes with φ-irreducible transition probabilities. See, e.g., Jain and Jamison (1967), Orey (1971), Tweedie (1974), (1975) and Revuz (1984). There is, however, no general theory for the nonirreducible case. In the present context, the latter arises, for example, when P is discrete. For some examples of nonirreducible models in biology and economics, see Reed (1974), Bhattacharya and Majumdar (1984), (1988) and Rosenblatt (1980). Our main interest in this article is to look at one such class of Markov processes, to find general conditions under which there exist unique invariant probabilities π, to study the stability of such measures and to identify broad classes of functions f in $L^2(S, \pi)$ for which the functional central limit theorem (FCLT) holds, i.e., the sequence of stochastic processes

$$Y_n(t) \equiv n^{-1/2}\left[\sum_{j=0}^{[nt]}\left(f(X_j) - \int f\,d\pi\right) + \left(t - \frac{[nt]}{n}\right)\left(f(X_{[nt]+1}) - \int f\,d\pi\right)\right] \tag{1.4}$$

converges in distribution to a Brownian motion under every initial distribution.

In the class of problems considered in this article, S is a topologically complete subspace of $\mathbb{R}^k$, i.e., the relativized topology on S may be metrized so as to make S complete. The Borel σ-field of S is $\mathscr{B}(S)$. For Γ one takes a set of measurable monotone nondecreasing functions $\gamma = (\gamma^{(1)}, \dots, \gamma^{(k)})$ on S into itself. In other words, $\gamma^{(i)}(x^{(1)}, \dots, x^{(k)})$ is monotone nondecreasing in each coordinate $x^{(1)}, \dots, x^{(k)}$. Make the assumption on P:

There exists x_0 and a positive integer m such that

$$Q(X_m(x) \le x_0\ \forall\, x) > 0, \qquad Q(X_m(x) \ge x_0\ \forall\, x) > 0. \tag{1.5}$$

It is then shown that there exists a unique invariant probability to which $p^{(n)}(x, dy)$ converges exponentially fast in a metric stronger than the Kolmogorov distance; this convergence is uniform for all $x \in S$ (Theorem 2.1). This generalizes an earlier result of Dubins and Freedman (1966) and Yahav (1975) who considered the case $k = 1$, S a compact interval. A necessary condition for compact S and arbitrary k is given by Lemma 2.6. Theorem 3.1 provides an FCLT of the type mentioned earlier. Section 4 contains two applications, one to mathematical economics and the other to nonlinear autoregressive models; both are new results.

2. Existence of a unique invariant probability. Let $S \subset \mathbb{R}^k$ be topologically complete in its relativized Euclidean topology and let Γ be a set of measurable monotone nondecreasing maps $\gamma = (\gamma^{(1)}, \dots, \gamma^{(k)})$ on S into S. We shall often write γx for $\gamma(x)$.

Let $\mathscr{C}$ be a σ-field on Γ such that the map $(\gamma, x) \to \gamma x$ is measurable on $(\Gamma \times S, \mathscr{C} \otimes \mathscr{B}(S))$ into $(S, \mathscr{B}(S))$.

Let $\mathscr{A}$ be the class of all sets $A \subset S$ of the form

$$A = \{y \in S: \gamma(y) \le x\}, \tag{2.1}$$

where γ varies over the class of all continuous monotone nondecreasing functions on S into itself and x varies over $\mathbb{R}^k$.

On the space $\mathscr{P}(S)$ of all probability measures on $(S, \mathscr{B}(S))$, define the distance d by

$$d(\mu, \nu) = \sup\{|\mu(A) - \nu(A)|: A \in \mathscr{A}\}, \qquad \mu, \nu \in \mathscr{P}(S). \tag{2.2}$$

This defines a topology on $\mathscr{P}(S)$ that is stronger than the weak-star topology.

Our first main result is

THEOREM 2.1. *Suppose there exists a positive integer m and some $x_0 \in S$ such that* (1.5) *holds. Then there exists a unique invariant probability π and*

$$\sup\{d(p^{(n)}(x, dy), \pi(dy)): x \in S\} \to 0 \tag{2.3}$$

exponentially fast as $n \to \infty$.

First let us show

LEMMA 2.2. *The space $\mathscr{P}(S)$ is complete under the distance d defined by* (2.2).

PROOF. It is known that $\mathscr{P}(S)$ is topologically complete under the weak-star topology [see Parthasarathy (1967), page 46], which is weaker than its topology under d. Hence if μ_n is a sequence in $\mathscr{P}(S)$ such that $d(\mu_n, \mu_m) \to 0$ as $n, m \to \infty$, then there exists $\mu \in \mathscr{P}(S)$ such that μ_n converges weak-star to μ. Fix a continuous monotone nondecreasing γ on S into S and write F_n and F for the cumulative distribution functions of $\mu_n \circ \gamma^{-1}$ and $\mu \circ \gamma^{-1}$, respectively. Then $F_n(x)$ converges to $F(x)$ at all points x of continuity of F. On the other hand, $\sup\{|F_n(x) - F_m(x)|: x \in \mathbb{R}^k\} \le d(\mu_n, \mu_m)$. Hence F_n converges uniformly to a function that is necessarily right continuous. This implies that this limit function is F and that $F_n(x)$ converges to $F(x)$ uniformly for all x. This being true for every continuous nondecreasing γ, $\mu_n(A)$ converges to $\mu(A)$ for every $A \in \mathscr{A}$. But μ_n converges uniformly on $\mathscr{A}$. Hence $d(\mu_n, \mu) \to 0$. □

We now introduce a distance d_1 stronger than d. For $a \ge 0$, let $\mathscr{G}_a$ denote the class of all real-valued Borel measurable nondecreasing functions f on S satisfying $0 \le f(x) \le a$ for all $x \in S$. Define

$$d_a(\mu, \nu) = \sup\left\{\left|\int f\,d\mu - \int f\,d\nu\right|: f \in \mathscr{G}_a\right\}, \qquad \mu, \nu \in \mathscr{P}(S). \tag{2.4}$$

Clearly, $d_a(\mu, \nu) = a d_1(\mu, \nu)$ for all $a \ge 0$.

Let the linear map $T^{*n} = (T^n)^*$ be defined on $\mathscr{M}(S)$ by

$$(T^{*n}\mu)(B) = \int p^{(n)}(x, B)\mu(dx), \qquad n \ge 1, \mu \in \mathscr{M}(S), B \in \mathscr{B}(S). \tag{2.5}$$

In order to state the next lemma, fix $x_0 \in S$ and a positive integer m. Write

$$\Gamma_1 = \{(\gamma_1,\ldots,\gamma_m) \in \Gamma^m: \gamma_m \cdots \gamma_1 x \le x_0 \ \forall\, x\},$$
$$\Gamma_2 = \{(\gamma_1,\ldots,\gamma_m) \in \Gamma^m; \gamma_m \cdots \gamma_1 x \ge x_0 \ \forall\, x\}. \tag{2.6}$$

LEMMA 2.3. *If* Γ_1, Γ_2 *are defined by* (2.6), *then*

$$d_1(T^{*n}\mu, T^{*n}\nu) \le \delta^{[n/m]} d_1(\mu,\nu), \tag{2.7}$$

where

$$\delta = \max\{1 - P^m(\Gamma_1), 1 - P^m(\Gamma_2)\}. \tag{2.8}$$

If (1.5) *holds, then* $\delta < 1$.

PROOF. Let $f \in \mathscr{G}_1$. Then

$$\begin{aligned}
0 &\le h_1(x) \equiv \int_{\Gamma_1 \setminus (\Gamma_1 \cap \Gamma_2)} f(\gamma_m \cdots \gamma_1 x) P^m(d\gamma_1 \cdots d\gamma_m) \\
&\le f(x_0)(P^m(\Gamma_1) - P^m(\Gamma_1 \cap \Gamma_2)), \\
0 &\le h_2(x) \equiv \int_{\Gamma_2 \setminus (\Gamma_1 \cap \Gamma_2)} (1 - f(\gamma_m \cdots \gamma_1 x)) P^m(d\gamma_1 \cdots d\gamma_m) \\
&\le (1 - f(x_0))(P^m(\Gamma_2) - P^m(\Gamma_1 \cap \Gamma_2)), \\
0 &\le h_3(x) \equiv \int_{\Gamma \setminus (\Gamma_1 \cup \Gamma_2)} f(\gamma_m \cdots \gamma_1 x) P^m(d\gamma_1 \cdots d\gamma_m) \\
&\le 1 - P^m(\Gamma_1 \cup \Gamma_2), \\
&\int_{\Gamma_1 \cap \Gamma_2} f(\gamma_m \cdots \gamma_1 x) P^m(d\gamma_1 \cdots d\gamma_m) = f(x_0) P^m(\Gamma_1 \cap \Gamma_2).
\end{aligned} \tag{2.9}$$

Now,

$$\begin{aligned}
&\int f\, dT^{*m}\mu - \int f\, dT^{*m}\nu \\
&\quad = \int h_1(x)\mu(dx) - \int h_1(x)\nu(dx) + \int h_2(x)\nu(dx) \\
&\qquad - \int h_2(x)\mu(dx) + \int h_3(x)\mu(dx) - \int h_3(x)\nu(dx).
\end{aligned} \tag{2.10}$$

Let a_1, a_2, a_3 denote the constants appearing on the right sides in (2.9) bounding h_1, h_2, h_3. Then, $h_1, a_2 - h_2, h_3$ belong to $\mathscr{G}_{a_i}$, $i = 1,2,3$. Therefore,

$$\begin{aligned}
d_1(T^{*m}\mu, T^{*m}\nu) &\le \sup_{f \in \mathscr{G}_1} \big[\{ f(x_0)(P^m(\Gamma_1) - P^m(\Gamma_1 \cap \Gamma_2)) \\
&\qquad + (1 - f(x_0))(P^m(\Gamma_2) - P^m(\Gamma_1 \cap \Gamma_2)) \\
&\qquad + (1 - P^m(\Gamma_1 \cup \Gamma_2))\} d_1(\mu,\nu)\big] \\
&\le \big[\max\{P^m(\Gamma_1) - P^m(\Gamma_1 \cap \Gamma_2), P^m(\Gamma_2) - P^m(\Gamma_1 \cap \Gamma_2)\} \\
&\qquad + 1 - P^m(\Gamma_1) - P^m(\Gamma_2) + P^m(\Gamma_1 \cap \Gamma_2)\big] d_1(\mu,\nu) \\
&= \max\{1 - P^m(\Gamma_2), 1 - P^m(\Gamma_1)\} d_1(\mu,\nu).
\end{aligned} \tag{2.11}$$

For the last equality, if $P^m(\Gamma_1) \geq P^m(\Gamma_2)$, then

$$\max\{P^m(\Gamma_1) - P^m(\Gamma_1 \cap \Gamma_2), P^m(\Gamma_2) - P^m(\Gamma_1 \cap \Gamma_2)\} = P^m(\Gamma_1) - P^m(\Gamma_1 \cap \Gamma_2).$$

Thus (the sum on) the left side of the equality in (2.11) is $1 - P^m(\Gamma_2)$. But the right side also equals $1 - P^m(\Gamma_2)$ in this case. The case $P^m(\Gamma_2) > P^m(\Gamma_1)$ is exactly similar. Hence

$$d_1(T^{*m}\mu, T^{*m}\nu) \leq \delta d_1(\mu, \nu). \tag{2.12}$$

Also,

$$\begin{aligned} d_1(T^*\mu, T^*\nu) &= \sup\left\{\left|\int\left[\int f(y)p(x, dy)\right]\mu(dx) - \int\left[\int f(y)p(x, dy)\right]\nu(dx)\right| : f \in \mathscr{G}_1\right\} \\ &\leq d_1(\mu, \nu). \end{aligned} \tag{2.13}$$

Combining (2.12) and (2.13) one arrives at (2.7). If (1.5) holds, it is trivial to check that $\delta < 1$. □

Since $d(\mu, \nu) \leq d_1(\mu, \nu) \leq 1$, the following is immediate from Lemma 2.3:

$$d(T^{*n}\mu, T^{*n}\nu) \leq \delta^{[n/m]}, \qquad n = 1, 2, \dots. \tag{2.14}$$

Corollary 2.4 is a consequence of Lemma 2.2 and (2.14).

COROLLARY 2.4. *If* (1.5) *holds for some* $x_0 \in S$ *and some positive integer* m, *then there exists a unique probability measure* π *on* $(S, \mathscr{B}(S))$ *such that*

$$\sup_{x \in S} d\big(p^{(n)}(x, dy), \pi(dy)\big) \leq \delta^{[n/m]} \to 0 \quad \text{as } n \to \infty. \tag{2.15}$$

PROOF. For $n' > n$, one has

$$d\big(p^{(n)}(x, dy), p^{(n')}(x, dy)\big) = d(T^{*n}\mu, T^{*n}\nu) \leq \delta^{[n/m]}, \tag{2.16}$$

with $\mu = \delta_x$ (point mass at x) and $\nu = T^{*(n'-n)}\delta_x$. Hence $p^{(n)}(x, dy)$ is a Cauchy sequence in the metric d. Let π be its limit, which exists by Lemma 2.2. Letting $n' \to \infty$ in (2.16) one arrives at (2.15). □

If the probability measure π in Corollary 2.4 can be shown to be invariant, then the proof of Theorem 2.1 would be complete. The next result shows this.

LEMMA 2.5. (i) *Suppose there exist* $a = (a^{(1)}, \dots, a^{(k)})$ *and* $b = (b^{(1)}, \dots, b^{(k)})$ *in* S *such that* $a \leq x \leq b$ *for all* $x \in S$. *If, in this case,* $p^{(n)}(x, dy)$ *converges weakly to the same probability measure* $\pi(dy)$ *on* S *for every* $x \in S$, *then* π *is the unique invariant probability for* p.

(ii) *The probability measure* π *in Corollary* 2.4 *is the unique invariant probability for* p, *whether or not there exist* a *and* b *as in part* (i).

PROOF. (i) Let

$$X_n(x) = \alpha_n \cdots \alpha_1 x, \qquad Y_n(x) = \alpha_1 \cdots \alpha_n x, \qquad x \in S, \tag{2.17}$$

where $\alpha, \alpha_1, \alpha_2, \ldots$ is an i.i.d. sequence of random maps (on S into S) with common distribution P and defined on some probability space $(\Omega, \mathscr{F}, Q)$. The distribution of $Y_n(x)$ is the same as that of $X_n(x)$, namely, $p^{(n)}(x, dy)$. Now $Y_n(a)$ increases and $Y_n(b)$ decreases, respectively, to $\underline{Y}$ and $\overline{Y}$, say. Since $Y_n(a) \le Y_n(b)$ for all n, $\underline{Y} \le \overline{Y}$. Under the hypothesis, however, the distributions of $\underline{Y}$ and $\overline{Y}$ are the same, namely, π. Hence $\underline{Y} = \overline{Y}$, almost surely. Therefore,

$$\begin{aligned} p^{(n+1)}(a, S \cap [a, x]) &= Q(\alpha Y_n(a) \le x) \ge Q(\alpha \underline{Y} \le x) \\ &= \int p(z, S \cap [a, x]) \pi(dz) \\ &= Q(\alpha \overline{Y} \le x) \ge Q(\alpha Y_n(b) \le x) \\ &= p^{(n+1)}(b, S \cap [a, x]). \end{aligned} \tag{2.18}$$

If x is a point of continuity of the cumulative distribution function (c.d.f.) of π, then the two extreme sides of (2.18) have the same limit $\pi(S \cap [a, x])$. Hence one must have the equality

$$\pi(S \cap [a, x]) = \int p(z, S \cap [a, x]) \pi(dz). \tag{2.19}$$

Since the class of sets $S \cap [a, x]$ for which (2.19) holds is closed under finite intersections and generates $\mathscr{B}(S)$, it follows that [see, e.g., Billingsley (1979), Theorem 3.3, page 34]

$$\pi(B) = \int p(z, B) \pi(dz) \qquad \forall B \in \mathscr{B}(S), \tag{2.20}$$

i.e., π is invariant for p. If π' is also invariant, then

$$\pi'(S \cap [a, x]) = \int p^{(n)}(z, S \cap [a, x]) \pi'(dz) \qquad \forall x. \tag{2.21}$$

In particular, for points x of continuity of the c.d.f. of π, one may take limits to get $\pi'(S \cap [a, x]) = \pi(S \cap [a, x])$. This implies $\pi' = \pi$, proving uniqueness.

(ii) First consider the case $m = 1$. In case there do not exist a and/or b as in part (i), reduce the problem to that of a bounded S, by an increasing homeomorphism. Let now $a^{(i)} = \inf\{x^{(i)}\colon x \in S\}$ and $b^{(i)} = \sup\{x^{(i)}\colon x \in S\}$, $1 \le i \le k$. Write $a = (a^{(1)}, \ldots, a^{(k)})$, $b = (b^{(1)}, \ldots, b^{(k)})$. Let $\overline{S} = S \cup \{a, b\}$. For $\gamma \in \Gamma_1$, set $\gamma(a) = a$ and $\gamma(b) = x_0$; for $\gamma \in \Gamma_2$, set $\gamma(a) = x_0$ and $\gamma(b) = b$; for $\gamma \notin \Gamma_1 \cup \Gamma_2$, set $\gamma(a) = a$ and $\gamma(b) = b$. Then the hypothesis (1.5), with $m = 1$, still applies on the new state space $\overline{S}$. Therefore, by Corollary 2.4 and the preceding part (i), there exists a unique invariant probability $\bar{\pi}(dy)$ to which $p^{(n)}(x, dy)$ converges in the d-metric, for all $x \in S$. Since $p^{(n)}(x, dy)$ converges to $\pi(dy)$ for all $x \in S$, $\bar{\pi} = \pi$.

To deal with the case $m > 1$, take for Γ the set $\Gamma^{(m)}$ of all compositions $\gamma_m \cdots \gamma_1$ with $\gamma_i \in \Gamma$, $1 \leq i \leq m$. For the σ-field $\mathscr{C}^{(m)}$ on $\Gamma^{(m)}$, take the class of all sets B whose inverse images under the map $(\gamma_1 \cdots \gamma_m) \to \gamma_m \cdots \gamma_1$ are in $\mathscr{C}^m$. Let $P^{(m)}$ be the induced probability measure on $(\Gamma^{(m)}, \mathscr{C}^{(m)})$. The (one-step) transition probability arising from the map $(\gamma, x) \to \gamma x$ on $\Gamma^{(m)}$ into S is then $p^{(m)}(x, dy)$, with the associated adjoint operator T^{*m}. By the preceding paragraph, π is the unique fixed point of T^{*m}: $T^{*m}\pi = \pi$. Also, one has

$$T^*\pi = T^*(T^{*mn}\pi) = T^{*(mn+1)}\pi \to \pi$$

in the d-metric. Hence $T^*\pi = \pi$. □

This completes the proof of Theorem 2.1.

Remark 2.5.1. If one can show that $\mathscr{P}(S)$ is complete in the metric d_1 defined by (2.4), then the contraction mapping theorem immediately yields $T^*\pi = \pi$. This is true for $k = 1$ and we are uncertain for $k > 1$.

Remark 2.5.2. Theorem 2.1 and its proof go over to a topologically complete $S \subset \mathbb{R}^\infty$.

In case $k = 1$ and S is compact, the hypothesis of Theorem 2.1 is also necessary, leaving aside the case $P(\{\gamma(M) = M\}) = 1$ for some unique M [see Dubins and Freedman (1966) for the continuous case].

More generally, one has the following result. As before, S is always taken to be topologically complete.

Lemma 2.6. *Let $S \subset \mathbb{R}^k$, Γ a set of measurable nondecreasing functions on S and let P be a probability measure on $(\Gamma, \mathscr{C})$ such that $p^{(n)}(x, dy)$ converges weakly for each x to the same probability $\pi(dy)$. Assume that there are two points $a, b \in S$ such that $a \leq x \leq b$ for all $x \in S$. Then* (1.5) *holds for some x_0 and some m, provided there are two points $c = (c^{(1)}, \dots, c^{(k)})$ and $d = (d^{(1)}, \dots, d^{(k)})$ in the support of $\pi(dy)$ such that $c^{(i)} < d^{(i)}$ for $1 \leq i \leq k$.*

Proof. Let $Y_n(a) \uparrow \underline{Y}$, $Y_n(b) \downarrow \overline{Y}$ [see (2.17)]. Since $p^{(n)}(a, dy)$ and $p^{(n)}(b, dy)$ converge weak-star to the same limit, $\underline{Y} = \overline{Y}$ a.s. Choose $\theta > 0$ such that $c^{(i)} + \theta < d^{(i)} - \theta$ for $1 \leq i \leq k$. Writing $e = (1, 1, \dots, 1)$, there exists a positive integer m such that $\text{prob}(X_m(b) \leq c + \theta e) = \text{prob}(Y_m(b) \leq c + \theta e) > 0$ and $\text{prob}(X_m(a) \geq d - \theta e) = \text{prob}(Y_m(a) \geq d - \theta e) > 0$. Then (1.5) holds for this m and any $x_0 \in [c + \theta e, d - \theta e]$. □

3. A functional central limit theorem. One of the principal objectives in this article is to obtain functional central limit theorems for

$$Y_n(t) \equiv n^{-1/2} \sum_{j=0}^{[nt]} \left(f(X_j) - \int f \, d\pi \right), \qquad 0 \leq t < \infty, \tag{3.1}$$

or its polygonal version defined by (1.4), for broad classes of functions f in $L^2(S, \pi)$ under the general assumptions made in Section 2. In many situations, especially when P is discrete, the Markov processes X_n considered here are not φ-irreducible with respect to any nontrivial σ-finite measure φ. As a consequence, the processes, even though ergodic, are not even strongly mixing. Indeed, the tail σ-field may be nontrivial [see Rosenblatt (1980) for an example].

The process Y_n defined by (3.1) or (1.4) takes values in the space $D[0, \infty)$ of real-valued right continuous functions on $[0, \infty)$ having left-hand limits with the Skorohod topology. The distribution of Y_n is then a probability measure on the Borel σ-field of $D[0, \infty)$, and its convergence in distribution to a Brownian motion means the weak-star convergence of this sequence of distributions to a Wiener measure [see, e.g., Parthasarathy (1967), Chapter 7].

THEOREM 3.1. *Let the hypothesis of Theorem* 2.1 *hold.*

(a) *Then for every f that may be expressed as the difference between two monotone nondecreasing functions in $L^2(S, \pi)$, $f - \int f\,d\pi$ belongs to the range of $T - I$.*

(b) *Whatever the initial distribution, the functional central limit theorem holds if f is as in part* (a), *and the variance parameter of the limiting Brownian motion is given by $\int g^2\,d\pi - \int (Tg)^2\,d\pi$, where g is an element of $L^2(S, \pi)$ satisfying $(T - I)g = f - \int f\,d\pi$.*

For the proof let us begin with two simple but crucial lemmas. Let $\|\cdot\|_2$ denote the norm in $L^2(S, \pi)$.

LEMMA 3.2. *Let μ be a probability measure on $(\mathbb{R}^1, \mathscr{B}(\mathbb{R}^1))$ such that $\int x^2 \mu(dx) < \infty$. Then*

$$\int x^2\mu(dx) - \left(\int x\mu(dx)\right)^2 = \tfrac{1}{2}\int\int (x-y)^2\mu(dx)\mu(dy).$$

PROOF. Expand the right-hand side and integrate. □

LEMMA 3.3. *Let $f \in L^2(S, \pi)$ and write*

$$\bar{f} = \int f\,d\pi. \tag{3.2}$$

If $\sum_{n=0}^{\infty}\|(T^n(f - \bar{f}))\|_2 < \infty$, then $f - \bar{f}$ belongs to the range of $T - I$; indeed, $(T - I)g = f - \bar{f}$, where

$$g = -\sum_{n=0}^{\infty} T^n(f - \bar{f}). \tag{3.3}$$

PROOF. Apply $T - I$ to the right side of (3.3). □

PROOF OF THEOREM 3.1. Let $f \in L^2(S, \pi)$ be monotone nondecreasing. By Lemma 3.2,

$$\begin{aligned}
&\|T^m(f - \bar{f})\|_2^2 \\
&= \int\Big(\int(f(y) - \bar{f})p^{(m)}(x, dy)\Big)^2 \pi(dx) \\
(3.4)\quad &= \int\Big[\int(f(y) - \bar{f})^2 p^{(m)}(x, dy) \\
&\quad - \tfrac{1}{2}\int\int(f(y) - f(z))^2 p^{(m)}(x, dy)p^{(m)}(x, dz)\Big]\pi(dx) \\
&= \|f - \bar{f}\|_2^2 - \tfrac{1}{2}\int\Big[\int\int(f(y) - f(z))^2 p^{(m)}(x, dy)p^{(m)}(x, dz)\Big]\pi(dx).
\end{aligned}$$

Now

$$\begin{aligned}
&\int\int(f(y) - f(z))^2 p^{(m)}(x, dy)p^{(m)}(x, dz) \\
&\geq \int_{\{z \geq x_0\}}\int_{\{y \leq x_0\}}(f(y) - f(x_0))^2 p^{(m)}(x, dy)p^{(m)}(x, dz) \\
&\quad + \int_{\{z \leq x_0\}}\int_{\{y > x_0\}}(f(y) - f(x_0))^2 p^{(m)}(x, dy)p^{(m)}(x, dz) \\
(3.5)\quad &\geq P^m(\Gamma_2)\int_{\{y \leq x_0\}}(f(y) - f(x_0))^2 p^{(m)}(x, dy) \\
&\quad + P^m(\Gamma_1)\int_{\{y > x_0\}}(f(y) - f(x_0))^2 p^{(m)}(x, dy) \\
&\geq \min\{P^m(\Gamma_1), P^m(\Gamma_2)\}\int(f(y) - f(x_0))^2 p^{(m)}(x, dy),
\end{aligned}$$

where Γ_1 and Γ_2 are defined by (2.6). Hence

$$\begin{aligned}
&\int\Big[\int\int(f(y) - f(z))^2 p^{(m)}(x, dy)p^{(m)}(x, dz)\Big]\pi(dx) \\
(3.6)\quad &\geq \min\{P^m(\Gamma_1), P^m(\Gamma_2)\}\int\Big[\int(f(y) - f(x_0))^2 p^{(m)}(x, dy)\Big]\pi(dx) \\
&= \min\{P^m(\Gamma_1), P^m(\Gamma_2)\}\int(f(y) - f(x_0))^2 \pi(dy) \\
&\geq \min\{P^m(\Gamma_1), P^m(\Gamma_2)\}\|f - \bar{f}\|_2^2 \geq (1 - \delta)\|f - \bar{f}\|_2^2,
\end{aligned}$$

where δ, defined by (2.8), is less than 1. Using (3.6) in (3.4) one gets

$$(3.7)\qquad \|T^m(f - \bar{f})\|_2 \leq c\|f - \bar{f}\|_2,$$

where

$$c = \left(1 - \tfrac{1}{2}(1 - \delta)\right)^{1/2} < 1. \tag{3.8}$$

Next note that if f is monotone nondecreasing, so is Tf and therefore $T^m f$. Hence iteration of (3.7) yields

$$\|T^{jm}(f - \bar{f})\|_2 \le c^j \|f - \bar{f}\|_2, \qquad j = 1, 2, \dots. \tag{3.9}$$

Since T is a contraction on $L^2(S, \pi)$, one has, finally,

$$\|T^n(f - \bar{f})\|_2 \le c^{[n/m]} \|f - \bar{f}\|_2 \qquad \forall\, n. \tag{3.10}$$

It now follows from Lemma 3.3 that $f - \bar{f}$ belongs to the range of $T - I$. This proves part (a).

In order to prove part (b), let $(T - I)g = f - \bar{f}$. Then

$$\begin{aligned} \sum_{j=0}^{n} \left(f(X_j) - \bar{f} \right) &= \sum_{j=0}^{n} \left(Tg(X_j) - g(X_j) \right) \\ &= \sum_{j=1}^{n+1} \left(Tg(X_{j-1}) - g(X_j) \right) + \left(g(X_{n+1}) - g(X_0) \right). \end{aligned} \tag{3.11}$$

Since $Tg(X_{j-1}) - g(X_j)$, $j \ge 0$, is (under the initial distribution π) a stationary ergodic sequence of martingale differences, the functional central limit theorem follows [see Billingsley (1968), Theorem 23.1; Gordon and Lifsic (1978) and Bhattacharya (1982), Theorem 2.1]. In this case the variance parameter of the limiting Brownian motion is $E(Tg(X_{j-1}) - g(X_j))^2 = \|g\|_2^2 - \|Tg\|_2^2$.

It remains to prove the functional central limit theorem starting from an arbitrary initial state x. Let $f \in L^2(S, \pi)$ be monotone nondecreasing. Let $\{X_j\}$ denote the process with initial distribution π. Write

$$\begin{aligned} S_{m,m'}(x) &= n^{-1/2} \sum_{j=m}^{m'} \left(f(X_j(x)) - \bar{f} \right), \\ S_{m,m'} &= n^{-1/2} \sum_{j=m}^{m'} \left(f(X_j) - \bar{f} \right). \end{aligned} \tag{3.12}$$

Then $S_{0,n}(x) = S_{0,n_0-1}(x) + S_{n_0,n}(x)$. Now, for every n_0,

$$S_{0,n_0-1}(x) \to 0 \quad \text{a.s. as } n \to \infty. \tag{3.13}$$

Also, for all $r \in \mathbb{R}^1$,

$$Q\left(S_{n_0,n}(x) > r\right) = Eh_n\left(X_{n_0}(x)\right) = \int h_n(y) p^{(n_0)}(x, dy), \tag{3.14}$$

where Q is the probability measure on the basic probability space and

$$h_n(y) = Q\left(S_{0,n-n_0}(y) > r\right) \tag{3.15}$$

is an increasing function of y. Hence, by Lemma 2.3,

$$\sup_{n>n_0}\left|\int h_n(y)p^{(n_0)}(x,dy) - \int h_n(y)\pi(dy)\right| \to 0 \quad \text{as } n_0 \to \infty. \tag{3.16}$$

Therefore, given $\varepsilon > 0$, one may choose $n_0 = n_0(\varepsilon)$ such that the left side of (3.16) is less than $\varepsilon/3$. Then choose $n(\varepsilon)$ such that for all $n \geq n(\varepsilon)$,

$$\begin{aligned} &\left|Q\left(S_{n_0,n}(x) > r\right) - Q\left(S_{0,n}(x) > r\right)\right| < \varepsilon/3,\\ &\left|Q\left(S_{0,n} > r\right) - Q\left(S_{0,n-n_0} > r\right)\right| < \varepsilon/3. \end{aligned} \tag{3.17}$$

It follows that

$$\left|Q\left(S_{0,n}(x) > r\right) - Q\left(S_{0,n} > r\right)\right| < \varepsilon \qquad \forall\, n \geq n(\varepsilon). \tag{3.18}$$

Hence the distribution of $S_{0,n}(x)$ converges in the weak-star topology to the appropriate Gaussian law. In this manner one proves convergence of the finite dimensional distributions of $Y_n(t)$ to those of a Brownian motion when the initial state is x. It remains to prove that the distributions of Y_n, $n = 1, 2, \ldots$, form a precompact set. To prove the latter, for an arbitrary set of positive integers $n_0 < n_1 < \cdots < n_{N+1} = n$ and a positive number r, write

$$\begin{aligned} A(y) &= \left\{\left[\max_{0\leq i\leq N} S_{n_i-n_0,\,n_{i+1}-n_0-1}(y)\right] > r\right\},\\ B(y) &= \left\{\left[\max_{0\leq i\leq N} S_{n_i-n_0,\,n_{i+1}-n_0-1}(y)\right] \geq -r\right\}. \end{aligned} \tag{3.19}$$

Let A, B denote the corresponding events for the sequence $\{X_j\}$. Since $Q(A(y))$ and $Q(B(y))$ are increasing in y, Lemma 2.3 may be used again to show that, as $n_0 \to \infty$,

$$\begin{aligned} &Q\left[\left[\max_{0\leq i\leq N} S_{n_i,\,n_{i+1}-1}(x)\right] > r\right] - Q\left[\left[\max_{0\leq i\leq N} S_{n_i,\,n_{i+1}-1}\right] > r\right]\\ &\qquad = \int Q(A(y))p^{(n_0)}(x,dy) - \int Q(A(y))\pi(dy) \to 0, \end{aligned} \tag{3.20}$$

uniformly for all N, n_i and r. A similar relation holds for the min and $B(y)$. Since the partial sum process under the initial distribution π converges to a Brownian motion, it now follows by Prohorov's theorem [see Billingsley (1968), Section 15] that Y_n converges in distribution to the same Brownian motion.

Finally, in case $f = f_1 - f_2$ with f_i monotone nondecreasing and in $L^2(S,\pi)$, $i = 1, 2$, the preceding argument easily extends to the joint distribution of the processes $Y_n^{(1)}$ and $Y_n^{(2)}$ associated with f_1 and f_2, respectively. Instead of the function (3.15), one now looks at $Q(S_{0,n-n_0}^{(1)}(y) > r_1, S_{0,n-n_0}^{(2)}(y) > r_2)$, where $S^{(1)}$ and $S^{(2)}$ are partial sums corresponding to f_1 and f_2, respectively. Hence $Y_n = Y_n^{(1)} - Y_n^{(2)}$ converges in distribution to the appropriate Brownian motion when $X_0 \equiv x$. It follows, on integration with respect to x, that this convergence holds under an arbitrary initial distribution. □

4. Two examples.

EXAMPLE 4.1. We shall write vectors in bold face in this example in order to distinguish them from scalars. In mathematical economics it is quite common to take $S = (0, \infty)^k$, Γ a set of nondecreasing and continuously differentiable maps $\gamma = (\gamma^{(1)}, \gamma^{(2)}, \ldots, \gamma^{(k)})$ such that each $\gamma^{(i)}$ is strictly concave, which may indicate, e.g., a law of diminishing returns. For simplicity, we take P to have finite support Γ. Assume, in addition, that for each $\gamma \in \Gamma$, (i) $\gamma(\mathbf{x}) \downarrow \mathbf{0}$ as $\mathbf{x} \downarrow \mathbf{0}$, (ii) $\lim_{\mathbf{x}\downarrow 0} D_i\gamma^{(i)}(\mathbf{x}) > 1$, $1 \le i \le k$, (iii) $\lim D_i\gamma^{(i)}(\mathbf{x}) < 1$ as $x^{(j)} \uparrow \infty$ for all j, $1 \le j \le k$, $1 \le i \le k$, (iv) $\lim D_i\gamma^{(i')}(\mathbf{x}) = 0$ for $i \neq i'$, as $x^{(j)} \uparrow \infty$ for all j, $1 \le j \le k$, $1 \le i \neq i' \le k$. Here $D_i = \partial/\partial x^{(i)}$.

Let us show that for each $\gamma \in \Gamma$ there exist two points $\mathbf{x}_1 < \mathbf{x}_2 \in S$ such that the range of γ on $[\mathbf{x}_1, \mathbf{x}_2]$ is contained in $[\mathbf{x}_1, \mathbf{x}_2]$. First note that $\gamma^{(i)}(\mathbf{x}) = \gamma^{(i)}(\mathbf{x}) - \gamma^{(i)}(\mathbf{0}) \ge \sum x^{(j)} D_j \gamma^{(i)}(\mathbf{x})$, which is greater than $x^{(i)}$ for all sufficiently small $\mathbf{x}$ in view of (ii). Hence $\gamma(\mathbf{x}) > \mathbf{x}$ for all sufficiently small $\mathbf{x}$. Choose $\mathbf{x}_1$ such that $\gamma(\mathbf{x}) > \mathbf{x}$ for all $\mathbf{x} \le \mathbf{x}_1$. Next, let the limit in (iii) be $\beta_i < 1$ and take $\beta = \max\{\beta_1, \ldots, \beta_k\}$. Let $0 < \varepsilon < (1 - \beta)/2$. Choose $a > 0$ so that $D_i\gamma^{(i)}(\mathbf{x}) < \beta + \varepsilon/2k$ and $D_j\gamma^{(i)}(\mathbf{x}) < \varepsilon/2k$ for $i \neq j$, if $\mathbf{x} \ge (a, a, \ldots, a)$. For all $b > a$, one has $\theta = \theta(a, b) \in [0, 1]$ so that

$$
\begin{aligned}
\gamma^{(i)}(b, \ldots, b) &= \gamma^{(i)}(a, a, \ldots, a) \\
&\quad + (b - a)\sum_j D_j\gamma^{(i)}(a + \theta(b - a), \ldots, a + \theta(b - a)) \\
&\le \gamma^{(i)}(a, a, \ldots, a) + (b - a)(\beta + \varepsilon/2) \\
&\le \gamma^{(i)}(a, a, \ldots, a) + b(\beta + \varepsilon) \\
&\le \gamma^{(i)}(a, \ldots, a) + b(1 + \beta)/2,
\end{aligned}
\tag{4.1}
$$

which is smaller than b for all sufficiently large b. Hence $\gamma(b, b, \ldots, b) < (b, b, \ldots, b)$ for all large b. Let $\mathbf{x}_2 = (b, \ldots, b)$ for such a large b. Then $\mathbf{x}_1$ and $\mathbf{x}_2$ satisfy the requirement mentioned previously.

Using the Brouwer fixed point theorem on $[\mathbf{x}_1, \mathbf{x}_2]$, it follows that γ has a fixed point $\mathbf{x}_\gamma \in [\mathbf{x}_1, \mathbf{x}_2]$. If $\mathbf{x}_* \le \mathbf{x}_1$ and $\mathbf{x}^* \equiv (b, b, \ldots, b) \ge \mathbf{x}_2$ for all $\gamma \in \Gamma$, then every γ maps $[\mathbf{x}_*, \mathbf{x}^*]$ into itself. In particular, $\mathbf{x}_\gamma \in [\mathbf{x}_*, \mathbf{x}^*]$ for all $\gamma \in \Gamma$. Since the range of γ^m on $[\mathbf{x}_*, \mathbf{x}^*]$ is contained in $[\gamma^m(\mathbf{x}_*), \gamma^m(\mathbf{x}^*)]$ and $\gamma^m(\mathbf{x}_*) \uparrow \mathbf{x}_\gamma$ and $\gamma^m(\mathbf{x}^*) \downarrow \mathbf{x}_\gamma$ as $m \uparrow \infty$, the distance between the range of γ^m and $\{\mathbf{x}_\gamma\}$ goes to zero as $m \to \infty$. Here we have used the fact that a strictly concave γ cannot have more than one fixed point in $[\mathbf{x}_1, \mathbf{x}_2]$ since $\gamma(\mathbf{0}) = \mathbf{0}$.

Assume finally that (v) there are $\gamma, \gamma' \in \Gamma$ such that $x_\gamma^{(i)} < x_{\gamma'}^{(i)}$ for $1 \le i \le k$. It follows from the preceding paragraph that if $\mathbf{x}_0$ is any given point in $(\mathbf{x}_\gamma, \mathbf{x}_{\gamma'})$, then the ranges of γ^m and γ'^m are contained in $[\mathbf{x}_*, \mathbf{x}_0]$ and $[\mathbf{x}_0, \mathbf{x}^*]$, respectively, for all sufficiently large m. Thus (1.5) holds. Hence, by Theorem 2.1, there exists a unique invariant probability π on the new state space $[\mathbf{x}_*, \mathbf{x}^*]$ such that $T^{*n}\mu$ converges in the d-metric to π uniformly for all probability measures μ on $[\mathbf{x}_*, \mathbf{x}^*]$. Since $\mathbf{x}_*$ can be taken arbitrarily small and $\mathbf{x}^*$ arbitrarily large, the invariant measure π is unique on $S = (0, \infty)^k$ and $T^{*n}\mu$ converges weakly to π for every μ on S, although an exponential rate of convergence may not hold in general, unless the support of μ is compact.

The assumption of finite Γ may be easily relaxed to the assumption of compactness of the support of P, where the topology on Γ is that of uniform convergence on compact subsets of $(0, \infty)^k$. In particular, it is enough to require, in addition to (i)–(v), that (vi) for some $x \in S$ the set $\{\gamma(x): \gamma \in \Gamma\}$ is bounded and (vii) the sets $\{D_j\gamma^{(i)}: \gamma \in \Gamma\}$, $1 \le i, j \le k$, are bounded on every compact subset of $(0, \infty)^k$.

The case $k = 1$ and Γ finite is known in mathematical economics and is described in Bhattacharya and Majumdar (1984) and Mirman (1980).

We now turn to nonlinear autoregressive models. An autoregressive process of order $q \ge 1$ is a sequence of random variables U_n with values in $\mathbb{R}^r$ satisfying a relationship of the form

$$U_{n+q} = \varphi(U_n, U_{n+1}, \dots, U_{n+q-1}) + \eta_{n+q}, \qquad n = 0, 1, \dots, \tag{4.2}$$

where φ is a measurable function on $(\mathbb{R}^r)^q$ into $\mathbb{R}^r$ and η_n, $n = q, q+1, \dots$, is an i.i.d. sequence with values in $\mathbb{R}^r$ independent of the initial variables $U_0, U_1, \dots, U_{q-1}$. Then the process $X_n = (U_n, U_{n+1}, \dots, U_{n+q-1})$, $n = 0, 1, \dots$, is a Markov process on the state space $S = (\mathbb{R}^r)^q$.

EXAMPLE 4.2 (Nonlinear autoregressive models with φ nondecreasing). Suppose $\varphi = (\varphi^{(1)}, \dots, \varphi^{(r)})$ is a bounded nondecreasing function of its arguments and that $a^{(i)} \le \varphi^{(i)} \le b^{(i)}$, $1 \le i \le r$. Assume

$$\begin{aligned} &\operatorname{prob}\big(\eta_n \le (c^{(1)}, \dots, c^{(r)})\big) > 0, \\ &\operatorname{prob}\big(\eta_n \ge (d^{(1)}, \dots, d^{(r)})\big) > 0, \end{aligned} \tag{4.3}$$

where the constants $c^{(i)}$ and $d^{(i)}$ satisfy

$$d^{(i)} - c^{(i)} \ge b^{(i)} - a^{(i)}, \qquad 1 \le i \le r. \tag{4.4}$$

Write $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ for $(a^{(1)}, \dots, a^{(r)}), (b^{(1)}, \dots, b^{(r)}), (c^{(1)}, \dots, c^{(r)}), (d^{(1)}, \dots, d^{(r)})$. Let us show that the Markov process $X_n = (U_n, \dots, U_{n+q-1})$ then admits a unique invariant probability and Theorems 2.1 and 3.1 apply. For $q = 1$ condition (1.5) applies with $m = 1$, since $\operatorname{prob}(X_1(x) \le \mathbf{b} + \mathbf{c}\ \forall\, x) > 0$, $\operatorname{prob}(X_1(x) \ge \mathbf{a} + \mathbf{d}\ \forall\, x) > 0$ and one may take any $x_0 \in [\mathbf{b} + \mathbf{c}, \mathbf{a} + \mathbf{d}]$. In general it may be shown that (1.5) holds with $m = q$. For example, in the case $q = 2$,

$$X_{n+1} = (U_{n+1}, U_{n+2}) = \psi(X_n) + \varepsilon_{n+1}, \tag{4.5}$$

where $\psi(x^{(1)}, x^{(2)}) = (x^{(2)}, \varphi(x))$ for $x = (x^{(1)}, x^{(2)}) \in \mathbb{R}^r \times \mathbb{R}^r$ and $\varepsilon_{n+1} = (0, \eta_{n+1})$. Hence

$$\begin{aligned} X_0(x) &\equiv x = (x^{(1)}, x^{(2)}), \\ X_1(x) &= (x^{(2)}, \varphi(x) + \eta_2), \\ X_2(x) &= (\varphi(x) + \eta_2, \varphi(X_1(x)) + \eta_3) \\ &= (\varphi(x) + \eta_2, \varphi(x^{(2)}, \varphi(x) + \eta_2) + \eta_3), \end{aligned} \tag{4.6}$$

so that

$$\operatorname{prob}(X_2(x) \le (\mathbf{b}+\mathbf{c}, \mathbf{b}+\mathbf{c})\ \forall\, x) \ge \operatorname{prob}(\eta_2 \le \mathbf{c}, \eta_3 \le \mathbf{c}) = (\operatorname{prob}(\eta_2 \le \mathbf{c}))^2 > 0$$

and

$$\operatorname{prob}(X_2(x) \ge (\mathbf{a}+\mathbf{d}, \mathbf{a}+\mathbf{d})\ \forall\, x) \ge (\operatorname{prob}(\eta_2 \ge \mathbf{d}))^2 > 0.$$

Thus one may take x_0 to be any point of $(\mathbb{R}^r)^2$ in

$$[(\mathbf{b}+\mathbf{c}, \mathbf{b}+\mathbf{c}), (\mathbf{a}+\mathbf{d}, \mathbf{a}+\mathbf{d})] = [\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{d}]^2.$$

The general case is now clear.

Since U_n is a nondecreasing function of X_n, it follows that for every integer $s \ge 0$, as $n \to \infty$ the (joint) distribution of $(U_n, U_{n+1}, \dots, U_{n+s})$ under an arbitrary initial distribution of $(U_0, \dots, U_{q-1})$ converges in the d-metric on $(\mathbb{R}^r)^s$ to its steady state distribution (i.e., its distribution when the initial distribution is the invariant distribution π).

If, in addition to (4.3) and (4.4), one assumes that $E|\eta_n|^2 < \infty$, then by Theorem 3.1 applied to the function $f(x) = x^{(1)}$, $x = (x^{(1)}, x^{(2)}, \dots, x^{(q)}) \in (\mathbb{R}^r)^q$, the functional central limit theorem holds for the summands U_n.

It may be noted that (4.4) means that the error distribution is well spread out. Indeed, if η_n has a distribution whose support is unbounded in each coordinate (e.g., if it has full support $\mathbb{R}^r$), then this hypothesis is automatically satisfied and the support of the invariant probability in $(\mathbb{R}^r)^q$ is noncompact.

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Note added in proof. A recent unpublished manuscript by H. Hopenhayn and E. Prescott entitled "Invariant distributions for monotone Markov processes" has come to our attention. In this, the authors prove a result similar to our Theorem 2.1.

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10.2 "Random iterations of two quadratic maps"

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Random Iterations of Two Quadratic Maps

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Abstract. We study invariant measures of Markov processes obtained by the action of successive independent iterations of a map chosen at random from a set of two quadratic maps.

1. Introduction.

Markov processes may be viewed as random perturbations of dynamical systems. Indeed, if the state space S is a Borel subset of a Polish space one may represent a Markov process with any prescribed transition probability and an arbitrary initial distribution as $\boldsymbol{\alpha}_n \boldsymbol{\alpha}_{n-1} \cdots \boldsymbol{\alpha}_1 X_0$, where $\{\boldsymbol{\alpha}_n : n \geq 1\}$ is an i.i.d. sequence of random maps on S into itself and X_0 is independent of $\{\boldsymbol{\alpha}_n : n \geq 1\}$ (see Kifer [7], p.8). In the case of a dynamical system $\boldsymbol{\alpha}_n$ is degenerate, i.e., $P(\boldsymbol{\alpha}_n = f) = 1$ for a given single map f on S. This point of view of a Markov process is useful for the study of Markov processes as well as dynamical systems. Often a chaotic dynamical system admits uncountably many ergodic invariant probabilities only one of which, the so-called Kolmogorov measure, is physically relevant. This measure is the limit of the invariant probabilities of Markov processes obtained as appropriate random perturbations of the dynamical system, as the distribution of $\boldsymbol{\alpha}_1$ approaches the Dirac measure at f (see Kifer [8], Ruelle [9], and Katok and Kifer [6]). This, however, is not the focus of the present article.

Consider the quadratic family of functions $\{F_\mu : 0 \leq \mu \leq 4\}$, where F_μ is the map on [0,1] defined by

$$F_\mu(x) := \mu x(1-x), \qquad 0 \leq x \leq 1. \tag{1.1}$$

Dynamical systems with $f = F_\mu$, and similar ones, have been extensively studied in the literature (see, e.g., Devaney [4] and Collet and Eckman [3]). Given a pair of parameter values $\mu < \lambda$ and a number $\gamma \in (0,1)$ we consider an i.i.d. sequence of maps $\{\boldsymbol{\alpha}_n : n \geq 1\}$ with $P(\boldsymbol{\alpha}_1 = F_\mu) = \gamma, P(\boldsymbol{\alpha}_1 = F_\lambda) = 1 - \gamma$. For certain choices of μ, λ, we study the uniqueness and other properties of invariant probabilities of the resulting Markov processes. It turns out that even for those F_μ (and F_λ) which are simple as dynamical systems, the above randomization often leads to Markov processes with interesting invariant probabilities some times supported on Cantor sets of Lebesgue measure zero.

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Section 2 on iterated random monotone maps on $[0,1]$ is based largely on Dubins and Freedman [5], and provides the basic tool for deriving the main results. In Section 3 we review certain aspects of the quadratic maps $F_\mu(0 \le \mu \le 1+\sqrt{5})$, such as attracting and repelling fixed points and period–two orbits, and identify pairs F_μ, F_λ which have a common invariant interval on which they are both monotone. Section 4 contains the main results, summarized in Theorem 4.1. It will be clear from the proofs that some of the results extend to more general classes of maps than the family (1.1), but we do not pursue such extensions in this article.

2. Iterations of i.i.d monotone maps.

Let $a < b$ be given reals, and $(\Omega, \mathcal{F}, P)$ a probability space on which is defined a sequence of i.i.d. continuous maps $\alpha_n(n \ge 1)$ on $[a,b]$ into $[a,b]$. This means (i) for each $\omega \in \Omega, x \to \alpha_n(\omega)x$ is continuous (for all $n \ge 1$), (ii) for each B belonging to the Borel sigmafield $\mathcal{B}$ on $[a,b]$, $\{(\omega, x) : \alpha_n(\omega)x \in B\} \in \mathcal{F} \otimes \mathcal{B}$, and (iii) for every finite set $\{x_1, x_2, \ldots, x_k\} \subset [a,b]$, the sequence of random vectors $(\alpha_n x_1, \alpha_n x_2, \ldots, \alpha_n x_k)$, $n \ge 1$, are i.i.d. If X_0 is a random variable (with values in $[a,b]$) independent of $\{\alpha_n : n \ge 1\}$ (i.e., of $\sigma\{\alpha_n x : x \in [a,b], n \ge 1\}$), then $X_0, X_n \equiv \alpha_n \ldots \alpha_1 X_0 (n \ge 1)$, is a Markov process on $[a,b]$ having transition probability $p(x,B) := P(\alpha_1 x \in B)$ and initial distribution $\mu(B) := P(X_0 \in B), B \in \mathcal{B}$. In particular, if $X_0 \equiv x$ then we write $X_n(x)$ for this Markov process. The n–step transition probability may then be expressed as $p^n(x,B) = P(X_n(x) \in B)$. Note that the continuity of $\alpha_1(\omega)$ implies $x \to p(x,dy)$ is weakly continuous. For weakly continuous transition probabilities (on some metric space) a well known elementary criterion for the existence of an invariant probability for p is the following: *If for some x and some sequence of integers $n_1 < n_2 < \ldots < n_k < \ldots$, there exists a probability measure π such that*

$$\frac{1}{n_k}\sum_{m=1}^{n_k} p^m(x,dy) \overset{weakly}{\longrightarrow} \pi(dy), \tag{2.1}$$

then π is invariant. If for some x, the sequence $\frac{1}{n}\sum_{m=1}^{n} p^m(x,dy)$ is tight, then (2.1) *holds for some sequence $n_k(k \ge 1)$ and some probability measure π.*

We now state a basic result due to Dubins and Freedman [5] for monotone maps on $[a,b]$. For this case the *splitting condition* is said to hold if there exist x_0 and a positive integer m such that

$$P(X_m(x) \le x_0 \forall x) > 0, \;\; P(X_m(x) \ge x_0 \forall x) > 0. \tag{2.2}$$

Let p^* denote the adjoint operator on the space of all finite signed measures on $[a,b]$,

$$(p^*\nu)(B) := \int p(x,B)\nu(dx), \;\; B \in \mathcal{B}, \tag{2.3}$$

with norm

$$\text{(2.4)} \qquad \begin{aligned} \|\nu\| &:= \sup\{|\nu([a,x])| : a \le x \le b\}, \\ \|p^*\nu\| &= \sup\{|\int p(y,[a,x])\nu(dy)| : a \le x \le b\}. \end{aligned}$$

Write $p^{*n}\nu = p^*(p^{*(n-1)}\nu)(n \ge 2), p^{*1} = p^*$.

PROPOSITION 2.1. (Dubins and Freedman [5]). *Suppose $\alpha_n (n \ge 1)$ are i.i.d. monotone continuous maps on $[a,b]$ into $[a,b]$.* (a) *If the splitting condition holds then $\|p^{*n}\nu_1 - p^{*n}\nu_2\| \equiv \|p^{*n}(\nu_1 - \nu_2)\|$ goes to zero exponentially fast as $n \to \infty$, uniformly for every pair of probability measures ν_1, ν_2; and there exists a unique invariant probability π which is the limit of $p^{*n}\nu$ for every probability ν.* (b) *If α_1 is strictly increasing a.s., and there is no c such that $P(\alpha_1(\omega)c = c) = 1$, then splitting is also necessary for the conclusion in* (a) *to hold.*

REMARK 2.1.1. Under the hypothesis of part (a) the invariant probability is nonatomic, i.e., its distribution function is continuous. For this take ν_1 nonatomic and $\nu_2 = \pi$ in the statement and note that the continuous distribution functions of $p^{*n}\nu_1$ converge uniformly to that of π.

REMARK 2.1.2. Part (a) of the theorem holds if the state space is an arbitrary interval not necessarily compact. Indeed, this result can be extended to appropriate subsets of $\mathbb{R}^k$ and coordinatewise monotone maps (see Bhattacharya and Lee [2]).

For our purposes a different version of this result will be useful. To state it define $Y_n(x) := \alpha_1 \cdots \alpha_n x$. If α_1 is increasing on $[a,b]$ then $Y_n(a) \uparrow$ and $Y_n(b) \downarrow$ as $n \uparrow$. Let $\underline{Y}$, $\bar{Y}$ denote the respective limits. Note that $X_n(x)$ and $Y_n(x)$ have the same distribution, namely, $p^n(x,dy)$. A proof of part (b) of Proposition 2.1 is included in the proof of the following result.

PROPOSITION 2.2. *Let α_1 be a.s. continuous and increasing on $[a,b]$. Consider the following statements:* (i) *$\underline{Y} = \bar{Y}$ a.s.* (ii) *There exists a unique invariant probability.* (iii) *Splitting holds.* (iv) *$\underline{Y} = \bar{Y}$ a.s. and $\underline{Y}$ is not constant a.s.* (v) *There exists a unique invariant probability and it is nonatomic.* (a) *The following implications hold:* (v) $\Longrightarrow$ (iv) $\Longrightarrow$ (iii) $\Longrightarrow$ (ii) $\Leftrightarrow$ (i). (b) If α_1 is strictly increasing a.s. then (iii) $\Leftrightarrow$ (iv) $\Leftrightarrow$ (v).

Proof. (a) By criterion (2.1), the distributions of $\underline{Y}$ and $\bar{Y}$ are both invariant. Since $\underline{Y} \le \bar{Y}$, these invariant probabilities are the same if and only if $\underline{Y} = \bar{Y}$ a.s. Also, $Y_n(a) \le Y_n(x) \le Y_n(b)$ for all x. Therefore, $\underline{Y} = \bar{Y}$ a.s. implies $Y_n(x) \to \underline{Y}$ a.s., so that $p^n(x,dy)$ converges weakly to the common distribution of $\underline{Y}$ and $\bar{Y}$, *for all* x. This easily implies uniqueness of the invariant probability. Hence (i) $\Leftrightarrow$ (ii). Also, (iii) $\Rightarrow$ (ii) by Proposition 2.1(a).

Now assume (iv) holds. Then there exists x_0 such that $P(\underline{Y} < x_0)(= P(\bar{Y} < x_0)) > 0$ and $P(\underline{Y} > x_0) > 0$. This implies (2.2) for all sufficiently large m. Thus (iv) $\Rightarrow$ (iii). Since (ii) $\Rightarrow$ (i), clearly (v) $\Rightarrow$ (iv).

(b) Assume (iii) holds. Then (i) holds. If $\underline{Y} = \bar{Y} = c$ a.s. for some constant c then the Dirac measure δ_c is invariant, which implies $P(\alpha_1 c = c) = 1$. This in turn implies $P(X_n(c) = c) = 1$ for all $n \geq 1$. Since α_1 is strictly increasing, so is $x \to X_n(x)$ (for every $n \geq 1$). Therefore, if $a \leq x_0 \leq c < b$ then $P(X_n(b) \leq x_0) = 0$, and if $a < c \leq x_0 \leq b$ then $P(X_n(a) \geq x_0) = 0$. Hence splitting does not occur. Thus (iii) $\Rightarrow$ (iv), so that (by (a)) (iii) $\Rightarrow$ (iv). By Remark 2.1.1, (iii) $\Rightarrow$ (v), so that (iii) $\Leftrightarrow$ (v). □

Suppose now that α_1 is decreasing a.s. Then $\alpha_1\alpha_2$ is increasing a.s. and $\underline{Z} := \lim Y_{2n}(a)$, $\bar{Z} := \lim Y_{2n}(b)$ (as $n \to \infty$) exist. Proposition 2.2 then holds for the two-step transition probability p^2 (in place of p), if $\underline{Y}$ and $\bar{Y}$ are replaced by $\underline{Z}$ and $\bar{Z}$, respectively. Since every invariant probability for p is invariant for p^2, the following corollary is immediate.

COROLLARY 2.2. *Suppose* α_1 *is continuous and either strictly increasing a.s. or strictly decreasing a.s. on* $[a, b]$. *In addition assume that there does not exist a* c *such that* $P(\alpha_1 c = c) = 1$. *Then splitting is a necessary and sufficient condition for the existence of a unique invariant probability. This probability is nonatomic.* **3. Quadratic maps.**

We will henceforth confine our attention to the family of maps $F_\mu(0 \leq \mu \leq 4)$ defined by (1.1). If $\mu \neq 0, F_\mu$ is strictly increasing on $[0, \frac{1}{2}]$ and strictly decreasing on $[\frac{1}{2}, 1]$ attaining its maximum value $\mu/4$ at $x = \frac{1}{2}$.

If $0 \leq \mu \leq 1$, then $F_\mu(x) < x$ for $x \in (0, 1]$. Hence $F_\mu^n(x) \downarrow$ as $n \uparrow$. The limit must be a fixed point. But the only fixed point is $x = 0$. Hence 0 is an *attracting fixed point*: $F_\mu^n(x) \to 0$ as $n \to \infty$, for all $x \in [0, 1]$.

If $1 < \mu \leq 4$, then F_μ has a second fixed point $p_\mu = 1 - \frac{1}{\mu}$. Suppose $1 < \mu \leq 2$. Then $F_\mu(x) > x$ for $x \in (0, p_\mu)$ and F_μ is increasing on $(0, p_\mu)$. Hence $F_\mu^n(x)$ increases to the fixed point p_μ as n increases. For $x \in (p_\mu, 1), F_\mu(x) < x$. Thus either $F_\mu^n(x)$ decreases to p_μ as n increases, or there exists n_0 such that $F_\mu^{n_0}(x) \in (0, p_\mu]$ and $F_\mu^n(x) F_\mu^{n_0}(x) \uparrow p_\mu$ as $n \uparrow$. Therefore, $F_\mu^n(x) \to p_\mu$ for all $x \in (0, 1)$, so that p_μ is an attracting fixed point.

For $\mu > 2$ one has $p_\mu > 1/2$, and the above approach fails. Let us try to find an interval $[a, b]$ on which F_μ is monotone, and which is left invariant by $F_\mu : F_\mu([a, b]) \subset [a, b]$. One must have $\frac{1}{2} \leq a \leq b \leq 1$. It is simple to check that $[\frac{1}{2}, \mu/4]$ is such an interval provided $F_\mu(\mu/4) \equiv F_\mu^2(\frac{1}{2}) \geq 1/2$.

This holds iff $2 \leq \mu \leq 1+\sqrt{5}$. For such a μ, F_μ is strictly decreasing, and F_μ^2 strictly increasing, on $[\frac{1}{2}, \mu/4]$. Hence $F_\mu^{2n}(1/2) \uparrow$ and $F_\mu^{2n}(\mu/4) \downarrow$ as $n \uparrow$. Let $\alpha \equiv \alpha(\mu), \beta \equiv \beta(\mu)$ be the respective limits. Then $F_\mu^{2n}(x) \to \alpha$ for $x \in [\frac{1}{2}, \alpha], F_\mu^{2n}(x) \to \beta$ for $x \in [\beta, \mu/4]$. In particular, $\alpha \leq \beta$ are fixed points of F_μ^2. Since, for $2 < \mu \leq 3, F_\mu^2$ has no fixed points other than $0, p_\mu$, it follows that in this case $\alpha = \beta = p_\mu$, so that $F_\mu^n(x) \to p_\mu$ for all $x \in (0,1)$.

Consider $3 < \mu \leq 1+\sqrt{5}$. In this case $|F'_\mu(p_\mu)| = \mu - 2 > 1$. Therefore, p_μ is a repelling fixed point, so that $\alpha < p_\mu < \beta$. This implies that $\{\alpha, \beta\}$ is an *attracting period-two orbit* of F_μ. Since F_μ^2 is a fourth degree polynomial, $\{0, \alpha, p_\mu, \beta\}$ are the only fixed points for it. Since $0, p_\mu$ are repelling, it follows that $F_\mu^{2n}(x) \to \alpha$ or β for all $x \neq 0, 1$ or a preimage of p_μ. Note that $F_\mu^2(x) - x$ does not change sign on (α, p_μ) or on (p_μ, β). This analysis does not extend beyond $1+\sqrt{5}$. We conjecture that for $\mu > 1+\sqrt{5}$ a stable period-four orbit appears, while the period-two orbit (as well as the fixed points) becomes unstable.

For later purposes we consider intervals $[a, b]$ contained in $[0, \frac{1}{2}]$ or $[\frac{1}{2}, 1]$ and the set $I(a,b) := \{\mu \in [0,4] : F_\mu([a,b]) \subset [a,b]\}$. Straight forward calculations show

$$(3.1a) \qquad I(0,b) = \left[0, \frac{1}{1-b}\right] \text{ if } 0 \leq b \leq \frac{1}{2},$$

$$(3.1b) \qquad I(a,b) = \left[\frac{1}{1-a}, \frac{1}{1-b}\right] \text{ if } 0 < a \leq b \leq \frac{1}{2},$$

$$(3.1c) \qquad I(a,b) = \left[\frac{a}{b(1-b)}, \frac{b}{a(1-a)}\right] \text{ if } \frac{1}{2} \leq a \leq b \leq 1 \text{and } a^2(1-a) \leq b^2(1-b).$$

The second requirement in (3.1c) may be expressed as

$$(3.1c)' \qquad a \leq b \leq b^*(a) := \frac{1-a}{2} + \frac{1}{2}\sqrt{(1-a)(1+3a)},$$

which implies the further restriction

$$(3.1c)'' \qquad \frac{1}{2} \leq a \leq \frac{2}{3}.$$

The maximum value of $\mu \in [0,4]$ in the union of the sets $I(a,b)$ in (3.1c) (subject to (3.1c)′, (3.1c)″) is $\mu = 1+\sqrt{5}$. In particular,

$$(3.2) \qquad I\left(\frac{1}{2}, \frac{\mu}{4}\right) = \left[\frac{8}{\mu(4-\mu)}, \mu\right], \qquad 2 < \mu \leq 1+\sqrt{5}.$$

4. Main results: random iterations of two quadratic maps.

In this section we consider the Markov process X_n as defined in section 2, with $P(\alpha_1 = F_\mu) = \gamma$ and $P(\alpha_1 = F_\lambda) = 1 - \gamma$ for appropriate pairs $\mu < \lambda$ and $\gamma \in (0,1)$. If $0 \le \mu, \lambda \le 1$, then it follows from Section 3 that $Y_n(x) \to 0$ a.s. for all $x \in [0,1]$, so that the Dirac measure δ_0 is the unique invariant probability. Now take $1 < \mu < \lambda \le 2$, and let $a = p_\mu \equiv 1 - 1/\mu$ and $b = p_\lambda$ in (3.1b). Then F_μ, F_λ are both strictly increasing on $[p_\mu, p_\lambda]$ and leave this interval invariant. Since p_μ, p_λ are attracting for F_μ, F_λ, respectively, (2.2) holds for any $x_0 \in (p_\mu, p_\lambda)$ if m is large enough. It follows from Proposition 2.1 (or, Proposition 2.2) that there exists a unique invariant probability π on $[p_\mu, p_\lambda]$. Since $P(X_n(x) \in [p_\mu, p_\lambda]$ for some $n) = 1$ for all $x \in (0, p_\mu) \cup (p_\lambda, 1)$ it follows that the Markov process has a unique invariant probability, namely, π on the state space $(0,1)$ and that π is nonatomic. It is clear that both p_μ and p_λ belong to the *support* $S(\pi)$ *of* π as do the set of all points of the form

$$(4.1) \qquad \begin{aligned} &F_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k} p_\mu \equiv f_{\varepsilon_1} f_{\varepsilon_2} \cdots f_{\varepsilon_k} p_\mu \quad (f_0 := F_\mu, f_1 := F_\lambda), \\ &F_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k} p_\lambda \quad (k \ge 1), \end{aligned}$$

for all k–tuples $(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_k)$ of 0's and 1's and for all $k \ge 1$. Write $\text{Orb}(x; \mu, \lambda) = \{F_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k} x : k \ge 0, \varepsilon_i = 0 \text{ or } 1 \forall i\}$ ($k = 0$ corresponds to x). It is easy to see that if $x \in S(\pi)$ then $S(\pi) = \overline{Orb(x; \mu, \lambda)}$. This support, however, need not be $[p_\mu, p_\lambda]$. Indeed, if $F_\lambda(p_\mu) > F_\mu(p_\lambda)$, i.e.,

$$(4.2) \qquad \frac{1}{\lambda^2} - \frac{1}{\lambda^3} < \frac{1}{\mu^2} - \frac{1}{\mu^3} \qquad (1 < \mu < \lambda \le 2),$$

then $S(\pi)$ is a *Cantor subset* of $[p_\mu, p_\lambda]$. Before proving this assertion we identify pairs μ, λ satisfying (4.2). On the interval $[1,2]$ the function $g(x) := x^{-2} - x^{-3}$ is strictly increasing on $[1, 3/2]$ and strictly decreasing on $[3/2, 2]$, and $g(1) = 0, g(3/2) = 4/27, g(2) = 1/8$. Therefore, (4.2) holds iff

$$(4.3) \qquad \lambda \in (3/2, 2] \text{ and } \mu \in [\hat{\lambda}, \lambda),$$

where $\hat{\lambda} \le 3/2$ is uniquely defined for a given $\lambda \in (3/2, 2]$ by $g(\hat{\lambda}) = g(\lambda)$. Since the smallest value of $\hat{\lambda}$ as λ varies over $(3/2, 2]$ is $\sqrt{5} - 1$ which occurs when $\lambda = 2$ ($g(2) = 1/8$), it follows that μ can not be smaller than $\sqrt{5} - 1$ if (4.2) (or, (4.3)) holds.

To show that $S(\pi)$ is a Cantor set (i.e., a closed, no where dense set having no isolated point) for μ, λ satisfying (4.2), or (4.3), write $I = [p_\mu, p_\lambda], I_0 = F_\mu(I), I_1 = F_\lambda(I), I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k} = F_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}(I)$ for $k \ge 1$ and k–tuples $(\varepsilon_1\varepsilon_2\cdots\varepsilon_k)$ of 0's and 1's. Here $F_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k} = f_{\varepsilon_1} f_{\varepsilon_2} \cdots f_{\varepsilon_k}$ as defined in (4.1). Under the present hypothesis $F_\lambda(p_\mu) > F_\mu(p_\lambda)$ (or, (4.2)), the 2^k intervals $I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ are disjoint, as may be easily shown by induction, using the fact that F_μ, F_λ are strictly increasing on $[p_\mu, p_\lambda]$. Let $J_k = \cup I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ where the union is over the 2^k k-tuples $(\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_k)$. Since $X_k(x) \in J_k$ for all $x \in I$, and $J_k \downarrow$ as $k \uparrow, S(\pi) \subset J_k$ for all k, so that $S(\pi) \subset J := \cap_{k=1}^{\infty} J_k$. Further, F_μ is a *strict contraction* on $[p_\mu, p_\lambda]$ while $F_\lambda^n(I) \downarrow \{p_\lambda\}$ as $n \uparrow \infty$. Hence the lengths of $I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ go to zero as $k \to \infty$, for a sequence $(\varepsilon_1, \varepsilon_2, \cdots)$ which has only finitely many 0's or finitely many 1's. If there are infinitely many 0's and infinitely many 1's in $(\varepsilon_1, \varepsilon_2, \cdots)$ then for large k with $\varepsilon_k = 0$ one may express $f_{\varepsilon_1} f_{\varepsilon_2} \cdots f_{\varepsilon_k}$ as a large number of compositions of functions of the type F_μ^n or $F_\lambda^n F_\mu (n \geq 1)$. Since for all μ, λ satisfying (4.2) the derivatives of these functions on $[p_\mu, p_\lambda]$ are bounded by $F_\lambda'(p_\mu) F_\mu'(p_\mu) < 1$ (use induction on n and the estimate $F_\lambda'(F_\lambda p_\mu) < 1$) it follows that the lengths of the nested intervals $I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ go to zero as $k \to \infty$ (for every sequence $(\varepsilon_1, \varepsilon_2, \cdots)$). Thus, J does not contain any (nonempty) open interval. Also, $J \subset \overline{Orb(p_\mu; \mu, \lambda)} = \overline{Orb(p_\lambda; \mu, \lambda)}$ by the same reasoning, so that $J = S(\pi)$. Since π is nonatomic, $S(\pi)$ does not include any isolated point, completing the proof that $S(\pi)$ is a Cantor set.

Write $|A|$ for the Lebesgue measure of A. If, in addition to (4.2),

$$\lambda < \left(\frac{\mu - 1}{2 - \mu}\right) \mu, \tag{4.4}$$

then $|J| = 0$. Indeed, for any subinterval I' of I one has $|F_\lambda(I')| \leq F_\lambda'(p_\mu)|I'|$, $|F_\mu(I')| \leq F_\mu'(p_\mu)|I'|$, from which it follows that $|J_{k+1}| \leq (2 - \mu)(1 + \lambda/\mu)|J_k|$. If (4.4) holds then $c \equiv (2 - \mu)(1 + \lambda/\mu) < 1$, so that $|J| = 0$ if (4.2), (4.4) hold.

Note that the proof that $|I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}| \to 0$ depends only on the facts that on $[p_\mu, p_\lambda]$, (i) F_μ is a contraction, (ii) $F_\lambda^n(I) \downarrow \{p_\lambda\}$, and (iii) $F_\lambda'(F_\lambda p_\mu) < 1, F_\lambda'(p_\mu) F_\mu'(p_\mu) < 1$. The last condition (iii) may be expressed as

$$\lambda - 2\lambda^2(\mu - 1)/\mu^2 < 1, \ \lambda < \mu/(2 - \mu)^2 \ \ (1 < \mu < \lambda \leq 2). \tag{4.5}$$

If (4.5) holds, but (4.2) does not, then the 2^k intervals $I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ cover $I = [p_\mu, p_\lambda]$. Since the endpoints of $I_{\varepsilon_1\varepsilon_2\cdots\varepsilon_k}$ are in $S(\pi)$, it follows that $S(\pi) = [p_\mu, p_\lambda]$.

A point of additional interest is that if (4.2) (or (4.3)) holds then the Markov process X_n restricted to the invariant set $J = S(\pi)$ is isomorphic to one on $\{0, 1\}^{\mathbb{N}}$ having the transition probability

$$(\varepsilon_1, \varepsilon_2, \cdots) \to \begin{cases} (0, \varepsilon_1, \varepsilon_2, \cdots) & \text{with probability } \gamma, \\ (1, \varepsilon_1, \varepsilon_2, \cdots) & \text{with probability } 1 - \gamma. \end{cases} \tag{4.6}$$

The isomorphism is defined by $y \to (\varepsilon_1, \varepsilon_2, \cdots)$ where

$$y = \lim_{k\to\infty} f_{\varepsilon_1} f_{\varepsilon_2} \cdots f_{\varepsilon_k} p_\mu$$

In this representation for a fixed $\gamma \in (0,1)$ the Markov processes on $J = J_{\mu,\lambda}$ are the same for all μ, λ satisfying (4.2).

Next consider the case $2 < \mu < \lambda \le 3$. If $\mu \in I(\frac{1}{2}, \lambda/4) \equiv [8/\lambda(4-\lambda), \lambda)$ (see (3.2)) then F_μ, F_λ may be restricted to $[1/2, \lambda/4]$ and are strictly decreasing on it. Since p_μ, p_λ are attracting for F_μ, F_λ, respectively, (2.2) holds for any $x_0 \in (p_\mu, p_\lambda)$ if m is sufficiently large. It follows from Section 2 that there exists a unique invariant probability in $[p_\mu, p_\lambda]$ and it is nonatomic.

Finally, if $2 < \mu \le 3 < \lambda < 1+\sqrt{5}$ and $\mu \in I(1/2, \lambda/4) \equiv [8/\lambda(4-\lambda), \lambda)$, then p_μ is attracting for F_μ and $\beta \equiv \beta(\lambda)$ (see Section 3) is an attracting fixed point for F_λ^2. It follows that (2.2) holds on $[p_\mu, p_\lambda]$ in this case also if $x_0 \in (p_\lambda, \beta)$ and m is even and sufficiently large, so that the invariant probability on $[p_\mu, p_\lambda]$ (and also on $(0,1)$) is unique and nonatomic.

We state the main results proved above as a theorem. Note that δ_0 is invariant on $[0,1]$ for all $0 \le \mu < \lambda \le 4$.

THEOREM 4.1. (a) *If* $0 \le \mu < \lambda \le 1$, *then* δ_0 *is the unique invariant probability on* $[0,1]$. (b) *If* $1 < \mu < \lambda \le 2$ *then there exists a unique invariant probability* π *on* $(0,1)$. *This probability is nonatomic. If* μ, λ *satisfy* (4.2) *(or* (4.3)*) then the support* $S(\pi)$ *of* π *is a Cantor subset* $J \equiv J_{\mu,\lambda}$ *of* $[p_\mu, p_\lambda]$. *If,* (4.2) *and* (4.4) *both hold, then* $|J| = 0$. (c) *If the inequality* (4.2) *does not hold, but* (4.5) *holds, then* $S(\pi) = [p_\mu, p_\lambda]$. (d) *If* $2 < \mu < \lambda < 1+\sqrt{5}$ *and* $\mu \in [8/\lambda(4-\lambda), \lambda)$ *then there exists a unique invariant probability on* $(0,1)$, *which is nonatomic and has its support contained in* $[1/2, \lambda/4]$.

EXAMPLES.

1. If $\mu = \sqrt{5} - 1 = 1.232\cdots, \lambda = 2$, then (4.2) holds, but (4.4) does not, and $S(\pi) = J$ is a Cantor set.

2. If $\lambda = 2, -\frac{1}{2} + \frac{1}{2}\sqrt{17} < \mu < 2$, then (4.2), (4.4) both hold, and $S(\pi)$ is a Cantor set of Lebesgue measure zero.

3. If $\lambda = 3/2, 6/(3+\sqrt{5}) < \mu < 3/2$, then (4.2) does not hold, but (4.5) does, and $S(\pi) = [p_\mu, p_\lambda]$.

4. Suppose $0 < \mu < 1, 1 < \lambda < 2$. Theorem 4.1 does not apply. But if $\gamma \in (0,1)$ is such that $\mu^\gamma \lambda^{1-\gamma} < 1$, then δ_0 is the unique invariant probability (see Barnsley and Elton [1]).

We conclude with two remarks.

Remark 4.1.1 If $[a, b]$ is an invariant interval under F_μ and $F_\lambda (\mu < \lambda)$, then $[a, b]$ is invariant under F_γ for all $\gamma \in [\mu, \lambda]$. In particular, if $1 \leq \mu < \lambda \leq 2$, then the maps $F_\gamma(\gamma \in [\mu, \lambda])$ are all increasing on the invariant interval $[p_\mu, p_\lambda]$, and the splitting condition is satisfied by the Markov process on $[p_\mu, p_\lambda]$ corresponding to every randomization of F_γ's, $\gamma \in [\mu, \lambda]$. Thus there exists a unique invariant probability in this case on $[p_\mu, p_\lambda]$ (and on $(0, 1)$). If the support of the distribution of the random parameter γ is $[\mu, \lambda]$, then the support of the invariant probability is $[p_\mu, p_\lambda]$. A similar consideration applies to $2 < \mu < \lambda < 1 + \sqrt{5}$ if $\mu \in [8/\lambda(4 - \lambda), \lambda]$.

Remark 4.1.2. Let $1 < \mu < 2 < \lambda < 4$ be arbitrary. The interval $[1 - \frac{1}{\mu}, \frac{\lambda}{4}]$ is invariant under F_γ for all $\gamma \in [\mu, \lambda]$. Let F_γ be chosen at random such that the distribution of γ has a positive density with respect to Lebesgue measure m on $[\mu, \lambda]$. One may then show that the coresponding Markov process is m-irreducible on $[1 - \frac{1}{\mu}, \frac{\lambda}{4}]$. It follows from standard Markov process theory that in this case there exists a unique invariant probability. If, moreover, $\lambda > \frac{16}{\mu^3} - \frac{16}{\mu^2} + 4$, then one can show that the transition probability density $p(x, y)$ is no smaller than a nonzero, non-negative function $f(y)$ for all x in $[1 - \frac{1}{\mu}, \frac{\lambda}{4}]$. It is then easy to check that the n-step transition probability density $p^{(n)}(x, y)$ converges in L^1 to the invariant probability uniformly in x.

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10.3 "On a theorem of Dubins and Freedman"

On a theorem of Dubins and Freedman. Journal of Theoretical Probability. 12 (1999), 1067–1087 (with M. Majumdar).

On a Theorem of Dubins and Freedman[1]

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Under a notion of "splitting" the existence of a unique invariant probability, and a geometric rate of convergence to it in an appropriate metric, are established for Markov processes on a general state space S generated by iterations of i.i.d. maps on S. As corollaries we derive extensions of earlier results of Dubins and Freedman;(17) Yahav;(30) and Bhattacharya and Lee(6) for monotone maps. The general theorem applies in other contexts as well. It is also shown that the Dubins–Freedman result on the "necessity" of splitting in the case of increasing maps does not hold for decreasing maps, although the sufficiency part holds for both. In addition, the asymptotic stationarity of the process generated by i.i.d. nondecreasing maps is established without the requirement of continuity. Finally, the theory is applied to the random iteration of two (nonmonotone) quadratic maps each with two repelling fixed points and an attractive period-two orbit.

KEY WORDS: Iteration of i.i.d. maps; monotone maps; quadratic maps; Markov processes; asymptotic stationarity.

1. INTRODUCTION

A familiar method of construction Markov processes on a measurable state space $(S, \mathscr{S})$ is by means of a sequence of i.i.d. random maps α_n $(n = 1, 2,...)$ on S into S, defined on some probability space (Ω, F, P). For a given initial state $x \in S$ one defines the Markov process

$$X_0 = x, \qquad X_1 \equiv X_1(x) = \alpha_1 x,..., X_n \equiv X_n(x) = \alpha_n X_{n-1}$$
$$= \alpha_n \alpha_{n-1} \cdots \alpha_1 x \qquad (n \geq 1) \tag{1.1}$$

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Here, for each $\omega \in \Omega$, $\alpha_n(\omega)$ is a map on S and $\alpha_n(\omega)\, x$ is the value of $\alpha_n(\omega)$ at x. Also, $\alpha_n \alpha_{n-1} \cdots \alpha_1$ denotes the random composition whose realization at $\omega \in \Omega$ is $\alpha_n(\omega) \circ \alpha_{n-1}(\omega) \circ \cdots \circ \alpha_1(\omega)$.

Markov processes defined in this manner commonly occur in the context of linear and nonlinear autoregressive and ARMA models [See e.g., Bhattacharya and Waymire;(9) pp. 166 184; and Tong(27)]. For some other applications, see Athreya;(1) Barnsley and Demko;(3) Barnsley and Elton;(4) Mirman;(25) Majumdar *et al.*;(22) Bhattacharya and Majumdar(7) and other references listed. It may be noted that a Markov process with any given transition probability $p(x, B)$ ($x \in S$, B Borel) may be constructed in this manner, provided the state space S is a Borel subset of a Polish space [see e.g., Kifer,(19) p. 8; or Bhattacharya and Waymire,(9) p. 228], although such a construction is not unique.

The main focus of the present article is the class of Markov processes generated, as in (1.1), by i.i.d. *monotone* maps on a state space $S \subset \mathbb{R}$. An important result of Dubins and Freedman(17) for i.i.d. monotone continuous maps α_n ($n \geqslant 1$) on a compact interval $S = [a, b]$ is the following. Suppose the so-called *splitting condition* (**H**) is satisfied:

(**H**) There exist a number x_0, a positive integer N, and a constant $\delta > 0$, such that

$$\begin{aligned} &P(\alpha_N \alpha_{N-1} \cdots \alpha_1 x \leqslant x_0 \ \forall x \in S) \geqslant \delta, \\ &P(\alpha_N \alpha_{N-1} \cdots \alpha_1 x \geqslant x_0 \ \forall x \in S) \geqslant \delta \end{aligned} \tag{1.2}$$

Theorem (5.10) in Dubins and Freedman(17) then asserts that there exists a unique invariant probability π for the Markov process and that the n-step transition probability $p^{(n)}(x, B) := P(X_n(x) \in B)$ converges to π exponentially fast in the *Kolmogorov distance*, uniformly for all initial states x:

$$\begin{aligned} &\sup_{x \in S,\, y \in \mathbb{R}} |p^{(n)}(x, (-\infty, y] \cap S) - \pi((-\infty, y] \cap S)| \\ &\qquad \leqslant (1-\delta)^{[n/N]}, \qquad n \geqslant 1 \end{aligned} \tag{1.3}$$

where $[n/N]$ is the integer part of n/N.

For the case i.i.d. monotone nondecreasing maps α_n on a compact interval $S = [a, b]$, Yahav(30) proved the existence of a unique invariant probability π, without the requirement of continuity of α_n. These results were extended to multidimensional state spaces S in Bhattacharya and Lee(6) [also see Correction, ibid., (1997)], assuming (**H**) holds; here (i) S is an arbitrary closed subset of an Euclidean space, or an open or semiclosed rectangle, and (ii) α_n ($n \geqslant 1$) are i.i.d. monotone nondecreasing measurable maps on S. It is shown that $p^{(n)}(x, dy)$ converges exponentially fast in a Kolmogorov type distance to a unique invariant probability π, uniformly for all initial states x.

In Section 2 we extend the Dubins–Freedman result by (a) allowing $S \subset \mathbb{R}^1$ to be an arbitrary interval or an arbitrary closed set, and (b) dispensing with the requirement of continuity of the monotone i.i.d. maps α_n. This is obtained as a corollary (Corollary 1) of a general result Theorem 1 on an abstract measurable space $(S, \mathscr{S})$ on which are defined a sequence of i.i.d. maps satisfying a splitting type condition. A second corollary (Corollary 2) considers continuous i.i.d. maps on $S \subset \mathbb{R}^k$, and extends the main result in Bhattacharya and Lee[6] to monotone maps on $S \subset \mathbb{R}^k$ which may be nondecreasing and nonincreasing, each with positive probability. Example 1 provides a derivation of the Doeblin-type geometric ergodicity based on Theorem 1. It would be interesting to explore the connection between Theorem 1 and Tweedie's useful criteria for *geometric ergodicity*. [See Tweedie;[28,29] Meyn and Tweedie,[24] Chap. 15].

Dubins and Freedman[6] have also shown that for the case of strictly increasing and continuous (i.i.d.) α_n on $S = [a, b]$ such that there is no common fixed point of $\alpha_1(\omega)$, $\omega \in \Omega$, the splitting condition (**H**) is also *necessary* for the existence of a unique invariant probability π. This "necessity" was extended to compact subsets S of an Euclidean space in Bhattacharya and Lee[6] for nondecreasing α_n, again without the requirement of continuity. A natural question is: what happens if α_n are monotone *nonincreasing*? We show that the splitting condition (H) is no longer necessary for the existence of a unique invariant probability, even for $S = [a, b]$ and continuous α_n. (See the example in Section 4.)

Section 3 deals with the following question on the *asymptotic stationarity* of the Markov process $X_n(x)$ $(n \geq 0)$ in (1.1). Does the process $X_m^+(x) := (X_m(x), X_{m+1}(x),...)$ converge in distribution, as $m \to \infty$, to the distribution of the stationary Markov process $(X_0, X_1,...)$, where X_0 has the invariant distribution? The point is that $x \to p(x, dy)$ is not necessarily weakly continuous here without the requirement of continuity of α_n, and there are examples (we provide one of Liggett) in which the n-step transition probability $p^{(n)}(x, dy)$ of a Markov process on a compact state space converges to a probability π as $n \to \infty$ for every x, and yet π is not invariant. Theorem 3 says that if the α_n $(n \geq 0)$ are i.i.d. monotone nondecreasing on $S \subset \mathbb{R}$ (but not necessarily continuous), $X_n(x)$, $n \geq 0$, is asymptotically stationary. Although this is a result for a one-dimensional S, the proof of this seems nontrivial and requires the use of the multidimensional results of Bhattacharya and Lee.[6]

The final Section 4 deals with an example in which two *quadratic maps* $F_{\theta_i}(x) := \theta_i x(1-x)$ $(i = 1, 2)$ on $S = (0, 1)$, $3 < \theta_1 < \theta_2 < 1 + \sqrt{5}$, are chosen at random with probabilities η and $1-\eta$ $(0<\eta<1)$. Each map has an attractive period-two orbit encompassing a repelling fixed point. Although these maps are not monotone, the asymptotics of the Markov process $X_n(x)$, $n \geqslant 0$, can be completely analyzed by the theory for monotone maps. It may be shown that after an a.s. finite number of transitions the process $X_n(x)$ $(x \in (0, 1))$ lands in an invariant interval $[\frac{1}{2}, \theta_2/4]$. On this interval both F_{θ_i} are monotone decreasing. But the splitting condition does not hold for this process, restricted now to $[\frac{1}{2}, \theta_2/4]$. This Markov chain has a periodic behavior with cyclic transitions from one interval I_1 to another I_2, $I_1 \cap I_2 = \phi$. The n-step transition probability $p^{(n)}(x, dy)$ converges in *Caesaro mean* to a unique invariant π, exponentially fast in the Kolmogorov distance.

Random iterations of two quadratic maps have been studied in Bhattacharya and Rao[8] for cases where the splitting condition does hold on an invariant compact subinterval S of $(0, 1)$ on which F_{θ_i} are monotone $(i = 1, 2)$. The invariant probabilities here are often of the *Cantor type*. Further examples, with applications to economics, are considered in Bhattacharya and Majumdar.[7] The present example is the first one studied in which both F_{θ_i} have period-two orbits. Recently interesting necessary conditions for the existence of invariant probabilities on $(0, 1)$ have been obtained by Athreya and Dai.[2]

2. A GENERAL THEOREM UNDER A SPLITTING TYPE CONDITIONS

Let $(S, \mathscr{S})$ be a measurable space. Let α_n $(n \geqslant 1)$ be a sequence i.i.d. random maps on S defined on a probability space $(\Omega, \mathscr{F}, P)$, with a common distribution Q on (Γ, Σ). Here Γ is a set of maps on S (into itself), Σ is a sigmafield on Γ, and the map $(x, \gamma) \to \gamma x \equiv \gamma(x)$ is measurable on $(S \times \Gamma, \mathscr{S} \otimes \Sigma)$ into $(S, \mathscr{S})$. For $\gamma = (\gamma_1, ..., \gamma_n) \in \Gamma^n$, write $\tilde{\gamma}$ for the composition

$$\tilde{\gamma} := \gamma_n \gamma_{n-1} \cdots \gamma_1 \tag{2.1}$$

Suppose there exists a class of sets $\mathscr{A} \subset \mathscr{S}$ such that the following set of conditions $(\mathbf{H}_1)$ hold. Define the (pseudo) metric d on the *set* $\mathscr{P}(S)$ *of all probability measures on* $(S, \mathscr{S})$ by

$$d(\mu, \nu) := \sup_{A \in \mathscr{A}} |\mu(A) - \nu(A)| \qquad (\mu, \nu \in \mathscr{P}(S)) \tag{2.2}$$

($\mathbf{H}_1$) (1) $(\mathscr{P}(S), d)$ is a complete metric space;

(2) there exists a positive integer N such that for all $\gamma \in \Gamma^N$, one has

$$d(\mu\ \tilde{\gamma}^{-1}, \nu\ \tilde{\gamma}^{-1}) \leqslant d(\mu, \nu) \qquad (\mu, \nu \in \mathscr{P}(S)) \tag{2.3}$$

(3) there exists $\delta > 0$ such that $\forall A \in \mathscr{A}$, and with N as in (2) one has

$$P(\alpha_N \cdots \alpha_1^{-1} A = S \text{ or } \varphi) \geqslant \delta \tag{2.4}$$

Theorem 1. Assume the hypothesis ($\mathbf{H}_1$). Then there exists a unique invariant probability π for the Markov process $X_n := \alpha_n \cdots \alpha_1 X_0$, where X_0 is independent of $\{\alpha_n : n \geqslant 1\}$. Also, one has

$$d(T^{*n}\mu, \pi) \leqslant (1-\delta)^{[n/N]} \qquad (\mu \in \mathscr{P}(S)) \tag{2.5}$$

where $T^{*n}\mu$ is the distribution of X_n when X_0 has distribution μ.

Proof. Let $A \in \mathscr{A}$. Then (2.4) holds, which one may express as

$$Q^N(\{\gamma \in \Gamma^N : \tilde{\gamma}^{-1} A = S \text{ or } \varphi\}) \geqslant \delta \tag{2.6}$$

Then, $\forall \mu, \nu \in \mathscr{P}(S)$,

$$|(T^{*N}\mu)(A) - (T^{*N}\nu)(A)| = \left| \int_{\Gamma^N} (\mu(\tilde{\gamma}^{-1}A) - \nu(\tilde{\gamma}^{-1}A))\, Q^N(d\gamma) \right| \tag{2.7}$$

Denoting the set in curly brackets in (2.6) by Γ_1, one then has

$$|(T^{*N}\mu)(A) - (T^{*N}\nu)(A)|$$

$$= \left| \int_{\Gamma_1} (\mu(\tilde{\gamma}^{-1}A) - \nu(\tilde{\gamma}^{-1}A))\, Q^N(d\gamma) + \int_{\Gamma^N \setminus \Gamma_1} (\mu(\tilde{\gamma}^{-1}A) - \nu(\tilde{\gamma}^{-1}A))\, Q^N(d\gamma) \right|$$

$$= \left| \int_{\Gamma^N \setminus \Gamma_1} (\mu(\tilde{\gamma}^{-1}A) - \nu(\tilde{\gamma}^{-1}A))\, Q^N(d\gamma) \right| \tag{2.8}$$

since on Γ_1 the set $\tilde{\gamma}^{-1}A$ is S or φ, so that $\mu(\tilde{\gamma}^{-1}A) = 1 = \nu(\tilde{\gamma}^{-1}A)$, or $\mu(\tilde{\gamma}^{-1}A) = 0 = \nu(\tilde{\gamma}^{-1}A)$. Hence, using (2.3) and (2.4)

$$|(T^{*N}\mu)(A) - (T^{*N}\nu)(A)| \leqslant (1-\delta)\, d(\mu, \nu) \tag{2.9}$$

Thus

$$d(T^{*N}\mu, T^{*N}\nu) \leqslant (1-\delta)\, d(\mu, \nu) \tag{2.10}$$

Since $(\mathscr{P}(S), d)$ is a complete metric space by assumption $(\mathbf{H}_1)(1)$, and T^{*N} is a strict contraction on $\mathscr{P}(S)$ by (2.10), there exists a unique *fixed point* π of T^{*N}, i.e., $T^{*N}\pi = \pi$ [see Friedman,[18] p. 119], and

$$\begin{aligned} d(T^{*kN}\mu, \pi) &= d(T^{*N}(T^{*(k-1)N}\mu), T^{*N}\pi) \\ &\leqslant (1-\delta)\, d(T^{*(k-1)N}\mu, \pi) \leqslant \cdots \leqslant (1-\delta)^k\, d(\mu, \nu) \end{aligned} \tag{2.11}$$

Also,

$$\begin{aligned} d(T^*\pi, \pi) &= d(T^*T^{*kN}\pi, \pi) = d(T^{*kN}T^*\pi, \pi) \\ &\leqslant (1-\delta)^k\, d(T^*\pi, \pi) \to 0 \qquad \text{as} \quad k \to \infty \end{aligned}$$

Hence $d(T^*\pi, \pi) = 0$, which implies $T^*\pi = \pi$. Thus π is a fixed point of T^*. If π_1 is another fixed point of T^* then π_1 is a fixed point of T^{*N}. By the uniqueness of the fixed point of T^{*N}, $\pi_1 = \pi$. Finally, since $d(\mu, \nu) \leqslant 1$ one has, with $n = [n/N]\, N + r$,

$$(T^{*n}\mu, \pi) = d(T^{*[n/N]N}T^{*r}\mu, T^{*[n/N]N}\pi) \leqslant (1-\delta)^{[n/N]} \tag{2.12}$$

□

For (2.4), we have assumed the set within parentheses to be measurable. If it is not, then assume that there exists $F_A \in \mathscr{F}$, with $P(F_A) \geqslant \delta$, on which $\alpha_N \cdots \alpha_1^{-1} A = S$ or φ.

We now derive two corollaries of Theorem 1 applied to i.i.d. monotone maps. Corollary 1 extends a result of Dubins and Freedman,[17] [Thm. (5.10)], to more general state spaces in $\mathbb{R}$ and relaxes the requirement of continuity of α_n. The set of monotone maps may include both nondecreasing and nonincreasing ones.

Corollary 1. Let S be an interval or a closed subset of $\mathbb{R}$. Suppose α_n $(n \geqslant 1)$ is a sequence of i.i.d. monotone maps on S satisfying the splitting condition (**H**) in Section 1. Then there exists a unique invariant probability π for the Markov process X_n generated by α_n $(n \geqslant 1)$ and (1.3) holds for the n-step transition probabilities $p^{(n)}(x, dy)$.

Proof. First let S be a closed set. To apply Theorem 1, let $\mathscr{A}$ be the class of all sets $A = (-\infty, y] \cap S$, $y \in \mathbb{R}$. Completeness of $(\mathscr{P}(S), d)$ may be established directly, but also follows from a more general result in Bhattacharya and Lee[6] [Correction (1997)]. Hence the condition (1) of $(\mathbf{H}_1)$ holds.

To check condition (2) of $(\mathbf{H}_1)$ note that if γ is monotone nondecreasing and $A = (-\infty, y] \cap S$, then $\gamma^{-1}((-\infty, y] \cap S) = (-\infty, x] \cap S$ or

$(-\infty, x) \cap S$, where $x = \sup\{z: \gamma(z) \leqslant y\}$. Thus $|\mu(\gamma^{-1}A) - \nu(\gamma^{-1}A)| = |\mu((-\infty, x] \cap S) - \nu((-\infty, x] \cap S)|$ or, $|\mu((-\infty, x) \cap S) - \nu((-\infty, x) \cap S)|$. In either case, $|\mu(\gamma^{-1}A) - \nu(\gamma^{-1}A)| \leqslant d(\mu, \nu)$, since $\mu((-\infty, x - 1/n] \cap S) \uparrow \mu((-\infty, x) \cap S)$ (and the same holds for ν). If γ is monotone nonincreasing, then $\gamma^{-1}A$ is of the form $[x, \infty) \cap S$ or $(x, \infty) \cap S$, where $x := \inf\{z: \gamma(z) \leqslant y\}$. Again it is easily shown, $|\mu(\gamma^{-1}A) - \nu(\gamma^{-1}A)| \leqslant d(\mu, \nu)$. Finally, (2.4) holds for all $A = (-\infty, y] \cap S$, by (1.2).

If S is an interval which is not closed then there is a strictly increasing (continuous) homeomorphism h on S onto one of the following closed subsets of $\mathbb{R}$: $(-\infty, \infty)$, $(-\infty, a]$, $[a, \infty)$, depending on whether S is an open interval or semi-closed $(c, d]$, $[c, d)$. Since h preserves both the order and the topology of S, one may lift the state space to the closed set $h(S)$. □

To state the next corollary, let S be either a closed subset of $\mathbb{R}^k$ or a homeomorphic image of a closed subset by a strictly increasing (continuous) map h. Define $\mathscr{A}$ to be the class of all sets of the form

$$A = \{y: \phi(y) \leqslant x\}, \ \phi \text{ continuous and monotone on } S, \ x \in \mathbb{R}^k \tag{2.13}$$

Also, we will mean by "$\leqslant$" the *partial order*: $x = (x_1, ..., x_k) \leqslant y = (y_1, ..., y_k)$ iff $x_i \leqslant y_i$ $\forall i = 1, 2, ..., k$. In the following corollary we will interpret (**H**) (i.e., (1.2)) to hold with this partial order $\leqslant$, and with "$x \geqslant y$" meaning $y \leqslant x$.

Corollary 2. Let S and $\mathscr{A}$ be as before. If α_n $(n \geqslant 1)$ is a sequence of i.i.d. monotone maps which are continuous a.s., and the splitting condition (**H**) holds, then there exists a unique invariant probability π and

$$d(T^{*n}\mu, \pi) \leqslant (1-\delta)^{[n/N]} \qquad \forall \mu \in \mathscr{P}(S), \qquad n \geqslant 1 \tag{2.14}$$

where $d(\mu, \nu) := \sup\{|\mu(A) - \nu(A)|: A \in \mathscr{A}\}$.

Proof. As in the proof of Corollary 1, it is enough to prove the result for S closed. Then the completeness of $(\mathscr{P}(S), d)$ follows from Bhattacharya and Lee,[6] [Correction (1997)], where the proof of completeness does not depend on whether the ϕ in (2.13) are only monotone nondecreasing, or simply monotone. Condition (2) in $(\mathbf{H}_1)$ is immediate. For if $A = \{y: \phi(y) \leqslant x\}$, and γ is continuous and monotone, then $\gamma^{-1}A = \{y: (\phi \circ \gamma)\, y \leqslant x\} \in \mathscr{A}$ since $\phi \circ \gamma$ is monotone and continuous.

It remains to verify $(\mathbf{H}_1)(3)$. Let A in (2.13) be such that ϕ is monotone nondecreasing. If $\phi(x_0) \leqslant x$, then, by the splitting condition (**H**), (1.2),

$$\begin{aligned} \delta &\leqslant P(\alpha_N \cdots \alpha_1 z \leqslant x_0\ \forall z \in S) \leqslant P(\phi\alpha_N \cdots \alpha_1 z \leqslant \phi(x_0)\ \forall z \in S) \\ &\leqslant P(\phi\alpha_N \cdots \alpha_1 z \leqslant x\ \forall z \in S) = P(\alpha_N \cdots \alpha_1 z \in A\ \forall z \in S) \end{aligned} \tag{2.15}$$

If x in the definition of A in (2.13) is such that $\phi(x_0) \nleqslant x$ (i.e., at least one coordinate of $\phi(x_0)$ is larger than the corresponding coordinate of x), then

$$\begin{aligned} \delta &\leqslant P(\alpha_N \cdots \alpha_1 z \geqslant x_0 \; \forall z \in S) \leqslant P(\phi\alpha_N \cdots \alpha_1 z \geqslant \phi(x_0) \; \forall z \in S) \\ &\leqslant P(\phi\alpha_N \cdots \alpha_1 z \nleqslant x \; \forall z \in S) \leqslant P(\alpha_N \cdots \alpha_1 z \in A^c \; \forall z \in S) \end{aligned} \tag{2.16}$$

Now let ϕ in the definition of A in (2.13) be monotone decreasing. If $\phi(x_0) \leqslant x$, then

$$\begin{aligned} \delta &\leqslant P(\alpha_N \cdots \alpha_1 z \geqslant x_0 \; \forall z \in S) \\ &\leqslant P(\phi\alpha_N \cdots \alpha_1 z \leqslant \phi(x_0) \; \forall z \in S) \leqslant P(\phi\alpha_N \cdots \alpha_1 z \leqslant x \; \forall z \in S) \\ &= P(\alpha_N \cdots \alpha_1 z \in A \; \forall z \in S) \end{aligned} \tag{2.17}$$

If $\phi(x_0) \nleqslant x$, then

$$\begin{aligned} \delta &\leqslant P(\alpha_N \cdots \alpha_1 z \leqslant x_0 \; \forall z \in S) \leqslant P(\phi\alpha_N \cdots \alpha_1 z \geqslant \phi(x_0) \; \forall z \in S) \\ &\leqslant P(\phi\alpha_N \cdots \alpha_1 z \nleqslant x \; \forall z \in S) = P(\alpha_N \cdots \alpha_1 z \in A^c \; \forall z \in S) \end{aligned} \tag{2.18}$$

Thus $(\mathbf{H}_1)(3)$ is verified for all $A \in \mathscr{A}$. □

Remark 1. Corollary 2 extends the main theorem in Bhattacharya and Lee[6] [Correction, ibid, (1997)] to i.i.d. monotone maps which may include both types—increasing as well as decreasing.

Remark 2. For a deeper study of the completeness of $\mathscr{P}(S)$ under a metric somewhat stronger than d see Chakraborty and Rao.[12]

As an indication that Theorem 1 may be applied in contexts other than those of monotone maps, we give the following example.

Example 1. Let $p(x, A)$ be a transition probability on a Borel subset S of a Polish space with $\mathscr{S}$ as the Borel sigmafield on S. Suppose there exists a nonzero measure λ on S and a positive integer m such that

$$p^{(m)}(x, A) \geqslant \lambda(A) \qquad \forall x \in S, \quad A \in \mathscr{S} \tag{2.19}$$

Then it is known that there exists a unique invariant probability π for $p(\cdot, \cdot)$ such that

$$\sup_{x, A} |p^{(n)}(x, A) - \pi(A)| \leqslant (1 - \delta)^{[n/m]}, \qquad \delta := \lambda(S) \tag{2.20}$$

For a proof of this result of Doeblin and for some applications see Doob[16] [p. 197], or Bhattacharya and Waymire[9] [pp. 180, 181, 198, 199]. We now show that (2.20) is an almost immediate consequence of Theorem 1. For this express $p^{(m)}(x, A)$ as

$$p^{(m)}(x, A) = \lambda(A) + (p^{(m)}(x, A) - \lambda(A)) = \delta\lambda_\delta(A) + (1-\delta)\, q_\delta(x, A) \tag{2.21}$$

where

$$\lambda_\delta(A) := \frac{\lambda(A)}{\delta}, \qquad q_\delta(x, A) = \frac{p^{(m)}(x, A) - \lambda(A)}{1-\delta} \tag{2.22}$$

Let $\beta_n (n \geq 1)$ be an i.i.d. sequence of maps on S constructed as follows. For each n, with probability δ let $\beta_n x \equiv Z_n$ where Z_n is a random variable with values in S and distribution λ_δ; and with probability $1-\delta$, let $\beta_n = \alpha_n$ where α_n is a random map on S such that $P(\alpha_n x \in A) = q_\delta(x, A)$ [see Kifer,[19] p. 8; or Bhattacharya and Waymire,[9] p. 228, for constructing α_n]. Then Theorem 1 applies for the transition probability $p^{(m)}(x, A)$ (for $p(x, A)$), and with $\mathscr{A} = \mathscr{S}$, $N = 1$. Note that $P(\beta_1^{-1} A = S \text{ or } \varphi) \geq P(\beta_1(\cdot) \equiv Z_1) = \delta$. Hence (2.4) holds. Since $\mathscr{A} = \mathscr{S}$ in this example, completeness of $(\mathscr{P}(S), d)$ and the condition (2.3) obviously hold. It would be interesting to explore the connections between the present approach and Tweedie's general criteria for geometric ergodicity. [See Tweedie;[28, 29] Meyn and Tweedie,[24] Chap. 15].

As this example and corollaries indicate, the significance of Theorem 1 stems form the fact that it provides geometric rates of convergence in *appropriate metrics* for different classes of irreducible as well as non-irreducible Markov processes. The metric d depends on the structure of the process.

We now turn to the *necessity* of the splitting condition (**H**) for the existence of a unique invariant probability. For α_n ($n \geq 1$) i.i.d. nondecreasing and continuous on $S = [a, b]$ it was proved by Dubins and Freedman[16] [Thm. (5.17)], that, barring the case of a.s. all maps having a common fixed point, the splitting condition (**H**) is necessary for the existence of a unique invariant probability. An extension to compact $S \subset \mathbb{R}^k$ and measurable nondecreasing maps is given in Bhattacharya and Lee,[6] [Lemma 2.6]. It turns out that *if the maps are a.s. nonincreasing then splitting is not in general necessary for the existence of a unique invariant probability*, even in the case $S = [a, b]$ and α_n continuous. In Section 4, we construct an example in which two continuous decreasing maps F_{θ_1}, F_{θ_2} on an interval $[a, b]$ are randomly chosen with probabilities η and $1-\eta$, respectively $(0<\eta<1)$. The corresponding Markov process has a period-two cycle and a unique invariant probability, but the splitting condition (**H**) does not hold.

3. ASYMPTOTIC STATIONARITY OF MONOTONE STOCHASTIC DYNAMICAL SYSTEMS

Let (S, ρ) be a metric space, $\mathscr{S}$ its Borel sigmafield. Let $p(x, dy)$ be a transition probability on S, i.e., (i) for every $x \in S$, $B \to p(x, B)$ $(B \in \mathscr{S})$ is a probability measure on $(S, \mathscr{S})$ and (ii) for every $B \in \mathscr{S}$, $x \to p(x, B)$ is Borel measurable. Suppose that, for every x, the n-step transition probability $p^{(n)}(x, dy)$ converges weakly to a probability measure π on $(S, \mathscr{S})$ as $n \to \infty$, π being independent of x. It is well known that if, in addition, $x \to p(x, dy)$ is *weakly continuous*, then π is invariant and is the unique invariant probability for $p(x, dy)$. The following simple counter example due to Liggett,[21] communicated to us by E. Waymire, shows that the provision of weak continuity of $p(x, dy)$ can not in general be omitted in the last statement.

Example 2. (Liggett). Consider the compact state space $S = \{0, 1\} \cup \{m/(m+1)\colon m = 1, 2,...\}$, $\mathscr{S}$ the Borel sigmafield ($\mathscr{S}=$ class of all subsets). Let $p(0, \{\frac{1}{2}\}) = 1$, $p(m/(m+1), \{(m+1)/(m+2)\}) = 1$ $\forall m = 1, 2,...,$ $p(1, \{0\}) = 1$. Then $p^{(n)}(x, dy)$ converges weakly to δ_1 (the point mass at 1) as $n \to \infty$, irrespective of the initial x. But δ_1 is not invariant and, indeed, there does not exist any invariant probability. This is of course a degenerate Markov process, where starting at any $x \in S$, X_n converges (pointwise) to 1. However, it is easy to modify the example so that the transition probability is not degenerate. For example, $p(0, \{\frac{1}{2}\}) = \theta$, $p(0, \{\frac{2}{3}\}) = 1-\theta$, $p(m/(m+1), \{(m+1)/(m+2)\}) = \theta$, $p(m/(m+1), \{(m+2)/(m+3)\}) = 1-\theta$ $\forall m = 1, 2,...,$ and $p(1, \{0\}) = \theta$, $p(1, \{\frac{1}{2}\}) = 1-\theta$ $(0 \leqslant \theta \leqslant 1)$.

Remark 3. It is simple to check that if, for all x in a metric space S, $(1/n)\sum_{m=1}^{n} p^{(m)}(x, B) \to \pi(B)$, as $n \to \infty$, for *all Borel B*, then π is invariant. Breiman[11], [pp. 133–135], gives a proof in the case $p^{(n)}(x, B) \to \pi(B)$ for al Borel B as $n \to \infty$. Essentially the same proof applies to the case of the convergence of the Caesaro mean $(1/n)\sum_{m=1}^{n} p^{(m)}(x, B)$.

It may be noted that in Theorem 1 no topological assumption is made on S. In Corollary 1 S is a metric space but $x \to p(x, dy)$ is in general not weakly continuous. The existence (and uniqueness) of an invariant probability in these cases is established by showing that T^{*N} is a strict contraction (and T^* is a contraction) on the complete metric space $(\mathscr{P}(S), d)$.

In the present section we investigate the asymptotic stationarity of the Markov process X_n $(n \geq 1)$.

Let (S, ρ) be a metric space, $\mathscr{S}$ its Borel sigmafield, and $p(x, dy)$ a transition probability on S. Let X_n $(n \geq 0)$ be a Markov spaces with transition probability $p(x, dy)$ and an arbitrary initial distribution (of $X(0)$). We will say X_n $(n \geq 0)$ is *asymptotically stationary* if $X_m^+ := (X_m, X_{m+1}, \ldots, X_{m+1}, \ldots)$ converges in distribution to a stationary Markov process, as $m \to \infty$.

Note that the distribution of X_m^+ is a probability measure, say Q_m^+, on $(S^\infty, \mathscr{S}^{\otimes\infty})$, where S^∞ is the space of all sequences $(x_0, x_1, \ldots)$ in S, and $\mathscr{S}^{\otimes\infty}$ is the usual product sigmafield on S^∞. The product topology on S^∞ is metrized by

$$\rho^\infty(\mathbf{x}, \mathbf{y}) := \sum_{n=0}^{\infty} \frac{1}{2^n} \frac{\rho(x_n, y_n)}{1 + \rho(x_n, y_n)} \qquad (\mathbf{x} = (x_0, x_1, \ldots), \quad \mathbf{y} = (y_0, y_1, \ldots)) \tag{3.1}$$

On the question of asymptotic stationary, the following result is perhaps well known. We therefore omit its proof.

Theorem 2. Let (S, ρ) be a separable metric space, and $p(x, dy)$ a weakly continuous transition probability on it. Suppose $p^{(n)}(x, dy)$ converges weakly to a probability measure π as $n \to \infty$, irrespective of x. Then π is invariant, and the Markov process starting at an arbitrary initial distribution is asymptotically stationary.

Our main result in this section says that Markov processes generated by i.i.d. monotone maps on an interval S, and satisfying the splitting condition (**H**), (see (1.2)) are asymptotically stationary. This is significant since $p(x, dy)$ may not be weakly continuous. In certain classes of models arising in optimization problems in economics, the maps α_n are increasing but not continuous [see Majumdar *et al.*[22]].

Theorem 3. Let S be either an interval or a closed subset of $\mathbb{R}$, and let α_n $(n \geq 1)$ be a sequence of i.i.d. monotone nondecreasing maps on S. If the splitting condition (**H**) in (1.2) holds, then the Markov process $X_n := \alpha_n \cdots \alpha_1 x$ $(n \geq 1)$, $X_0 = x$, is asymptotically stationary, no matter what the initial state x may be.

Two main components in the proof of Theorem 3 are (1) the fact that the weak convergence of finite dimensional distributions implies weak convergence on $\mathscr{P}(S^\infty)$ (see Lemma 1) and (2) an extension of the Dubins–

Freedman theorem to measurable monotone nondecreasing maps on arbitrary closed subsets S of Euclidean space [Bhattacharya and Lee,[6] Correction, ibid., (1997)]. For (2) the splitting condition (1.2) reads the same, provided one uses the partial order: "$(x_1, x_2,..., x_k) \leqslant (y_1, y_2,..., y_k)$" if $x_i \leqslant y_i$ $\forall i = 1, 2,..., k$.

Lemma 1. Let (S, ρ) be a separable metric space, and S^∞ the space of all sequences $\mathbf{x} = (x_0, x_1, x_2,...)$ of elements of S, with the product topology. Let $C_f(S^\infty)$ be the set of all real-valued bounded continuous functions on S^∞ depending only on finitely many coordinates. If P_n $(n \geqslant 1)$, P are probability measures on the Borel σ-field $\mathscr{S}^{\otimes\infty}$ such that

$$\int h\, dP_n \to \int h\, dP \qquad \text{for all} \quad h \in C_f(S^\infty), \qquad \text{as} \quad n \to \infty \tag{3.2}$$

then P_n converges weakly to P.

Lemma 1 is well known and its proof is therefore omitted [see Billingsley,[10] p. 22, Problem 7].

Proof of Theorem 3. For specificity, write $X_n(x) := \alpha_n \cdots \alpha_1 x$. In view of Lemma 1 it is enough now to show that for every $k \geqslant 0$, the distribution $Q_{n,k}(x)$, say, of $Z_{n,k}(x) := (X_{n-k}(x), X_{n-k+1}(x),..., X_n(x))$ converges weakly to the distribution Q_k of $Z_k := (X_0, X_1,..., X_k)$, as $n \to \infty$. Here X_0 has the invariant distribution π, so that $(X_0, X_1,...)$ is the stationary Markov process with $X_n := \alpha_n \cdots \alpha_1 X_0$ $(n \geqslant 1)$. Fix $k \geqslant 0$. Define the following sequence of i.i.d. maps β_n on S^{k+1} into S^{k+1}.

$$\beta_n(y_0, y_1,..., y_k) := (y_1, y_2,..., y_k, \alpha_n y_k) \qquad (n \geqslant 1) \tag{3.3}$$

Then

$$\begin{aligned}
\beta_1(y_0, y_1,..., y_k) &= (y_1, y_2,..., y_k, \alpha_1 y_k),\\
\beta_2\beta_1(y_0, y_1,..., y_k) &= (y_2, y_3,..., y_k, \alpha_1 y_k, \alpha_2\alpha_1 y_k),\\
\beta_{k+1} \cdots \beta_1(y_0, y_1,..., y_k) &= (\alpha_1 y_k, \alpha_2\alpha_1 y_k,..., \alpha_{k+1} \cdots \alpha_1 y_k),\\
\beta_n \cdots \beta_1(y_0, y_1,..., y_k) &= (\alpha_{n-k} \cdots \alpha_1 y_k,..., \alpha_n \cdots \alpha_1 y_k) \qquad (n \geqslant k+1)
\end{aligned} \tag{3.4}$$

Note that the map (3.3) is (a.s.) monotone nondecreasing on S^{k+1} into S^{k+1}, and that

$$Z_{n,k}(x) = \beta_n \cdots \beta_1(x, x,..., x) \qquad (x \in S, n \geqslant k+1) \tag{3.5}$$

Now, with x_0 and N as in (**H**),

$$\begin{aligned}
&P(\beta_{N+k}\cdots\beta_1(y_0, y_1,..., y_k)\\
&\geqslant (x_0, x_0,..., x_0) \qquad \forall (y_0, y_1,..., y_k)\in S^{k+1})\\
&= P(\alpha_N\cdots\alpha_1 y_k \geqslant x_0, \alpha_{N+1}\alpha_N\cdots\alpha_1 y_k\geqslant x_0,..., \alpha_{N+k}\cdots\alpha_1 y_k\geqslant x_0, \forall y_k\in S)\\
&\geqslant P(\{\alpha_N\cdots\alpha_1 y\geqslant x_0\ \forall y\in S\}\cap\{\alpha_{N+1}x_0\geqslant x_0\}\cap\cdots\cap\{\alpha_{N+k}x_0\geqslant x_0\})\\
&\geqslant \delta\cdot\delta_1^k
\end{aligned}\tag{3.6}$$

where $\delta := P(X_N(y)\geqslant x_0\ \forall y\in S)>0$ by (**H**), and $\delta_1 = P(\alpha_{N+1}x_0\geqslant x_0) = \cdots = P(\alpha_{N+k}x_0\geqslant x_0)$. Note that if $P(\alpha_{N+1}x_0\geqslant x_0)=0$ then $P(\alpha_{N+1}x_0<x_0)=1$, so that $P(\alpha_i x_0<x_0)=1\ \forall i$ and $P(\alpha_N\cdots\alpha_1 x_0<x_0)=1$, contradicting (**H**). Thus $\delta_1>0$. Similarly,

$$\begin{aligned}
&P(\beta_{N+k}\cdots\beta_1(y_0, y_1,..., y_k)\\
&\qquad \leqslant (x_0, x_0,..., x_0)\ \forall (y_0, y_1,..., y_k)\in S^{k+1})>0
\end{aligned}\tag{3.7}$$

Now (3.6) and (3.7) imply the splitting condition for the maps $\{\beta_n\}_{n\geqslant 1}$, with $\underline{x}_0 := (x_0, x_0,..., x_0)$, $N+k$ and $\delta\cdot\delta_1^k$ in the role of x_0, N, and δ respectively, in (**H**). Hence, by fact (2) mentioned after the statement of Theorem 3 [see Bhattacharya and Lee,[6] Thm. 2.1, and Correction, ibid. (1997)], $Q_{n,k}(x)\to Q_k$ weakly as $n\to\infty$. □

4. RANDOM ITERATION OF TWO QUADRATIC MAPS WITH PERIOD-TWO ORBITS

There are many examples in the literature of Markov processes generated by i.i.d. monotone random maps. They may arise in economics as *models of survival* or *growth*, or as *models of optimal transition of stocks* from one period to the next under uncertainty (Mirman;[25] Majumdar and Radner;[23] Majumdar *et al.*[22]) An exposition of these classes of problems in economics may be found n Bhattacharya and Majumdar.[7]

A different kind of application related to the generation of *random continued fractions* is provided by the decreasing maps $F_\varepsilon(x) := \varepsilon + (1/x)$ on $S=(0, \infty)$, where ε is chosen at random according to any given distribution on $[0, \infty)$. Interesting invariant distributions have been computed in this case for special distributions of ε [see Letac and Sheshadri;[20] Chassiang *et al.*;[14] Chamayou and Letac;[13] and Bhattacharya and Goswami[5]].

Another interesting application is to the study of Markov processes on $S=(0, 1)$ obtained by the random iteration of two *quadratic maps*

$F_{\theta_i}(x) = \theta_i x(1-x)$ $(i = 1, 2)$, choosing F_{θ_1} with probability η and F_{θ_2} with probability $1-\eta$, $0 < \eta < 1$. Although F_{θ_i} is not monotone $(i = 1, 2)$, for certain classes of pairs (θ_1, θ_2) of parameter values the Markov process enters an interval $I \subset (0, 1)$ after a finite (a.s.) number of steps with the properties: (1) I is *invariant* under F_{θ_i} $(i = 1, 2,)$ and (2) F_{θ_i} is monotone on I $(i = 1, 2,)$. One may then study the asymptotics of the Markov process on I as the new state space, since for large times the process will be in I a.s. Various interesting aspects of these asymptotics have been studied in Bhattacharya and Rao[8] and Bhattacharya and Majumdar.[7] In the present section we analyze the asymptotics for a pair (θ_1, θ_2) not covered earlier. Here F_{θ_i} $(i = 1, 2)$ both have attractive period-two orbits. Among other things, it is shown below that the resulting Markov process has a unique invariant probability, but does not satisfy the splitting condition (H). Thus, unlike the case of i.i.d. increasing maps, for Markov processes generated by i.i.d. iterations of decreasing maps splitting is *not necessary* for the existence of a unique invariant probability.

Assume that $3 < \theta_1 < \theta_2 \leqslant 1 + \sqrt{5}$. It is know [see Devaney;[15] pp. 31 39; or Sandefur,[26] pp. 172 181] that in this case F_{θ_1} has an unstable, or repelling, fixed point $q_{\theta_i} := 1 - \theta_i^{-1}$ encompassed by an attractive, or stable, period-two orbit $\{p_{\theta_i}, r_{\theta_i}\}$, $\frac{1}{2} < p_{\theta_i} < q_{\theta_i} < r_{\theta_i} < \theta_i/4$ $(i = 1, 2)$. The *interval* $I = [\frac{1}{2}, \theta_2/4]$ is easily seen to be *invariant* under each F_{θ_i}, and F_{θ_i} is *decreasing* on $[\frac{1}{2}, \theta_2/4]$ $(i = 1, 2)$. To be specific, one has [see Sandefur,[26] p. 201]

$$p_{\theta_i} = \sqrt{\theta_i + 1}\left(\frac{\sqrt{\theta_i + 1} - \sqrt{\theta_i - 3}}{2\theta_i}\right) < q_{\theta_i} = 1 - \frac{1}{\theta_i} < r_{\theta_i}$$
$$= \sqrt{\theta_i + 1}\left(\frac{\sqrt{\theta_i + 1} + \sqrt{\theta_i - 3}}{2\theta_i}\right) \qquad (i = 1, 2) \tag{4.1}$$

For our main example take

$$\theta_1 = 3.15, \qquad \theta_2 = 3.2 \tag{4.2}$$

and consider the Markov process generated by i.i.d. random iterations of F_{θ_1} and F_{θ_2}, chosen with probabilities η and $1-\eta$, respectively, $0 < \eta < 1$. It follows from (4.1) and (4.2), that the fixed points of $F^2_{\theta_i} := F_{\theta_i} \circ F_{\theta_i}$ $(i = 1, 2)$ are (up to four decimal points)

$$\frac{1}{2} < p_{\theta_2} = 0.5130 < p_{\theta_1} = 0.5335 < q_{\theta_1} = 0.6825 < q_{\theta_2} = 0.6875$$
$$< r_{\theta_1} = 0.7840 < r_{\theta_2} = 0.7994 < \frac{\theta_2}{4} = 0.8 \tag{4.3}$$

To clearly specify the stochastic dynamics the following features of the maps F_{θ_i} should be noted (see Figs. 1–5)

$$\begin{aligned} &\text{(a)} \quad F_{\theta_i} \text{ decreases strictly on } \left[\frac{1}{2}, \frac{\theta_2}{4}\right] \qquad (i=1,2), \\ &\text{(b)} \quad F_{\theta_i} \circ F_{\theta_j} \text{ increases strictly on } \left[\frac{1}{2}, \frac{\theta_2}{4}\right] \qquad (i,j=1,2) \end{aligned} \tag{4.4}$$

and (see Figs. 3–5)

$$F^2_{\theta_i}(x) = \begin{cases} > x & \text{on } [\frac{1}{2}, p_{\theta_i}), \\ < x & \text{on } (p_{\theta_i}, q_{\theta_i}), \\ > x & \text{on } (q_{\theta_i}, r_{\theta_i}), \\ < x & \text{on } (r_{\theta_i}, \theta_2/4], \qquad (i=1,2) \end{cases} \tag{4.5}$$

As a consequence of (4.4) and (4.5), writing $F^n_{\theta_i}$ for the n-th iterate of F_{θ_i}, one has

$$F^{2n}_{\theta_i}(x) = \begin{cases} \uparrow p_{\theta_i} & \text{as } n \uparrow \text{ on } [\frac{1}{2}, p_{\theta_i}], \\ \downarrow p_{\theta_i} & \text{as } n \uparrow \text{ on } (p_{\theta_i}, q_{\theta_i}), \\ \uparrow r_{\theta_i} & \text{as } n \uparrow \text{ on } (q_{\theta_i}, r_{\theta_i}], \\ \downarrow r_{\theta_i} & \text{as } n \uparrow \text{ on } (r_{\theta_i}, \theta_2/4], \qquad (i=1,2) \end{cases} \tag{4.6}$$

Denote $I_1 = [p_{\theta_2}, p_{\theta_1}]$, $I_2 = [r_{\theta_1}, r_{\theta_2}]$. Since $F_{\theta_i}(p_{\theta_i}) = r_{\theta_i}$ and $F_{\theta_i}(r_{\theta_i}) = p_{\theta_i}$, it follows that (1) $F_{\theta_i}(I_1) \subset I_2$, $F_{\theta_i}(I_2) \subset I_1$ $(i=1,2)$, so that (2) $F_{\theta_i} \circ F_{\theta_j}$ leaves each of the intervals I_1 and I_2 invariant, for every pair (i, j), $i, j = 1, 2$. Thus the Markov process X_{2n} $(n = 0, 1, 2,...)$ may be restricted to the state space I_1, and the first two relations in (4.6) imply that this process satisfies the splitting condition (H) with an arbitrary $x_0 \in (p_{\theta_2}, p_{\theta_1})$, N sufficiently large, $\delta = \min\{\eta^N, (1-\eta)^N\}$. Let π_1 denote the unique invariant probability for X_{2n} $(n \geq 0)$ on I_1. Similarly, X_{2n} $(n \geq 0)$ is a Markov process on I_2 which, in view of the last two relations in (4.6), satisfies the splitting condition for any $x_0 \in (r_{\theta_1}, r_{\theta_2})$ and N sufficiently large. Let π_2 denote the unique invariant probability of X_{2n} $(n \geq 0)$ on I_2. Note that $I_1 \cap I_2 = \phi$, $I_1 \cup I_2 \subset [\frac{1}{2}, \theta_2/4]$. Then X_{2n} $(n \geq 0)$, considered as a Markov process on $[\frac{1}{2}, \theta_2/4]$, has *two ergodic invariant probabilities* π_1 and π_2. This, of course, implies that X_{2n} $(n \geq 0)$ on $[\frac{1}{2}, \theta_2/4]$ does not satisfy the splitting condition. Also note that, no matter what the initial state of X_{2n} $(n \geq 0)$, a.s. after a finite time the process enters $I_1 \cup I_2$. Thus it has no ergodic invariant probability other than π_1 and π_2.

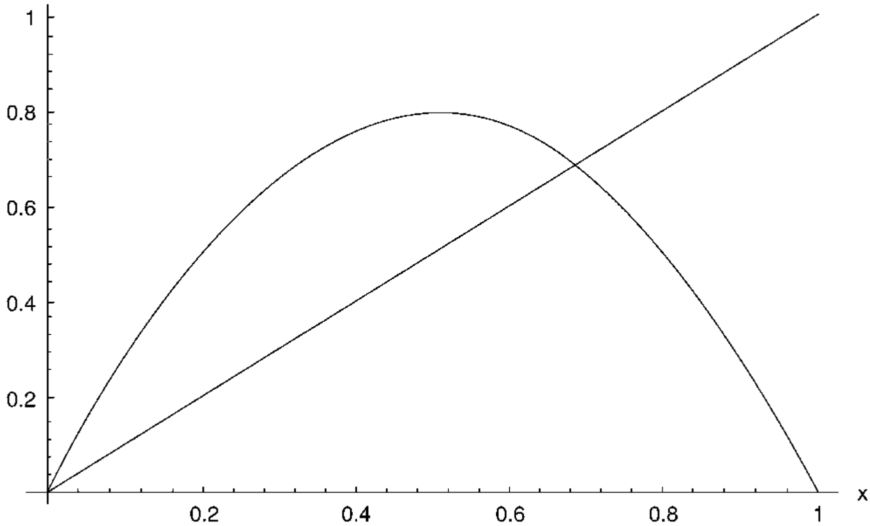


Fig. 1. Graph of $f(x) = 3.2x(1-x)$.

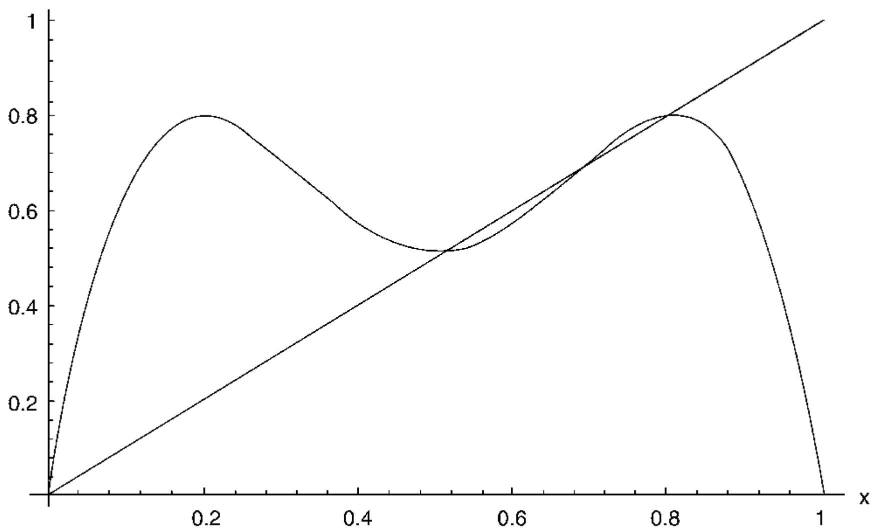


Fig. 2. Second Iterate of $f(x) = 3.2x(1-x)$.

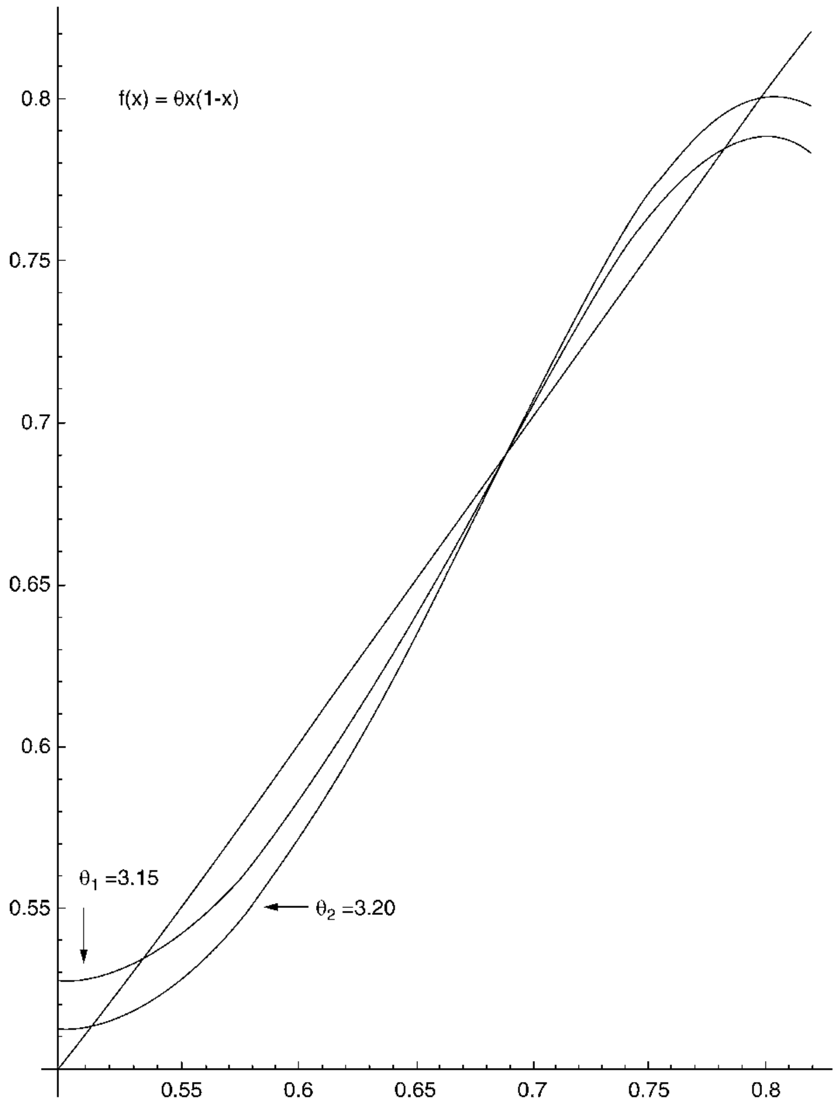


Fig. 3 Second Iterate of f.

Consider now the Markov process X_n $(n \geqslant 0)$ on $[\frac{1}{2}, \theta_2/4]$. This process *does not satisfy the splitting condition*. One way to see this is to note that $p^{(2n)}(x, I_j) = 0$ if $x \in I_i$ $(i \neq j)$, $p^{(2n)}(x, I_i) = 1$ if $x \in I_i$ $(i = 1, 2)$, $p^{(2n+1)}(x, I_j) = 1$ if $x \in I_i$ $(i \neq j)$, $p^{(2n+1)}(x, I_i) = 0$ if $x \in I_i$. The Markov process X_n $(n \geqslant 0)$ on $[\frac{1}{2}, \theta_2/4]$ is, however, *ergodic* with a *two-period cycle*

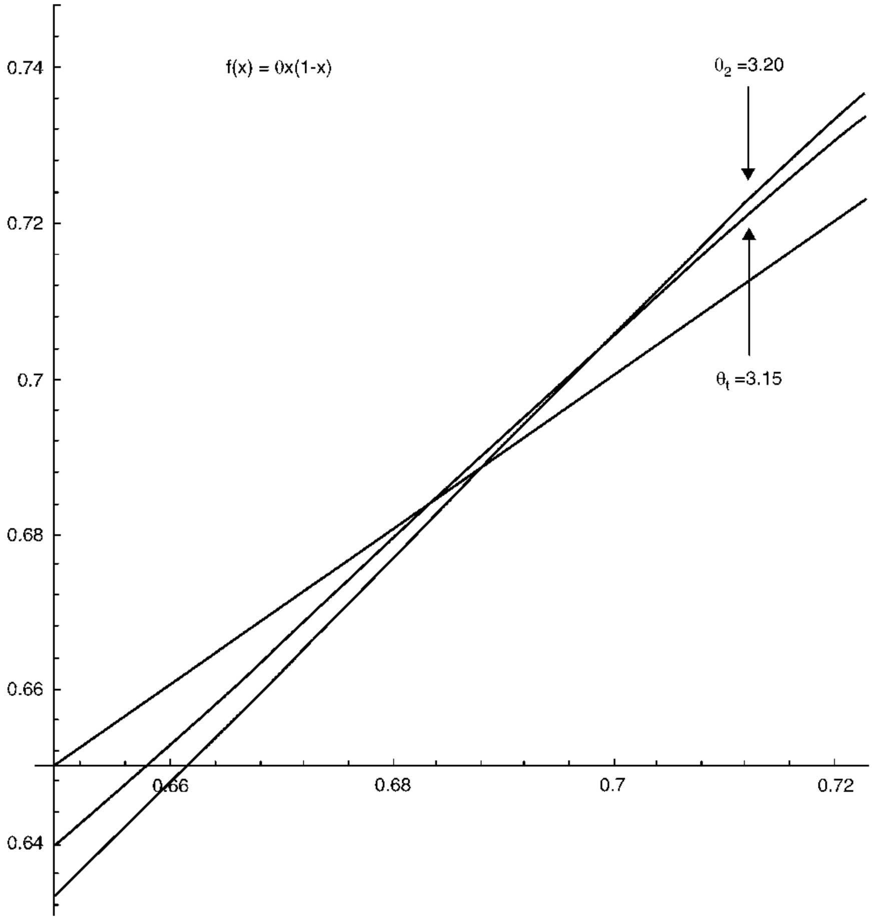
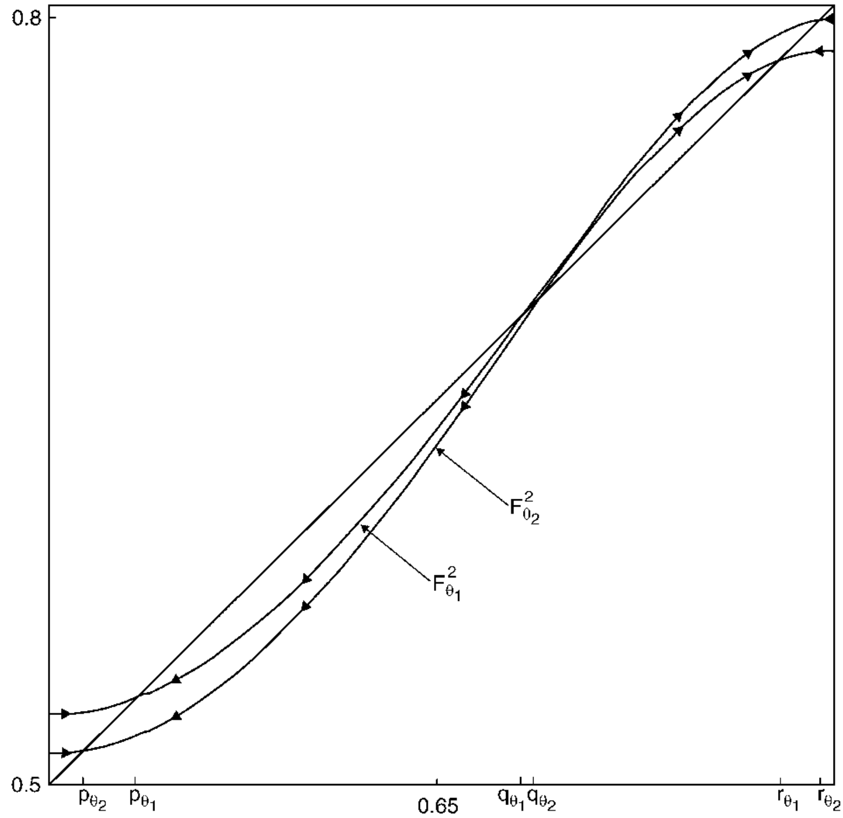


Fig. 4. Second Iterates of $f(0.65 < x < 0.73)$.

and has the unique invariant probability $\pi = \frac{1}{2}\pi_1 + \frac{1}{2}\pi_2$. To see this use the fact that X_{2n} $(n \geqslant 0)$ satisfies the splitting condition one each of I_1, I_2 and, therefore,

$$\sup_{\substack{x \in I_i \\ y \in \mathbb{R}}} |\, p^{(2n)}(x, (-\infty, y] \cap I_i) - \pi_i((-\infty, y] \cap I_i)| \leqslant (1-\delta)^{[n/N]} \qquad (i = 1, 2;\, n \geqslant 1) \tag{4.7}$$



Arrows show directions of trajectories depending upon the position of the initial point

Fig. 5. Schematic Diagram

Therefore , on the state space $S_0 := I_1 \cup I_2$ one has

$$\sup_{\substack{x \in S_0 \\ y \in \mathbb{R}}} \left| \frac{1}{2M} \sum_{n=1}^{2M} [\, p^{(n)}(x, (-\infty, y] \cap S_0) - \pi((-\infty, y] \cap S)] \right|$$

$$\leqslant (1-\delta)^{[M/N]} \qquad (M \geqslant 1) \tag{4.8}$$

In particular,

$$\frac{1}{n} \sum_{m=1}^{n} p^{(m)}(x, dy) \xrightarrow{\text{weakly}} \pi = \frac{1}{2}\pi_1 + \frac{1}{2}\pi_2 \qquad \forall x \in S_0 = I_1 \cup I_2 \tag{4.9}$$

Because $x \to p(x, dy)$ is weakly continuous (since F_{θ_i} are continuous), (4.9) implies π is the unique invariant probability for X_n $(n \geqslant 0)$ on $S_0 = I_1 \cup I_2$. Since it is easy to see (use (4.6)) that, whatever the initial state $x \in [\frac{1}{2}, \theta_2/4]$, the process X_{2n} (and, therefore, X_n) enters $I_1 \cup I_2 = S_0$ after a finite (a.s.) time, it follows that the weak convergence in (4.9) holds for all $x \in [\frac{1}{2}, \theta_2/4]$. Thus we have an example, where α_n $(n \geqslant 1)$ are i.i.d. monotone decreasing and continuous on a compact interval $[a, b] = [\frac{1}{2}, \theta_2/4]$, the corresponding Markov process X_n $(n \geqslant 0)$ has a unique invariant probability π, but the splitting condition does not hold.

To conclude the asymptotic analysis in this example, note that the Markov process X_n $(n \geqslant 0)$ on the state space $S = (0, 1)$ generated by the (nonmonotone) quadratic maps F_{θ_1}, F_{θ_2} on (0, 1) (chosen with probabilities η, $1 - \eta$, respectively) has the unique invariant probability $\pi = \frac{1}{2}\pi_1 + \frac{1}{2}\pi_2$. For no matter what the initial state $x \in (0, 1)$ may be, the process X_n enters the invariant interval $[\frac{1}{2}, \theta_2/4]$ after a finite (a.s.) number of steps. If one takes $S = [0, 1]$, then the Markov process starting at 0 remains at 0 for all times; if it starts from 1 then it moves to 0 in the next step. Thus 0 is an absorbing state, and δ_0 (the point mass at 0) is trivially an ergodic invariant probability of X_n $(n \geqslant 0)$, in addition to π. If the Markov process starts at any $x \neq 0, 1$, then $(1/n) \sum_{m=1}^{n} p^{(m)}(x, dy) \to \pi$ weakly as $n \to \infty$.

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10.4 "An approach to the existence of unique invariant probabilities for Markov processes"

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An Approach to the Existence of Unique Invariant Probabilities for Markov Processes*

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A notion of *localized splitting* is introduced as a further extension of the splitting notions for iterated monotone maps introduced earlier by Dubins and Freedman [16] and more generally by Bhattacharya and Majumdar [5]. We will see that under quite general conditions, *localized splitting theory* is a natural extension of the minorization theory [15], [14], recurrence theory [18], splitting theory of Nummelin [22] and regeneration theory of Athreya and Ney [3], under which we can prove the existence of a unique invariant probability. The paper is concluded with some new applications of splitting theory to random iterated quadratic maps.

1. Introduction and Some Background Results

The focus of this paper is the ergodic theory of Markov processes on a general state space viewed as actions of iterated random maps. In the case that S is a Borel subset of a Polish space a Markov process $\{X_n\}_{n=0}^{\infty}$ on $(S, \mathcal{S})$ with arbitrarily prescribed transition probability $p(x, dy)$ and initial state $x \in S$ may be represented by means of a sequence of *i.i.d.* random maps α_n on S into S, $n \geq 1$, defined on some probability space $(\Omega, \mathcal{F}, P)$ as:

$$X_0 = x, \quad X_1 = \alpha_1 x, \ldots, X_n = \alpha_n \cdots \alpha_1 x, \quad n \geq 1. \tag{1}$$

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Here $\alpha_n(\omega)$ is a map on S, for each $\omega \in \Omega$, whose value at $x \in S$ is denoted $\alpha_n x$ under the usual probability convention of suppressing ω. Also $\alpha_n \cdots \alpha_1$ denotes the n-fold composition of the maps $\alpha_n, \ldots, \alpha_1$.

Although the representation is not unique, the familiar "inverse distribution function method" used to generate simulations from a given distribution on the real number line lies at the heart of this representation; see [20] or [7, p. 228]. However another way in which Markov processes on a general state space with such representation occur, and which need not involve topological conditions on the state space, is simply as a *model* in some specific context, e.g., linear/nonlinear autoregressive and ARMA models, Markov Chain Monte Carlo, Bayesian statistics, economics, temporal discretization of diffusion, fractal image compression, etc. For an expository orientation to the breadth of applications accommodated by this viewpoint see the excellent recent article by Diaconis and Freedman [13], as well as Bhattacharya and Waymire [7], Bhattacharya and Waymire [8]. The article by Diaconis and Freedman [13] differs from the present approach in exploiting *contractive properties* of the maps on average, whereas our focus is on certain *splitting properties* of the maps which occur with positive probability.

So one may either assume at the outset that S is a Borel subset of a Polish space, or assume that one is given a Markov process on a measurable state space $(S, \mathcal{S})$ with the representation (1). It is most convenient for exposition to simply make the former assumption, which we will set as the framework for this paper.

Let us now attempt to give some background from the general ergodic theory for Markov processes for perspective on the framework being developed here. The reader is referred to Meyn and Tweedie [21] for a thorough and state of the art account of general minorization and small set theory, to Diaconis and Freedman [13] for the contractive mapping theory, and to Bhattacharya and Majumdar [5] for the recent splitting theory which spawned the present work.

When applicable *Doeblin's minorization* condition provides a powerful approach to check for the existence of a unique invariant probability, which also gives uniform exponential rates of convergence in total variation distance. In fact, Doeblin's minorization is also necessary for uniform exponential rates in total variation distance; see [23, Theorem 6.15], [25, Proposition 2], [21, Theorem 16.2.3]. Doeblin's minorization requires a probability measure ν on $(S, \mathcal{S})$, a positive integer N, and a positive real number δ such that

$$(2) \qquad p^{(N)}(x,B) \geq \delta\nu(B), \quad x \in S,\ B \in \mathcal{S},$$

where $p^{(m)}(x,dy)$ denotes the m-step transition probability defined inductively by

$$(3)\ p^{(0)}(x,dy) = \delta_x(dy), \quad p^{(m+1)}(x,B) = \int_X p(y,B)p^{(m)}(x,dy), \quad m \geq 0.$$

Theorem 1.1 (Doeblin's Minorization). *Under Doeblin's minorization condition* (2) *there is a unique invariant probability* π *on* $(S,\mathcal{S})$. *Moreover, for all* $x \in S$ *and* $B \in \mathcal{S}$,

$$\left|p^{(n)}(x,B) - \pi(B)\right| \leq (1-\delta)^{[\frac{n}{N}]} \quad n \geq 1.$$

We will derive Theorem 1.1 as a special case of Theorem 1.4 below involving a notion of splitting (see Remark 1.2 following the statement of Theorem 1.4).

The notion of a *small set* A_0 provides a *localized minorization* condition defined by a subset $A_0 \in \mathcal{S}$ of the state space S, a probability measure ν on $(A_0, A_0 \cap \mathcal{S})$, a positive integer N, and a positive real number δ such that

$$(4) \qquad p^{(N)}(x,B) \geq \delta\nu(B), \quad x \in A_0,\ B \in A_0 \cap \mathcal{S};$$

see [21] for a treatment of small sets. These are also the so-called C-sets in [24]. We simply refer to (4) as *local minorization on* A_0, where we will assume further that this occurs on a *recurrent set* A_0 in the sense that

$$(5) \qquad P_x\Big(\bigcup_{n=0}^{\infty}[X_n \in A_0]\Big) = 1, \quad x \in S.$$

Here and elsewhere P_x denotes probability, and E_x denotes expectation, when $X_0 \equiv x$. It was pointed out to the authors by K. B. Athreya (personal communication) that local minorization on a recurrent set is an equivalent condition for Harris' familiar notion of *φ-recurrence* whenever $\mathcal{S}$ is countably generated; necessity is proved in [24] and sufficiency is straightforward to check.

A formulation in terms of iterated maps may be obtained along the lines introduced by Athreya and Ney [3] to identify regeneration structure in locally minorized Markov processes on a recurrent set A_0.

Proposition 1.2 (Local Minorization). *The local minorization condition* (4) *on a recurrent set* A_0 *is equivalent to the existence of a representation by i.i.d. maps* $\alpha_1, \alpha_2, \ldots,$ *of the form* (1) *such that* $\alpha_N \ldots \alpha_1$ *is a constant map on* A_0 *into* A_0 *with probability* δ.

Proof. One may restrict attention to the case $N = 1$. Otherwise $p^{(N)}(x, B)$ is treated as a one-step transition probability. First observe that if such maps exist then for $x \in A_0$, $B \in \mathcal{S}$, one has

$$p(x,B) = P(\alpha_1 x \in B) \geq P(\alpha_1 \in \Gamma_c, \alpha_1 x \in B) = \delta P(\alpha_1 x \in B \,|\, \alpha_1 \in \Gamma_c),$$

where Γ_c denotes the collection of constant maps on A_0 into A_0. Conversely, suppose that local minorization holds on a recurrent set A_0. Let α_n be a representation by *i.i.d.* maps and define an alternative representation by *i.i.d.* maps β_n, $n \geq 1$ constructed as follows: Toss a coin with probability δ of heads. If head occurs then select a random point in A_0 distributed as ν and define $\beta_1 x$ as this constant value for all $x \in A_0$, but if tail occurs then for each $x \in A_0$ let $\beta_1 x$ be distributed as $(1-\delta)^{-1}\big(p(x,dy) - \delta\nu(dy)\big)$. If $x \in S - A_0$, then define $\beta_1 x = \alpha_1 x$. Now let β_n be an *i.i.d.* sequence of maps distributed. Then by such a construction

$$p(x,dy) = P(\beta_n x \in dy), \quad x \in S.$$

We leave the detailed construction of the probability space etc. to the reader; or see [9]. ■

The following theorem is a centerpiece of general Markov process theory based on various notions of Harris recurrence by Orey [24], regeneration by Athreya and Ney [3], or so-called Nummelin splitting [22]; see [21] for a comprehensive treatment. In Remark 3.3 in Section 3 we derive Theorem 1.3 as a special case of our Theorem 2.1 (and Lemma 2.3).

Theorem 1.3. *Assume the local minorization condition* (4) *on a recurrent set* A_0. *In addition assume that*

$$\sup_{x \in A_0} \mathbf{E}_x \tau_{A_0} < \infty,$$

where $\mathbf{E}_x$ *denotes expectation when* $X_0 = x$, *and*

$$\tau_{A_0} = \inf\{n \geq 1 \,:\, X_n \in A_0\}.$$

Then there is a unique invariant probability π *on* $(S, \mathcal{S})$. *Moreover for all* $x \in S$,

$$\sup_{B \in \mathcal{S}} \left| \frac{1}{n} \sum_{m=1}^{n} p^{(m)}(x, B) - \pi(B) \right| \to 0 \quad \text{as} \quad n \to \infty.$$

Remark 1.1. Recurrence of A_0 and the finiteness of the expected time to renew a visit to A_0 may often be checked by Foster–Tweedie *drift conditions,* or equivalently, *stochastic Lyapunov conditions;* see [21].

Finally let us record a generalization of the [16] splitting condition for monotone maps given by Bhattacharya and Majumdar [5]. This condition is defined by a sub-collection $\mathcal{A}$ of $\mathcal{S}$, a positive integer N and a positive real number δ such that

$$P\big((\alpha_N \cdots \alpha_1)^{-1} A = S \text{ or } \emptyset\big) \geq \delta \quad \text{for all} \quad A \in \mathcal{A}. \tag{6}$$

We will refer to this condition as *full splitting* and to the parameter N as a *splitting scale.* The sub-collection $\mathcal{A}$ of $\mathcal{S}$ will be called the *splitting class* of sets.

With a remarkably simple proof, Bhattacharya and Majumdar [5] obtained the following theorem. Denote by Q the distribution of α_1 on an appropriate space Γ of measurable maps γ of S into S.

Theorem 1.4. *Assume the full splitting condition* (6).

(i) *Assume that* $(\mathcal{P}(S), d)$ *is a complete metric space under*

$$d(\mu, \nu) = \sup_{B \in \mathcal{A}} \big|\mu(B) - \nu(B)\big|, \quad \mu, \nu \in \mathcal{P}(S),$$

where $\mathcal{P}(S)$ *denotes the space of probability measures on* $(S, \mathcal{S})$.

(ii) *Also with* N *as the splitting scale, assume that for every* N*-tuple of maps* $(\gamma_1, \ldots, \gamma_N)$ *outside a* Q^N*-null set,*

$$d\big(\mu \circ (\gamma_N \cdots \gamma_1)^{-1}, \nu \circ (\gamma_N \cdots \gamma_1)^{-1}\big) \leq d(\mu, \nu), \quad \mu, \nu \in \mathcal{P}(S).$$

Then there is a unique invariant probability π *on* $(S, \mathcal{S})$. *Moreover*

$$\sup_{x \in S, B \in \mathcal{A}} \big|p^{(n)}(x, B) - \pi(B)\big| \leq (1 - \delta)^{[\frac{n}{N}]}.$$

Remark 1.2 (Proof of Theorem 1.1). To derive Theorem 1.1 from Theorem 1.4 it is enough to consider the case $N = 1$. (Otherwise treat

$p^{(N)}(x, dy)$ as a one-step transition probability). Write $p(x, B) = \delta\nu(B) + (1-\delta)q(x, B)$, where $q(x, B) = \big(p(x, B) - \delta\nu(B)\big)/(1-\delta)$. Let $\{Z_n : n \geq 1\}$ be an i.i.d. sequence with common distribution ν. Define an i.i.d. sequence of maps $\{\alpha_n : n \geq 1\}$ such that (i) $\alpha_n x \equiv Z_n$ with probability δ, and (ii) with probability $1 - \delta$, $\alpha_n x$ has distribution $q(x, dy)$. Then (6) holds with $\mathcal{A} = \mathcal{S}$ and Theorem 1.4 applies.

Remark 1.3. It is known that the sufficient condition in Theorem 1.3 is necessary if the process is aperiodic ([21, p. 384]). Also, in the aperiodic case one may replace the Caesaro mean $\frac{1}{n}\sum_{m=1}^{n} p^{(m)}(x, B)$ by $p^{(n)}(x, B)$ by making use of the renewal theorem.

This is the starting point for the present paper. The remainder is organized as follows. In Section 2 we introduce a localized version of splitting and state our main theorem (Theorem 2.1) asserting the existence and uniqueness of an invariant probability under localized splitting conditions. This is followed by the proof of existence. The proof of uniqueness is taken up in Section 3. In the end we have a generalization of Theorem 1.4. Also, Theorem 1.4 and/or the Dubins and Freedman theory have found interesting applications to random iterations of (nonmonotone) quadratic maps, eg. see [6], [5], [1], [11]. These results are essentially obtained by finding an invariant set on which the maps are monotone, but may involve some delicate considerations of a splitting class of sets. This is illustrated in Section 4 with the introduction of a notion of *strict splitting* in the context of quadratic maps to extend previously known results significantly.

2. A Localized Splitting and Existence

Let us begin by introducing a localized version of the splitting condition (6).

Definition 2.1. The Markov process $\{X_n\}_{n=0}^{\infty}$ on $(S, \mathcal{S})$ is said to have a *locally splitting* representation by *i.i.d.* maps $\alpha_1, \alpha_2, \ldots$ if there is a *recurrent set* $A_0 \in \mathcal{S}$, a sub-collection $\mathcal{A}$ of $\mathcal{S}$, and a positive real number δ such that for each $A \in \mathcal{A}_0 \equiv A_0 \cap \mathcal{A}$,

$$P\big(A_0 \cap (\alpha_{\tau_{A_0}} \cdots \alpha_1)^{-1}A = A_0 \text{ or } \emptyset\big) \geq \delta. \tag{7}$$

Here τ_{A_0} is the first return time to A_0 so that, for $\omega \in \{\tau_{A_0} = n\}$, $\beta_1(\omega) := (\alpha_{\tau_{A_0}} \cdots \alpha_1)(\omega) = \alpha_n(\omega)\alpha_{n-1}(\omega) \cdots \alpha_1(\omega)$. The collection $\mathcal{A}_0$ is the *local splitting class.*

One may easily check from Proposition 1.2 that local minorization on a recurrent set A_0 implies local splitting on A_0 with $\mathcal{A} = \mathcal{S}$, i.e., with local splitting class $\mathcal{A}_0 = A_0 \cap \mathcal{S}$. We will consider a localization of splitting which generalizes this framework. We will require the local splitting class to be such that the space $\mathcal{P}(A_0)$ of probability measures on $(A_0, A_0 \cap \mathcal{A})$ is a complete metric space under

$$(8) \qquad d_0(\mu,\nu) = \sup_{B\in\mathcal{A}_0} \left|\mu(B) - \nu(B)\right|, \quad \mu,\nu \in \mathcal{P}(A_0).$$

Our main objective in this section and in Section 3 is to prove

Theorem 2.1. *Assume the local splitting condition* (7) *with local splitting class $\mathcal{A}_0 = A_0 \cap \mathcal{A}$ such that A_0 is a recurrent set and $\big(\mathcal{P}(A_0), d_0\big)$ is a complete metric space. If, in addition,*

$$\sup_{x\in A_0} \mathbf{E}_x\tau_{A_0} < \infty, \quad P_x(\tau_{A_0} < \infty) = 1 \quad \textit{for all } x \in A_0^c,$$

then there is a unique invariant probability π on $(S, \mathcal{S})$.

To prepare for the proof define

$$(9) \quad \tau_{A_0}^{(0)} := 0, \quad \tau_{A_0}^{(n+1)} := \inf\left\{ k > \tau_{A_0}^{(n)} : X_k \in A_0\right\}, \quad n = 0,1,2,\ldots.$$

Also we write $\tau_{A_0} \equiv \tau_{A_0}^{(1)}$. The process viewed only on its returns to A_0 will be denoted

$$(10) \qquad \tilde{X}_n = X_{\tau_{A_0}^{(n)}}, \quad n = 1,2,\ldots.$$

Define the kernel $p_{A_0}(x,B)$, $x \in S$, $B \in \mathcal{S}$, by

$$(11) \qquad p_{A_0}(x,B) = \sum_{n=1}^{\infty} P_x(X_n \in B,\ X_k \in A_0^c,\ 1 \le k < n).$$

It is well-known that the process $\{\tilde{X}_n\}_{n=0}^{\infty}$ is a Markov process with transition probabilities obtained from $p_{A_0}(x,B)$ by restricting x to A_0, and B to $\mathcal{S} \cap A_0$ (e.g. see [24]).

For $x \in A_0, B \in \mathcal{S}\cap A_0$, let $p_{A_0}^{(n)}(x,B)$ denote the n-step transition probability for the process on A_0 (with one-step transition probability p_{A_0}). For general $B \in \mathcal{S}$, we will write $p_{A_0}^{(n+1)}(x,B)$ for $\int_{A_0} p_{A_0}(y,B)p_{A_0}^{(n)}(x,dy)(n \ge 1)$, with $p_{A_0}^{(1)}(y,B) \equiv p_{A_0}(y,B)$ as defined in (11).

It will be important to observe that for each $x \in S$, the kernel $B \to p_{A_0}(x, B)$ defines a measure on the sigma-field $\mathcal{S}$. The probabilistic interpretation is that $p_{A_0}(x, B)$ is the expected number of visits to $B \in \mathcal{S}$ prior to revisiting A_0. In particular under the assumption

$$\sup_{x \in A_0} \mathbf{E}_x \tau_{A_0} < \infty, \tag{12}$$

one sees that

$$p_{A_0}(x, S) = \mathbf{E}_x \tau_{A_0} < \infty, \qquad x \in A_0. \tag{13}$$

Remark 2.1. One may check, as a warm-up exercise to Lemma 2.2, that if $p(x, dy)$ satisfies local minorization (4) on A_0 then $p_{A_0}(x, dy)$, $x \in A_0$, will satisfy Doeblin minorization (2) on A_0.

Lemma 2.2. *Under the conditions of Theorem 2.1, the process $\{\tilde{X}_n\}_{n=0}^{\infty}$, started at $\tilde{X}_0 = x \in A_0$, has a unique invariant probability π_{A_0} on $(A_0, A_0 \cap \mathcal{S})$. Moreover,*

$$\sup_{x \in A_0, B \in \mathcal{A}_0} \left| p_{A_0}^{(n)}(x, B) - \pi_{A_0}(B) \right| \le (1 - \delta)^n, \quad n \ge 1.$$

Proof. In view of Theorem 1.4 it suffices to show that the process $\{\tilde{X}_n\}_{n=0}^{\infty}$, started at $\tilde{X}_0 = x \in A_0$, has a full splitting representation on A_0. For this first let $\{\alpha_n\}_{n=1}^{\infty}$ denote a localized splitting representation of $\{X_n\}_{n=0}^{\infty}$. Define a random map β_1 on A_0 as follows: For $\omega \in \Omega$, define $\beta_1(\omega)$: $A_0 \to A_0$, as before, by

$$\beta_1(\omega) y = \alpha_{\tau_{A_0}(y)(\omega)}(\omega) \cdots \alpha_1(\omega) y, \qquad y \in A_0.$$

Now let $\beta_1, \beta_2, \ldots$ be an *i.i.d.* sequence of maps. This provides a representation since both $\{\tilde{X}_n\}_{n=0}^{\infty}$ and the process generated by the *i.i.d.* maps $\beta_1, \beta_2, \ldots$ are Markov processes with the same transition probabilities. To see that this is a full splitting representation on A_0 simply note that by (7),

$$P(\beta_1^{-1} A = A_0 \text{ or } \emptyset) \ge \delta \qquad \forall\, A \in \mathcal{A}_0 = A_0 \cap \mathcal{A}. \tag{14}$$

The other required conditions for Theorem 1.4 follow, with $N = 1$, immediately from the conditions of Theorem 2.1, since $\mathcal{A} = \mathcal{S}$. ■

Remark 2.2. One may notice from the proof of Lemma 2.2 that it is the condition (ii) of Theorem 1.4 that is the reason for our restriction on the local splitting class. Nonetheless, as will be seen, this localization significantly extends the applicability of Theorem 1.4.

With Lemma 2.2 the proof of the existence part of Theorem 2.1 may be completed by spreading π_{A_0} to $\mathcal{S}$ by defining

$$\pi(B) = c\int_{A_0} p_{A_0}(x,B)\pi_{A_0}(dx), B \in \mathcal{S}, \tag{15}$$

where

$$c^{-1} = \mathbf{E}_{\pi_{A_0}}\tau_{A_0} > 0,$$

and $\mathbf{E}_{\pi_{A_0}}$ denotes expectation when X_0 has distribution π_{A_0}. Note that on A_0, $\pi = c\pi_{A_0}$. Now the proof of existence is completed by virtue of the following straightforward lemma.

Lemma 2.3. *Under the conditions of Theorem* 2.1, (15) *defines an invariant probability on* $(S,\mathcal{S})$ *for* $p(x,dy)$. *Moreover, if* $\mathcal{A} = \mathcal{S}$, *then for* $x \in A_0$, $B \in \mathcal{S}$, $a := c\sup\{E_y\tau_{A_0} : y \in A_0\}$,

$$\left|cp_{A_0}^{(n+1)}(x,B) - \pi(B)\right| \le a(1-\delta)^n, \quad n \ge 1.$$

Proof. Let $B \in \mathcal{S}$. Then using Lemma 2.2,

$$\begin{aligned}
&\int_S p(y,B)\pi(dy) \\
&= \int_S p(y,B)c\int_{A_0} p_{A_0}(x,dy)\pi_{A_0}(dx) \\
&= c\int_S\int_{A_0}\sum_{n=1}^{\infty} p(y,B)P_x(X_n \in dy, X_k \in A_0^c \text{ for } 1 \le k < n)\pi_{A_0}(dx) \\
&= c\int_{A_0}\sum_{n=1}^{\infty} P_x(X_{n+1} \in B, X_k \in A_0^c \text{ for } 1 \le k < n)\pi_{A_0}(dx) \\
&= c\int_{A_0}\Big\{p_{A_0}(x,B) - p(x,B) \\
&\quad + \sum_{n=1}^{\infty} P_x(X_{n+1} \in B, X_n \in A_0, X_k \in A_0^c \text{ for } 1 \le k < n)\Big\}\pi_{A_0}(dx)
\end{aligned} \tag{16}$$

$$= \pi(B) - c\int_{A_0} p(x,B)\pi_{A_0}(dx)$$

$$+ c\int_{A_0}\int_{A_0} p(y,B)p_{A_0}(x,dy)\pi_{A_0}(dx) = \pi(B).$$

In addition, if $\mathcal{A} = \mathcal{S}$, note that for $x \in A_0$, $B \in \mathcal{S}$,

$$\left|cp_{A_0}^{(n+1)}(x,B) - \pi(B)\right| = \left|c\int_{A_0} p_{A_0}(y,B)\{p_{A_0}^{(n)}(x,dy) - \pi_{A_0}(dy)\}\right|$$
$$\leq \sup_{B\in A_0\cap\mathcal{S}} \left|p_{A_0}^{(n)}(x,B) - \pi_{A_0}(B)\right|,$$

so the convergence follows from Lemma 2.2, since $cp_{A_0}(y,B) \leq cp_{A_0}(y,S) \leq a$. ∎

3. Localized Splitting and Uniqueness

Let us suppose that π is an arbitrary invariant probability. The following lemma will be useful for extrapolating from stationarity on A_0 with respect to $P_{\pi_{A_0}}$. Let $\mathcal{F}$ denote the sigmafield of events $\sigma\{X_n : n \geq 0\}$.

Lemma 3.1. *Suppose π_{A_0} is the unique invariant probability for the process $\{\tilde{X}_n\}_{n=0}^{\infty}$ on the recurrent set A_0. Also assume (12) holds. If π is any invariant probability for $p(x,dy)$ then $\pi = c'\pi_{A_0}$ on $A_0 \cap \mathcal{S}$ with $c' = \pi(A_0)$. In particular,*

$$P_\pi(E) \geq c'P_{\pi_{A_0}}(E), \qquad E \in \mathcal{F},$$

i.e., $P_{\pi_{A_0}}$ is absolutely continuous with respect to P_π.

Proof. In view of recurrence it follows from [21, Theorem 10.4.7, p. 243] that π restricted to A_0 is invariant under $p_{A_0}(x,dy)$. Thus the first assertion follows from the uniqueness of π_{A_0}, and the second by

$$P_\pi(E) \geq \int_{A_0} P_y(E)\pi(dy) = c'\int_{A_0} P_y(E)\pi_{A_0}(dy) = c'P_{\pi_{A_0}}(E). \qquad ∎$$

Proof of Uniqueness in Theorem 2.1. Without loss of generality assume that π is an ergodic invariant probability; else, in view of the topological structure of S, one may take an ergodic component in the ergodic decomposition. The idea for proving uniqueness is to use the ergodic theorem to show that for bounded measurable functions $f : S \to \mathbf{R}$, $\int_S f d\pi$ is determined by f and expected values with respect to π_{A_0}. In particular, first note that by ergodicity of the process $\{X_n\}_{n=0}^{\infty}$ under P_π one has P_π-a.s. that

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} f(X_j) \to \int_S f\, d\pi. \tag{17}$$

In particular, taking $f = \mathbf{1}[A_0]$, one has P_π-a.s.

$$\lim_{n\to\infty} \frac{N_n}{n} = \pi(A_0), \tag{18}$$

where

$$N_n = \sum_{j=1}^{n} \mathbf{1}[X_j \in A_0] \tag{19}$$

denotes the number of visits to A_0 during $[1, n]$. Now, for arbitrary bounded measurable functions $f : S \to \mathbf{R}$ we have P_π-a.s.

$$\frac{1}{n} \sum_{j=1}^{n} f(X_j) - \frac{N_n}{n} \cdot \frac{1}{N_n} \sum_{m=1}^{N_n} Z_m \to 0 \tag{20}$$

as $n \to \infty$, where, for times $\tau^{(m)} := \tau_{A_0}^{(m)}$ ($\tau^{(0)} = 0$) defined by (9),

$$Z_m := \sum_{j=\tau^{(m-1)}+1}^{\tau^{(m)}} f(X_j), \qquad m \geq 1. \tag{21}$$

It follows from (17), (18) and (20) that the limit $\lim_{n\to\infty} \frac{1}{N_n} \sum_{m=1}^{N_n} Z_m$ exists P_π-a.s. and is given by $\frac{1}{\pi(A_0)} \int_S f d\pi$. But $\{Z_m\}_{m=1}^{\infty}$ is a stationary process under $P_{\pi_{A_0}}$, and therefore the sequence $\left\{ \frac{1}{N} \sum_{m=1}^{N} Z_m \right\}_{N=1}^{\infty}$ will converge $P_{\pi_{A_0}}$-a.s. and in L^1 to $E_{\pi_{A_0}} Z_1$. On the other hand, in view of Lemma 3.1, these imply that $P_{\pi_{A_0}}$-a.s.

$$E_{\pi_{A_0}} Z_1 = \lim_{N\to\infty} \frac{1}{N} \sum_{m=1}^{N} Z_m = \lim_{n\to\infty} \frac{1}{N_n} \sum_{m=1}^{N_n} Z_m = \frac{1}{\pi(A_0)} \int_S f\, d\pi. \tag{22}$$

Taking $f = 1$ in (22) identifies $\pi(A_0)$ as

$$\pi(A_0) = c \equiv \frac{1}{\mathbf{E}_{\pi_{A_0}} \tau_{A_0}}. \tag{23}$$

Thus we finally arrive at the unique determination of π via the formula

$$\int_S f\, d\pi = c\mathbf{E}_{\pi_{A_0}} Z_1 \tag{24}$$

for all bounded measurable functions f on S. ∎

Remark 3.1. To prove (20), note that the magnitude of the left side is no more than $M\big(\tau^{(k+1)} - \tau^{(k)}\big)/\tau^{(k)}$ with $k = N_n$ and $M = \sup\big\{\,|f(x)|\, : x \in S\big\}$. Now

$$\frac{\tau^{(k+1)} - \tau^{(k)}}{\tau^{(k)}} = \left(\frac{k}{\tau^{(k)}} - \frac{k+1}{\tau^{(k+1)}}\right)\cdot\frac{\tau^{(k+1)}}{k+1} + \frac{\tau^{(k+1)}}{k+1}\cdot\frac{k}{\tau^{(k)}}\cdot\frac{1}{k} \longrightarrow 0 \quad \text{a.s.} \quad (P_\pi)$$

as $k \to \infty$, taking $n = \tau^{(k)}$ and $n = \tau^{(k+1)}$, respectively, in (17) with $f = \mathbf{1}[A_0]$.

Remark 3.2. It is not necessary to use the ergodic decomposition in the above proof. For any invariant probability π, the convergence in (17) is replaced by convergence to a random variable a.s. and in L^1 (w.r.t. P_π). Hence one may take expectations on both sides to arrive at (24).

Remark 3.3 (Proof of Theorem 1.3.). Under the hypothesis of Theorem 1.3, and using a representation by i.i.d. iterated random maps α_n $(n \geq 1)$ (See Proposition 1.2), the assumptions of Theorem 2.1 are satisfied with $\mathcal{A}_0 = A_0 \cap \mathcal{S}$ (or, $\mathcal{A} = \mathcal{S}$). Hence the existence and uniqueness of an invariant probability follows from Theorem 2.1. The convergence $\pi(B)$ of $\left(\sum_{m=1}^{n} p^{(m)}(x, B)\right)/n$ uniformly for all $B \in \mathcal{S}$ is easily derived by the convergence to the invariant probability π_{A_0} of $p_{A_0}^{(n)}(x, dy)$ (on $(A_0, \mathcal{A}_0)$) in total variation distance given by Lemma 2.3.

Remark 3.4. Suppose A_0 is a closed, or invariant, set, i.e., $\alpha_n x \in A_0$ $\forall\, x \in A_0$ (a.s.). Then $\tau_{A_0} = 1$ (a.s. P_x) $\forall\, x \in A_0$, and β_n is the restriction of α_n to A_0. One may then apply Theorem 1.4 directly with $N = 1$, localized to A_0, to derive the conclusion of Theorem 2.1. In this case $\pi(B) = \pi_{A_0}(B \cap A_0)$ $\forall\, B \in \mathcal{S}$. On the other hand if, for some constant $N > 1$, $\alpha_N \cdots \alpha_1 x \in A_0$ $\forall\, x \in A_0$ (a.s.), one may replace the local splitting condition (7) by

$$P\big((\alpha_N \cdots \alpha_1)^{-1} A = A \text{ or } \emptyset\big) \geq \delta \qquad \forall\, A \in \mathcal{A}_0 = A_0 \cap \mathcal{A}. \tag{25}$$

Then the conclusion of Theorem 2.1 holds, i.e., there exists a unique invariant probability. If the constant $N > 1$ is the smallest such integer for which (25) holds, then typically the Markov process has a N-period cycle, (7) and (25) are the same with $\tau_{A_0} = N$. This is the case in Example 4 in Section 4.

5. Applications to Quadratic Maps

In this section Theorem 1.4 is applied to iterations of *i.i.d.* quadratic maps $\alpha_n = F_{\eta_n}(n \geq 1)$, where η_n $(n \geq 1)$ are *i.i.d.* random variables taking values in the parameter space $[0, 4]$ and, for each $\theta \in [0, 4]$,

$$F_\theta(x) = \theta x(1 - x), \qquad 0 \leq x \leq 1. \tag{26}$$

Since 0 is a common fixed point of all F_θ, the Dirac measure δ_0 is always an invariant probability for the Markov process $X_n(x) := \alpha_n \cdots \alpha_1 x$ $(n \geq 1)$, $X_0(x) = x$, on the state space $[0, 1]$. We focus on the existence and uniqueness of an invariant probability other than δ_0. The appropriate state space is then $S = (0, 1)$ left invariant by all F_θ.

We begin by recalling a few basic facts about the quadratic family $\{F_\theta : \theta \in [0, 4]\}$, shared by other unimodal families as well; see [10] and [12] for proofs and further properties. It is easily checked that for $0 \leq \theta \leq 1$ the map F_θ has the unique attracting fixed point 0. For $\theta > 1$, 0 is repelling for F_θ and a new fixed point $p_\theta = 1 - \frac{1}{\theta}$ appears, which is attractive for $1 < \theta \leq 3$, and repelling for $\theta > 3$. A period two orbit for F_θ appears for $\theta > 3$, which remains attractive for $3 < \theta \leq 1 + \sqrt{6}$, becoming repelling for $\theta > 1 + \sqrt{6}$, at which point a period-four orbit appears. In this manner period-doubling bifurcations take place for all periods $2^n (n \geq 0)$. Beyond this, other periods appear each with a period doubling sequence of its own. For $\theta \simeq 3.8284$ there appears an attractive period-three orbit. A well-known theorem of Sarkovskii (see [12, p. 60]) says that a continuous map with a period-three orbit has periodic orbits of all periods. Beyond the period-three regime, there are θ values which have no attractive periodic orbits, and chaos sets in. Although the set of θ's for which F_θ has an attractive periodic orbit is dense in $[0, 4]$, the set of θ's for which F_θ is chaotic or even has an absolutely continuous invariant probability, has positive Lebesgue measure ([19], [17]).

Turning to the Markov process $X_n := \alpha_n \cdots \alpha_1 X_0 (n \geq 1)$, with X_0 independent of $\{\alpha_n = F_{\theta_n} : n \geq 1\}$, the following lemma allows one to extend earlier results of Bhattacharya and Rao [6] and Bhattacharya and Majumdar [5]. In order to state it, we will recast the splitting class as $\mathcal{A} = \{[c,x] : c \le x \le d\}$ for the case of *i.i.d.* monotone maps $\{\alpha_n : n \ge 1\}$ on an interval $[c,d]$ as follows. The Markov process $X_n(x)$, $(n \ge 1)$, $X_0(x) = x$, $x \in [c,d]$ is said to have the splitting property if there exists $\delta > 0$, $x_0 \in [c,d]$, and an integer N such that

$$(27) \qquad P\big(X_N(x) \le x_0 \forall x \in [c,d] \text{ or } X_N(x) \ge x_0 \forall x \in [c,d]\big) \ge \delta.$$

It is shown in [16] that (27) implies the existence and uniqueness of an invariant probability π on $[c,d]$; i.e. Theorem 1.3 holds. If the inequalities '$\le x_0$' and '$\ge x_0$' appearing within parenthesis in (27) are replaced by strict inequalities '$< x_0$' and '$> x_0$', respectively, then the above property will be referred to as a *strict splitting property.* Note that (27), or its strict version, is a property of the distribution Q of η_n. Denote by Q^N the (product) probability distribution of $(\eta_1, \ldots, \eta_N)$.

Lemma 4.1. *Let $\theta_1 < \theta_2$ and $m \ge 1$ be given.*

(a) *If, for all $\theta^i \in \{\theta_1, \theta_2\}$, $1 \le i \le m$, the range of $F_{\theta^1} \cdots F_{\theta^m}$ on an interval $I_1 = [u_1, v_1]$ is contained in $I_2 = [u_2, v_2]$, then the same is true for all $\theta^i \in [\theta_1, \theta_2]$. In particular, if $F_{\theta^1} \cdots F_{\theta^m}$ leaves an interval $[c,d]$ invariant for all $\theta^i \in \{\theta_1, \theta_2\}$, $1 \le i \le m$, then the same is true for all $\theta^i \in [\theta_1, \theta_2]$, $1 \le i \le m$.*

(b) *Suppose, for all $\theta^i \in \{\theta_1, \theta_2\}$, $1 \le i \le m$, $F_{\theta^1} \cdots F_{\theta^m}$ leaves invariant an interval $[c,d]$. Assume also that the strict splitting property above holds, with $N = km$ a multiple of m, for a distribution $Q = Q_0$ whose support is $\{\theta_1, \theta_2\}$. Then* (i) *$F_{\theta^1} \cdots F_{\theta^m}$ leaves $[c,d]$ invariant for all $\theta^i \in [\theta_1, \theta_2]$, and* (ii) *the strict splitting property holds for an arbitrary $Q = \hat{Q}$ whose support has θ_1 as the smallest point and θ_2 as its largest.*

Proof. (a) The proof is by induction on m. The assertion is true for $m = 1$, since in this case $u_2 \le \min\{F_{\theta_1}(y) : y \in [u_1, v_1]\} \le F_\theta(x) \le \max\{F_{\theta_2}(y) : y \in [u_1, v_1]\} \le v_2$, for all $x \in [u_1, v_1]$. Assume the assertion is true for some integer $m \ge 1$. Let $a = \min\{F_{\theta^2} \cdots F_{\theta^{m+1}}(x) : \theta^i \in \{\theta_1, \theta_2\}, 2 \le i \le m+1, x \in [u_1, v_1]\}$, and $b = \max\{F_{\theta^2} \cdots F_{\theta^{m+1}}(x) : \theta^i \in \{\theta_1, \theta_2\}, 2 \le i \le m+1, x \in [u_1, v_1]\}$. By the induction hypothesis, for arbitrary $\theta^2, \ldots, \theta^{m+1} \in [\theta_1, \theta_2]$, the range of $F_{\theta^2} \cdots F_{\theta^{m+1}}$ on $[u_1, v_1]$ is contained in $[a,b]$. On the other hand, $u_2 \le \min\{F_{\theta_1}(y) : y \in [a,b]\}$, $v_2 \ge \max\{F_{\theta_2}(y) : y \in [a,b]\}$. Hence, for arbitrary $\theta^1, \ldots, \theta^{m+1} \in [\theta_1, \theta_2]$, the range of $F_{\theta^1} \cdots F_{\theta^{m+1}}$ on $[u_1, v_1]$ is contained in $[u_2, v_2]$, thus completing the induction argument.

(b)(ii) Suppose a strict splitting property holds with $\delta > 0$, x_0, N. Define the continuous functions L, l on $[\theta_1, \theta_2]^N$ by

$$(28) \qquad \begin{cases} L(\theta^1, \ldots, \theta^N) := \max\limits_{c \le x \le d} F_{\theta^1} \cdots F_{\theta^N}(x), \\ \\ l(\theta^1, \ldots, \theta^N) := \min\limits_{c \le x \le d} F_{\theta^1} \cdots F_{\theta^N}(x) \end{cases}$$

By hypothesis, the open subset U of $[\theta_1, \theta_2]^N$ defined by $U := \{(\theta^1, \ldots, \theta^N) \in [\theta_1, \theta_2]^N : L(\theta^1, \ldots, \theta^N) < x_0\}$, includes a point $(\theta_0^1, \ldots, \theta_0^N) \in \{\theta_1, \theta_2\}^N$. Therefore U contains a rectangle $R = R_1 \times \cdots \times R_N$ where R_i is of the form $R_i = [\theta_1, \theta_1 + h_i)$ or $R_i = (\theta_2 - h_i, \theta_2]$ for some $h_i > 0 (1 \le i \le N)$, depending on whether $\theta_0^i = \theta_1$ or $\theta_0^i = \theta_2$. By the hypothesis on $\hat{Q}$, $\delta_1 := \hat{Q}^N(R) = \hat{Q}(R_1) \cdots \hat{Q}(R_N) > 0$. Hence the first inequality within parentheses in (27) (with '$< x_0$') holds with probability at least δ_1. Similarly, the second inequality in (27) holds (with '$> x_0$') with some probability $\delta_2 > 0$, since $V := \{(\theta^1, \ldots, \theta^N) \in [\theta_1, \theta_2]^N : l(\theta^1, \ldots, \theta^N) > x_0\}$ is an open subset of $[\theta_1, \theta_2]^N$, which includes a point $(\theta_0^1, \ldots, \theta_0^N) \in \{\theta_1, \theta_2\}^N$. Now take the minimum of δ_1, δ_2 for δ in (27). Finally, the invariance of $[c, d]$ under $F_{\theta^1} \cdots F_{\theta^N}$ for all $\theta^i \in [\theta_1, \theta_2]$, $1 \le i \le N$, follows from (a). ∎

In Examples 1–4 below the invariant interval $[c, d]$ is either contained in $\left(0, \frac{1}{2}\right]$ or in $\left[\frac{1}{2}, 1\right)$ to insure monotonicity of $\alpha_n = F_{\eta_n}$, so that the theorem of [16], i.e. Theorem 1.4 with $\mathcal{A} = \{[c, x] : c \le x \le d\}$, can be applied to the process $\{Y_k := X_{km}\}_{k=0}^{\infty}$. The distribution Q of θ_n in the case $m = 1$ in Lemma 4.1, or Q^m in case $m > 1$, is assumed to have support with θ_1, θ_2 its smallest and largest points, respectively. This generalizes the case of support precisely $\{\theta_1, \theta_2\}$ considered in [6] and [5]. It is also true in these examples that the probability of reaching $[c, d]$ in finite time, starting from any $x \in (0, 1)$ is one. One may then show, by Theorem 2.1 (see Remark 3.4), that there is a unique invariant probability on $S = (0, 1)$.

Example 1. Take $1 < \theta_1 < \theta_2 \le 2, m = 1$. Then F_{θ_i} has an attractive fixed point $p_{\theta_i} = 1 - \frac{1}{\theta_i} (i = 1, 2)$. Here $[c, d] = [p_{\theta_1}, p_{\theta_2}] \subset \left(0, \frac{1}{2}\right]$, $x_0 \in (c, d)$, and N is a sufficiently large integer such that $F_{\theta_1}^N p_{\theta_2} < x_0$, and $F_{\theta_2}^N p_{\theta_1} > x_0$. The Markov process on $S = (0, 1)$ then has a unique invariant probability π and $X_n(x)$ converges in distribution to π geometrically fast in the Kolmogorov distance, as $n \to \infty$, for every $x \in (0, 1)$.

Example 2. Take $2 < \theta_1 < \theta_2 \le 3$, $m = 1$. Then F_{θ_i} has an attractive fixed point $p_{\theta_i} = 1 - \frac{1}{\theta_i}$ $(i = 1, 2)$ and $[c, d] = [p_{\theta_1}, p_{\theta_2}] \subset \left[\frac{1}{2}, 1\right)$. The same conclusion as in Example 1 holds in this case as well.

Example 3. Take $2 < \theta_1 \leq 3 < \theta_2 \leq 1 + \sqrt{5}$, $\theta_1 \in \left[\frac{8}{\theta_2(4-\theta_2)}, \theta_2\right)$, $m = 1$. Then F_{θ_1} has an attractive fixed point $p_{\theta_1} = 1 - \frac{1}{\theta_1}$, and F_{θ_2} has an attractive period-two orbit $\{q_1, q_2\}$, $q_1 < q_2$. The interval $[c, d] = \left[\frac{1}{2}, \frac{\theta_2}{4}\right]$ is invariant under $F_{\theta_i}(i = 1, 2)$, and strict splitting occurs with $x_0 \in (p_{\theta_2}, q_2)$ and N a sufficiently large even integer. Also with probability one, the Markov process $\{X_n(x)\}_{n=0}^{\infty}$ reaches $\left[\frac{1}{2}, \frac{\theta_2}{4}\right]$ in finite time, whatever be $x \in (0, 1)$. Thus there is a unique invariant probability π on $S = (0, 1)$ and $X_n(x)$ converges in distribution to π as $n \to \infty$, for every $x \in (0, 1)$.

Example 4. Take $\theta_1 = 3.18$, $\theta_2 = 3.20$, $m = 2$. Then F_{θ_i} has an attractive periodic orbit $\{q_{1i}, q_{2i}\}$, $q_{1i} < q_{2i}$ $(i = 1, 2)$. One may choose $[c, d] = [q_{21} - \varepsilon, q_{22} + \varepsilon]$ with $\varepsilon > 0$ sufficiently small and show that $F_{\theta^1} F_{\theta^2}(\theta^i \in \{\theta_1, \theta_2\})$ leaves $[c, d]$ invariant, and a (strict) splitting occurs for $x_0 \in (q_{21}, q_{22})$ and N a sufficiently large even integer. Also with probability one, the Markov process $\{X_n(x)\}_{n=0}^{\infty}$ reaches $[c, d]$ in finite time, whatever be $x \in (0, 1)$. Thus there is a unique invariant probability π on $S = (0, 1)$.

Examples 1–4 may be derived as special cases of the following result. As before, Q denotes the common distribution of the *i.i.d.* sequence η_n $(n \geq 1)$ and $X_n(x) = F_{\eta_n} \cdots F_{\eta_1} x$ $(n \geq 1)$.

Theorem 4.2. *Let θ_1, θ_2 denote the smallest and largest points of the support of Q, $1 < \theta_1 < \theta_2 < 4$. Assume that F_{θ_i} has an attractive periodic orbit of period $m_i \geq 1$ $(i = 1, 2)$. Assume that $\{q_1, q_2\}$ are points of the attractive orbits of F_{θ_1}, F_{θ_2} with the following properties:*

(i) *There is an interval I containing $\{q_1, q_2\}$ which is contained either in $\left(0, \frac{1}{2}\right]$ or in $\left[\frac{1}{2}, 1\right)$ such that $F_{\theta_i}^m$ leaves I invariant for some multiple m of both m_1 and m_2 $(i = 1, 2)$,*

(ii) *$F_{\theta_i}^{km} I \to \{q_i\}$ as $k \to \infty$ $(i = 1, 2)$, and*

(iii) *$P_x(\tau_I < \infty) = 1$ for all $x \in (0, 1)$. Then the Markov process $\{X_n\}_{n=0}^{\infty}$ has a unique invariant probability on $S = (0, 1)$.*

Proof. By Lemma 4.1(a), the Markov process $\{Y_k := X_{km}\}_{k=0}^{\infty}$ may be defined on the state space I, on which it is generated by *i.i.d.* monotone maps $\beta_k := \alpha_{km} \cdots \alpha_{(k-1)m+1}(k \geq 1)$. Let x_0 belong to the interior of the line segment joining q_1, q_2. Then the (strict) splitting condition (28) holds, with Y_N in place of X_N, if N is sufficiently large, by virtue of assumption (ii). Hence there exists a unique invariant probability π_0, say, of $\{Y_k\}_{k=0}^{\infty}$ on I. Under P_{π_0}, by considering the proportion of times spent in a set by $\{X_n\}_{n=0}^{\infty}$ in the first M stationary blocks $\left(X_{(k-1)m}, X_{(k-1)m+1}, \dots, X_{km-1}\right)$,

$1 \leq k \leq M$, as $M \to \infty$, one obtains an invariant probability π for $\{X_n\}_{n=0}^{\infty}$ on S given by $\pi(B) = \frac{1}{m}\sum_{n=0}^{m-1} P_{\pi_0}(X_n \in B)$. In view of (iii), the invariant probability π is unique. On may also mimic the proof of Theorem 2.1; however the steps are simpler here (Also see Remark 3.4). ∎

Remark 4.1. Given any integer $n \geq 0$, there exist $\theta_1 < \theta_2$ so that F_{θ_1}, F_{θ_2} have attractive periodic orbits of period 2^n. One may choose θ_1, θ_2 sufficiently close so that the largest points in their orbits, q_1, q_2, say, have no other periodic (or fixed) point of F_{θ_i} between them ($i = 1,2$), and so that q_1, q_2 both lie in $\left(\frac{1}{2}, 1\right)$ (or, $\left(0, \frac{1}{2}\right)$, in some cases with $n = 0$). The hypothesis of Theorem 4.2 hold in this case.

Suppose next that Q has a density component. Then under broad conditions one can show the existence of a unique invariant probability on $S = (0,1)$, as the following theorem shows.

Theorem 4.3. *Let $1 < \mu < \lambda < 4$. Suppose $Q\big([\mu,\lambda]\big) = 1$ and Q has a nonzero absolutely continuous component with a density bounded away from zero on some open interval (μ_1, μ_2) $(\mu_1 < \mu_2)$ containing a parameter value θ for which F_θ has an attractive periodic orbit of some period 2^n $(n \geq 0)$. Then the Markov process has a unique invariant probability on $S = (0,1)$.*

We first need a preliminary lemma.

Lemma 4.4. *Let $1 < \mu < \lambda < 4$. Let $u = \min\left\{1 - \frac{1}{\mu}, F_\mu\left(\frac{\lambda}{4}\right)\right\}$, $v = \frac{\lambda}{4}$. Then for every $\theta \in [\mu,\lambda]$, $[u,v]$ is invariant under F_θ.*

Proof. We need to prove that (i) $\max\left\{F_\theta(x) : u \leq x \leq v\right\} \leq v$ for $\theta \in [\mu,\lambda]$ and (ii) $\min\left\{F_\theta(x) : u \leq x \leq v\right\} \geq u$ for $\theta \in [\mu,\lambda]$. The first of these follows from the relations $\max\left\{F_\theta(x) : u \leq x \leq v\right\} \leq \max\left\{F_\lambda(x) : u \leq x \leq v\right\} \leq \frac{\lambda}{4}$. For (ii) note that by unimodality, $\min\left\{F_\theta(x) : u \leq x \leq v\right\} = \min\left\{F_\theta(u), F_\theta(v)\right\} \geq \min\left\{F_\mu(u), F_\mu(v)\right\}$. If $u = 1 - \frac{1}{\mu} \leq F_\mu\left(\frac{\lambda}{4}\right)$, then the last minimum is $F_\mu(u) = 1 - \frac{1}{\mu} = u$. If $u = F_\mu\left(\frac{\lambda}{4}\right) < 1 - \frac{1}{\mu}$, then $\min\left\{F_\mu(u), F_\mu\left(\frac{\lambda}{4}\right)\right\} = F_\mu\left(\frac{\lambda}{4}\right) = u$, since on $\left(0, 1 - \frac{1}{\mu}\right)$, $F_\mu(x) > x$. ∎

Proof of Theorem 4.3. We will sketch only the main ideas behind the proof. Under the hypothesis there exist $n \geq 0$ and an interval $[\gamma_1, \gamma_2] \subset (\mu_1, \mu_2)$, $\gamma_1 < \gamma_2$, such that for every $\theta \in [\gamma_1, \gamma_2]$, F_θ has an attractive periodic orbit of period $m = 2^n$. For simplicity assume that Q is absolutely continuous with a continuous density h which is positive on $[\delta_1, \delta_2]$. Let q_1, q_2 be the largest points on the attractive orbits of F_{γ_1} and F_{γ_2}, respectively.

One may choose γ_1, γ_2 sufficiently close to each other so that (1) there is no other periodic (or fixed) point of F_{γ_i} in the line segment joining q_1, q_2, and (2) there is an interval I containing $\{q_1, q_2\}$ which is left invariant by $F^m_{\gamma_i}$ and $F^{km}_{\gamma_i} I \to \{q_i\}$ as $k \to \infty$ $(i = 1, 2)$. It follows from Lemma 4.1(a) that I is left invariant by $F_{\theta^1} \cdots F_{\theta^m}$ for all $\theta^i \in [\gamma_1, \gamma_2]$, $1 \le i \le m$.

The m-step transition probability density $p^{(m)}(x,y)$ of the Markov process $\{X_n\}_{n=0}^{\infty}$ is easily shown to be given by

$$\begin{aligned} p(x,y) &= \frac{1}{x(1-x)} h\left(\frac{y}{x(1-x)}\right), \\ p^{(2)}(x,y) &= \frac{1}{x(1-x)} \int_{[u,v]} \frac{1}{z(1-z)} h\left(\frac{y}{z(1-z)}\right) h\left(\frac{z}{x(1-x)}\right) dz, \\ p^{(n+1)}(x,y) &= \int_{[u,v]} \frac{1}{z(1-z)} h\left(\frac{y}{z(1-z)}\right) p^{(n)}(x,z)\, dz \\ &\qquad (n \ge 1), \quad (u \le x,\ y \le v). \end{aligned}$$

Here u, v are as in Lemma 4.4. Using the fact that $F^m_\theta q = q$ for a point q on the attractive 2^n- periodic orbit of F_θ, with $\theta \in [\gamma_1, \gamma_2]$, one may show that $p^{(m)}(x,y) > 0$ for all $x, y \in I$ (if γ_1, γ_2 are sufficiently close). This implies that the restriction $\{\tilde{X}_n\}_{n=0}^{\infty}$ of the process $\{X_n\}_{n=0}^{\infty}$ to I at times of visits to I satisfies Doeblin's local minorization. Also, using the compactness of $[u,v]$ and the fact that every point in $[u,v]$ belongs to an interval of attraction to a point in the attractive orbit of some F_θ with $\theta \in (\gamma_1, \gamma_2)$, one can show $\sup\{\mathbf{E}_x \tau_I : x \in I\} < \infty$. Similarly one proves $P_x(\tau_I < \infty) = 1$ for all $x \in S = (0,1)$. ∎

Remark 4.2. It has recently been shown by Dai [11], generalizing an earlier result of Bhattacharya and Rao [6, Remark 4.1.2], that if Q has an absolutely continuous component with a positive density on a subinterval of $(1,3)$ then the Markov process is Harris recurrent and, therefore, the invariant probability is unique. One may arrive at this by an application of Theorem 1.2.

Remark 4.3. Lemma 4.2 corrects an oversight in [6] and in [11], where u is taken to be $1 - \frac{1}{\mu}$.

Remark 4.4. Finally, in a recent article Athreya and Dai [1] have proved the existence (but not uniqueness) of an invariant probability on $S = (0,1)$ under the assumption that $\mathbf{E} \ln \eta_1 > 0$, $\mathbf{E}\big|\ln(4 - \eta_1)\big| < \infty$. Athreya and

Dai [1] also have shown that '$\mathbf{E}\ln\eta_1 > 0$' is a necessary condition for the existence of an invariant probability π on $(0,1)$, by using the functional equation $X_{n+1} = \eta_{n+1}X_n(1-X_n)$ to point out that an invariant π must satisfy the equation $-\int \ln(1-x)\pi(dx) = \mathbf{E}\ln\eta_1$.

Remark 4.5. In view of Theorem 4.2, and the density of the set of θ's such that F_θ has an attractive periodic orbit, one may conjecture that if the Athreya–Dai sufficiency condition holds and Q has a nonzero absolutely continuous component with a density which is positive on some interval $(1,4)$, then there exists a unique invariant probability on $S = (0,1)$.

Remark 4.6. Recently, Athreya and Dai [2] have produced an example of a Q with a two-point support for which the Markov process has more than one invariant probability on $S = (0,1)$.

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Part IV
Stochastic Foundations in Applied Sciences I: Economics

Chapter 11
Stability Analysis for Random Dynamical Systems in Economics

Takashi Kamihigashi and John Stachurski

Abstract Random dynamical systems encountered in economics have certain distinctive characteristics that make them particularly well suited to analysis using the tools for studying Markov processes developed by Rabi N. Bhattacharya and his coauthors over the last few decades. In this essay we discuss the significance of these tools for both mathematicians and economists, provide some historical perspective, and review some recent related contributions.

11.1 Introduction

The foremost concern within the field of economics is allocation of scarce resources among alternative and competing uses. Such resources must be allocated not only contemporaneously but also across time. Allocating resources over time necessarily involves uncertainty over possible future states of the world. These facts have led economists to maintain a deep interest in the properties of random dynamical systems.

The random processes of interest to economists have a special characteristic: Their laws and properties are generated to a large extent by the decisions of economic agents—the choices of human beings. These choices are made according to a variety of concerns, such as profit maximization by firms, utility maximization by households and consumers and social welfare maximization by policy makers (should they be so inclined).

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Putting humans in models is inherently problematic. Nonetheless, a broad approximation to many kinds of human behavior can be obtained by assuming that agents respond to incentives, which in the language of mathematics means that they optimize (taking into account the constraints they face, their predictions of future outcomes, and perhaps their bounded knowledge and information processing capabilities). As a result, economic models almost always contain agents who optimize given their constraints, and the random dynamic systems economists analyze are determined partly by their resulting policy functions. (A "policy function" in this context usually means a map from current state to current actions.) In particular, the policy functions of the agents combine with other elements of the system (equilibrium constraints, physical laws of motion, exogenous shocks, etc.) to determine the evolution of the state variables.

Policy functions are often the solution to complex optimization problems and are typically nonlinear. (One example is threshold behavior caused by fixed costs or indivisibilities, as seen in the lumpy investment behavior of firms or oscillations in asset prices.) In many settings their exact properties are difficult to discern. If the law of motion for a given system depends on a policy function that is formally defined as the solution to a dynamic programming problem but has no analytical solution, then pinning down the exact properties of the law of motion (continuity, smoothness, etc.) becomes a difficult problem. Hence the approach to studying economic dynamics sometimes differs from methods adopted for other kinds of systems.

One particular problem associated with the issues described above is that many models either fail to be irreducible or cannot be shown to be irreducible under standard assumptions. For example, in the nonlinear models on continuous state spaces routinely treated in economics, systematic approaches to irreducibility require a considerable amount of smoothness (see, e.g., Chapter 4 of [33]). It can be almost impossible to extract such fine grained information from our limited knowledge of policy functions that are defined in a formal sense but cannot be written down explicitly.

Without irreducibility, many results from the classical theory of Markov processes (see, e.g., [33, 24]) cannot be applied. Given this scenario, it is perhaps not surprising that Rabi Bhattacharya's seminal work on Markov processes without the irreducibility assumption and his subsequent research with his coauthors on these and related topics [3, 4, 14, 10, 7, 6, 9, 8, 12, 11] have turned out to be ideally suited to the study of random dynamical systems in economics.

In the rest of this essay we discuss the significance of Rabi Bhattacharya's contributions through the lens of economic applications. We begin by introducing two canonical applications, extensions of which serve as workhorse models for economic research. Next we turn to theory. We also fill in some of the historical background of related work in economics, as well as subsequent developments.[1]

[1] We focus on discrete time systems since they are more commonly observed in models of economic dynamics. Analysis of continuous time systems can be found, for example, in [13, 2].

11.2 Basic Economic Models

In this section we review two standard economic models that are routinely employed in economic applications (after adding in frictions or additional features that the modelers wish to study). We strip the models down to their most essential features for expositional convenience. While this eliminates some of the complications mentioned in the introduction, references are included for those who wish to dig deeper.

11.2.1 Optimal Growth

Foundational models in the field of growth theory analyze the dynamics of output, income, savings, and consumption in a setting where growth is driven through the accumulation of productive capital [15, 34]. These models have been extended in many directions, in order to account for the role of research and development, the impact of precautionary savings, dynamics of labor through the business cycle, and so forth. We present only a classical one-sector optimal growth model, where a representative agent chooses a policy for consuming and saving in order to solve

$$\max_{\{c_t\}_{t=0}^{\infty}} \mathbb{E} \sum_{t=0}^{\infty} \delta^t u(c_t) \tag{11.1}$$

$$\text{s.t.} \quad c_t + k_t \leq y_t, \quad y_t = \xi_t f(k_{t-1}), \quad k_0 \text{ given.} \tag{11.2}$$

Here $u\colon (0,\infty) \to \mathbb{R}$ is a utility function, δ is a subjective discount factor taking values in $(0,1)$, f is a production function, c_t is consumption, k_t is capital (which equals savings in our simple model), y_t is output, and all variables are nonnegative. The stochastic sequence $\{\xi_t\}$ is taken to be IID with distribution ϕ having support on some subset of $(0,\infty)$. As is standard in the literature, we take u to be bounded, increasing, and strictly concave, with $u'(0) = \infty$. The function f is also assumed to be strictly increasing and strictly concave with $f'(0) = \infty$, $f(0) = 0$ and $f'(\infty) = 0$.

Under these conditions it is well known that a unique optimal savings policy σ exists. Optimality means that if we let income evolve according to $y_{t+1} = f(\sigma(y_t))\xi_{t+1}$ and consume according to $c_t = y_t - \sigma(y_t)$, then the resulting consumption process maximizes (11.1) under the stated constraints [15, 27, 36]. In general no analytical expression exists for the optimal policy σ.

The slope conditions on u and f at zero are used partly to ensure stability and partly to generate interior choices. Regarding the first point, if $f'(0) < \infty$, then it is possible that output converges to zero with probability one. We return to this point below. Regarding interiority, the slope conditions at zero are enough to imply that $0 < \sigma(y) < y$ for all $y > 0$, and, as a consequence, that σ satisfies the Euler equation

$$u' \circ c(y) = \delta \int u' \circ c[f(\sigma(y))z] f'(\sigma(y)) z \phi(dz) \qquad (y > 0) \tag{11.3}$$

where $c(y) := y - \sigma(y)$. For a proof, see, for example, [42, Prop. 12.1.24]. This equation is very useful for inferring properties of σ and the optimal income dynamics.

To study the dynamics of the optimal process, we take y_t as the state variable, and consider the process $y_{t+1} = f(\sigma(y_t))\xi_{t+1}$. A natural state space is $(0, \infty)$ or some subinterval. Key questions are the existence and uniqueness of stationary distributions for the state variable, convergence of marginal distributions to the stationary distribution under some suitable topology, and ergodicity and central limit theorems for the time series. Answering these questions is of fundamental importance when comparing predictions with data.

11.2.2 Stability Arguments

In the simple version of the model we have presented, irreducibility can be established after assuming enough smoothness on ϕ, the distribution of the shock process. This is because the shock ξ_{t+1} appears outside the policy function in the law of motion $y_{t+1} = f(\sigma(y_t))\xi_{t+1}$. However, this property is easily lost if we alter the timing or include additional complications such as correlated productivity shocks or elastic labor supply (see, e.g., [25, 17]). Although we omit such complications here, their existence implies that general stability results need to be built on top of more robust features of the dynamics.

Two such features are continuity and monotonicity. For example, consumers typically save more when income goes up. In the context of our optimal growth model, it is certainly true that the optimal savings function $y \mapsto \sigma(y)$ is continuous and increasing, and, since f preserves these properties, the associated Markov process $y_{t+1} = f(\sigma(y_t))\xi_{t+1}$ is both stochastically monotone and Feller [43, 15, 34].

These properties were exploited in the first proof of stability for the model discussed above, due to Brock and Mirman [15]. They showed that the model has a unique and stable stationary distribution whenever the shocks have compact support $[a, b]$ with $0 < a < b$. The same properties were also exploited in subsequent related work by Mirman and Zilcha [34] and Razin and Yahav [40]. A summary of the approach that combines monotonicity and continuity can be found in [43].[2]

However, continuity is not a robust feature that can be relied upon for stability proofs in more general cases. For example, if we drop the concavity assumption on f, the optimal policy can contain jumps [21, 25, 36]. Seminal work by Rabi Bhattacharya and his coauthors showed that for existence, uniqueness, and stability in models such as this one sector stochastic optimal growth model, continuity of the optimal policy is unnecessary: it is sufficient to require the optimal policy to be monotone and to satisfy an appropriate mixing condition, as we discuss in Section 11.3.

[2] Subsequently the stability analysis was extended to the case of unbounded shocks by [41, 37, 28, 47].

11.2.3 Overlapping Generations

Another foundational class of models in economic theory is the models of production and growth with overlapping generations. Here we discuss a simple example loosely based on Galor and Ryder [23] and Wang [45]. The framework is as follows. Agents live for two periods, working in the first and living off savings in the second. Savings in the first period forms capital stock, which in the following period will be combined with the labor of a new generation of young agents for production under the technology $y_t = F(k_t, \ell_t)\epsilon_t$. Here y_t is income, k_t is capital, and ℓ_t is the number of young agents, all of whom supply inelastically one unit of labor. For convenience we assume that population is constant ($\ell_t = \ell = 1$), and set $f(k) = F(k, 1)$. Following Galor and Ryder [23, p. 362] we assume that $f \colon \mathbb{R}_+ \to \mathbb{R}_+$ has the usual properties $f(0) = 0$, $f' > 0$, $f'' < 0$, $f'(0) = \infty$, $f'(\infty) = 0$, as well as the extended Inada condition

$$\lim_{k \downarrow 0} [-kf''(k)] > 1. \tag{11.4}$$

The shocks $\{\epsilon_t\}$ are IID on $\mathbb{R}_+$ according to density ϕ.

As Galor and Ryder point out [23, Lemma 1, p. 365], restrictions on the utility function are necessary to obtain unique self-fulfilling expectations. Here we assume that young agents maximize utility

$$U(c_t, c'_{t+1}) = \ln c_t + \beta \mathbb{E}(\ln c'_{t+1}), \quad \beta \in (0, 1), \tag{11.5}$$

subject to the budget constraint

$$s_t = w_t - c_t, \quad c'_{t+1} = s_t R_{t+1},$$

where s is savings from wage income, c (respectively, c') is consumption while young (respectively, old), w is the wage rate, and R is the gross rate of return on savings. Competitive markets imply that firms pay inputs their marginal factor product. Thus, the gross interest rate and wage rate are

$$R_t(k_t, \epsilon_t) = f'(k_t)\epsilon_t, \quad w_t(k_t, \epsilon_t) = [f(k_t) - k_t f'(k_t)]\epsilon_t. \tag{11.6}$$

At time t, households choose s_t to maximize

$$\ln(w_t(k_t, \epsilon_t) - s_t) + \beta \mathbb{E} \ln[s_t R_{t+1}(k_{t+1}, \epsilon_{t+1})], \tag{11.7}$$

using their knowledge of the distribution ϕ of ϵ_t to evaluate the expectations operator, as well as their current belief that next period capital stock will be k_{t+1}. In self-fulfilling expectations equilibrium their beliefs are realized, with

$$k_{t+1} = s_t = \frac{\beta}{1+\beta} h(k_t)\epsilon_t, \tag{11.8}$$

where $h(k) = [f(k) - kf'(k)]$. The role of condition (11.4) is to ensure that $h'(0) > 1$, implying that capital will not collapse to zero as long as the distribution of the shock is sufficiently favorable.

The first aim of dynamic analysis is to establish existence of a unique and stable stationary distribution for capital $\{k_t\}$ under reasonable assumptions on the shock process $\{\epsilon_t\}$. The most notable property of h is monotonicity, as follows directly from concavity of the production function f. This makes the system amenable to analysis using the methods of Bhattacharya and Lee [3] described below.

11.2.4 Other Applications

We have mentioned only two simple applications. For more applications amenable to analysis using related stability conditions, see, for example, the infinite horizon incomplete market models typified by [26], stochastic endogenous growth models such as that found in [20], a wide variety of OLG models, such as those as found in [1, 39, 38] and [35], and industry models such as [16] and [19].

11.3 Stability Conditions

In this section we discuss sufficient conditions for stability, starting with the monotonicity and "splitting" conditions introduced by Bhattacharya and Lee [3].[3]

11.3.1 Splitting

The framework adopted by Bhattacharya and Lee [3] consists of a sequence of IID random maps $\{\gamma_t\}_{t\geq 1}$ on some probability space $(\Omega, \mathscr{F}, \mathbb{P})$, each map γ_t sending a subset S of $\mathbb{R}^n$ into itself, and an S-valued process $\{X_t\}_{t\geq 0}$ generated by

$$X_t = \gamma_t X_{t-1} = \gamma_t \circ \cdots \circ \gamma_1(x)$$

where $x \in S$ is the initial condition. The key assumption of their stability analysis is the existence of a $c \in S$ and $m \in \mathbb{N}$ such that
(S1) $\mathbb{P}\{\gamma_m \circ \cdots \circ \gamma_1(x) \geq c, \ \forall x \in S\} > 0$; and
(S2) $\mathbb{P}\{\gamma_m \circ \cdots \circ \gamma_1(x) \leq c, \ \forall x \in S\} > 0$.
The order $\leq$ here is the usual pointwise order for vectors in $\mathbb{R}^n$.

Conditions (S1) and (S2) are often referred to collectively as a "splitting condition." They have a natural interpretation of mixing in an order-theoretic sense. Under this split-

[3] The work of Bhattacharya and Lee builds to some degree on earlier work by Dubins and Freedman [22] and Yahav [46].

ting condition and the assumption that all maps γ_t are increasing, it was shown that the Markov process $\{X_t\}$ has a unique invariant distribution and is globally asymptotically stable; see [3, 5, 18]. Stability is with respect to a metric that is weaker than total variation convergence but equivalent to the Kolmogorov metric in one dimension (and implies weak convergence in higher dimensions under mild restrictions).

These simple and intuitive conditions can easily be applied to the optimal growth model described in Subsection 11.2.1 whenever the shock is bounded. No continuity is required, so variations that induce jumps in the policy function can also be treated. Monotonicity is known to hold, as already discussed.

Conditions (S1) and (S2) can also be used to prove stability for the overlapping generations model described in Subsection 11.2.3. In particular, provided that the shock distribution is chosen to be supported on a bounded subset of $(0, \infty)$, the state space S for k_t can be taken to be a bounded closed interval $[K_a, K_b] \subset (0, \infty)$. The splitting condition (S1) can then be checked by showing that, starting from $k_0 = K_a$, sufficiently positive shocks can drive the state k_m above some point $c \in [K_a, K_b]$ with positive probability. In view of monotonicity, the same shocks will drive the state above c in m periods from *any* initial condition. A proof along these lines gives (S1), and (S2) can be checked in a similar way.

Further results pertaining to the splitting conditions (S1) and (S2) were obtained by Rabi Bhattacharya and coauthors in a sequence of studies subsequent to the original paper by Bhattacharya and Lee [3]. These relate to processes that are monotone but not necessarily increasing, to the connections between splitting and classical minorization conditions, and to the implications of splitting for ergodicity and central limit theorems [4, 6, 7, 10, 12]. For example, Theorem 3.1 of Bhattacharya, Majumdar, and Hashimzade [12] tells us that when the overlapping generations model satisfies the splitting conditions as described above, the equilibrium capital stock process $\{k_t\}$ satisfies

$$\sqrt{n}\left\{\frac{1}{n}\sum_{t=1}^{n} g(k_t) - \int g(x)\mu(dx)\right\} \xrightarrow{d} N(0, \sigma^2)$$

for some $\sigma \geq 0$ where $\xrightarrow{d}$ means convergence in distribution. Here μ is the stationary distribution of the process (11.8) and $g\colon [K_a, K_b] \to \mathbb{R}$ is any function of bounded variation (and therefore representable as the difference between two monotone increasing functions).

11.3.2 Monotone Mixing

The existence of many economic models lacking irreducibility but possessing a certain monotone structure led to considerable interest in understanding the stability properties of non-irreducible random dynamical systems arising from economic models.

One well-known example in the economic literature is due to Hopenhayn and Prescott [25]. They studied monotone processes that exist on a compact metric space with a closed partial order. The space S is assumed to contain a least element a and greatest element b.[4]

[4] That is, $a \leq x \leq b$ for all $x \in S$.

Monotonicity means that the stochastic kernel

$$P(x, B) := \mathbb{P}\{X_{t+1} \in B \mid X_t = x\}$$

has the property that $x \mapsto P(x, B)$ is increasing for every measurable increasing set B in S. They require a "monotone mixing condition," which states that there exists a $c \in S$ and $m \in \mathbb{N}$ such that $P^m(a, [c, b]) > 0$ and $P^m(b, [a, c]) > 0$. This condition, combined with monotonicity, implies the splitting conditions (S1) and (S2) discussed above. Thus, although the proofs are rather different, the work of Hopenhayn and Prescott can be thought of as extending at least some of the results of Bhattacharya and Lee to abstract compact metric spaces.

11.3.3 Order Mixing

Recently there has been a surge of interest in developing results analogous to Bhattacharya and Lee [3] but with weaker mixing assumptions (paired, of course, with weaker conclusions in terms of uniformity and rates of convergence). To see why this might be useful, consider, for example, the stochastic optimal growth model $y_{t+1} = f(\sigma(y_t))\xi_{t+1}$ and suppose now that the productivity shock ξ is lognormal, say, or has any other unbounded distribution. In such a setting, the splitting conditions (S1) and (S2) are too strict. To see this, recall that the map $y \mapsto f(\sigma(y))$ is continuous and zero at $y = 0$. Hence if we fix any $c > 0$ and any $m \in \mathbb{N}$, the probability that $y_m \geq c$ conditional on y_0 can be made arbitrarily small by taking $y_0 \downarrow 0$.

Weaker mixing conditions maintaining an order theoretic flavor were introduced by Bhattacharya and Waymire in [14], who studied local splitting conditions in conjunction with a recurrence condition ensuring drift back to the set where splitting occurs. An alternative but related approach was suggested by Szeidl in [44].

An even weaker mixing condition was considered in [29], called *order mixing*. Loosely speaking, a Markov process on a partially ordered set $(S, \preceq)$ is defined to be order mixing if, given any two independent sequences $\{X_t\}_{t\geq 0}$ and $\{X'_t\}_{t\geq 0}$ generated by the model, we have

$$\mathbb{P}\{\exists t \geq 0 \text{ s.t. } X_t \preceq X'_t\} = 1. \tag{11.9}$$

The initial conditions X_0 and X'_0 are permitted to be distinct, but both processes are updated according to the same transition law.[5] While order mixing is not strong enough to imply existence of a stationary distribution, it does imply uniqueness and convergence, where convergence means that if $\{X_t\}$ and $\{X'_t\}$ are two copies of the process with different initial conditions then

$$|\mathbb{E}h(X_t) - \mathbb{E}h(X'_t)| \to 0 \quad \text{as } t \to \infty \tag{11.10}$$

for any bounded measurable increasing function h.

Order mixing is implied by the splitting conditions (S1) and (S2). These conditions tell us that $X_t \preceq X'_t$ occurs once over m periods with positive probability. Hence $X_t \preceq X'_t$

[5] Note that $\mathbb{P}\{\exists t \geq 0 \text{ s.t. } X'_t \preceq X_t\} = 1$ must also hold by interchanging the two processes.

eventually with probability one by the Borel-Cantelli lemma. To see that order mixing is strictly weaker than (S1) and (S2), consider two processes generated by the same Markov model, in this case AR(1) processes on $\mathbb{R}$ defined by $X_{t+1} = \rho X_t + \xi_{t+1}$ with $X_0 = x$ and $X'_{t+1} = \rho X'_t + \xi'_{t+1}$ with $X'_0 = x'$. Here $\{\xi_t\}$ and $\{\xi'_t\}$ are IID, standard normal, and independent of each other. While (S1) and (S2) fail, it is easy to see that $\mathbb{P}\{X_1 \le X'_1\}$ is strictly positive, regardless of (x, x'). Hence the process is order mixing.

11.3.4 Order Reversing

A still weaker mixing condition was introduced in [31]. This condition combined with a technical condition implies order mixing.

To be more precise, a Markov process $\{X_t\}$ on a partially ordered set $(S, \preceq)$ is called *order reversing* if, for any given x and x' in S with $x \ge x'$, and any independent copies $\{X_t\}$ and $\{X'_t\}$ of the process starting at x and x' respectively, there exists a $t \in \mathbb{N}$ with $\mathbb{P}\{X_t \le X'_t\} > 0$. In other words, there exists a point in time at which the initial ordering is reversed with positive probability. Evidently, order reversing is considerably easier to check than order mixing in applications.

A Markov process $\{X_t\}$ is called *bounded in probability* if, for any initial condition $x \in S$ and any $\epsilon > 0$, there exists a compact set $C \subset S$ such that $\mathbb{P}\{X_t \in C\} \ge 1 - \epsilon$ for all t; see, e.g., [33] or [31] for a more precise definition. If the state space itself is compact, then any stochastic process is bounded in probability. Hence this condition allows for non-compact state spaces since a Markov process on a non-compact space can be bounded in probability.

Boundedness in probability is itself not trivial to show for models like the optimal growth model discussed above, but it can be established under reasonable assumptions by exploiting the Euler equation (11.3). For example, if we take $w_1 := (u' \circ c)^{1/2}$, where c is the consumption policy as in (11.3), then some manipulations of the Euler equation lead us to

$$\int w_1[f(\sigma(y))z]\phi(dz) \le \left[\int \frac{1}{\delta f'(\sigma(y))z}\phi(dz)\right]^{1/2} w_1(y).$$

This is a kind of drift condition, which can be used to check boundedness in probability. In this case it tells us that when income is small, the value of w_1 tends to decline (recall our assumption that $f'(0) = \infty$). Since w_1 is large near zero, this means that the state moves away from zero—which is one half of boundedness in probability in this context. See [27, 36] for further discussion of these issues.

It has been shown [31, Lemma 6.5] that for monotone processes that are bounded in probability, order reversing implies order mixing. One advantage of this approach is that, at least for monotone processes, once we have boundedness in probability and order reversing, existence of a stationary distribution requires only mild additions to the assumptions. For example, if, in addition, the stochastic kernel of the process has either a deficient or an excessive distribution (where the marginal distribution of the state is shifted up or down in the stochastic dominance ordering over one unit of time), then a stationary distribution exists, is unique, and is globally stable in a topology stronger than the weak topology [31, Theorem 3.1]. The essence of this fixed point argument was explored in [30] in an abstract setting.

One can introduce still simpler mixing conditions that imply order reversing. For example, in [31] a Markov process $\{X_t\}$ is called *upward reaching* if, given any initial condition x and any other point c in S, there exists a $t \in \mathbb{N}$ such that $\mathbb{P}\{X_t \geq c\} > 0$. The process is called *downward reaching* if given any initial condition x and any other point c in S, there exists a $t \in \mathbb{N}$ such that $\mathbb{P}\{X_t \leq c\} > 0$. It can be shown [31, Proposition 3.2] that if a monotone process is bounded in probability and either upward or downward reaching, then it is order reversing. Related ideas are presented in [32].

11.4 Conclusion

The tools for studying possibly non-irreducible Markov processes introduced and refined over the past few decades by Rabi Bhattacharya and his coauthors have significantly raised the ability of economists to elicit sharp predictions from their models and compare them with data. Much interesting work remains to be done. For example, it seems likely that a more unified approach to the various order-theoretic mixing conditions discussed above can be obtained. Further, the relationship between the weaker mixing conditions and properties like laws of large numbers and central limit theorems are only starting to be investigated. On the applied side, economists are continuously generating interesting random dynamical systems and seeking the input of experts to determine their asymptotic properties.

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Chapter 12
Some Economic Applications of Recent Advances in Random Dynamical Systems

Santanu Roy

12.1 Introduction

The analysis of resource allocation over time under conditions of uncertainty occupies a central place in economics. A very widely used framework for the study of such dynamic resource allocation problems is one where stocks of “capital” or other assets accumulate over time through investment, and the accumulation process is subject to random “shocks.” Important economic problems studied in this framework include economic growth under productivity shocks, household accumulation of wealth with uncertain returns on savings, depletion of renewable and other natural resources whose natural growth is subject to environmental or climate related shocks, and the growth of pests and other invasive biological species whose expansion rates are affected by uncertainty. Though the economic models used to study these problems can be fairly elaborate, they often generate random dynamical systems where the intertemporal transition of capital or a related stock variable is determined by a “transition” function that depends on the previous period’s capital as well as the realizations of an exogenously specified stochastic process of “shocks.” The important problem for the economist is to then understand the asymptotic or limiting behavior of this dynamical system and how it depends on initial conditions, the nature of the transition function and the distribution of shocks. This naturally leads to the question of existence and (local or global) stability of a stochastic steady state i.e., an invariant distribution of the random dynamical system. Economists tend to view the limiting stochastic steady state of the dynamical system as a long run “equilibrium.” The rate of convergence to the limiting steady state is important for the strength of predictions made on the basis of this long run equilibrium. It is also important to be able to estimate the long run distribution of capital

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or resource stocks on the basis of finite data. Finally, whether or not similar economic systems that differ only in initial conditions may exhibit very different long run behavior depends on global stability of the steady state.

The purpose of this chapter is to provide a brief exposition of the manner in which some recent advances in random dynamical systems and in particular, some of the contributions made by Prof. Rabi Bhattacharya and his coauthors, have provided useful tools of analysis and insights for economists studying problems of capital accumulation under uncertainty. I will focus on applications related to random dynamical system generated by iterated i.i.d. monotone maps.

12.2 A Simple Economic Model of Capital Accumulation under Uncertainty

Time is denoted by $t = 0, 1, 2 \ldots$. The model is one with a single good. The total stock of "output" available at the beginning of each period t, denoted by y_t, depends on the size of capital (input) at the end of the previous period. Let $\{r_t\}_{t=1}^{\infty}$ be a sequence of independent and identically distributed random variables with common distribution function G. The distribution G is nondegenerate and the support of the distribution is an interval $[a, b], a < b < \infty$. Further, $G(r) = 0$ for all $r < a, G(r) = 1$ for all $r > b$ and $0 < G(r) < 1$ for all $r \in (a, b)$. We interpret the random variable r_t as a "shock" that affects the output realized from any input of capital in period $(t - 1)$.

A (time stationary) production function $f(x, r)$ determines how the capital stock x and realization r of the current random shock generates output next period. In particular, $f(x, r) : \mathbb{R}_+ \times [a, b] \to \mathbb{R}_+$ is assumed to be strictly increasing in x. Further, $f(0, r) = 0$ for all $r \in [a, b]$. To rule out unbounded expansion of output, it is assumed that there exists $K > 0$ such that for all $r \in [a, b]$, $f(K, r) \le K$ and $f(x, r) < x$ for all $x > K$. The economic system begins with an initial stock

$$y_0 \in (0, K]. \tag{12.1}$$

In every period t, an amount $x_t, 0 \le x_t \le y_t$, is invested in capital accumulation. Assume that capital depreciates fully every period. As a result, x_t is also the size of capital at the end of period t. This generates output y_{t+1} in period $t + 1$:

$$y_{t+1} = f(x_t, r_{t+1}) \tag{12.2}$$

(to be clear, r_{t+1} is realized after investment is made in period t). Though this is by no means necessary, for ease of exposition we will assume that for each $x \ge 0$, $f(x, r)$ is nondecreasing in r on $[a, b]$.

This simple framework has been used to study a variety of economic problems. In models of economic growth under uncertainty, x_t represents the investment in physical capital and $y_t - x_t$ is the amount of available output used for current consumption in period t; the production function f represents the production technology and r_t is the random shock that captures fluctuations in exogenous factors that affect productivity of capital.[1] In stochastic models of renewable resource harvesting, y_t is the resource stock or biomass of a specie at the beginning of period t, $y_t - x_t$ is the part of the stock that is harvested in period t, x_t is the part of the stock that remains after harvesting and is allowed to regenerate or grow to next period's stock, f captures the natural growth (renewal or biological reproduction) process of the resource, and the random shock r_t captures environmental and other exogenous fluctuations that affects this process.[2] In models of control and spread of invasive species or pests, y_t is the biomass of the specie or the size of invasion (for instance, area covered) at the beginning of period t, $y_t - x_t$ is the part that is removed through various "controls" in period t, x_t is the stock of the specie or the size of invasion that remains after current control, f captures the natural expansion or growth of the invasion size or biomass and the random shock r_t captures fluctuations that affect the expansion process.[3] In a large class of these models, it is natural to assume (as we have done in our simple framework) that the expansion process is bounded above; for instance, natural resource expansion is bounded above by the carrying capacity of the ecosystem and economic growth may be bounded because of technological limitations.

Let $x(y):\mathbb{R}_+ \to \mathbb{R}_+$, $x(y) \leq y$ denote a (time stationary) investment function which specifies current investment as a function of current output. Then, using the fact that $x_t = x(y_t)$, we have from (12.2)

$$y_{t+1} = f(x(y_t), r_{t+1}). \tag{12.3}$$

In descriptive models of capital accumulation, the investment function is specified exogenously as being one of the fundamentals of the economic system and the focus is then on understanding how the properties of the investment function $x(y)$, the production function f, and distribution of shocks G determine the dynamics generated by (12.3). In these models, "plausible" assumptions are directly imposed on the function $x(y)$ and one of the common assumptions is that $x(y)$ is nondecreasing on $\mathbb{R}_+$.

In other positive and normative economic models of capital accumulation, the function $x(y)$ is generated endogenously through the behavior of economic agents, their preferences, their interaction structure, and the nature of economic institutions. While these latter elements often vary according to the specific economic problem that the model wishes to address, in a very large class of these models with a single capital good (and under reasonable assumptions on the structure of the model), one can show that the investment function $x(y)$ generated by the model is nondecreasing on $\mathbb{R}_+$. However, in many of these settings, one cannot ensure that $x(y)$ is continuous.

In models of optimal economic growth under uncertainty as well as models of optimal resource management, $x(y)$ is generated as the optimal policy function of a stochastic stationary dynamic optimization problem of maximizing the expected discounted sum of immediate returns from consumption or resource harvests over time. Depending on the context, the immediate return can be viewed as social welfare, the consumption utility of a representative agent or the net profit of a private firm that harvests the resource. Under strict concavity and other reasonable restrictions on the immediate return function, one can

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1 See, for instance, the survey by Olson and Roy [17].

2 See, for instance, Olson and Roy [15], Mitra and Roy [13].

3 See, for instance, Olson and Roy [16].

show that the optimal investment policy function $x(y)$ is nondecreasing. However, if the production function f is not concave in capital input, then the feasible set for the dynamic optimization problem is non-convex and in that case, one cannot ensure continuity of the optimal policy function. Non-concavity of the production function f in capital input is necessary to allow for important features such as increasing returns to scale in production technology and "depensation" in resource growth (for instance, the growth rate of a specie may decline if the stock size is reduced below a threshold).[4]

In models of optimal control of pests and invasive species, $x(y)$ is generated as the optimal decision rule in a dynamic optimization problem where one minimizes the expected discounted sum of control costs over time; once again, $x(y)$ can be shown to be increasing under some restrictions on the cost of controlling the invasion but without requiring additional restrictions on f. However, continuity of the optimal decision rule $x(y)$ cannot be ensured if $f(x, r)$ is not convex in x.[5]

In dynamic games of common property resource harvesting by multiple economic agents, each agent decides on her own harvest of the commonly owned resource stock over time so as to maximize her own expected discounted sum of net benefit from resource harvests. The amount of the stock left over in each period after all agents have harvested, is the current investment. In a Markov-perfect equilibrium of such a game, each agent uses a time stationary decision rule that depends only on the size of the resource stock y at the beginning of the period, and this generates the equilibrium investment function $x(y)$. Under certain assumptions, one can show the existence of Markov-perfect equilibria where $x(y)$ is increasing. However, one cannot in general ensure continuity of $x(y)$ even if one assumes that the production f is concave.[6]

So, let us assume that $x(y)$ is nondecreasing on $\mathbb{R}_+$. For $y \in \mathbb{R}_+$ and $r \in [a, b]$, let h be the transition function that determines the output next period as a function of current output y and realization r of the random shock, and defined by

$$h(y, r) = f(x(y), r).$$

Using (12.3), the stochastic process of output $\{y_t\}$ is now determined by the random dynamical system

$$y_{t+1} = h(y_t, r_{t+1}). \tag{12.4}$$

Observe that for every $r \in [a, b]$, as $f(., r)$ is increasing and $x(.)$ is nondecreasing, $h(., r)$ is nondecreasing on $\mathbb{R}_+$. In other words, the random dynamical system (12.4) is one generated by iterates of a monotone map. Also, note that

$$h(y, r) = f(x(y), r) \leq f(y, r) \leq f(K, r) \leq K \text{ for all } y \in [0, K].$$

Thus, given (12.1), for all $t = 0, 1, 2, \ldots.$

$$y_t \in [0, K] \text{ with probability one.}$$

[4] See, among others, Majumdar, Mitra, and Nyarko [11], Olson and Roy [15], and Mitra and Roy [13].

[5] Olson and Roy [16].

[6] See, for instance, Sundaram [18].

Observe that $h(0, r) = 0$ for all $r \in [a, b]$ so that 0 is an absorbing state for the stochastic process $\{y_t\}$. As $f(x, r)$ has been assumed to be nondecreasing in r, $h(y, r)$ is nondecreasing in r for any $y > 0$.

Finally, note that the function $h(y, r)$ is not necessarily continuous in y either because, as discussed above, the investment function $x(y)$ is not continuous in y or because the production function $f(x, r)$ is not necessarily continuous in capital input x; the latter may reflect features such as lumpiness, indivisibility, and threshold effects in the production technology.

12.3 Long Run Behavior of the Economic System

Consider the Markov process $\{y_t\}$ defined by the law of motion (12.4) on the state space $[0, K]$. As zero is an absorbing state, the degenerate distribution at zero is an invariant distribution. If the process $\{y_t\}$ converges in distribution to this degenerate distribution at zero, then we have long run extinction. In this case, it is impossible for the economic system to sustain consumption or harvests above any fixed threshold $\epsilon > 0$ in the long run. Therefore, in models of economic growth or resource harvesting, we are often interested in a limiting invariant distribution whose support is a subset of $\mathbb{R}_{++}$ (a so-called "regular" invariant distribution).

Suppose there exists a closed interval $S = [\underline{y}, \overline{y}], 0 < \underline{y} < \overline{y} \leq K$ such that:

$$h(\underline{y}, a) \geq \underline{y}, \text{ and } h(y, a) < y \text{ for all } y \in (\underline{y}, \overline{y}] \tag{12.5}$$

$$h(\overline{y}, b) \leq \overline{y}, \text{ and } h(y, b) > y \text{ for all } y \in [\underline{y}, \overline{y}). \tag{12.6}$$

This implies that for any $y \in S$ and for all $r \in (a, b)$

$$\underline{y} \leq h(\underline{y}, a) \leq h(y, a) \leq h(y, r) \leq h(y, b) \leq h(\overline{y}, b) \leq \overline{y}$$

so that $y_0 \in S$ implies that $y_t \in S$ for all t with probability one.

Consider the random dynamical system defined by (12.4) on the state space $S = [\underline{y}, \overline{y}]$. In a series of research papers, Prof. Rabi Bhattacharya and his coauthors have developed various sufficient conditions for the existence of a unique and stable invariant distribution for a Markov process defined by i.i.d. random monotone maps on some suitably defined subset of $\mathbb{R}^k$. In particular, when the state space is an interval such as S and the i.i.d. maps are nondecreasing, it has been shown that there is a unique stable invariant distribution (on S) if, and only if, a certain "splitting condition" is satisfied. This splitting condition is due to Dubins and Freedman [9] who showed that it ensures a stable and unique invariant distribution when the state space is a compact interval and the Markov process is generated by i.i.d. monotone and continuous maps; further, it ensures that the n-step transition probability converges to the invariant probability exponentially fast in the Kolmogorov distance, uniformly for all initial states. Yahav [19] showed the existence of a unique invariant distribution even if the maps are not continuous as long as they are increasing. Bhattacharya and Lee [3] extend this result to a broader class of multidimensional state spaces and show that the exponential convergence result in Dubins and Freedman [9] holds. Independently and using a somewhat less general notion of "splitting," Hopenhayn and Prescott [10] establish similar results on existence and stability; however they do not establish any result on the speed of convergence. Bhattacharya and Majumdar [4, 5] show that the Dubins-Freedman result can be established for monotone i.i.d. maps (increasing or decreasing) when the state space is either an arbitrary interval or an arbitrary closed set in $\mathbb{R}$.[7]

Now, suppose that the probability distribution G of the random shocks assigns strictly positive probability to a and b. Then for any fixed $z \in (\underline{y}, \overline{y})$, (12.5) and (12.6) imply that there exists $N \geq 1$ such that starting from initial state $\overline{y}$, the process reaches a state below z if the worst realization a of the random shock occurs for the first N consecutive periods and further, starting from initial state $\underline{y}$, the process reaches a state above z if the best realization b of the random shock also occurs for the first N consecutive periods. Let $\delta > 0$ be the minimum of the probability of these two events. This implies that starting from any initial state in the interval S, we can show that in N steps, the process reaches a state below z and a state above z with probability at least as large as δ. This allows us to establish the splitting condition.

In the argument outlined in the previous paragraph, one can easily dispense with the requirement of having strictly positive probability mass on the best and worst shocks under slightly stronger restrictions on the function $h(y, r)$. Further, though we have assumed the function $f(x, r)$, and therefore the function $h(y, r)$, to be strictly increasing in r this is by no means necessary; the argument can easily be extended to the case where the transition functions $h(., r)$ are not necessarily ordered by the realization r of the shock.

The existence of a unique invariant distribution on the set S implies that the dynamical system has a strictly positive stochastic steady state. In particular, for any initial stock $y_0 \in [\underline{y}, \overline{y}]$, the economic system eventually attains the limiting stochastic steady state and it is one where output and capital are bounded away from zero i.e., the system is capable of sustaining (with probability one) a strictly positive level of consumption in the long run. If, in addition to (12.5) and (12.6),

$$h(y, a) > y \text{ for all } y \in (0, \underline{y}), \tag{12.7}$$

then from any initial stock $y_0 \in (0, \underline{y})$, the stochastic process $\{y_t\}$ eventually enters and remains in the interval $[\underline{y}, \overline{y}]$ with probability one; therefore, the unique invariant distribution on $[\underline{y}, \overline{y}]$ is also the limiting distribution of y_t's for any initial state in $(0, \overline{y}]$. If, further,

$$h(y, b) < y \text{ for all } y > \overline{y}, \tag{12.8}$$

then from any initial stock $y_0 > \overline{y}$, the stochastic process $\{y_t\}$ eventually enters and remains in the interval $[\underline{y}, \overline{y}]$ with probability one. Thus, under (12.5)–(12.8), the unique invariant distribution on $[\underline{y}, \overline{y}]$ is globally stable on $(0, K]$, i.e., the long run (or limiting) behavior of y_t's is independent of initial state. In the classical optimal growth framework where the

[7] See also, Athreya [1] and Bhattacharya et al. [8].

production function $f(x,r)$ is assumed to be concave in x and the optimal investment rule $x(y)$ is derived by maximizing the discounted sum of utility or net benefits from consumption where the utility function is strictly concave, it has been shown that (12.5)–(12.8) are satisfied under certain restrictions on the behavior of $f(.,r)$ near zero.[8]

If (12.7) does not hold then output need not be bounded away from zero with probability one in the long run and, in some cases, may converge to zero (the extinction outcome).[9] Indeed, in nonclassical models of optimal economic growth that allow for technological nonconvexities and in models of optimal renewable resource management where the growth function of the resource may be characterized by depensation, it has been shown that (12.7) may not hold and extinction may occur from small initial stocks though from initial stocks above a critical level, the system converges to a strictly positive steady state.[10] Further, in these models, (12.8) may not hold and in particular, there may be multiple nonoverlapping intervals like $[\underline{y},\overline{y}]$ that satisfy (12.5) and (12.6) so that the splitting condition is satisfied and there is distinct unique invariant distribution on each of these intervals. This corresponds to a situation of multiple nontrivial (strictly positive) long run steady states of the economy and a situation where the long run destiny depends on the initial condition.[11] These are situations where there is an economic case for policy intervention to modify initial conditions so that the system can be guided to a preferred long run steady state.

The contributions by Bhattacharya and his coauthors have made it possible to analyze and characterize long run properties of a rich class of dynamic economic models that generate random dynamical systems of i.i.d. iterated monotone maps where the maps are not necessarily continuous. Further, their results on exponential convergence has strengthened the extent to which we can rely on predictions based on these long run properties. However, there are some problems that remain. For instance, even for the simple framework described above, we may often have a situation where

$$h(y,a) < y \text{ for all } y > 0$$

but (12.6) holds. A natural question that arises here is whether there is a unique invariant distribution on $(0,\overline{y}]$ in which case one think of a long run steady state that is not bounded away from zero that assigns zero probability mass at zero. However, because $h(y,a) \to 0$ as $y \to 0$, the number of steps it takes to cross any fixed positive stock can be arbitrarily large if one starts from stocks close enough to zero (zero itself is of course an absorbing state). It is then difficult to verify a condition like the "splitting condition." Some recent advances in the study of global stability suggest alternative conditions that may be useful in addressing this kind of question.[12]

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[8] See, for instance, Brock and Mirman [2].

[9] See, Mitra and Roy [14].

[10] See, Mitra and Roy [13].

[11] See, Majumdar et al. [11].

[12] See, for instance, Kamihigashi and Stachurski [12].

Finally, it is important to extend the analysis to the case where the exogenous random shocks $\{r_t\}$ are not necessarily independent over time. For many of the economic applications, it is natural to allow $\{r_t\}$ to be any "well-behaved" stationary Markov process, while retaining the monotone structure of the transition function h. It will be useful to develop conditions for existence of a unique stable invariant distribution that generalize the splitting condition for i.i.d. monotone maps to such settings.

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Chapter 13
Reprints: Part IV

R.N. Bhattacharya and Coauthors

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13.1 "Dynamical systems subject to random shocks: an introduction"

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Dynamical systems subject to random shocks: An introduction

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1 Preface

In his influential article Frisch (1933) suggested alternative routes for research on macrodynamics and remarked:

"One way which I believe is particularly fruitful and promising is to study what would become of the solution of a deterministic dynamic system if it were exposed to a stream of erratic shocks that constantly upsets the ... evolution, and by so doing introduce into the system the energy necessary to maintain the swings. If fully worked out, I believe that this idea will have an interesting synthesis between the stochastical point of view and the point of view of rigidly determined dynamical laws."

The pioneering efforts of Goodwin, Hicks, Samuelson, Tinbergen, Metzler and others (see the collection by Gordon and Klein, 1965) led to a class of deterministic models for "explaining" the cyclical behavior ("swings") of an economy, often with a particular emphasis on processes described by second order difference or differential equations, or with nonlinear processes with reflecting boundaries. There were also a few articles in which random shocks were explicitly introduced. Samuelson's brief summary of stochastic models in his *Foundations* (1947, pp. 342–349), referred to Slutsky's pioneering paper and other work on time series by Davis, Wold and Haavelmo. The difficulties in dealing with nonlinear systems were duly stressed, and their potential in developing formal models capable of providing a firm theoretical foundation for policy-oriented empirical research was also clearly recognized by him.

Advances in the study of dynamic processes described by a "simple" first order nonlinear difference equation have resulted in a better understanding of the possibilities of complex behavior and the difficulties of long run prediction and of deriving results on comparative dynamics. The collection of articles in this Sym-

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posium can be best viewed as an attempt to continue with the important direction of research so clearly suggested by Frisch some seventy years ago, and to bring together a number of relatively recent mathematical results that add to the toolbox of economic theorists.

Consider a random dynamical system (S, Γ, Q) where S is the state space, Γ an appropriate family of maps on S into itself (interpreted as the family of all possible laws of motion) and Q is a probability distribution on (some σ-field of) Γ. The evolution of the system is described as follows: initially, the system is in some state x of S. Tyche chooses an element α_1 of Γ according to the probability distribution Q, and the system moves to the state $X_1 = \alpha_1(x)$ in period one. Again, independently of α_1, an element α_2 of Γ is chosen according to Q, and the state of the system in period two is given by $X_2 = \alpha_2(\alpha_1(x))$. In general, starting from x in S, one has

$$X_{n+1}(x) = \alpha_{n+1}(X_n(x)) \tag{1.1}$$

where the maps (α_n) are independent and identically distributed according to the distribution Q. The initial state x can also be chosen (independently of (α_n)) as a random variable X_0. The sequence (X_n) of states obtained in this manner is a Markov process with a stationary transition probability

$$p(x, A) \equiv Q(\{\gamma \epsilon \Gamma : \gamma(x) \epsilon A\}) \tag{1.2}$$

The formulation (1.1) has been particularly convenient for modeling dynamic processes subjected to random shocks in a variety of contexts in economics and other disciplines. On the other hand, every discrete time Markov process on a 'standard' state space admits a representation of the form (1.1) (see Kifer, 1986, p. 8, or Bhattacharya and Waymire, 1990, p. 220).

It is worthwhile to comment on the significance of the study of random dynamical systems from several perspectives. First, by endowing (S, Γ, Q) with some special structures (for example, $S = [0, 1]$, Γ a family of monotone maps...), one hopes to throw light on the long run behavior and steady states of the system. Secondly, as has been stressed by Eckmann and Ruelle (1985), physical systems are often "stochastically excited", and in such situations, a randomly perturbed dynamical system as a stochastic process is a more relevant object of study than a deterministic system. Neither the law of motion nor the initial state may be known with certainty, when we model an economic process, and there is, quite justifiably, a rich literature in economics – both at the micro and macro levels – in which random exogenous shocks are explicitly introduced. The process (1.1) can be interpreted as a *descriptive* stochastic model. Alternatively, one may start with a stochastic dynamic programming model of optimization under uncertainty, and directly arrive at a stationary optimal policy function, which together with the given law of transition describes the *optimal* evolution of states in the form (1.1). Of particular interest in this context are some results on the "inverse optimal problem under uncertainty" due to Mitra (1998) and Montrucchio and Privileggi (1999) which assert that a broad class of random dynamical systems (1.1) can be so generated.

Thirdly, random dynamical systems figure prominently in a vast and unavoidably technical literature on the search for the Kolmogorov - SRB measure for chaotic dynamic systems. A chaotic dynamical system f with a compact state space $K \subset \mathbb{R}^d$, by definition, has sensitive dependence on initial conditions (Devaney, 1989, p. 50). Since an "exact" measurement of a state at some point of evolution (call it the 'initial state') is virtually impossible, states in the distance future are unpredicdtable. For most applications, however it is enough to know the long run statistical behavior of the trajectory : $\{f^n x : n \geq 0\}$. That is, one needs to know if the empirical process $\frac{1}{n}\sum_{n=0}^{n-1} \delta_f n_x$ converges as $n \to \infty$ to some limit, say β, independent of x for almost all x (with respect to the Lebesgue measure), and, if so, what this limit is. If it exists, this limit is necessarily an invariant probability for the dynamical system: $\beta f^{-1} = \beta$, and it is ergodic. But there are infinitely many ergodic invariant probabilities for a chaotic dynamical system. In particular, the uniform distribution on a (necessarily repelling, or unstable) periodic orbit is an ergodic, i.e., extremal, invariant probability, and there are infinitely many such invariant probabilities on distinct periodic orbits (Devaney, 1989, pp. 49, 50), none of which can be β. Long time ago Kolmogorov suggested that one should randomly perturb the dynamical system by adding an absolutely continuous noise component so that the resulting Markov process has a unique invariant probability, say π. The limit of π, as the noise goes to zero, should be β. Kolmogorov's conjecture has been proved for Axiom A diffeomerphisms independently by Sinai, Ruelle and Bowen (see Eckmann and Ruelle, 1985, or Kifer, 1988, for a precise statement), and the limit β is called the *SRB measure* in this case. We will refer to it more generally as the *Kolmogorov measure*. In the context of quadratic maps $F_\theta = \theta x(1-x)$ on $[0,1]$, where $\theta \epsilon [0,4]$, the existence of such a measure has been proved by Katok and Kifer (1986) for those values of θ which satisfy the Misiurewicz condition: F_θ has no stable periodic orbit and $\frac{1}{2}$ does not belong to the closure of the trajectory $\{F_\theta^n \frac{1}{2} : n \geq 1\}$. It was shown by Misiurewicz (1981) that under this condition F_θ has a unique absolutely continuous invariant probability β, and that this condition is satisfied by uncountably many parameter values θ. Indeed, Jakobson (1981) proved that the set of such parameter values has positive Lebesgue measure. It may be noted that, except in special cases, β is virtually impossible to compute analytically. On the other hand viewed as an approximation of β, π is more tractable and, at the least, has approximations $\frac{1}{N}\sum_{n=1}^{N} p^{(n)}(x, dy)$ where $p^{(n)}$ [the n-step transition probability of $\{X_n,\ n \geq 0\}$] may be expressed analytically by recursion.

2 Basic issues and criteria for stability in distribution

Consider a random dynamical system (S, Γ, Q) where the state space is a metric space (denote this meteric by ρ), and let $\mathcal{P}(S)$ be the set of all probability measures on (the Borel σ-field $\mathcal{S}$ of) S. Now, for any $\mu \varepsilon \mathcal{P}(S)$, let $T^*\mu$ be the probability distribution obtained as (using 1.2)

$$T^*\mu(A) = \int_S p(x, A)\mu(dx) \equiv \int_\Gamma \mu(\gamma^{-1}(A))Q(d\gamma) \tag{2.1}$$

An element π of $\mathcal{P}(S)$ is an *invariant distribution* for $p(x, A)$ (or, for the Markov process X_n generated according to (1.1)) if π is a fixed point of T^*, i.e.,

$$\pi\ is\ invariant\ iff\ T^*\pi = \pi \tag{2.2}$$

Denote by $p^{(n)}(x, dy)$ the n-step transition probability generated by $p(x, dy)$. Write T^{*n} as the n-th iterate of T^*, i.e., for $n \geq 2$

$$T^{*n}\mu(A) = \int_S p^{(n)}(x, A)\mu(dx) .$$

$T^{*n}\mu$ is the distribution of X_n when X_0 has distribution μ.

One can think of an invariant distribution as a steady state or equilibrium of the process X_n generated according to (1.1). A major thrust of the present Symposium is on criteria for a form of stability of the random dynamical system (1.1) which allows one to predict the long-run future based on past data: the system (1.1) or the process (X_n) is *stable in distribution* if it converges in distribution to a steady state distribution π, irrespective of the initial state X_0. If this convergence is for the time averages of the distributions of $X_1, ..., X_n$, then the process is said to be *stable in distribution on the average*. There exists a comprehensive theory for a stronger form of stability for the so-called "Harris irreducible processes", in which the convergence is in total variation distance, i.e., is uniform over all measurable sets in the state space (see, e.g., the books by Orey, 1971, Nummelin, 1984, and Meyn and Tweedie, 1993). Typically, this holds if the transition probabilities have appropriate densities with respect to some reference measure such as the Lebesgue measure. It is true that in many interesting situations it is quite non-trivial to verify Harris-irreducibility (see, e.g., Bhattacharya and Majumdar, 2002, which deals with random iterations of quadratic maps). But the criteria described in the present collection apply to processes (1.1) which may *not* be irreducible, as typically is the case when Q has a finite support $\{f_1, f_2, ..., f_k\}$. Two important classes of random dynamical systems for which the criteria for stability in distribution may be derived without requiring Harris irreducibility arise from random iterations of (1) Lipschitz maps on a metric space satisfying an average (in geometric mean) contraction criterion (see the articles by Bhattacharya-Majumdar (*B-M*) and Carlsson), and (2) monotone maps satisfying a "splitting" condition (see (*B-M*) and Goswami).

Another important problem is to understand the nature of the steady state distribution π, since it is rarely the case that π can be computed or specified analytically (two surprising exceptions are provided in the article by Goswami). It is of interest to know, for example, if π is absolutely continuous with respect to Lebesgue measure, or singular, when the transition probabilities do not have densities. In particular, this turns out often to be a difficult problem even in the case when Q has the support $\{f_1, f_2\}$, i.e., one randomly picks one of the two functions f_1, f_2 (with probabilities $p > 0$ and $1 - p$ respectively) in every period. It is astonishing that, in what may appear to be the simplest of cases, the determination of whether π is absolutely continuous or singular when the randomization is between two affine contractions $a_i + b_i x (i = 1, 2)$ on $S = [0, 1]$, had been a famous open problem for more than half a century, until a breakthrough was achieved by Solomyak (1995). Solomyak's theory is reviewed in this Symposium by Mitra, Montrucchio and Privileggi who also provide recent extensions including their own.

Finally, a basic question that precedes any consideration of stability in distribution is whether there exists an invariant probability for (X_n) at all. A well known general result is that in the case of a compact state space and a weakly (Feller) continuous transition probability function $p(x,\cdot)$, there exists at least one invariant probability. The proof is by a fixed point argument. The Feller continuity is guaranteed if, with Q-probability one, the functions in Γ are continuous. To point out the inadequacy of this otherwise useful result, consider the case of Γ consisting of quadratic or logistic maps $F_\theta(x) = \theta x(1-x)$, $x \in S = [0,1]$, $\theta \in [0,4]$. The point mass at 0, δ_0, is obviously invariant, since 0 is a fixed point of every element of Γ. An important question then is: if the state space is restricted to the open interval $S = (0,1)$, does there exist an invariant probability π on S? The article by Athreya deals with the problem of existence of an invariant π on open intervals such as $S = (0,1)$ for a general class of maps including the logistic family.

3 Sufficient conditions for uniqueness and stability of the steady state

The general theory of Markov processes alerts us of the possibilities of multiple steady states, and of the complexity of the long run behavior. A landmark paper on identifying conditions under which uniqueness and stability hold on compact state spaces is that of Dubins and Freedman (1966). In this section we will review in some detail two important cases discussed by them.

3.1 Iteration of Random Lipschitz maps

Let (S,ρ) be a complete separable metric space, Γ a set of Lipschitz maps on S (into S) and Q a probability measure on an appropriate sigmafield $\mathcal{G}$ on Γ. On a basic probability space $(\Omega,\mathcal{F},P)$ are defined a sequence of i.i.d. random maps $\{\alpha_n : n \geq 1\}$ with (common) distribution Q. A general criterion for the existence of a unique invariant probability for (X_n) defined by (1.1) and for the stability in distribution is given by the following two conditions, which only require α_n to be continuous and not necessarily Lipschitz (see the proof of Theorem 3.3 in *B-M*):

(a) $\sup\{\rho(\alpha_n\alpha_{n-1}...\alpha_1 x,\ \alpha_n\alpha_{n-1}...\alpha_1 y) : \rho(x,y) \leq M\} \to 0$ *in probability, as* $n \to \infty$, *for every* $M > 0$, *and*

(b) *for some* $x_0 \epsilon S$, *the sequence of distributions of* $\rho(X_n(x_0), x_0) \equiv \rho(\alpha_n...\alpha_1 x_0, x_0)$ *is relatively weakly compact.*

For simplicity, assume that S is *compact*. Then (b) is automatic, since the sequence $\rho(X_n(x_0), x_0)$ is bounded by the diameter of S, whatever be x_0 and n. We now show that in this case (a) implies stability in distribution. Obviously here one may simplify the statement of (a) by taking just one M, namely, the diameter of S:

(a)$'$: *diam* $(\alpha_n\alpha_{n-1}...\alpha_1 S) \to 0$ *in probability as* $n \to \infty$.

It is to be proved that in the case of a compact metric space (S,ρ), (a)$'$ is sufficient for stability in distribution. This follows immediately if one lets X_0 be a random variable independent of the sequence $\{\alpha_n\}$ and considers an invariant distribution π, which exists due to the compactness of S and continuity of α_n. Then $X_n(X_0) \equiv \alpha_n...\alpha_1 X_0$ has the distribution π for all n, and (a)$'$ implies that for every real-valued Lipschitz f on S, with Lipschitz constant ℓ, one has

$$\left|Ef(X_n(x)) - \int f d\pi\right| = |E\{f(\alpha_n...\alpha_1 x) - f(\alpha_n...\alpha_1 X_0)\}|$$
$$\leq \ell E\rho(\alpha_n...\alpha_1 x, \alpha_n...\alpha_1 X_0) \leq \ell E\ diam(\alpha_n...\alpha_1 S) \to 0, \quad (3.1)$$

as $n \to \infty$, whatever $x \in S$. This implies the weak convergence of $X_n(x)$ to π for every x (see, e.g., Dudley, 1989, p. 317).

For i.i.d. random Lipschitz maps α_n on a compact metric space (S, ρ), Theorem 3.2 in *B-M* verifies (a)$'$ under the assumption of contraction on the (geometric) average in the following sense:

$$-\infty \leq E\ \log\ L_1^r < 0, \text{ for some } r \geq 1, \quad (3.2)$$

where L_1^r is the random Lipschitz constant of $\alpha_1\alpha_2...\alpha_r$:

$$L_1^r := \sup\{\rho(\alpha_1...\alpha_r x,\ \alpha_1...\alpha_r y)/\rho(x,y) : x \neq y\}.$$

The criterion (a)$'$ may also be used to prove the following basic result of Dubins and Freedman (1966). Here γ is defined to be a *contraction* if $\rho(\gamma x, \gamma y) \leq \rho(x, y)$ for all $x, y \in S$, and it is a *strict contraction* if there is strict inequality $\rho(\gamma x, \gamma y) < \rho(x, y)$ for all $x \neq y$.

Proposition 1 *Let (S, ρ) be compact metric and Γ the set of all contractions on S. Let Q be a probability measure on the Borel sigmafield of Γ (w.r.t. the 'supremum' distance) such that the support of Q contains a strict contraction. Then the Markov process X_n defined by (1.1) has a unique invariant probability and is stable in distribution.*

Proof Let γ be a *strict contraction* in the support of Q, *i.e.*, $\rho(\gamma x, \gamma y) < \rho(x, y) \forall x \neq y$. The j-th iterate of γ is denoted γ^j. Since $\gamma^{j+1}S = \gamma^j(\gamma S) \subset \gamma^j S$, it follows that $\gamma^j S$ decreases as j increases. Indeed

$$\gamma^j S \ decreases\ to\ \cap_{j=1}^{\infty} \gamma^j S = \text{ a singleton } \{x_0\}. \quad (3.3)$$

To see this, first note that the limit is nonempty, by the finite intersection property of (S, ρ). Assume, if possible, that there are points x_0, y_0 in the limit set, $x_0 \neq y_0$. Let $\delta := \rho(x_0, y_0)$. The continuous function $(x, y) \to \rho(\gamma x, \gamma y)/\rho(x, y)$ on the compact set $K_\delta = \{(x, y) : \rho(x, y) \geq \delta\} (\subset S \times S)$ attains a maximum $c < 1$. Let x_1, y_1 be two pre-images of x_0, y_0, respectively, under γ *i.e.*, $(x_1 \epsilon \gamma^{-1}\{x_0\},\ y_1 \epsilon \gamma^{-1}\{y_0\})$, $\gamma x_1 = x_0, \gamma y_1 = y_0$. Since γ is a contraction, $\rho(x_1, y_1) \geq \rho(\gamma x_1, \gamma y_1) = \rho(x_0, y_0) = \delta$. Therefore, $\rho(x_0, y_0) \leq c\rho(x_1, y_1), or, \rho(x_1, y_1) \geq \delta/c$. In general, let $x_j,\ y_j$ be two pre-images under γ of $x_{j-1},\ y_{j-1}$, respectively. Then, by induction, $\rho(x_j, y_j) \geq \rho(x_{j-1}, y_{j-1})/c \geq ... \geq \rho(x_0, y_0)/c^j \to \infty$ as $j \to \infty$, which contradicts the fact that S is bounded.

By the same kind of reasoning one shows that

$$diam(\gamma^j S) \downarrow 0 \text{ as } j \uparrow \infty. \quad (3.4)$$

For, if (3.4) is not true, there exists $\delta > 0$ such that $diam(\gamma^j S) > \delta > 0$ for all j. Thus there exist $x_j, y_j \epsilon \gamma^j S$ such that $\rho(x_j, y_j) \geq \delta$ which implies, using pre-images, that there exist $x_0, y_0 \epsilon S$ satisfying $\rho(x_0, y_0) \geq \delta / c^j \to \infty$ as $j \to \infty$, a contradiction.

Now fix j and let $\gamma_1, \gamma_2, ..., \gamma_n$, $n > j$, be such that $\gamma_{i+1}, ..., \gamma_{i+j}$ are within a distance ε from γ, *i.e.*, $\|\gamma_{i+k} - \gamma\|_\infty < \varepsilon$, $k = 1, ..., j$, where $1 \leq i+1 < i+j \leqq n$. We shall show:

$$diam(\gamma_n \gamma_{n-1} ... \gamma_1 S) \leq diam(\gamma^j S) + 2j\varepsilon \tag{3.5}$$

For this note that the contraction $\gamma_n \gamma_{n-1} ... \gamma_{i+j+1}$ does not increase the diameter of the set $\gamma_{i+j} ... \gamma_{i+1} \gamma_i ... \gamma_1 S$. Also, $\gamma_{i+j} ... \gamma_{i+1}(\gamma_i ... \gamma_1 S) \subset \gamma_{i+j} ... \gamma_{i+1} S$. Hence the left side of (3.5) is no more than $diam(\gamma_{i+j} ... \gamma_{i+1} S)$. Now, whatever be x, y, one has, by the triangle inequality,

$$\rho(\gamma_{i+j} ... \gamma_{i+2} \gamma_{i+1} x, \gamma_{i+j} ... \gamma_{i+2} \gamma_{i+1} y) \leq 2\varepsilon + \rho(\gamma_{i+j} ... \gamma_{i+2} \gamma x,\ \gamma_{i+j} ... \gamma_{i+2} \gamma y).$$

Applying the same argument with γx, γy in place of x, y, and replacing γ_{i+2} by γ, and so on, one arrives at (3.5).

We are now ready to verify (a)$'$. Choose $\delta > 0$ arbitrarily. Let j be such that $diam(\gamma^j S) < \delta/2$. Let $\varepsilon = \delta/4j$, so that the right side of (3.5) is less than δ. Define the events

$$A_m = \{\left\|\alpha_{j(m-1)+k} - \gamma\right\|_\infty < \varepsilon \quad \forall k = 1, 2, ..., j\} (m = 1, 2, ...) \tag{3.6}$$

Note that $P(A_m) = b^j$, where $b := P(\|\alpha_1 - \gamma\|_\infty < \varepsilon)$. Since γ is in the support of Q, $b > 0$. The events $A_m (m = 1, 2, ...)$ form an independent sequence, and $\sum_{m=1}^\infty P(A_m) = \infty$. Hence, by the second Borel-Cantelli Lemma, $P(A_m$ occurs for some $m) \geq P(A_m$ occurs for infinitely many $m) = 1$. But on A_m, $diam(\alpha_{mj} \alpha_{mj-1} ... \alpha_{mj-j+1} S) < \delta$ so that, with probability one, $diam(\alpha_n ... \alpha_1 S) < \delta$ for all sufficiently large n. Since $\delta > 0$ is arbitrary, (a)$'$ holds.

The proof given above is merely an amplification of the rather terse derivation given in the original article by Dubins and Freedman (1966). It may be noted that this result does not follow from Theorem 3.2 (or Theorem 3.3) in *B-M*, since one may easily construct strict contractions with Lipschitz constant one. On the other hand, Theorems 3.2 and 3.3 in *B-M* apply to sets Γ which contain (noncontracting) maps with Lipschitz constant larger than one in the support of Q, but still satisfies the criterion (a) and (b) for stability in distribution. An important case in point is the model $X_{n+1} = A_{n+1} X_n + B_{n+1}$ on $S = \mathbb{R}^k$, with (A_n, B_n), $n \geq 1$, i.i.d., A_n being a random $(k \times k)$-matrix and B_n a k-dimensional random vector. Theorem 4.2 in *B-M* (originally proved by Berger, 1992, by a different method) provides a criterion for stability based on (a) and (b), extending an earlier result of Brandt (1986). The autoregressive model of order k follows as a special case of this.

Finally, Carlsson provides another interesting criterion involving average contraction.

3.2 Random iteration of monotone maps and a spliting condition

In addition to the preceding theory concerning random dynamical systems governed by random contractions or by random Lipschitz maps with an average (geometric mean) contraction, there exists a fairly general theory for iterations of random monotone maps.

Its study was also pioneered by Dubins and Freedman (1966). In their work $S = [0,1]$, Γ a family of continuous monotone maps, and the process satisfies the 'splitting' condition (H):

(H) *there exist a finite positive integer* N, *some* $z_0 \epsilon S$ *and positive numbers* δ_1, δ_2 *such that*:

$$P(\alpha_N \dots \alpha_1 x \leq z_0 \quad \forall\, x \epsilon S) \geq \delta_1$$
$$P(\alpha_N \dots \alpha_1 x \geq z_0 \quad \forall\, x \epsilon S) \geq \delta_2$$

Let $d_K(\mu, \nu)$ be the Kolmogorov distance on $\mathcal{P}(S)$, i.e., if F_μ and F_ν are the distribution functions of μ, ν then

$$d_K(\mu, \nu) \equiv \sup_{x \epsilon S} |F_\mu(x) - F_\nu(x)| \equiv \sup_{x \epsilon R} |F_\mu(x) - F_\nu(x)|$$

We now have the following:

Proposition 2 *Let* $S = [0,1]$, *and* Γ *be a family of monotone maps. Assume that the splitting condition (H) holds.*

Then, (i) *the distribution* $T^{*n}\mu$ of X_n *converges to a probability* π:

$$d_K(T^{*n}\mu, \pi) \leq (1-\delta)^{[n/N]} \tag{3.7}$$

where $\delta = \min(\delta_1, \delta_2)$ and $[n/N]$ is the integer part of n/N.

(ii) π *is the unique invariant distribution.*

A contraction mapping theorem can be used to prove this result. The main steps are:

(a) show that $(\mathcal{P}(S),\, d_K)$ is a complete metric space and $d_K(T^*\mu,\, T^*\nu) \leq d_K(\mu,\, \nu)$
(b) using the splitting property verify that $d_K(T^{*N}\mu,\, T^{*N}\nu) \leqq (1-\delta) d_K(\mu, \nu)$
(c) Then, some calculation leads to:$\forall n \geq N$

$$d_K(T^{*n}\mu,\, T^{*n}\nu) \leq (1-\delta)^{[n/N]} d_K(\mu, \nu)$$

(d) T^{*N} is a uniformly strict contraction, hence there is a unique π such that $T^{*N}\pi = \pi$, but $T^{*N}(T^*\pi) = T^*(T^{*N}\pi) = T^*\pi$, i.e., $T^*\pi$ is invariant under T^{*N}. So $\pi = T^*\pi$,. This means that π is an invariant distribution. But every fixed point π' of T^* is also a fixed point of T^{*N}. Hence π is the unique fixed point of T^*. Taking $\nu = \pi$ in (c) we get (3.7).

To generalize the result one needs to find some meetric $\hat{d}$ relative to which (a) holds. Moreover, one also must verify relative to this metric $\hat{d}$ that (b) holds when d_K is replaced by $\hat{d}$. Finally, while it is easy to show that convergence in d_K implies weak convergence, one must ensure that convergence in $\hat{d}$ ensures weak or some other meaningful convergence of (X_n). Such generalizations are reviewed in detail in *B-M* along with applications to random quadratic maps $F_\theta = \theta x(1-x)$ on $S = (0,1)$, with appropriate conditioins on the parameter θ, which allow one to restrict attention to an invariant interval (either contained in $(0, 1/2]$ or $[1/2, 1)$) on which each F_θ is monotone and the splitting condition holds.

4 The nature of the steady state

As mentioned in the Preface, understanding the nature of steady states of random dynamical systems is of theoretical as well as practical interest. More often than not, however, this is a difficult enterprise.

Consider, for example, the apparently simple case of randomly choosing one of two affine linear strict contractions on $S = [0,1] : f_0(x) = rx$, $f_1(x) = rx + (1-r)$, $p \equiv Q(\{f_0\}) = P(\alpha_1 = f_0)$, $1-p = Q(\{f_1\}) = P(\alpha_1 = f_1)$. Here $0 < r < 1$, $0 < p < 1$. By Proposition 3.1, or Proposition 3.2, in the previous section, there exists a unique steady state or invariant probability π_r for the random dynamical system (1.1). It follows from the uniform convergence of the distribution function of X_n to that of π_r, irrespective of the initial distribution μ of X_0 (see 3.7), that π is nonatomic , i.e., it has a continuous distribution function. To go further, note that the range of f_0 is $I_0 = [0,r]$ and that of f_1 is $I_1 = [1-r, 1]$. If $0 < r < 1/2$, I_0 and I_1 do not overlap, and the range of X_1 is contained in $I_0 \cup I_1$. The range of X_2 is contained in the union of four nonoverlapping closed intervals $I_{00} = f_0(I_0)$ and $I_{01} = f_0(I_1)$ both contained in I_0, and $I_{10} = f_1(I_0)$ and $I_{11} = f_1(I_1)$ both contained in I_1. The range of X_3 is contained in 2^3, or eight, nonoverlapping closed intervals obtained by splitting each one of the preceding four into two nonoverlapping closed intervals, and so on. As is familiar in analysis, there arises in this fashion a limiting *Cantor set* as the support of $\pi_r (0 < r < 1/2)$.

What happens in this example if $r = 1/2$? In the symmetric case $p = 1/2$, a simple computation verifies that the uniform distribution is invariant and, because of the guaranteed stability, it is the unique steady state $\pi_{1/2}$. This is, however, just a lucky occurrence, since for $1/2 < r < 1$ even the basic question of whether π_r is absolutely continuous (with respect to Lebesgue measure) or singular had remained open for more than half a century. Finally, in a breakthrough, Solomyak (1995) proved an old conjecture that, if $p = 1/2$, π_r is *absolutely continuous* for all r in $[1/2, 1)$ outside a set of Lebesgue measure zero. It has been known for many years that there are infinitely many values of r in $(1/2, 1)$ for which π_r is singular. One such value is $r = (\sqrt{5}-1)/2 = .617...$. It is not known if the latter set is countable. The article by Mitra, Montrucchio and Privileggi provides an overview of this deep theory and its more recent extensions, especially to the case $p \neq 1/2$. They also prove some interesting new results, including the mutual singularity of π_r, for a given r, as p ranges over $(0,1)$. They point out that the random dynamical system considered in the preceding paragraphs governs an affine logarithmic transformation of the *optimal (growth in) production* $\{X_n\}$ in a dynamical optimization problem in a one-sector Cobb-Douglas economy with a logarithmic utility function.

One may inquire about the nature of steady states of nonlinear random dynamical systems, especially those for which the support of Q has only two functions. Not a great deal is known here. In the case of *quadratic maps* $F_\theta(x) = \theta x(1-x)$, with the support of Q as $\{F_{\theta_1}, F_{\theta_2}\}$, under stringent restrictions such as $1 < \theta_1 < \theta_2 \leq 2$, e.g., one can prove that the unique invariant probability π on $S = (0,1)$ is singular and its support is a Cantor set (Bhattacharya and Rao, 1993). The proof of singularity here is analogous to that outlined for the case of affine contractions above.

Next, consider the *random continued fractions* on $S = (0,\infty)$ considered in the article by Goswami, with $\Gamma = \{f_0, f_1\}$, $p = Q(\{f_0\})$, $1-p = Q(\{f_1\})$, $0 < p < 1$, and $f_0(x) = \frac{1}{x}$, $f_1(x) = \frac{1}{x} + \theta$. The parameter $\theta \epsilon (0,\infty)$. One may express the process $\{X_n\}$ recursively as $X_{n+1} = \frac{1}{X_n} + \varepsilon_{n+1}$, $n \geq 0$, where $\{\varepsilon_n : n \geq 1\}$ is an i.i.d. Bernoulli type sequence, $P(\varepsilon_n = 0) = p$, $P(\varepsilon_n = \theta) = 1-p$. The maps $f_i (i = 0,1)$ are monotone decreasing on $S = (0,\infty)$ and the hypotheses of Proposition 3.2 in Section 3 are satisfied. Hence there exists a unique invariant probability π_θ, and one has stability in distribution. It is shown that the support of π_θ is (i) full (i.e., $(0,\infty)$) if $0 < \theta \leq 1$, and (ii) a Cantor set if $\theta > 1$. Amazingly, π_1 has been explicitly computed (originally by Chassaing et al., 1984, and by a different method by Bhattacharya and Goswami, 1999). The distribution function of π_1 is given by (see Theorem 5.2 in Goswami)

$$\pi_1((0,x]) = \sum_{i=0}^{\infty} \left(-\frac{1}{p}\right)^i \left(\frac{p}{1+p}\right)^{a_1+..+a_{i+1}}, \quad 0 < x \leq 1,$$
$$\pi_1((0,x]) = 1 - \frac{1}{p}\pi_1\left(\left(0, \frac{1}{x}\right]\right), \quad x > 1. \tag{4.1}$$

Here, for $0 < x \leq 1$, the sequence of positive integers $a_1, a_2, ...$ are the ones that occur in the classical continued fraction expansion of x, i.e., $x = [a_1, a_2, ...]$. For rational x, such an expansion terminates after a finite number of steps and (4.1) reduces to a finite sum. This is an interesting example of a singular probability measure with full support on $S = (0,\infty)$. Whether for some $\theta \epsilon (0,1)$, or almost all such θ, π_θ is absolutely continuous with respect to Lebesgue measure is an interesting open problem.

As a final remark, note that in case of stability in distribution, the random dynamical system (1.1) has the unique invariant probability π characterized as follows: If X has distribution π, then $\alpha(X)$ has distribution π where α has distribution Q and is independent of X. The derivation (4.1) may be arrived at using this relation, which in this case reads: X has the same distribution (π) as $\frac{1}{X} + \varepsilon$ where ε is Bernoulli (with $P(\varepsilon = 0) = p$, $P(\varepsilon = 1) = 1-p$), and is independent of X. The only other distribution of ε for which π has been computed explicitly, is a two-parameter gamma distribution. In this case π turns out to have a two-parameter *inverse Gaussian distribution* (for this result of Letac and Seshadri, 1983, see Theorem 5.1 in Goswami).

5 Estimation of long-run averages

Ostensiby, the practical goal in studying criteria for stability in distribution of a time series such as (1.1) is to estimate long-run averages of some characteristics $v(X_n)$ of X_n based on past data. If the process $\{X_n\}$ is stable in distribution (on the average) and $\int |v|\, d\pi < \infty$ then, according to the ergodic theorem, $\bar{v}_n := \frac{1}{n}\sum_{j=0}^{n-1} v(X_j)$ converges to (the long-run average) $\int v d\pi$ with probability one, for π-*almost all initial states* $X_0 = x$. But one does not know π and, in general, there is no apriori guarantee that the initial state x belongs to *the* distinguished set. Indeed, we have seen in Sections 2 and 4, the support of π may be quite small, e.g., a Cantor set of Lebesgue measure zero. If π is widely spread out, as is the case, e.g., if π has a strictly positive density with respect to Lebesgue measure on an Euclidean state space S, then one may be reasonably assured of convergence.

A second important problem is to determine the *speed of convergence* of $\bar{v}_n$ to $\int v d\pi$. One knows from general considerations, such as the central limit theorem, that this convergence is no faster than $0_p(n^{-1/2})$. Is this optimal speed achieved, irrespective of the initial state? An approach towards resolving these issues is illustrated in B-M, which follows a general method given in Bhattacharya and Majumdar (2001) and Athreya and Majumdar (2002). Consider, for specificity, S to be $\mathbb{R}^k$ or a closed subset of $\mathbb{R}^k$, and $\{\alpha_n\}$ a sequence of i.i.d. continuous increasing maps on S, and assume that 'splitting' holds. It is shown in Bhattacharya and Lee (1988) that if v is a real-valued function of bounded variation on S and $\int |v|\, d\pi < \infty$, then

$$\bar{v}_n = \int v d\pi + 0_p(n^{-1/2}), \tag{5.1}$$

whatever be the initial state $X_0 = x$. The condition $\int |v|\, d\pi < \infty$ is satisfied, in particular, if v is bounded. Thus, if S is compact and v is continuously differentiable, then (5.1) holds.

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13.2 "Random iterates of monotone maps"

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ORIGINAL PAPER

Random iterates of monotone maps

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Abstract In this paper we prove the existence, uniqueness and stability of the invariant distribution of a random dynamical system in which the admissible family of laws of motion consists of monotone maps from a closed subset of a finite dimensional Euclidean space into itself.

Keywords Random dynamical systems · Invariant distribution · Convergence · Markov processes

JEL Classification C1 · C6 · D6 · D8 · D9

1 Introduction

This paper is dedicated to Leonid Hurwicz. Hurwicz (1944) was a contributor to the literature on stochastic models of growth and cycles. In collaboration with Kenneth Arrow he also set the tenor of research on multi-sector dynamic models [see Part III of Arrow and Hurwicz (1977)]. We focus on a class of stochastic or random dynamic processes that have been of particular interest in the context of optimization problems in—to use his terminology—"non-classical" environments. A formal statement of the main result is in Sect. 2. But we begin with a few informal remarks to provide the motivation. The mathematical model of discounted stochastic dynamic programming has become the basic tool in exploring optimal decision making under uncertainty both at the micro- and macro-levels. In "classical" models, by imposing appropriate (strict) convexity, continuity and monotonicity properties on the primitives (technological

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constraints involved in specifying the law of motion, return functions...), one is able to assert that *the* optimal policy function is *monotone* and *continuous*. Once, however, one attempts to step out of the "classical" environment (for example, to allow for a Knightian S-shaped production function that exhibits an initial phase of increasing returns), the standard proof of *continuity* of *the* optimal policy function fails. Indeed, even in a deterministic non-classical model of intertemporal optimization, an example of discontinuity (in which the production function is S-shaped, the return function is linear) was given in Majumdar and Mitra (1983). However, in a large class of stochastic models one can still prove that there is *an* optimal policy function that is *monotonic* [see Majumdar et al. (1989) for an elaboration of the finer points of *selection* and a comprehensive account of dynamic optimization under uncertainty with non-concave production functions]. This monotonicity property turns out to be crucial in making significant progress in understanding the evolution of an optimal process, and in establishing some long run convergence properties. The analysis is simpler when the state space is an interval (in the real line). Exploring the implications of monotonicity (with possible discontinuity) when the state space is a closed subset of a finite dimensional Euclidean space is the point of departure of this paper. Consider a *random dynamical system* (S, Γ, Q) where S is the *state space* (for example, a closed subset of $\mathbb{R}^k$, Γ an appropriate family of maps on S into itself and Q is a probability measure on (some σ-field of) Γ.

The evolution of the system can be described as follows: initially, the system is in some state x; an element α_1 of Γ is chosen randomly according to the probability measure Q and the system moves to the state $X_1 = \alpha_1(x)$ in period one. Again, independently of α_1, an element α_2 of Γ is chosen according to the probability measure Q and the state of the system in period two is obtained as $X_2 = \alpha_2(\alpha_1(x))$. In general, starting from some x in S, one has

$$X_{n+1}(x) = \alpha_{n+1}(X_n(x)) \tag{1.1}$$

where the maps (α_n) are independent and identically distributed according to the measure Q. The initial point x can also be chosen (independently of (α_n)) as a random variable X_0. The sequence X_n of states obtained in this manner is a *Markov process* and has been of particular interest in economics (and other disciplines).

For describing "convergence to a long run steady state", perhaps the most widely used results identify conditions under which there is some time invariant probability measure π such that, *no matter what the initial* x_0 *is,* X_n *converges in distribution to* π. In this case we say that the (Markov) process is *stable in distribution*.

2 The main result

In this section we extend an important old result of Dubins and Freedman (1966) on i.i.d. iterations of monotone maps to multi-dimensional state spaces, and improve upon some recent results in Bhattacharya and Majumdar (1999, 2007), by dispensing with the requirement of continuity of the maps. The state spaces of the Markov process we consider is assumed to be a subset of $\mathbb{R}^k (k \geq 1)$ satisfying the following assumption:

(A.1) *S is either a closed subset of* $\mathbb{R}^k$, *or a Borel subset which can be made homeomorphic to a closed subset of* $\mathbb{R}^k$, *by means of a strictly increasing continuous map on S into* $\mathbb{R}^k$.

It may be noted that every rectangle $X_{j=1}^k I_j$, where I_j's are arbitrary nondegenerate sub-intervals of the real line $\mathbb{R}$ satisfies the assumption (A.1). For, an interval $(a, b)(-\infty \le a < b \le \infty)$ is homeomorphic to $(-\infty, \infty)$ by an appropriate strictly increasing continuous map. An interval $(a, b](-\infty \le a < b < \infty)$ is similarly homeomorphic to $(-\infty, 0]$, etc.

To define the Markov process, let Γ be a set of measurable *monotone maps* $\gamma = (\gamma_1, \gamma_2, \ldots, \gamma_k)$ on S into S, under the *partial order*: $\mathbf{x} \le \mathbf{y}$ if $x_j \le y_j$ for $1 \le j \le k$; $\mathbf{x} = (x_1, \ldots, x_k), \mathbf{y} = (y_1, y_2, \ldots, y_k) \in \mathbb{R}^k$ (or S). That is, either γ is *monotone increasing*: $\gamma(\mathbf{x}) \le \gamma(\mathbf{y})$ if $\mathbf{x} \le \mathbf{y}$, or γ is *monotone decreasing*: $\gamma(\mathbf{y}) \le \gamma(\mathbf{x})$ if $\mathbf{x} \le \mathbf{y}$; $\mathbf{x}, \mathbf{y} \in S$. Let Γ be endowed with a σ-field $\mathcal{C}$, and let Q be a probability measure on $(\Gamma, \mathcal{C})$. Consider a sequence of i.i.d. maps $\{\alpha_n : n \ge 1\}$ with common distribution Q, defined on a probability space $(\Omega, \Im, P)$. For purposes of measurability, assume that the map $(\gamma, \mathbf{x}) \to \gamma(\mathbf{x})$ on $\Gamma X S$ into S is measurable with respect to the product σ-field $\mathcal{C} \otimes \mathcal{B}(S)$ on $\Gamma X S$ and the Borel σ-field $\mathcal{B}(S)$ on S. For each $\mathbf{y} \in S$, define the Markov process $\{X_n : n \ge 0\}$ by

$$X_0 = \mathbf{y}, \quad X_1 = \alpha_1 X_0, \ldots, X_n = \alpha_n X_{n-1} = \alpha_n \alpha_{n-1} \ldots \alpha_1 X_0, \tag{2.1}$$

where $\alpha_n \alpha_{n-1} \ldots \alpha_1$ denotes *composition of maps* in the indicated order. In general, X_0 can be any random variable with values in S, independent of the sequence $\{\alpha_n : n \ge 1\}$. The *transition probability* of the Markov process is $p(\mathbf{x}, B) = P(\alpha_1 \mathbf{x} \in B) = Q(\{\gamma \epsilon \Gamma : \gamma \mathbf{x} \in B\})$. In general, the *n-step transition probability* is given by the distribution of $X_n(\mathbf{x}) \equiv \alpha_n \alpha_{n-1} \ldots \alpha_1 \mathbf{x}$, and is denoted by $p^{(n)}(\mathbf{x}, .)$. It may also be expressed as

$$p^{(n)}(\mathbf{x}, B) = Q^n \left(\{\gamma \in \Gamma^n : \tilde{\gamma}\, \mathbf{x} \in B\} \right), \quad (\mathbf{x} \epsilon S, \ B \epsilon \mathcal{B}(S)), \quad n \ge 1, \tag{2.2}$$

where Q^n is the product probability on the product space $(\Gamma^n, \mathcal{C}^{\otimes n})$, and $\tilde{\gamma}$ is the composition

$$\tilde{\gamma}\, \mathbf{x} = \gamma_n \gamma_{n-1} \ldots \gamma_1 \mathbf{x} \quad (\gamma = (\gamma_1, \gamma_2, \ldots, \gamma_n) \in \Gamma^n). \tag{2.3}$$

Recall that π is an *invariant probability* for the Markov process, or for the transition probability p, if π is a probability measure on $(S, \mathcal{B}(S))$ satisfying

$$\pi(B) = \int p(\mathbf{x}, B) \pi(d\mathbf{x}) \quad \forall B \epsilon \mathcal{B}(S). \tag{2.4}$$

In turn, (2.4) implies that $\pi(B) = \int p^{(n)}(\mathbf{x}, B) \pi(d\, \mathbf{x})\ \forall B \epsilon \mathcal{B}(S)$, and $\forall n \ge 1$. If one denotes the distribution of X_n as $T^{*n}\mu$, where μ is the distribution of X_0, then T^{*n} is the n-fold composition of $T^* : T^{*n} = T^* T^{*(n-1)} (n \ge 2)$, $T^{*1} = T^*$. Note that T^* (as well as T^{*n}) is a map on the *space* $\wp(S)$ *of all probability measures on* $(S, \mathcal{B}(S))$:

$$(T^{*n}\mu)(B) = \int p^{(n)}(\mathbf{x}, B)\mu(d\mathbf{x}) \quad (\mu \in \wp(S), B \in \mathcal{B}(S)). \tag{2.5}$$

Clearly, an invariant probability π is just a *fixed point* of $T^* \equiv T^{*1}$, in which case it is a fixed point of T^{*n} for every n.

On the space $\wp(S)$, define, for each $a > 0$, the metric

$$d_a(\mu, \nu) = \sup_{g \in \mathcal{G}_a} \left| \int g d\mu - \int g d\nu \right|, \quad (\mu, \nu \in \wp(S)), \tag{2.6}$$

where $\mathcal{G}_a$ is the *class of all Borel measurable monotone* (increasing or decreasing) *functions g on S into* $[0, a]$. It is simple to check that (i) $d_a = ad_1$, and (ii) the distance (2.6) remains the same if $\mathcal{G}_a$ is restricted to monotone increasing Borel measurable functions on S into $[0, a]$. The following result is due to Chakraborty and Rao (1998), who derived a number of interesting results on the metric space $(\wp(S), d_a)$. One can show that convergence in the metric d_a implies weak convergence if (A1) holds (Bhattacharya and Majumdar 2007, pp. 287–288).

Lemma 1 *Under the hypothesis* (A.1), $(\wp(S), d_a)$ *is a complete metric space.*

The following *splitting condition* generalizes that in Dubins and Freedman (1966). To state it, let $\tilde{\gamma}$ be as in (2.3), but with $n = N : \tilde{\gamma} = \gamma_N \gamma_{N-1} \dots \gamma_1$ for $\gamma = (\gamma_1, \gamma_2, \dots, \gamma_N) \in \Gamma^N$.

(A.2) *There exist* $F_i \in \mathcal{C}^{\otimes N} (i = 1, 2)$ *for some* $N \geq 1$, *such that*
 (i) $\delta_i \equiv Q^N(F_i) > 0$ $(i = 1, 2)$, *and*
 (ii) *for some* $\mathbf{x_0} \in S$, *one has*

$$\tilde{\gamma}(\mathbf{x}) \leq \mathbf{x}_0 \quad \forall \mathbf{x} \in S, \quad \forall \gamma \in F_1,$$
$$\tilde{\gamma}(\mathbf{x}) \geq \mathbf{x}_0 \quad \forall \mathbf{x} \in S, \quad \forall \gamma \in F_2,$$

Also, assume that the set $H_+ = \{\gamma \in \Gamma^N : \tilde{\gamma}$ *is monotone increasing*$\} \in \mathcal{C}^{\otimes N}$.

Readers interested in the verification of the splitting condition in dynamic models in economics may turn to Bhattacharya and Majumdar (2007).

Our main result is the following:

Theorem 2 *Let* $\{\alpha_n : n \geq 1\}$ *be a sequence of i.i.d. measurable monotone maps with a common distribution Q. Assume* (A.1), (A.2) *hold. Then there exists a unique invariant probability* π *for the Markov process* (2.1) *and*

$$\sup_{\mathbf{x} \in S} d_1 \left(p^{(n)}(\mathbf{x}, \cdot), \pi \right) \leq (1 - \delta)^{[\frac{n}{N}]} \quad (n \geq 1), \tag{2.7}$$

where $\delta = \min\{\delta_1, \delta_2\}$, *and* $\left[\frac{n}{N}\right]$ *is the integer part of* $\frac{n}{N}$.

Proof The proof uses Lemma 1 and two steps. The first involves detailed calculations.
Step 1. T^{*N} is a uniformly strict contraction on $(\wp(S), d_1)$.

Let $F_{i+} = F_i \cap H_+$, $F_{i-} = F_i \cap H_-$, where H_+ is defined in (A.2), and $H_- = \Gamma^N \backslash H_+ (i = 1, 2)$. Define, for any given $g \in \mathcal{G}_1$, the functions

$$\begin{aligned}
h_{i+}(\mathbf{x}) &= \int\limits_{F_{i+}\backslash(F_{i+}\cap F_j)} g(\tilde{\gamma}\mathbf{x})Q^N(d\gamma),\\
h_{i-}(\mathbf{x}) &= \int\limits_{F_{i-}\backslash(F_{i-}\cap F_j)} g(\tilde{\gamma}\mathbf{x})Q^N(d\gamma), \qquad (i = 1, 2;\ j \neq i);\\
h_{3+}(\mathbf{x}) &= \int\limits_{H_+\cap(F_1\cup F_2)^c} g(\tilde{\gamma}\mathbf{x})Q^N(d\gamma),\\
h_{3-}(\mathbf{x}) &= \int\limits_{H_-\cap(F_1\cup F_2)^c} g(\tilde{\gamma}\mathbf{x})Q^N(d\gamma),\\
h_4(\mathbf{x}) &= \int\limits_{F_1\cap F_2} g(\tilde{\gamma}\mathbf{x})Q^N(d\gamma).
\end{aligned} \tag{2.8}$$

Then the functions $h_{i\pm}(i = 1, 2, 3)$, are monotone. To see this, let g be monotone increasing, then $h_{i+}(i = 1, 2, 3)$ are monotone increasing while $h_{i-}(i = 1, 2, 3)$ are monotone decreasing. If g is monotone decreasing, then the reverse holds. Now, for g monotone increasing ($g \in \mathcal{G}_1$),

$$\begin{aligned}
h_{1+}(\mathbf{x}) &\leq g(\mathbf{x}_0)\Big(Q^N(F_{1+}) - Q^N(F_{1+} \cap F_2)\Big) \equiv a_{1+},\\
h_{1-}(\mathbf{x}) &\leq g(\mathbf{x}_0)\Big(Q^N(F_{1-}) - Q^N(F_{1-} \cap F_2)\Big) \equiv a_{1-},\\
h_{2+}(\mathbf{x}) &\geq g(\mathbf{x}_0)\Big(Q^N(F_{2+}) - Q^N(F_{2+} \cap F_1)\Big),\\
h_{2-}(\mathbf{x}) &\geq g(\mathbf{x}_0)\Big(Q^N(F_{2-}) - Q^N(F_{2-} \cap F_1)\Big),\\
h_{3+}(\mathbf{x}) &\leq Q^N\left(H_+ \cap (F_1 \cup F_2)^c\right) \equiv a_{3+},\\
h_{3-}(\mathbf{x}) &\leq Q^N\left(H_- \cap (F_1 \cup F_2)^c\right) \equiv a_{3-}.
\end{aligned} \tag{2.9}$$

Also, write

$$\begin{aligned}
h'_{2+}(\mathbf{x}) &= \int\limits_{F_{2+}\backslash(F_{2+}\cap F_1)} (1 - g(\tilde{\gamma}\mathbf{x}))Q^N(d\gamma),\\
h'_{2-}(\mathbf{x}) &= \int\limits_{F_{2-}\backslash(F_{2-}\cap F_1)} (1 - g(\tilde{\gamma}\mathbf{x}))Q^N(d\gamma).
\end{aligned} \tag{2.10}$$

Then $h'_{2\pm}(\mathbf{x})$ are monotone and satisfy

$$\begin{aligned} h'_{2+}(\mathbf{x}) &\leq (1-g(\mathbf{x}_0))\Big(Q^N(F_{2+}) - Q^N(F_{2+}\cap F_1)\Big) \equiv a_{2+},\\ h'_{2-}(\mathbf{x}) &\leq (1-g(\mathbf{x}_0)\big(Q^N(F_{2-}) - Q^N(F_{2-}\cap F_1)\big) \equiv a_{2-}. \end{aligned} \tag{2.11}$$

Thus $h_{1\pm}\epsilon\mathcal{G}_{a_1\pm}$, $h'_{2\pm}\epsilon\,\mathcal{G}_{a_{2\pm}}$, $h_{3\pm}\epsilon\,\mathcal{G}_{a_{3\pm}}$. Also,

$$\left|\int h_{2\pm}(\mathbf{x})\mu(d\mathbf{x}) - \int h_{2\pm}(\mathbf{x})\nu(d\mathbf{x})\right| = \left|\int h'_{2\pm}(\mathbf{x})\mu(d\mathbf{x}) - \int h'_{2\pm}(\mathbf{x})\nu(d\mathbf{x})\right|, \tag{2.12}$$

and

$$\int h_4(\mathbf{x})\mu(d\mathbf{x}) - \int h_4(\mathbf{x})\nu(d\mathbf{x}) = 0 \quad (\mu,\nu\epsilon\wp(S)). \tag{2.13}$$

The last relation follows from the fact that $h_4(\mathbf{x}) = g(\mathbf{x}_0)Q^N(F_1\cap F_2)$, a constant function on S. For, on $F_1\cap F_2$, $\tilde{\gamma}(\mathbf{x}) = \mathbf{x}_0\forall\mathbf{x}\epsilon S$. Hence

$$\begin{aligned} &\left|\int gd(T^{*N}\mu) - \int gd(T^{*N}\nu)\right|\\ &= \left|\sum_{i=1}^{3}\left[\int h_{i+}(\mathbf{x})\mu(d\mathbf{x}) - \int_i h_{i+}(\mathbf{x})\nu(d\mathbf{x}) + \int h_{i-}(\mathbf{x})\mu(d\mathbf{x}) - \int h_{i-}(\mathbf{x})\nu(d\mathbf{x})\right]\right|\\ &\leq \sum_{i=1,3}\left|\int h_{i+}(\mathbf{x})\mu(d\mathbf{x}) - \int h_{i+}(\mathbf{x})\nu(d\mathbf{x})\right| + \sum_{i=1,3}\left|\int h_{i-}(\mathbf{x})\mu(d\mathbf{x}) - \int h_{i-}(\mathbf{x})\nu(d\mathbf{x})\right|\\ &\quad + \left|\int h'_{2+}(\mathbf{x})\mu(d\mathbf{x}) - \int h'_{2+}(\mathbf{x})\nu(d\mathbf{x})\right| + \left|\int h'_{2-}(\mathbf{x})\mu(d\mathbf{x}) - \int h'_{2-}(\mathbf{x})\nu(d\mathbf{x})\right|\\ &\leq (a_{1+} + a_{1-} + a_{2+} + a_{2-} + a_{3+} + a_{3-})d_1(\mu,\nu) \equiv \bar{b}d_1(\mu,\nu), \text{ say.} \end{aligned} \tag{2.14}$$

Note that

$$\begin{aligned} a_{1+} + a_{1-} &= g(\mathbf{x}_0)\Big(Q^N(F_1) - Q^N(F_1\cap F_2)\Big),\\ a_{2+} + a_{2-} &= (1-g(\mathbf{x}_0))\Big(Q^N(F_2) - Q^N(F_1\cap F_2)\Big),\\ a_{3+} + a_{3-} &= Q^N((F_1\cup F_2)^c) = 1 - Q^N(F_1) - Q^N(F_2) + Q^N(F_1\cap F_2), \end{aligned}$$

so that, adding these terms, one gets

$$\begin{aligned} \bar{b} &= 1 - \Big[(1-g(\mathbf{x}_0))Q^N(F_1) + g(\mathbf{x}_0)Q^N(F_2)\Big]\\ &\leq 1 - \min\Big\{Q^N(F_1),\ Q^N(F_2)\Big\} = 1 - \delta. \end{aligned} \tag{2.15}$$

Taking the supremum over all monotone increasing $g \in \mathcal{G}_1$ on the left in (2.14), one arrives at the inequality

$$d_1\left(T^{*N}\mu,\, T^{*N}\nu\right) \leq (1-\delta)d_1(\mu,\nu), \quad \forall\mu,\nu\in\wp(S). \tag{2.16}$$

Note that, the supremum in (2.6) over all of $\mathcal{G}_a$ is the same as the supremum over the subset of all monotone increasing functions in $\mathcal{G}_a$, since $a - g \in \mathcal{G}_a$ and is monotone increasing if g is monotone decreasing, $g \in \mathcal{G}_a$. Thus T^{*N} is a uniformly strict contraction on $(\wp(S), d_1)$.

Step 2. Application of the Contraction Mapping Theorem.

From (2.16) and Lemma 1, it follows by the contraction mapping theorem that T^{*N} has a unique fixed point π in $\wp(S)$ and that, writing $n = \left[\frac{n}{N}\right]N + r$, one has

$$\begin{aligned} d_1(T^{*n}\mu,\,\pi) &= d_1\left(T^{*[\frac{n}{N}]N}T^{*r}\mu,\; T^{*[\frac{n}{N}]N}\pi\right) \leq (1-\delta)^{[\frac{n}{N}]}d_1(T^{*r}\mu,\pi) \\ &\leq (1-\delta)^{[\frac{n}{N}]} \quad \forall\mu,\nu\in\wp(S). \end{aligned} \tag{2.17}$$

In particular, (2.7) follows by letting $\mu = \delta_{\{\mathbf{x}\}}$ – the Dirac measure at $\mathbf{x}$ in (2.17). Note that $T^{*N}(T^*\pi) = T^*(T^{*N}\pi) = T^*\pi$, so that $T^*\pi$ is also a fixed point of T^{*N}. By uniqueness of the fixed point, $T^*\pi = \pi$. □

Remark 2.1 In order to derive confidence regions of (or tests for) useful functionals of π (e.g., the mean or dispersion), based on a finite set of observations $X_j (1 \leq j \leq n)$, one needs to derive asymptotic distributions of the corresponding functionals of the *empirical distribution* $\frac{1}{n}\sum_{j=1}^{n}\delta_{X_j}$. As in Bhattacharya and Majumdar (2007, Sections 5.3, 5.4), one can show that, under the assumptions (A.1), (A.2), for every bounded function g on S which may be expressed as the difference $g_1 - g_2$ of two bounded measurable monotone functions (or, equivalenty, for every finite linear combination of monotone functions), the central limit theorem (CLT) holds for its empirical mean $\frac{1}{n}\sum_{j=1}^{n} g(X_j)$, whatever the initial state. That is,

$$\sqrt{n}\left(\frac{1}{n}\sum_{j=1}^{n} g(X_j) - \int g\,d\pi\right) \underset{n\to\infty}{\overset{\mathcal{L}}{\to}} N(0,\sigma^2), \tag{2.18}$$

where $\overset{\mathcal{L}}{\to}$ denotes convergence in law, or distribution, and $N(0, \sigma^2)$ is the Normal distribution with mean 0 and variance σ^2. The variance parameter may be expressed as

$$\sigma^2 = \int f^2(\mathbf{y})\pi(d\mathbf{y}) - \int (Tf)^2(\mathbf{y})\pi(d\mathbf{y}), \tag{2.19}$$

where T is the *transition operator*: $Th(\mathbf{x}) = \int h(\mathbf{y})p(\mathbf{x}, d\mathbf{y})$ and f solves the *Poisson equation* in $L^2(S, \pi)$

$$(I - T)f = g - \int g d\pi. \tag{2.20}$$

Here $L^2(S, \pi)$ is the Hilbert space of functions on S which are square integrable (with respect to π). See Bhattacharya and Majumdar (2007, Chap. 5) for more details on this general theme. In the case S is non-compact and g is unbounded (e.g., $g(\mathbf{x}) = x_j$ for $\mathbf{x} = (x_1, \ldots, x_k)$), one requires that there exist a solution f to the Poisson equation (2.20). Certain broad conditions for this solvability may be found in Bhattacharya and Lee (1988), for the case of i.i.d. monotone increasing maps.

Remark 2.2 Instead of the metric d_1, one may use a somewhat weaker metric $d_{\mathcal{A}}$ defined by

$$d_{\mathcal{A}}(\mu, \nu) = \sup_{A \in \mathcal{A}} |\mu(A) - \nu(A)| \quad (\mu, \nu \in \wp(S)), \tag{2.21}$$

where $\mathcal{A}$ comprises all sets of the form

$$A = \{\mathbf{y} \in S : \varphi(\mathbf{y}) \leq \mathbf{x}\}, \quad \mathbf{x} \in S, \quad \varphi \text{ monotone measurable.} \tag{2.22}$$

One may prove the completeness of $(\wp(S), d_{\mathcal{A}})$ more or less following the steps of the proof of Lemma C5.1, p. 287, in Bhattacharya and Majumdar (2007), where $\mathcal{A}$ is restricted to the class of sets A in (2.22) with φ continuous and monotone increasing. The analog of Theorem 2.2, with $d_{\mathcal{A}}$ in place of d_1, may then be proved roughly along the lines of the proof of Corollary 5.1, pp. 257–258, in Bhattacharya and Majumdar (2007).

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Part V
Stochastic Foundations in Applied Sciences II: Geophysics

Chapter 14
Advection-Dispersion in Fluid Media and Selected Works of Rabi Bhattacharya

Enrique A. Thomann and Edward C. Waymire

Abstract In its broadest sense, understanding the dispersion of particles suspended in fluid media is a classic problem that has motivated a tremendous amount of laboratory and field experimentation as well as mathematical and physical theory for centuries. The theory traces back to celebrated work of such historically eminent scientists as Adolf Fick, Albert Einstein, Marian Smoluchowski, Jean Perrin, and Geoffrey I. Taylor, to name a few of the most prominent historic figures. The richness of the problem is reflected in the development of new mathematical, statistical, and computational tools that have resulted from continued explorations of this phenomena beyond the framework of advection-dispersion in a pure liquid. The work of Rabi Bhattacharya, in collaboration with hydrologist Vijay Gupta, stands out for the important theoretical insights provided to contemporary understanding of this phenomena in heterogeneous media over a range of space-time scales. This chapter is an attempt to provide some overview and context for the salient features of these contributions.

Keywords Diffusion, Dispersion Brownian motion, Multi-scale, Homogenization, Markov processes, Parabolic partial differential equations, Central limit theorems

14.1 Introduction

In its broadest sense, understanding the dispersion of particles suspended in fluid media is a classic problem that has motivated a tremendous amount of laboratory and field experimentation as well as mathematical and physical theory for centuries. The theory traces back to celebrated work of such historically eminent scientists as Adolf Fick, Albert Einstein, Marian Smoluchowski, Jean Perrin and Geoffrey I. Taylor, to name a few of the most prominent historic figures. The richness of the problem is reflected in the development of

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new mathematical, statistical, and computational tools that have resulted from continued explorations of this phenomena beyond the framework of advection-dispersion in a pure liquid. The work of Rabi Bhattacharya, in collaboration with hydrologist Vijay Gupta, stands out for the important theoretical insights provided to contemporary understanding of this phenomena in heterogeneous media over a range of space-time scales.

From the point of view of continuum mechanics, the modern theoretical understanding of dispersion of a dilute concentration of particles suspended in a fluid domain G is generally viewed (defined) as the solution to a linear parabolic partial differential equation governing particle concentration $c(y,t)$ at location y and time t of the general form

$$\frac{\partial c}{\partial t} = L^* c(y,t) \equiv \frac{1}{2}\nabla(D\nabla c) - \nabla \cdot vc, \quad t > 0, y \in G, \tag{14.1}$$

for a positive-definite symmetric matrix D (dispersion coefficient), fluid velocity vector field v (drift coefficient), and some initial concentration $c_0(y) = c(y, 0^+)$, and suitable boundary condition on ∂G, e.g., Dirichlet or Neumann. Here $\nabla = (\frac{\partial}{\partial x_j})_{1\le j\le k}$, and we have taken the liberty of a k-dimensional mathematical formulation. For practical purposes one is generally interested in $k = 1, 2$ or 3. In general D and/or v may be both space-time dependent; however, for the purposes of this chapter we restrict to the time-homogenous (autonomous) cases in which the dependence is at most on spatial variables. This class of equations is generally accepted as the result of mass conservation together with a localized linear phenomenological law governing particle flux (*Ficks law*) as being proportional to the gradient of particle concentration.

From the point of view of probability theory, the same phenomena can be viewed (defined) in terms of the stochastic processes $X^x = \{X^x(t) : t \ge 0\}$ governing particle motions as defined by corresponding stochastic differential equations of the form

$$dX^x(t) = \mu(X^x(t))dt + \sqrt{D(X^x(t))}dB(t), \quad t > 0, x \in G, \tag{14.2}$$

initiated at $X^x(0) = x \in G$ and stopped or reflected at the boundary of G, where $B = \{B(t) : t \ge 0\}$ is standard Brownian motion started at the origin, and

$$\mu_j = v_j + \nabla De_j, \quad 1 \le j \le k. \tag{14.3}$$

A relationship between these two views is most succinctly expressed in the case of free space $G = \mathbb{R}^k$ with the aid of Itô's lemma by the property that for a large class of sufficiently smooth functions g

$$g(X^x(t)) - \int_0^t Lg(X^x(s))ds = M_t^x(g), \quad t \ge 0, x \in \mathbb{R}^k, \tag{14.4}$$

is a martingale, in fact a stochastic integral with respect to B. Here $Lg = \frac{1}{2}\nabla \cdot D\nabla g + \mu \cdot \nabla g$ is the elliptic operator (formally) adjoint to L^* given in (14.1) via integration by parts. In particular, it follows upon taking $g = c_0$

$$g(x,t) = \mathbb{E}c_0(X^x(t)) = \int_{\mathbb{R}^k} c_0(y)p(t,x,dy), \quad t \ge 0, x \in G = \mathbb{R}^k, \tag{14.5}$$

where $p(t, x, dy)$ is the transition probability for the Markov processes X^x, and/or the fundamental solution to the adjoint to (14.1).

While the above sketch takes liberties with some technical conditions, the Stroock-Varadhan use of Itô's stochastic calculus in the formulation of the martingale problem for diffusions establishes this mathematical perspective as a powerful connection between (14.1) and (14.2) under very general conditions, see [27]. Of course there are other approaches, some heuristic and some rigorous. From the point of view of partial differential equations perhaps the greatest testimony to such connections of the latter type was captured by the late John Nash [22] in connection with his celebrated results on the existence of a smooth transition density $p(t, x, y)$ as a function of y under remarkably general conditions on the coefficients: "The methods used here were inspired by physical intuition, but the ritual of mathematical exposition tends to hide this natural basis. For parabolic equations, diffusion, Brownian movement, and flow of heat or electrical charges all provide helpful interpretations."

In the case of constant drift and dispersion coefficients, Donsker's functional central limit theorem firmly establishes Brownian motion as the appropriate model of stochastic particle motions in the sense of a scaling limit as anticipated by Einstein, Smoluchowski and an inspiration to Nash. As will be elaborated somewhat, this is a perspective clearly shared by Rabi in his efforts to understand and explain some specific dispersive phenomena of interest to hydrologists in multi-scale heterogeneous media.

Specifically for the case of homogeneous, dispersion matrix $DI_{k\times k}$ for a positive scalar D, and constant drift vector v, one may arrive at the representation

$$X^x(t) = x + vt + \sqrt{D}B(t), \quad t \geq 0, \tag{14.6}$$

via the central limit theorem applied to rescaled random walks in the limit of large frequency of collisions, e.g., see [16]. The appeal to "dilute" systems of particles is a formal appeal to weak interactions so that the law of large numbers may be applied to connect the probability density of an individual particle with particle concentrations.

The Ornstein-Uhlenbeck process provides an alternative approach to obtain a stochastic evolution of a heavy particle undergoing collisions with many relatively lighter fluid molecules based on considerations of velocity in place of position. For example, Holley [20] considered a motion in one coordinate direction of a solute particle of mass M bombarded by a Poisson distribution of lighter molecules of density $\rho(M) > 0$ moving independently according to (one-dimensional) velocities governed by simple symmetric random walk; i.e., velocity $\pm v(M)$ with equal probabilities, and assuming conservation of momentum and energy upon collision with the heavy particle. Molecules simply exchange velocities in collisions with one another. Denote the velocity process for the solute particle by $V_M = \{V_M(t) : t \geq 0\}$ with $V_M(0) = 1$. For a sufficiently high density and rate of collision with the lighter molecules relative to the size of the large solute particle, one has the following.

Theorem 1 (Holley). *Let* $v(M) = \sqrt{\frac{(M+1)D}{\beta}}$, *and* $\rho(M) = \frac{\beta}{4}\sqrt{\frac{(M+1)\beta}{D}}$. *Then* V_M *converges in distribution to* V *as* $M \to \infty$, *where* V *is the Gaussian process defined by the unique solution to the Langevin equation*

$$dV(t) = -\beta V(t)dt + \sqrt{D}dB(t), V(0) = 0.$$

Using Itô's lemma, for example, one arrives at the corresponding velocity process given by

$$V^v(t) = ve^{-\beta t} + \sqrt{D}\int_0^t e^{-\beta(t-s)}dB(s), \quad t \geq 0. \tag{14.7}$$

Integration by parts yields (for a deterministic integrand)

$$V^v(t) = ve^{-\beta t} + \sqrt{D}B(t) - \sqrt{D}\beta\int_0^t e^{-\beta(t-s)}B(s)ds, \ t \geq 0. \tag{14.8}$$

In particular V^v is a Gaussian Markov process with $\mathbb{E}V^v(t) = ve^{-\beta t}$ and $\mathrm{cov}(V^v(s), V^v(t)) = \frac{D}{2\beta}e^{-\beta(t-s)} - \frac{D}{2\beta}e^{-\beta(t+s)}, 0 < s < t$. For initial conditions $v = 0, x$ and integrating one obtains the (non-Markov) position process

$$X^x(t) = x + \sqrt{D}\int_0^t e^{-\beta(t-s)}B(s)ds, \quad t \geq 0. \tag{14.9}$$

Integration by parts provides the alternative formula by a stochastic integral

$$X^x(t) = x + \frac{\sqrt{D}}{\beta}B(t) - \frac{\sqrt{D}}{\beta}\int_0^t e^{-\beta(t-s)}dB(s) \tag{14.10}$$

Taking $\sqrt{D} = \beta\sqrt{D_0}$, one obtains convergence in distribution to Brownian motion with zero drift and diffusion coefficient D_0 in the limit as $\beta \to \infty$. In particular, in this case one has from Itô isometry that

$$\mathbb{E}|X^x(t) - x - \sqrt{D_0}B(t))|^2 = (2\beta)^{-1}(1 - e^{-2\beta t}) < \frac{1}{2\beta}. \tag{14.11}$$

Alternatively, on large time scales the Brownian motion is essentially equivalent to the integrated Ornstein-Uhlenbeck process in the sense that for

$$X_n^x(t) = n^{-\frac{1}{2}}\beta X^x(nt) = n^{-\frac{1}{2}}\beta x + n^{-\frac{1}{2}}\int_0^{nt}\beta V(s)ds \tag{14.12}$$

one has convergence in distribution

$$X_n^x \Rightarrow \sqrt{D}B \tag{14.13}$$

as $n \to \infty$. Although this particular (Gaussian) case may be treated by more elementary methods, it provides a simple illustration of a central limit theorem for ergodic Markov processes by Rabi [9] that has enjoyed remarkable applications to problems in hydrology and geophysics that will be elaborated upon in forthcoming sections. We quote his general theorem for the general context of progressively measurable ergodic Markov processes Y with arbitrary state space $(S, \mathcal{S})$ having unique invariant probability π. Let $(A, \mathcal{D}_A)$ denote the infinitesimal generator of the corresponding Markov process semigroup acting on $L^2(S, \pi)$.

Theorem 2 (Bhattacharya). *Let p be a transition probability of a Markov process Y admitting an invariant initial distribution π. Assume that $\|p(t, x, \cdot) - \pi(\cdot)\| \to 0$ as $t \to \infty$ for all $x \in S$. Let $h : S \to \mathbb{R} \in L^2(\pi)$ and assume h belongs to the range of A. Then regardless of the initial distribution of Y, the sequence of stochastic processes $n^{-\frac{1}{2}} \int_0^{nt} h(Y(s))ds, t \geq 0, n = 1, 2, \ldots$, converges weakly to a Brownian motion σB having zero drift and diffusion coefficient σ^2 given by*

$$\sigma^2 = -2\langle h, g\rangle = -2 \int_S h(y)g(y)\pi(dy)$$

for any $g \in \mathcal{D}_A$ such that $Ag = h$.

Returning to (14.13), $Y = V$ is the Ornstein-Uhlenbeck process whose generator is of the form $A = -\beta y \frac{\partial}{\partial y} + \sqrt{D} \frac{\partial^2}{\partial y^2}$. It is also easy to check that V has Gaussian invariant probability π with mean zero and variance $\frac{D}{2\beta}$. For $h(y) = \beta y$ in (14.12), one may take $g(y) = -y$, to compute $\sigma^2 = D$ as asserted in (14.13).

Remark 1. Deeper understanding of distinguished particle systems has been a subject of considerable interest from the point of view of *hydrodynamic limits*, but is outside the scope of the present essay, e.g., see [21]. The purpose here is simply to indicate the role of the Ornstein-Uhlenbeck process as the physical description of velocities of solute particles immersed in pure liquid; also see [29] for a perspective from physics.

14.2 Brownian Motion in Porous Media and Taylor-Aris Dispersion

Among Rabi's earliest considerations of dispersion of solutes in a porous media one finds the paper [13] involving an investigation of pore scale effects on the otherwise limiting Brownian dispersion of a dilute system of particles. More specifically, the authors consider a dilute suspension of particles in a homogeneous isotropic porous medium saturated by a pure fluid such as water. As typical in the framework for Brownian motion, the mass of the solute molecule is assumed to be much larger than that of a liquid molecule, and the particle's interactions are sufficiently weak to be viewed as statistically independent. Roughly, the particle suffers collisions with the solid phase (sometimes referred to as the "pore wall") at successive times, but in between collisions the velocity process is governed by the Ornstein-Uhlenbeck process; the effect of collision with the solid phase is to scatter the particle in a random direction.

Theorem 3 (Bhattacharya and Gupta). *Suppose that* $V = \{V(t) : t \geq 0\}$ *is the velocity process defined by*

$$dV(t) = -\beta(V(t) - u_0)dt + gdt + \sigma dB(t),\ \tau_j < t \leq \tau_{j+1}, j = 0, 1, 2 \ldots,$$
$$V(\tau_j^+) = \rho O_j V(\tau_j),\ i \geq 1,$$

where $\tau_0 = 0, \tau_{j+1} - \tau_j, j \geq 0$, *is an i.i.d. sequence of nonnegative random variables having finite fourth moments such that* $\mu = \mathbb{E}\tau_1$ *is a scale parameter for their common distribution, and* $O_1, O_2, \ldots$ *is an i.i.d. sequence of random orthogonal matrices distributed uniformly according to Haar measure over the group of all* 3×3 *real orthogonal matrices. Also* $0 \leq \rho \leq 1$, *and g is the (constant) gravitational acceleration vector. Let*

$$X^x(t) = x + \int_0^t V(s)ds, \quad t \geq 0.$$

Then, letting $\mu \downarrow 0$ *such that* $\beta\mu \to \delta > 0$, *and* $\sigma^2/\beta^2 \to D_1 > 0$, *one has that* $\sqrt{\mu}(X(t\mu^{-1}) - t\mu^{-1}), 0 \leq t \leq 1$, *converges weakly to Brownian motion with zero drift and diffusion coefficient matrix* $g(\delta)D_1$, *where*

$$g(\delta) = 1 - \frac{1}{\delta}\int_0^\infty \{2(1 - e^{-\delta s}) - \frac{1}{2}(1 - e^{-2\delta s})\} P(\tau_1 \in ds).$$

As noted in [13], at times far apart compared to μ, the position process X is (approximately) governed by a Brownian motion with drift $(u_0 + \beta^{-1}g)(1 - (\beta\mu)^{-1}\int_0^\infty (1 - e^{-\beta\mu s})P(\tau_1 \in ds))$ and diffusion coefficient $\frac{g(\beta\mu)}{\beta^2}\sigma^2$. In general, the basic parameters β, D, μ are regarded as functions of the convective flux u_0. In case $u_0 = 0$ and β and D are the same as in the classical case of diffusion in pure liquids, it follows that the diffusion coefficient in the porous medium is *smaller* than that in the pure liquid and in accordance with experimental observations; see [13] for references and further discussion.

G.I. Taylor's [28] determination of the time-asymptotic equation governing the dispersion of particles immersed in a pure cylindrical flow containing a pure fluid with constant advective velocity U in the longitudinal direction ranks among the most important practical results in the theory of advection-dispersion. While the formula was derived by somewhat formal asymptotic expansions applied to the governing pde, the derivation was eventually made mathematically rigorous by Rutherford Aris [2]. However, an extremely simple explanation[1] in terms of Rabi's central limit theorem (Theorem 2) was developed in [15, 14].

[1] It was not long after the publication of [15] that Rabi, and his coauthor Vijay Gupta, received a note of acknowledgment and congratulations from Rutherford Aris on finding the "right" approach. This idea was used in [24] to cover an application involving a discontinuous diffusion coefficient as well.

Theorem 4. *Let* $\mathbf{X} = (X, Y, Z)$ *be a Markov process having continuous paths in* $\mathbb{R}^3$ *and transition probabilities given by the fundamental solution to satisfying Kolmogorov's forward equation*

$$\frac{\partial c}{\partial t} = D_0 \Delta c - u_0 f(y,z)\frac{\partial c}{\partial x}, \ (x,y,z) \in \mathbb{R} \times E^0 \subset \mathbb{R}^3,$$

with Neumann boundary condition

$$\frac{\partial c}{\partial n} = 0, \quad (x,y,z) \in \mathbb{R} \times \Gamma,$$

where $E^0 = \{(y,z) : y^2 + z^2 \leq a^2\}$ *is the interior of a two-dimensional region* $E = E^0 \cup \Gamma$ *bounded by the smooth curve* $\Gamma = \{(y,z) : y^2 + z^2 = a^2\}$, D_0 *is a positive constant, and* $f(y,z) = 1 - \frac{y^2+z^2}{a^2}$ *is the parabolic flow rate obtained from incompressible Navier-Stokes equations in the cylinder such that* $(f(y,z)u_0, 0)$ *is the fluid velocity (drift). Let* $\overline{u} = \frac{1}{2}u_0$. *Then,*

$$X_n(t) = n^{-\frac{1}{2}}(X(nt) - \overline{u}nt), t \geq 0.$$

Then X_n *converges in distribution to Brownian motion with zero drift and diffusion coefficient*

$$D = 2D_0 + \frac{a^2 u_0^2}{96 D_0}.$$

Note that $D_0 = \frac{1}{2}(2D_0)$ in the Kolmogorov equation makes $2D_0$ the dispersion rate in the stochastic formulation (14.2). While we have stated the above theorem for the case of the cylinder, the general result of [15] allows for arbitrary shaped cross sections E^0 bounded by a smooth curve Γ. The limiting diffusion, suitably centered, remains a Brownian motion with zero drift and positive (effective) diffusion coefficient. For example, motivated by considerations of the stability of a viscous liquid to two-dimensional disturbances in a porous medium, Wooding [30] considered the Taylor-Aris analysis to obtain the corresponding formula for dispersion of a solute in a unidirectional parabolic flow between two parallel planes separated by a distance $2a$. This can be readily computed from Theorem 4 adapted to this geometry; related calculations will be given in 14.4.

14.3 Multiscale Dispersion

Rabi expressed a vision with regard to multi-scaling phenomena being reported by field hydrologists early on in collaborations with hydrologists Vijay Gupta and Garrison Sposito [19]: "The principal outcome of this construction is the fact that, in an appropriate asymptotic sense, the position process $\{X(t); t > 0\}$, as a time integral of the constructed velocity process, is asymptotically Markovian (a Brownian motion) with a mean drift vector, $\mu(U)$, and the dispersion matrix, $D(U)$. Because this result is asymptotic in nature it is valid at the time and space intervals over which a solute molecule undergoes a very large number of collisions with both the liquid molecules and the grains of the solid phase, i.e., at the macroscopic space and time scales. The Markovian nature of the position process, along with the assumption of weak interaction among solute molecules, then may be used to show rigorously that the macroscopic solute concentration, $c(x,t)$, is a solution of a parabolic partial differential equation. This equation differs from (14.1) in that the mean convective velocity of the solute, $\mu(U)$, which appears in it is not necessarily equal to U, the mean fluid velocity."

This was formulated primarily in response to laboratory and field experiments involving the *growth of dispersion* with velocity U. Much of the early thinking was by way of mathematical scaling/averaging principles that *should* hold and *should* explain the empirical observations. Quoting from [10]: "A commonly used experimental methodology is to fit Gaussians to the concentration $c(t,y)$ as a function of y, for successively larger scales of t. One may think of this as different Brownian motion approximations at different scales of time. It has been widely observed that the diagonal dispersion coefficients, or variances per unit time, increase steadily with the time scale, especially in the direction of flow. This phenomenon has been called the scale effect in dispersion." However it took a concentrated effort to develop the new mathematical theory that would precisely illustrate this thinking. The results are truly remarkable and perhaps even beyond expectations, [11, 12, 10, 8]. We include here a simple example to partially illustrate the theory.

From a mathematical perspective, Rabi [10] introduced the following considerations of two spatial scales of heterogeneity embodied in the flow velocity v,

$$v(y) = b(y) + \beta(y/a), \tag{14.14}$$

where a is a large positive scalar. The term $b(\cdot)$ represents the drift velocity at the local scale and $\beta(\frac{\cdot}{a})$ the large scale velocity in the defining k-dimensional stochastic differential equation

$$dX(t) = v(X(t))dt + \sigma(X(t))dB(t), \tag{14.15}$$

where b, β, σ are essentially assumed Lipschitz continuous, and the eigenvalues of $\sigma\sigma'$ are bounded away from zero and infinity. Here fluctuations in b represent the effect of a local (or small) scale heterogeneity in the aquifer geometry and soil characteristics, while fluctuations in v which manifest only at a larger scale of distance (of the order a) are represented in $\beta(a)$. It is assumed that the fluid media is *stratified* to the extent that the large scale velocity $\beta(x_1,\ldots,x_k)$ does not depend on x_1 and there is no small scale velocity in directions other than the x_1 direction, i.e., $b_j(x) = 0$, $j \geq 2$. In this context precise time scales ($t \ll a^{\frac{2}{3}}, t \ll a$, or $t \ll a^{\frac{4}{3}}$) are computed over which the local scale b dominates and large scale fluctuations may be ignored. The significance is that, regardless of the larger scale effects β, whenever a Gaussian approximation holds for the concentration corresponding to flow velocity $b(\cdot) + \beta(x_0)$, for an initial point injection at ax_0 the same holds over this time scale. That is, on this time scale the large scale effect is essentially felt as an additive constant. Beyond this the possibilities are fascinating, ranging from Brownian motion to possible non-Gaussian intermediate and larger scale effects. The reader is invited to consult [10] to appreciate the scope of this theory illustrating Rabi's multiscale theory in terms of a more comprehensive selection of theorems and examples.

Toward explaining the more specific scale effect (growth) of dispersion problem Rabi [10] obtains the following key result. Take $b = 0$ and assume that β is continuously differentiable, periodic with period lattice $\mathbb{Z}^k$, and divergence-free (zero divergence), the latter corresponding to an incompressible fluid. Assume σ is a constant non-singular matrix. X is defined by

$$dX(t) = u_0\beta(X(t))dt + \sigma B(t), \quad t \geq 0, \tag{14.16}$$

where u_0 is a large parameter scaling the magnitude of the (periodic) drift velocity. In view of the periodicity assumptions X is an ergodic diffusion on the k-dimensional torus having uniform invariant distribution $\pi(dx)$. Then, in the limit as $t \to \infty$, $t^{-\frac{1}{2}}(X(t) - X(0) - t\overline{\beta})$ is asymptotically Gaussian with mean zero and dispersion coefficient $K = K(u_0)$, depending on the parameter u_0. Here

$$\overline{\beta} = \int_{[0,1]^k} \beta(x)\pi(dx)$$

is simply the average of β over the torus, and

$$K = \int_{[0,1]^k} (\nabla\phi - I_k)(\nabla\phi - I_k)'dx, \tag{14.17}$$

for the unique mean zero solution $\phi \in L^2(\pi)$ of

$$A\phi_j = u_0(\beta_j - \overline{\beta}_j), \quad 1 \leq j \leq k. \tag{14.18}$$

Theorem 5. *Assume the above conditions on the drift and diffusion coefficients defining X. Let $D = \sigma\sigma'$ and $\mathcal{D} = \frac{1}{2}\sum_{i,j} D_{i,j}\frac{\partial^2}{\partial x_i \partial x_j}$ as an operator on the Sobolev space H^2. Then $i\mathcal{D}^{-1}\beta \cdot \nabla$ is a skew symmetric compact and self-adjoint operator on H^1 with null space N. Denoting projections of $f \in H^1$ onto N by f_N,*

1. *If $(\mathcal{D}^{-1}(\beta_j - \overline{\beta}_j))_N \neq 0$, then $\lim_{u_0\to\infty} \frac{K_{jj}}{u_0^2} = 2\|(\mathcal{D}^{-1}(\beta_j - \overline{\beta}_j))_N\|_1^2 > 0$*
2. *If $\beta_j - \overline{\beta}_j$ belongs to the range of $\beta(\cdot) \cdot \nabla$, say, $\beta(\cdot)\nabla h = \beta_j - \overline{\beta}_j$ for some $h \in H^1$, then $\lim_{u_0\to\infty} K_{jj} = 2\|h_0\|_1^2 + D_{jj}$, where h_0 is the projection of h onto $N^\perp$.*

In particular, under the hypothesis of the first part of this theorem one sees that the dispersion coefficient K_{jj} grows quadratically with u_0. Such behavior is in fact consistent with field observations; see [10] and references therein.

14.4 Discontinuous Coefficients and Skew Dispersion

In recent years there has been an interest in models of advection-dispersion in media under which interfaces defined by discontinuities in the diffusion coefficient occur; see [26] for rather comprehensive survey of applications. In the context of dispersion in porous media [6], for example, includes results of experiments on breakthrough times of an inert dye injected in a water saturated column of glass beads of two distinct sizes and separated by an interface. The results indicate a clear asymmetry in the time required to traverse one end of the column to the other, depending on the injection point. Such experiments prompted the development of new non-Fickean models in efforts to explain such phenomena; e.g., see [17]. Observations of this type prompted more thorough general analysis of the effect of discontinuities in the dispersion coefficient as reported in [6] and references therein. This includes an explanation for the breakthrough asymmetry within a Fickean diffusive framework as well as exploration of other phenomena such as Taylor-Aris dispersion; [1, 24].

While Rabi has laid out a robust approach to dispersion in heterogenous' media, the techniques are largely (although not exclusively) limited to continuous (Lipschitz) drift and dispersion coefficients. For example Theorem 2 could be used to compute the formula for the Taylor-Aris effective dispersion coefficient, but the stochastic calculus involves methods from semi-martingale theory, especially local time, not needed for the case of smooth coefficients.

As an illustration, consider the (interfacial) Taylor-Aris problem (Theorem 4) for Wooding's geometry (see [30]) of two parallel planes separated by $2a$ but assuming $D_0(x,y) = \begin{cases} D_0^+ & \text{if } 0 \le y \le h \\ D_0^- & \text{if } -h \le y < 0. \end{cases}$ Then, using Theorem 2 one finds that the first term of the effective dispersion involves an *arithmetic average* $D_a = (D_0^+ + D_0^-)/2$, while the second term involves a *harmonic average* $\frac{1}{D_h} = \frac{\frac{1}{D_0^+}+\frac{1}{D_0^-}}{2}$ given by

$$D = 2D_a + \frac{8u_0^2h^2}{945(2D_h)} = 2D_a + \frac{2\overline{u}^2h^2}{105(2D_h)}. \tag{14.19}$$

The details of the stochastic calculus needed to extend Theorem 4 to this setting are given in [24].[2]

While the manifestation of small scale discontinuities in the diffusion coefficients has been shown to manifest on larger scales in quite interesting ways, e.g., in occupation and first passage (breakthrough) times, this has largely involved applications that could be reduced to one-dimensional mathematical considerations. The technical limitations are tied to the use of local time in the analysis; see [25] for some other recent developments in this regard.

14.5 Concluding Remarks

The subject of solute transport in porous media is vast, and the survey of select results presented here represents a small but important approach to understanding upscaling in this context; see [18] for a much broader survey of mathematical approaches and perspective.

[2] There is a typo in the general formula of Corollary 2.2 in [24]. The integral in (2.12) should be with respect to Lebesgue measure in place of $\pi(dz)$ there.

The essential parameters that determine the model of advection-dispersion of solute concentrations are a drift rate μ and a dispersion rate $D = \sigma\sigma'$, together with some specification of initial conditions and possible boundary behaviors. However, these rates can be used to describe the phenomena in different ways: (i) to define local fluxes of solute concentration for (14.1), or (ii) to define local mean and variance-covariances of stochastic displacements of individual particles for a model of the type (14.2). In case (i) it is natural to refer to the factor D that, in addition to the drift, defines the flux locally in proportion to the concentration gradient as the *dispersion rate*, while in case (ii) for the same D, $\frac{1}{2}D$ is a local measure of the rate of spread in the distribution of particles. Beyond this, one may elect to analyze the phenomena of advection-dispersion from either mathematical perspective. For this Rabi generally selects the latter.

Regardless of the class of models, the questions generally involve approaches to understand how the rates defining models of type (i) or (ii) should be modified in passing to larger scale descriptions; a process known as *homogenization*. As illustrated by the results surveyed in the previous sections, the larger scale answer generally depends on various scales intrinsic to the defining model.

As evident in the theorems surveyed here, and all the more so in the comprehensive articles themselves, a key feature of the problems amenable to Rabi's approach is that of a *finite* number of *separated* scales; for contrast in which new phenomena occur for infinitely many separated scales see [3] and the discussion in [7]. Moreover, problems of homogenization are also of interest for models in which there is no such separation of scales; e.g., see [23, 5, 4].

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Chapter 15
Cascade Representations for the Navier–Stokes Equations

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15.1 Introduction

The basic equations governing the motion of a fluid are well understood. For simplicity, we shall refer to the case of an incompressible, constant density, viscous Newtonian fluid; the velocity vector field $u(t,x)$ and pressure scalar field $p(t,x)$ satisfy the classical Navier–Stokes equations (in dimension 3) with viscosity $\nu > 0$

$$\begin{aligned} \partial_t u + (u \cdot \nabla)u + \nabla p &= \nu \Delta u, \\ \operatorname{div} u &= 0, \end{aligned} \tag{15.1}$$

with appropriate initial and boundary conditions depending on the problem. For relatively simple fluid motions, these equations give us a very good tool for simulations and physical understanding. But there are complex fluid motions, those usually called turbulent, where special features are experimentally or numerically observed which do not have a clear explanation yet from the Navier–Stokes equations. In a sense, there is something at the foundation of fluid dynamics that is still unclear. For later reference, let us mention that this happens when a certain parameter R, called Reynolds number, is very large.

Andrej Nikolaevič Kolmogorov, in his celebrated paper on turbulence [18], where he exposed very innovative ideas referred to as the K41 theory, used the following sentences to describe something which is a sort of idealization of experimental observations: "on the averaged flow are superposed the 'pulsations of the first order' consisting in disorderly displacements of separate fluid volumes [...] of diameters of the order of magnitude $l^{(1)} = l$ [...]. The pulsations of the first order are for very large R in their turn unsteady, and on

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them are superposed the pulsations of the second order with mixing path $l^{(2)} < l^{(1)}$. [...] the pulsations of the first order absorb the energy of the motion and pass it over successively to pulsations of higher orders."

This is an intuitive description of the so-called *direct cascade*. Kinetic energy flows from larger scale structures (the "pulsations," often called eddies, which may be also thin vortex tubes or patches) to smaller ones, due to dynamical instabilities. Mathematics further idealizes these structures by means of the concept of Fourier component. So, opposite to regular fields, where Fourier components with small wave number k contain most of the energy and it decays very fast for large k's, in a turbulent fluid energy is distributed in a distinguished fashion between Fourier modes, with a sort of "long tail," also related to a poor regularity (at least in the limit of zero-viscosity).

At the same time, mostly in fluids with a 2D symmetry, it is experimentally observed that an *inverse cascade* takes place: energy contained in small scale structures cumulates to increase the energy of larger scale structures. Strictly speaking, in every nontrivial fluid there are both kind of cascade, direct and inverse, but their intensity may be different. We suggest to read U. Frisch [13] for an extensive discussion of cascade models, Kolmogorov theory, and turbulence.

The problem, thus, may be summarized as the question of understanding the interaction between modes, the exchange of energy between them, starting from the Navier–Stokes equations.

Without claiming that it solves this problem, we however like to review some "cascade representation" formulae for solutions to the Navier–Stokes equations, which are clearly based on the interaction between modes. Rabi Bhattacharya contributed to develop this interesting approach that we shall review in next pages.

15.2 Fourier Formulation of the Navier–Stokes Equations

For simplicity, let us consider equations (15.1) on the torus $[0, 2\pi]^3$. Write the Fourier series $u(t, x) = \sum_{k \in \mathbb{Z}^3} u_k(t) e^{ik \cdot x}$, $p(t, x) = \sum_{k \in \mathbb{Z}^3} p_k(t) e^{ik \cdot x}$ where $u_k(t)$ takes values in $\mathbb{C}^3$. The divergence-free condition $\operatorname{div} u = 0$ reads in Fourier variables as $k \cdot u_k(t) = 0$. By replacing the Fourier series into equations (15.1) and by projecting onto the plane orthogonal to k to get rid of the pressure, we get

$$\tfrac{d}{dt} u_k(t) + i \sum_{m+n=k} (u_m(t) \cdot k)\, \pi_k u_n(t) = -\nu\, |k|^2\, u_k(t), \tag{15.2}$$

where the projection is defined as $\pi_k v = (I - \frac{k \otimes k}{|k|^2}) v$, for $v \in \mathbb{R}^3$, and we have used the identity $u_{k_1}(t) \cdot k_2 = u_{k_1}(t) \cdot k$, following from the divergence free condition. These equations are already full of information about the interaction between modes. The difficulty lies in the nature of the bilinear map

$$(u_m, u_n) \longmapsto b_k(u_m, u_n) := i(u_m \cdot \tfrac{k}{|k|}) \pi_k u_n$$

which fulfills the easy bound $|b_k(u_m, u_n)| \leq |u_m|\,|u_n|$ but certainly has other more hidden algebraic properties of major importance, however not easy to exploit. From (15.2) one deduces the energy balance

$$\frac{1}{2}\frac{d}{dt}|u_k|^2 + |k| \sum_{m+n=k} c^u_{k,m,n}|u_k|\,|u_m|\,|u_n| = -\nu|k|^2|u_k|^2$$

where the coefficients $c^u_{k,m,n}(t)$, depending on the solution, are given by

$$c^u_{k,m,n}(t) = b_k(\widetilde{u}_m(t), \widetilde{u}_n(t)) \cdot \widetilde{u}_k(t)$$

where for any k we write $\widetilde{u}_k = \frac{u_k}{|u_k|}$. We have written the energy balance in this peculiar form for comparison with the identity (15.4) below. The difficulty here is that it is not clear when the energy flux is stronger in a direction more than another. As a comparison, let us mention the following simplified model (called dyadic model of turbulence, see [11, 3, 2]), made of scalar valued equation

$$\frac{d}{dt}X_n(t) = -\nu k_n^\alpha X_n(t) + k_{n-1}X_{n-1}^2(t) - k_n X_n(t)\, X_{n+1}(t) \qquad (15.3)$$

where it is possible to understand very well the flux of energy between components, at least when all $X_n(t)$ are positive. Indeed here

$$\frac{1}{2}\frac{d}{dt}|X_n(t)|^2 = -\nu k_n^\alpha |X_n(t)| + k_{n-1}X_{n-1}^2(t)\, X_n(t) - k_n |X_n(t)|^2 X_{n+1}(t) \qquad (15.4)$$

and thus, for solutions with all positive components, the energy $\frac{1}{2}|X_n(t)|^2$ of mode n increases due to mode $n-1$ and decreases due to mode $n+1$. The energy flux is from large scale to small scale structures.

For equations (15.2) this is still obscure. There are brilliant rigorous examples, however, in the literature, where something has been said. Let us mention A. Shnirelman [28], who uses the fact that Fourier pairs of modes (k_1, k_2), of the form $k_2 \sim -k_1$, or more precisely $k_2 = -k_1 + k_0$, with small $k_0 \in \mathbb{Z}^3$, produce an effect $b_{k_0}(u_{k_1}, u_{k_2})$ at mode k_0 close to the origin. For large $|k_1|$ (hence large $|k_2|$) we have a sort of inverse cascade, we have small scale structures which transfer energy to large scale structures. In [28] the inviscid equations are considered

$$\frac{d}{dt}u_k(t) + |k| \sum_{m+n=k} b_k(u_m, u_n) = f_k^N(t), \qquad u_k(0) = 0$$

with $f^N = \left(f_k^N\right)_{k\in\mathbb{Z}^3}$ having high amplitude Fourier components at some k_1 and $k_2 = -k_1 + k_0$ with $|k_1| \sim N$ and $|k_0| \sim 1$ (and $f_k^N = 0$ for the other k's). As $N \to \infty$ the forcing term converges weakly to zero and the solution u^N maintains, due to the inverse cascade, a nonzero amplitude at k_0, producing in the limit a nonzero solution which started from the zero initial condition, without forcing term (in particular, that solution is not energy preserving). The precise construction in [28] is obviously more elaborated than the short description given here.

15.3 Picard Iteration and Deterministic Cascade Representation

We may rewrite equation (15.2) as

$$u_k(t) = e^{-\nu|k|^2 t} u_k(0) + \int_0^t e^{-\nu|k|^2(t-s)} |k| \sum_{m+n=k} b_k(u_m(s), u_n(s))\, ds. \tag{15.5}$$

A natural scheme to prove for instance existence of solutions, or for the numerical approximation etc., is the iteration

$$u_k^{n+1}(t) = e^{-\nu|k|^2 t} u_k(0) + \int_0^t e^{-\nu|k|^2(t-s)} |k| \sum_{m+\ell=k} b_k\left(u_m^n(s), u_\ell^n(s)\right) ds, \tag{15.6}$$

with $u_k^0(t) := e^{-\nu|k|^2 t} u_k(0)$. We follow here the presentation given by Gallavotti [14], Ch. 1, Section 12. Advanced results on this approach can be found in the paper by Bhattacharya et al. [4]. Since b_k is bilinear, one can substitute $u_{k_1}^n(s)$ and $u_{k_2}^n(s)$ given in terms of $u_\cdot^{n-1}(\cdot)$ and $u_\cdot^0(\cdot)$ and so on, arriving at a series development based only on $u_\cdot^0(\cdot)$. For instance, just to have a rough idea, $u_k^2(t)$ is the sum of five terms, three of which are (the first one in place of the dots is just $u_k^0(t)$ but it is omitted for comparison with the picture below)

$$u_k^2(t) = \ldots + |k| \int_0^t e^{-\nu|k|^2(t-s)} \sum_{k_1+k_2=k} b_k(u_{k_1}^0(s), u_{k_2}^0(s))\, ds \tag{15.7}$$

$$\begin{aligned} &+ |k| \int_0^t e^{-\nu|k|^2(t-s)} \sum_{k_1+k_2=k} |k_2| \int_0^s e^{-\nu|k_2|^2(s-r)} \cdot \\ &\cdot b_k\Big(\sum_{k_{21}+k_{22}=k_2} b_{k_2}(u_{k_{11}}^0(r), u_{k_{12}}^0(r)), u_{k_2}^0(s)\Big)\, dr\, ds + \ldots \end{aligned} \tag{15.8}$$

$$\begin{aligned} &+ |k| \int_0^t e^{-\nu|k|^2(t-s)} \sum_{k_1+k_2=k} |k_1|\,|k_2| \int_0^s \int_0^s e^{-\nu|k_1|^2(s-r)} e^{-\nu|k_2|^2(s-r')} \cdot \\ &\cdot b_k\Big(\sum_{k_{11}+k_{12}=k_1} b_{k_1}(u_{k_{11}}^0(r), u_{k_{12}}^0(r)), \sum_{k_{21}+k_{22}=k_2} b_{k_2}(u_{k_{21}}^0(r'), u_{k_{22}}^0(r'))\Big), \end{aligned} \tag{15.9}$$

all given explicitly as suitable multi-linear combinations of $u_\cdot^0$. Figure 15.1 shows a (very rough) graphical representation of the three terms in equations (15.7), (15.8), and (15.9).

In [14] the expansion is written symbolically as

$$u_k^n(t) = u_k^0(t) + \sum_{1\le m\le 2^n} \sum_{\Theta\in m\text{-trees}} \Theta\left(k, t, u^0\right)$$

with a suitable definition of the set of all m-trees and of the operation $\Theta\left(k, t, u^0\right)$. Therefore, if a suitable limit takes place, we have the representation

$$u_k(t) = \sum_{m\ge 0} \sum_{\Theta\in m\text{-trees}} \Theta\left(k, t, u^0\right)$$

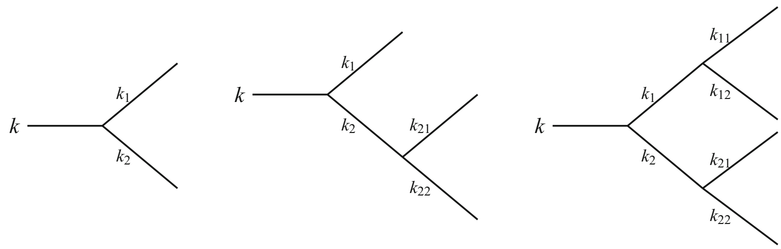

Fig. 15.1 Trees associated with the terms (15.7), (15.8), and (15.9).

where, by convention, we write $\Theta\left(k, t, u^0\right) = u_k^0(t)$ if Θ is the 0-tree. For conceptual comparison with the probabilistic representations detailed below, we see here that, under proper conditions, one can express the solution as a series in terms of the initial condition.

Beside [4], let us also mention the classical work of T. Kato [17] and the recent approach of Y. Sinai [30], see also [1, 29] and [15], which share something with the arguments above.

15.4 Stochastic Cascade and Majorizing Kernels

In the expressions above we see (up to a factor $|k|$) the function $\nu |k|^2 e^{-\nu|k|^2 t}$ which is the exponential density with average $\frac{1}{\nu|k|^2}$. Along with the splitting structure of modes $k \longleftrightarrow k_1 + k_2$, this resembles a probabilistic approach to PDEs, with exponential waiting times and random branching. The idea of using branching processes as the underlying engine of probabilistic representations is not new, let us mention H. P. McKean pioneering work [21], as well as [31, 16]. In these papers branching is coupled with diffusion, and the stochastic representation is derived directly in the physical space, so that the linear operator is limited to generators of diffusions and the nonlinearity is polynomial.

15.4.1 The Stochastic Cascade of Le Jan and Sznitman

Le Jan and Sznitman [19] have seen in these ingredients the opportunity to develop a probabilistic representation formula, which they have called stochastic cascade representation.

Let us give a brief outline of the method. Here we borrow the presentation of [6]. Consider PDEs on $\mathbb{R}^d$ with periodic boundary conditions, possibly vector valued with values in $\mathbb{R}^r$, of the type

$$\partial_t u = Au + F(u) + f, \tag{15.10}$$

where A is an operator with a complete set of eigenfunctions, F is a polynomial nonlinearity (that for simplicity here we assume quadratic) in u and its derivatives, and f is a given driving function. The case of full space can be considered with similar ideas.

In short, the solution u is expanded into Fourier series, and the PDE is transformed into a system of countably many ODEs for the possibly rescaled[1] Fourier coefficients $\chi(t) : \mathbb{Z}^d \to \mathbb{C}^r$ that solve an infinite dimensional system of $\mathbb{C}^r$-valued ODEs

$$\dot{\chi}_k = \lambda_k\Big[-\chi_k + C_b \sum_{m,n\in\mathbb{Z}^d} q_{k,m,n} B_{k,m,n}(\chi_m, \chi_n) + d_k \gamma_k(t)\Big]. \tag{15.11}$$

with $k \in \mathbb{Z}^d$. The constants $\lambda_k > 0$ (that will determine the rate of particle evolution), $q_{k,m,n}$, $d_k \in [0,1]$ (which will determine the probabilities of branching and dying), and $C_b \geq 0$ (the branching constant) are fixed, as are bilinear operators $B_{k,m,n} : \mathbb{C}^r \times \mathbb{C}^r \to \mathbb{C}^r$ satisfying

$$|B_{k,m,n}(\chi, \chi')| \leq |\chi|\,|\chi'|$$

for all $\chi, \chi' \in \mathbb{C}^r$. In view of the probabilistic representation we assume

$$q_k + d_k = 1, \quad k \in \mathbb{Z}^d, \qquad \text{and} \qquad q_k \to 0, \quad \text{as } |k| \to \infty$$

where $q_k = \sum_{m,n\in Z^d} q_{k,m,n}$, and we consider the system above in its mild formulation. There is considerable flexibility when choosing the coefficients of the ODE system, and one can adjust the probabilities $q_{k,m,n}$, and d_k by adjusting the constant C_b and considering rescaled forcing data γ. In particular, in an equation where the probabilities q_k, d_k do not add up to 1, it is always possible to adjust d_k and the forcing data so that this constraint holds. Similarly, an equation with C_b replaced by bounded functions of k can be recast into the same form by forcing the k dependence into the probabilities q_k and d_k.

We describe first the branching tree. Fix $k \in \mathbb{Z}^d$, a tree rooted at k is a system of particle positions, birth, branch, and death times, defined inductively over the particles. At the root the birth time is zero, and the branching and death times are exponential with rate λ_k. Given a tree, each particle, with position say k', either dies with probability $d_{k'}$, or disappear giving raise to two new independent particles, with positions m and n with probability $q_{k'mn}$. The new particles will have a lifespan distributed as independent exponential random variables with rates λ_m and λ_n. Notice that by construction, given a branching particle giving raise to two particles at positions m and n, and conditional to its genealogy, the two sub-trees generated are independent and with the same distribution of trees rooted at m and n. To ensure that the tree has only finitely many branches before a given time t, a sufficient condition is that $q_k \leq d_k$.

The solution of the system is represented by the expectation of a recursive functional R over a tree of branching particles. A branching event triggers the multiplication by $B_{k,m,n}$ of the two functionals corresponding to the two branches rooted at m, n, and a death event the evaluation of the external force. For instance if $r = 1$ and all the bilinear forms $B_{k,m,n}$ coincide with the usual product in $\mathbb{C}$, then the evaluation over a tree $\mathcal{T}$ rooted at k is

$$R_t(\mathcal{T}) = C_b^{B_t} \prod_{\alpha\in D_t} \gamma_{k_\alpha}(t - t_\alpha) \prod_{\alpha: t\in[s_\alpha, t_\alpha)} \chi_{k_\alpha}(0),$$

[1] For instance, following Le Jan and Sznitman [19], for the three-dimensional Navier–Stokes we set $\chi_k(t) = |k|^2 u_k(t)$.

where B_t and D_t are the number of particles that have branched and died, respectively, before time t. If $\chi(0) \in \ell^\infty(\mathbb{C}^r)$ and $\gamma \in L^\infty([0,T], \ell^\infty(\mathbb{C}^r))$, the representation formula for χ_k is given by the expectation of the functional on all trees rooted at k,

$$\chi_k(t) = \mathbb{E}_k[R_t],$$

whenever the expectation converges absolutely.

The Navier–Stokes equation in dimension three fit into the general scheme given above, with $d = r = 3$, and a suitable choice of the kernels q_{kmn} and of the products $B_{k,m,n}$ (here we take zero driving force). In particular, as we have already mentioned, Le Jan and Sznitman [19] take $\chi_k = |k|^2 u_k$.

15.4.2 Majorizing Kernels

Rabi Bhattacharya and his group have considerably contributed to the analysis with a generalization of the stochastic cascade introduced above, see among others the papers [4, 5] and [24, 26, 33, 32, 10, 25], adding in particular a degree of freedom of conceptual importance, namely the *majorizing kernels*.

Let $h : \mathbb{Z}^3\backslash\{0\} \to (0, \infty)$ be a function such that $(h * h)(k) \le C|k|h(k)$ for some $C > 0$. Up to other details and some additional generality, a function h with the previous property is called a *majorizing kernel* (with exponent one). It generalizes the case $h(k) = 1/|k|^2$ treated by [19]. Following [4], given such h, setting $\chi_k(t) := u_k(t)/h(k)$, from (15.5) we get

$$\chi_k(t) = e^{-\nu|k|^2 t}\chi_k(0) + \int_0^t \nu|k|^2 e^{-\nu|k|^2 s} \sum_{m+n=k} \frac{h(m)h(n)}{\nu|k|h(k)} b_k(\chi_m(t-s), \chi_n(t-s))\, ds.$$

We introduce the Markov kernel $H_k(m,n) := \frac{h(m)h(n)}{(h*h)(k)}$ with support on the set of pairs (m,n) such that $m + n = k$. Setting $m(k) := \frac{(h*h)(k)}{\nu|k|h(k)}$ we have

$$\chi_k(t) = e^{-\nu|k|^2 t}\chi_k(0) + \nu|k|^2 \int_0^t e^{-\nu|k|^2 s} m(k) \sum_{k_1+k_2=k} H_k(k_1,k_2) b_k(\chi_{k_1}(t-s), \chi_{k_2}(t-s)).$$

The property of majorizing kernel guarantees that $m(k) \le 1$. Recall also that $|b_k(\chi_m, \chi_n)| \le |\chi_m|\,|\chi_n|$, already mentioned above. These two properties are of basic importance to control the convergence of the expected values described below.

When the stochastic cascade probabilistic scheme is applied to the last equation above, the solution is given by

$$u_k(t) = h(k)\mathbb{E}_k[R_t].$$

Up to details, the main result of [4] states that when $\sup_{k\in\mathbb{Z}^3\backslash\{0\}} \frac{|u_k(0)|}{h(k)}$ is small enough (depending on ν), a unique solution exists of the Navier–Stokes equations, given by the probabilistic representation formula above. These theorems are competitive with those obtained by various authors using harmonic analysis tools, see for instance [9], and allow to capture several possible spaces of initial conditions, other than the pseudo-measures space of [19].

15.5 Pruning the Trees

The major limitation of the previous two approaches (the deterministic and stochastic cascade representations) is that they apply only for relatively small (in suitable norms) initial conditions, since the series or the expected values have to converge similarly to a geometric series. There are cancellations, but it is very difficult to use them. Thus one has to majorize the complex multi-linear expressions by products of positive quantities; at the end this requires restrictive assumptions on data.

For a very simple model of those problems, namely a one-dimensional differential equation with quadratic nonlinearity, it has been shown by F. Morandin [23] that Borel summability applies, a form of renormalization theory which takes advantage of cancellations. This approach allows one to treat arbitrary initial conditions. Unfortunately, at present, this technique did not find a proper extension even to two-dimensional ordinary differential equations.

The paper [6] provides both an explanation of the issue through a comparison equation, whose finiteness implies integrability of the recursive functional, and a way to avoid non-integrability by suitably pruning the tree.

15.5.1 The Comparison Equation

The comparison equation for the infinite dimensional system of ODEs is obtained essentially by neglecting any geometric information about the (vector) directions of the data in the system, namely, we consider a new infinite dimensional system by taking the norm of the data $|\chi_k(0)|$, γ_k and for the system (15.11), where each product $B_{k,n,m}$ is replaced by the standard product in $\mathbb{C}^r$, namely

$$\dot{\tilde{\chi}}_k = \lambda_k\Big(-\tilde{\chi}_k + C_b \sum_{m,n\in\mathbb{Z}^d} q_{k,m,n}\tilde{\chi}_m\tilde{\chi}_n + d_k|\gamma_k|\Big),$$

and let $\tilde{R}$ be the evaluation operator associated with the above equation. We now look for nonnegative real solutions $\tilde{\chi}_k$, so that there is no issue in the definition of the expectation of $\tilde{R}$, as it takes values in the positive real numbers. Clearly, when the expectation of $\tilde{R}$ is finite, it provides a mild solution of the comparison equation. A sort of converse holds, as given in the following comparison theorem, see [6, Theorem 4.1].

Theorem 1. *If the expectations of $\tilde{R}$ are finite for all $t \in [0, T]$ and $k \in \mathbb{Z}^d$, then the expected values define a mild solution of the comparison equation.*

Conversely if there exists a finite mild solution of the comparison equation on $[0, T]$, then the expectations of the evaluation operator are finite for all $t \in [0, T]$ and $k \in \mathbb{Z}^d$.

Moreover, the probabilistic representation is the smallest positive solution of the comparison equation. Finally, the comparison $\mathbb{E}_k[|R_t|] \le \mathbb{E}_k[\tilde{R}_t]$ holds, with equality whenever $|B_{k,m,n}(\chi,\chi')| = |\chi|\,|\chi'|$.

In other words the comparison equation essentially governs the convergence of the expectation of the original system (15.11), *but not the finiteness of the solutions of the original system* (15.10).

Let us consider a few examples. The first example is the most elementary, namely the one-dimensional ODE $\dot{x} = -x + x^2$. The comparison equation is the same ODE, but with positive initial data only. Now we see immediately why the probabilistic representation blows up for initial data below -1, while the solution is global for the same initial data.

For a PDE example, consider the one-dimensional Burgers equation

$$\partial_t u - \Delta u + (u \cdot \nabla)u = f,$$

with periodic boundary conditions and zero mean, where f is an external forcing. If we expand the solution in its Fourier coefficients u_k, define the weights $w_k = |k|^\alpha$, and set $\chi_k = w_k u_k$, $\lambda_k = |k|^2$ for $k \neq 0$, $q_{k,m,n} = C_b^{-1} \frac{|n| w_k}{\lambda_k w_m w_n}$, and $B_{k,m,n}(\chi, \chi') = -\mathtt{i}(\chi \cdot \frac{n}{|n|})\chi'$, whenever $m + n = k$ (and zero otherwise), then the Burgers system can be recasted in the general form (15.11), if we choose $\alpha > 1$, C_b sufficiently large that $q_k < 1$ and define $d_k = 1 - q_k$ and $\gamma_k = (f_k w_k / \lambda_k d_k)$ for $k \in \mathbb{Z}^d$, $k \neq 0$.

Let us obtain now the comparison equation associated with the Burgers system. By defining $\tilde{u}_k = w_k^{-1} \tilde{\chi}_k$, we obtain a comparison equation that in spatial coordinates reads

$$\partial_t \tilde{u} = \Delta \tilde{u} + \tilde{u}(-\Delta)^{\frac{1}{2}} \tilde{u} + \tilde{f}$$

where $\tilde{f}$ has Fourier coefficients $|f_k|$. Notice that this scalar comparison PDE is independent of the choice of weights, so in particular no majorizing kernel, as defined in the previous section, can fix the divergence. Similar conclusions can be given for the Navier–Stokes equations, but with a comparison equation that has a less simple and evocative comparison equation.

The scalar comparison equation associated with the Burgers system has quadratic growth and it is not difficult to show that, for instance with zero forcing and large enough initial data, solutions blow up in finite time, see for example [20] and the references therein for the case of branching with diffusion. Notice finally that, at least for $d = 1$, the equality in the last part of the theorem above holds. This implies that the stochastic representation is well defined if and only if the corresponding comparison equation has a solution with finite Fourier coefficients.

15.5.2 Pruning the Tree

To understand the idea of *pruning* introduced in [6], we consider the seemingly simple example $\dot{x} = -x + x^2$. The probabilistic representation of the solutions of this ODE is $x(t) = \mathbb{E}[u(0)^{N_t}]$, where N_t is the number of particles at time t of a simple rate one branching process starting from a single particle at time 0. The representation is well defined for all time $t \geq 0$ if and only if $|x(0)| \leq 1$, and is non-well defined if $x(0) < -1$, where the ODE has global solutions. The underlying reason is that the absolute convergence of the expectation destroys the possible cancellations.

In order to try to take into account those cancellations, we try to keep the number of particles finite, so to approximate the expectation with a finite sum. To this aim we formulate a first modification of the branching process. Assign to each particle a label from the positive integers. Whenever a particle branches, the two offspring have label $n-1$. A particle with label 0 dies if tries to branch. Notice that this approximation is already given in [19] for their uniqueness proof (see also [4]). Let x_n be the expectation of the evaluation operator for these pruned trees. It turns out that the functions $(x_n)_{n\geq 0}$ satisfy the explicit iterative scheme

$$\dot{x}_n = -x_n + x_{n-1}^2,$$

that is the one-dimensional counterpart of (15.6). Unfortunately, the limit as $n \to \infty$ of the above explicit iterative scheme fails to exist for large t if $x(0) < -1$.

To fully take into account the cancellations, we formulate a second and more effective modification. A branching particle with label n gives raise to two particles, one with label $n-1$ and one *with the same label of its parent*.[2] The expectation of the evaluation operator this time leads to the semi-implicit iterative scheme

$$\dot{x}_n = -x_n + x_{n-1}x_n,$$

and it is straightforward to check that $x_n(t)$ is well defined for all n and t. Moreover, x_n converges to the solution $x(t)$ of the original ODE problem for each initial condition $u(0) \leq 1$. In other words we have the stochastic representation

$$u(t) = \lim_{n\to\infty} \mathbb{E}[x(0)^{N_t(n)}],$$

where $N_t(n)$ is the number of particles at time t originated by a root particle with label n.

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Chapter 16
Reprints: Part V

R.N. Bhattacharya and Coauthors

On a statistical theory of solute transport in porous media. SIAM Journal on Applied Mathematics 37 (1979), 485–498. © 1979 Society for Industrial and Applied Mathematics (with V.K. Gupta).

On the Taylor-Aris theory of solute transport in a capillary. SIAM Journal on Applied Mathematics 44 (1984), 33–39. © 1984 Society for Industrial and Applied Mathematics (with V.K. Gupta).

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16.1 "On a statistical theory of solute transport in porous media"

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ON A STATISTICAL THEORY OF SOLUTE TRANSPORT IN POROUS MEDIA*

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Abstract. Consider the motion of a solute molecule in a homogeneous isotropic porous medium saturated with a pure liquid. The following assumptions are made on the velocity of the molecule: the time intervals between successive collisions of the molecule with the solid matter of the medium are i.i.d. random variables; the molecule is scattered by these collisions in random directions which are i.i.d. uniform and independent of the collision times; in between two successive collisions with the solid phase the velocity of the molecule is governed by the Langevin equation. Under these and mild additional assumptions it is proved that the position $\{X(t): t \geqq 0\}$ of the molecule is approximately a Brownian motion. If the solute molecules are weakly interacting among themselves, then the above result leads to a macroscopic parabolic equation (1.14) governing solute concentration. If the successive collision times with the solid phase are assumed to be exponential, then the velocity $\{v(t): t \geqq 0\}$ as well as $\{(v(t), X(t)): t \geqq 0\}$ are Markovian. This leads to laws of mass, momentum, and energy conservation for solute transport.

1. Introduction and main results. The point of view adopted in this article is essentially that of kinetic theory. The physical problem treated here may be described as follows. Solute molecules are carried by a pure liquid (say, water) moving with a constant macroscopic velocity u_0 (=flux divided by porosity) through a homogeneous isotropic porous medium. The different solute molecules are assumed to be in weak interaction among themselves, so that immiscible substances (like oil) or very high concentrations of miscible substances are not considered. The medium is assumed to be saturated with the liquid. The mass of the solute molecule is assumed to be much larger than that of a liquid molecule. The magnitude of the macroscopic velocity u_0 is assumed to be moderate. Under these circumstances the concentration of the solute, as a function of time and space coordinates, is generally taken to satisfy a parabolic equation with constant coefficients (see Fried and Combarnous (1971), where references to earlier literature may also be found). In this article such an equation will be derived from molecular considerations. The mathematical assumptions on the velocity $v(t) = (v^{(1)}(t), v^{(2)}(t), v^{(3)}(t))$, $t>0$, of the solute molecule are described in the following paragraph. Roughly, the particle suffers collisions with the solid phase (some times referred to as the 'pore wall') at successive times $\tau_1, \tau_2, \cdots$; in between collisions the velocity process is governed by a Langevin equation; the effect of collision with the solid phase is to scatter the particle in a random direction.

1.1. Assumptions. Consider a probability space $(\Omega, \mathcal{A}, P_\mu)$ on which are defined three independent stochastic processes:

(i) a three dimensional standard Brownian motion $B(t) = (B^{(1)}(t), B^{(2)}(t), B^{(3)}(t))$, $t \geqq 0$;

(ii) a sequence of independent and identically distributed (*i.i.d.*) nonnegative random variables $\{\eta_i\}_{i \geqq 1}$ having finite fourth moments and such that $\mu \equiv E\eta_i$ is a *scale parameter* for the common distribution function F_μ;

(iii) a sequence of i.i.d. random orthogonal matrices $\{O_i\}_{i \geqq 1}$ whose common distribution is the normalized Haar measure on the group of all real 3×3 orthogonal matrices. Define

$$(1.1) \qquad \tau_i = \sum_{j=1}^{i} \eta_j \qquad (i \geqq 1), \quad \tau_0 = 0.$$

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It is assumed that, conditionally given $\{\tau_n\}_{n\geqq 1}$, $\{O_n\}_{n\geqq 1}$, in the time interval $(\tau_i, \tau_{i+1}]$ the velocity $v(t)$ evolves as an *Ornstein–Uhlenbeck process*, i.e., it satisfies the following stochastic differential equation (also known as a *Langevin equation*) in the usual sense (see McKean (1969) or Nelson (1967)):

$$dv(t) = -\beta(v(t)-u_0)\,dt + g\,dt + \sigma\,dB(t) \qquad (\tau_i < t \leqq \tau_{i+1}), \tag{1.2}$$

where β is a positive constant, g is the acceleration (vector) due to gravity, and σ is a constant 3×3 nonsingular symmetric matrix. Also, assume that there is a constant ρ, $0 \leqq \rho \leqq 1$, such that

$$v(\tau_i+) = \rho O_i v(\tau_i) \qquad (i \geqq 1), \tag{1.3}$$

where $v(\tau_i+) = \lim_{t\downarrow 0} v(\tau_i + t)$. Finally, assume that

$$v(0) = v(0+) = v_0, \tag{1.4}$$

where v_0 is a random vector independent of the three stochastic processes (i)–(iii) mentioned above.

1.2. Main results. Write

$$\begin{gathered} w_0 = u_0 + g/\beta, \qquad f(z) = 1 - \frac{1}{z}\int_0^\infty (1-e^{-zs})F_1(ds), \\ \alpha = \left[1 - \frac{1}{\beta\mu}\int_0^\infty (1-e^{-\beta s})F_\mu(ds)\right] w_0 = f(\beta\mu) w_0, \end{gathered} \tag{1.5}$$

where F_1 is the distributing function of η_1/μ. Let $w_0' w_0$ denote the matrix whose (i, j) element is $w_0^{(i)} w_0^{(j)}$. Also write

$$\begin{gathered} g(z) = 1 - \frac{1}{z}\int_0^\infty \{2(1-e^{-zs}) - \tfrac{1}{2}(1-e^{-2zs})\}F_1(ds), \\ h(z) = \int_0^\infty \left\{s - \frac{1}{z}(1-e^{-zs})\right\}^2 F_1(ds) - \left(\int_0^\infty \{s - \tfrac{1}{2}(1-e^{-zs})\}F_1(ds)\right)^2, \\ D = \sigma^2, \qquad \tilde{D} = g(\beta\mu)\frac{1}{\beta^2}D + \mu h(\beta\mu) w_0' w_0. \end{gathered} \tag{1.6}$$

The position process $X(t) = (X^{(1)}(t), X^{(2)}(t), X^{(3)}(t))$, $t \geqq 0$, is defined by

$$X(t) = X_0 + \int_0^t v(s)\,ds \qquad (t \geqq 0), \tag{1.7}$$

where X_0 is any random vector. Also define

$$\begin{gathered} Y_i = \int_{\tau_{i-1}}^{\tau_i} v(s)\,ds \qquad (i \geqq 1), \\ S_\mu(t') = \mu^{1/2} \sum_{i=1}^{[t'/\mu^2]} (Y_i - \mu\alpha) \qquad (0 \leqq t' \leqq 1), \end{gathered} \tag{1.8}$$

where [a] is the *integer part of* a. The P_μ- distribution of $S_\mu(\cdot)$ is a probability measure on $D[0, 1]$—the space of all right continuous functions on [0, 1] into R^3 having left limits, endowed with the Skorokhod topology (see Billingsley (1968, Chap. 3)). Define

$$(1.9)\qquad \delta=\beta\mu,\qquad D_1=\frac{1}{\beta^2}D,$$

and regard δ, D_1, μ as *independent parameters*. This reparametrization (of β, D, and μ) amounts (physically) to an appropriate choice of scales for time and distance, as we argue after the statement of Theorem 1.

PROPOSITION 1. *As $\mu\downarrow 0$, while δ and D_1 remain fixed, the P_μ- distribution of $S_\mu(\cdot)$ converges weakly to the Wiener measure with zero drift vector and diffusion matrix $g(\delta)D_1$.*

Our first main result, Theorem 1, is deduced from this.

THEOREM 1. *As $\mu\downarrow 0$, while δ and D_1 remain fixed, the P_μ- distribution of the stochastic process $\mu^{1/2}(X(t'/\mu)-(t'/\mu)\alpha)$, $0\leqq t'\leqq 1$, converges weakly to the Wiener measure with zero drift vector and diffusion matrix $g(\delta)D_1$.*

It is important to understand the physical significance of the parametrization (1.9). Suppose we introduce new *scales* for time and distance:

$$(1.10)\qquad t'=ct,\qquad \bar{x}=c^{1/2}x\qquad (c>0),$$

or, equivalently, consider the new stochastic processes

$$(1.11)\qquad \bar{X}(t')=c^{1/2}X(t'/c),\qquad \bar{v}(t')=\frac{d}{dt'}\bar{X}(t')=c^{-1/2}v(t'/c)\qquad (t'\geqq 0).$$

Then the Langevin equation (1.2) becomes

$$(1.12)\qquad d\bar{v}(t')=-\bar{\beta}(\bar{v}(t')-\bar{u}_0)\,dt'+\bar{g}\,dt'+\bar{\sigma}\,d\bar{B}(t')\qquad (t'\in(c\tau_i,c\tau_{i+1}]),$$

where $\bar{B}(t')=c^{1/2}B(t'/c)$, $t'\geqq 0$, is again a standard Brownian motion, and

$$(1.13)\qquad \begin{aligned}&\bar{\beta}=\beta/c,\quad \bar{u}_0=u_0/c^{1/2},\quad \bar{g}=g/c^{3/2},\quad \bar{\sigma}=\sigma/c,\quad \bar{\mu}=c\mu,\\ &\bar{D}=\bar{\sigma}^2=\sigma^2/c^2.\end{aligned}$$

Note that $\overline{\beta\mu}=\beta\mu$ is independent of c. Hence if we take $c=\mu$ and let $\mu\downarrow 0$, $\overline{\beta\mu}$ does not change. The same is true of $\bar{D}/\bar{\beta}^2$. Theorem 1 implies that, when observed at time points far apart compared to μ, $X(\cdot)$ is approximately a diffusion with drift α and diffusion matrix $g(\beta\mu)\beta^{-2}D$. The multiplication by $\mu^{1/2}$ (in Theorem 1) of $[X(t'/\mu)-(t'/\mu)\alpha]$ merely prevents the latter from blowing up (i.e., brings it back to scale) as $\mu\downarrow 0$. In order that the theorem be of physical significance the neglected term in $\tilde{D}$ (namely, $\mu h(\beta\mu)w_0'w_0$) should be very small compared to $\tilde{D}$. It may be shown that in the typical physical problem $\tilde{D}$ (or, its smallest eigenvalue) is of the order of 10^{-4} while $|w_0|^2h(\beta\mu)\mu$ is of the order of 10^{-8}, when cgs units are used (see Gupta et al. (1979)).

To deduce the macroscopic equation governing *solute concentration* $c(t,x)$ assume now that the velocity processes of the different solute molecules are independent (although, in reality, they are weakly dependent—due to the diluteness of the concentration). Since given a fixed set of initial positions (i.e., given an initial concentration) the position processes are independent, one may invoke the law of large numbers (see, e.g., Bhattacharya et al. (1976, p. 506)) to assert that the concentration is macroscopically stable and satisfies the parabolic Fokker–Planck (or, forward) equation

$$(1.14)\qquad \frac{\partial c(t,x)}{\partial t}=-\langle\alpha,\operatorname{grad}_x c(t,x)\rangle+\frac{g(\beta\mu)}{2\beta^2}\sum_{k,l}D_{kl}\frac{\partial^2 c(t,x)}{\partial x^{(k)}\partial x^{(l)}}\,.$$

In general, the basic parameters β, D, μ should be regarded as functions of the convective flux u_0. In case $u_0 = 0$ it is reasonable to assume that β and D are the same as in the classical case of diffusion in pure liquids (see Nelson (1967) and Chandrasekhar's article in Wax (1954)). Then, for $u_0 = 0$, $D = d_0 I$ where d_0 is a scalar and I is the 3×3 identity matrix. Hence for this case the second order terms in (1.14) reduce to $g(\beta\mu)(d_0/\beta^2)$ times the Laplacian of c. Thus the 'diffusion coefficient' in the porous medium is $g(\beta\mu)$ times that in pure liquid. But, from (1.6), $0 < g(z) < 1$; for if $z > 0$, then $2(1 - e^{-zs}) - \frac{1}{2}(1 - e^{-2zs})$ is strictly positive for all $s > 0$. This leads to the conclusion that the diffusion coefficient in the porous medium is smaller than that in the pure liquid; this is in accordance with experimental observations (see, e.g., Fried and Cambarnous (1971, Fig. 12, p. 193)).

The assumption that the common distribution of O_i's is the Haar measure essentially means that the unit vector giving the direction cosines of the velocity of the solute molecule after collision (with the solid phase) is equidistributed on the unit sphere. This may be justified by a strict interpretation of isotropy of the porous medium. It should be noted that all we require of the common distribution is that

$$EO_i v = 0 \tag{1.15}$$

for every constant vector v. If the distribution is the Haar measure, then (1.15) follows from the fact that O_i and $-O_i = (-I)O_i$ have the same distribution (since $-I$ is an orthogonal matrix).

The assumption that $\mu \equiv E\eta_i$ is a scale parameter is also quite reasonable on physical grounds.

In case of diffusion in pure liquids a dynamical derivation of the Langevin equation for the case $u_0 = 0$ has been given by Mazur and Oppenheim (1970) starting from equations of motion and Gibbs distribution on the phase space of liquid molecules, under the assumption that certain correlation functions are short lived in time.

It is a significant feature of the present theory that the parameter ρ does not appear in (1.14) (or in the parameters of the limiting process occurring in Proposition 1 and Theorem 1). The concentration of the solute is thus insensitive to the nature of collision (elastic or inelastic) with the solid phase.

Turning to the velocity process, one may show without much difficulty that, conditionally given η_i's and O_i's it is Gaussian and Markovian with nonhomogeneous transitions. One may show that, under the additional assumption that η_i's are *exponentially distributed with parameter* $1/\mu$, the velocity process is (unconditionally) Markovian with homogeneous transitions. Although it is simple to establish this directly, we shall use an interesting and useful representation of the process $(v(t), X(t))$, $t \geqq 0$, as the solution of a *generalized Itô equation* (see Gihman and Skorohod (1972, pp. 288–300)). For this purpose let $\nu_1(\cdot, \cdot)$ be a Poisson random measure which

(a) is independent of $\{B(t) : t \geqq 0\}$ and

(b) is a Poisson process over (i.e., indexed by) the Borel sigma field of $[0, \infty) \times R^3$ such that

$$E(\nu_1([t_1, t_2], B)) = (t_2 - t_1)\pi_1(B), \tag{1.16}$$

where $\pi_1 = \mu^{-1} H_1$, H_1 denoting the uniform distribution on $S^2 = \{v \in R^3 : |v| = 1\}$. The statement (b), of course, implies that the process $\nu_1(\cdot, \cdot)$ has independent increments, each of which is a Poisson random variable with a parameter specified by (1.16). One may check without difficulty (see Gihman and Skorohod (1972)) that the unique nonanticipative solution of the stochastic differential equation

$$(1.17)\qquad \begin{aligned} dv(t) &= -\beta(v(t)-u_0-g/\beta)\,dt+\sigma\,dB(t)\\ &\quad+\int_{\{|a_1|=1\}}(\rho|v(t)|a_1-v(t))\nu_1(dt,da_1),\qquad v(0)=v_0, \end{aligned}$$

has the same law as that of the velocity process constructed earlier (with exponentially distributed η_i's). One may represent the $\{(v(t), X(t)): t \geqq 0\}$ process also by

$$(1.18)\qquad \begin{aligned} d\begin{pmatrix} v(t)\\ X(t)\end{pmatrix} &= \begin{pmatrix} -\beta(v(t)-u_0-g/\beta)\\ v(t)\end{pmatrix}dt+\Sigma\,d\tilde{B}(t)\\ &\quad+\int_{\{a=(a_1,0)\in R^3\times R^3\}}\begin{pmatrix}\rho|v(t)|a_1-v(t)\\ 0\end{pmatrix}\nu(dt,da),\\ v(0)&=v_0,\qquad X(0)=x_0, \end{aligned}$$

where $\Sigma=\left(\begin{smallmatrix}\sigma & 0\\ 0 & 0\end{smallmatrix}\right)$ is a 6×6 matrix, $\{\tilde{B}(t): t\geqq 0\}$ is a six dimensional standard Brownian motion, and $\nu(\cdot,\cdot)$ is a Poisson random measure on $[0,\infty)\times R^3\times\{0\}$ with $E(\nu([t_1,t_2], B)\times\{0\})=(t_2-t_1)\pi_1(B)$.

THEOREM 2. *Assume, in addition to the hypothesis of Theorem 1, that η_i's are exponentially distributed with common parameter μ^{-1}.*

(a) *Then the processes $\{v(t): t\geqq 0\}$, $\{(v(t), X(t)): t\geqq 0\}$ are both Markovian having homogeneous transition probability functions.*

(b) *If ψ is a function on $R^3\times R^3$ having bounded continuous derivatives of second and smaller orders, then the function*

$$(1.19)\qquad h(t,v',x')\equiv E_{v',x'}\psi(v(t),X(t))$$

satisfies the backward equation

$$(1.20)\qquad \frac{\partial h}{\partial t}=Lh\equiv L_1h+\sum_{i=1}^{3}v'^{(i)}\frac{\partial h}{\partial x'^{(i)}}-\mu^{-1}h+Bh,$$

where $E_{v',x'}$ denotes expectation when the initial state is (v',x') and

$$(1.21)\qquad L_1h(t,v',x')=\frac{1}{2}\sum_{i,j=1}^{3}D_{ij}\frac{\partial^2 h}{\partial v'^{(i)}\partial v'^{(j)}}-\beta\sum_{i=1}^{3}(v'^{(i)}-w_0^{(i)})\frac{\partial h}{\partial v'^{(i)}},$$

and

$$(1.22)\qquad Bh(t,v',x')=\mu^{-1}\int_{S^2}h(t,\rho|v'|a_1,x')H_1(da_1).$$

Remark. In case $\rho=0$, the transition probability of the velocity process has the density

$$(1.23)\qquad q(t,v|v')=e^{-t/\mu}q_0(t,v|v')+\sum_{n=1}^{\infty}e^{-t/\mu}\frac{(t/\mu)^n}{n!}\int_0^t\frac{ns^{n-1}}{t^n}q_0(t-s,v|0)\,ds,$$

where q_0 is the transition density of the Ornstein–Uhlenbeck process, i.e., $q_0(t,v|v')$ is the Gaussian density (at v) with mean $e^{-\beta t}(v'-w_0)+w_0$ and dispersion matrix $(1/(2\beta))\cdot(1-e^{-2\beta t})D$. The relation (1.23) is obtained by conditioning with respect to the number of collisions in a time interval of length t. Given that this number is n, the conditional distribution of the time of the last collision has the density ns^{n-1}/t^n, $0\leqq s\leqq t$ (see Karlin and Taylor (1975, p. 160)).

Section 2 contains proofs of Theorems 1, 2. In § 3 we derive the formal adjoint of the backward operator appearing on the right side of (1.20) and show how important conservation laws may be obtained, in case the transition probability is sufficiently well behaved.

2. Proofs. Throughout $E(\cdot\cdot|\{\cdot\cdot\})$ will denote conditional expectation given the sigma field (determined by) $\{\cdot\cdot\}$.

Proof of Theorem 1. Write

$$w_0 = u_0 + g/\beta, \qquad w(t) = \sigma^{-1}(v(t) - w_0), \tag{2.1}$$

and rewrite (1.2), (1.3) and (1.4) as,

$$\begin{aligned} &dw(t) = -\beta w(t)\,dt + dB(t) && (\tau_{i-1} < t \leqq \tau_i) \\ &w(\tau_i +) = \rho\sigma^{-1}O_i(\sigma w(\tau_i) + w_0) - \sigma^{-1}w_0 && (i \geqq 1) \\ &w(0+) = \sigma^{-1}(v_0 - w_0). \end{aligned} \tag{2.2}$$

It follows from the mathematical assumptions that conditionally given the sequences $\{\tau_i\}_{i\geqq 1}$, $\{O_i\}_{i\geqq 1}$, the process $w(t)$, $t>0$, is Markovian having a transition density q_1 given by (see Nelson (1967, pp. 55, 56))

$$\begin{aligned} &q_1(t, w; s, w') = \text{Gaussian density (in } w\text{) with mean vector} \\ &c(t-s)w' \text{ and covariance matrix } (1/(2\beta))\,(1-c^2(t-s))I \\ &(\tau_{i-1} < s < t \leqq \tau_{i+1}, \text{ or } s = 0+ \text{ and } 0 < t \leqq \tau_1) \end{aligned} \tag{2.3}$$

where I is the 3×3 identity matrix and

$$c(t) = e^{-\beta t}.$$

Also, in view of the "boundary condition" in (2.2), one has, for t in $(\tau_{i-1}, \tau_i]$, $i \geqq 2$,

$$\begin{aligned} &q_1(t, w; \tau_{i-1}, w') = \text{Gaussian density with mean vector} \\ &c(t-\tau_{i-1})\{\rho\sigma^{-1}O_{i-1}(\sigma w' + w_0) - \sigma^{-1}w_0\} \text{ and covariance} \\ &\text{matrix } (1/(2\beta))(1-c^2(t-\tau_{i-1}))I \quad (\tau_{i-1} < t < \leqq \tau_i). \end{aligned} \tag{2.4}$$

Now in view of (2.1), conditionally given $\{\tau_i\}_{i\geqq 1}$ and $\{O_i\}_{i\geqq 1}$, $\{v(t); t>0\}$ is also a Markov process whose transition density p is obtained on transformation of (2.3), (2.4) as

$$\begin{aligned} &p_1(t, v; s, u) = \text{Gaussian density (in } v\text{) with mean vector} \\ &c(t-s)(u-w_0) + w_0 \text{ and covariance matrix} \\ &(1/(2\beta))(1-c^2(t-s))D \text{ if } \tau_{i-1} < s < t \leqq \tau_i, \\ &p_1(t, v; \tau_i, u) = \text{Gaussian density with mean vector} \\ &\rho c(t-\tau_i)O_i u + (1-c(t-\tau_i))w_0, \text{ and covariance matrix} \\ &(1/(2\beta))(1-c^2(t-\tau_i))D \text{ if } \tau_i < t \leqq \tau_{i+1}. \end{aligned} \tag{2.5}$$

Write

$$N(t) = \sup\{n \geqq 0 : \tau_n \leqq t\}, \qquad t \geqq 0, \tag{2.6}$$

and let $\mathscr{E}_t$ denote the sigma field generated by $\{(B(s), N(s)) : 0 \leqq s \leqq t\}$. Then τ_i is a stopping time relative to $\{\mathscr{E}_t : t \geqq 0\}$. Let $\mathscr{E}_{\tau_i}$ be the pre τ_i sigma field. Finally, let $\mathscr{F}_i$

denote the sigma field generated by $\mathscr{E}_{\tau_i}$, η_{i+1} and $O_1, \cdots, O_{i-1}$ $(i \geqq 1)$, where $O_0 \equiv I$. Then by (2.5) and the facts that

(i) O_i is independent of $\mathscr{F}_i$,

(ii) $EO_i v = 0$ for every constant vector v,

one has

$$E(I_{\{\tau_{i-1}<s\leqq\tau_i\}}v(s)|\mathscr{F}_{i-1}) = (1-c(s-\tau_{i-1}))I_{\{\tau_{i-1}<s\leqq\tau_i\}}w_0,$$
$$E(Y_i|\mathscr{F}_{i-1}) = \left(\int_0^{\eta_i}(1-c(s))\,ds\right)w_0 = \left(\eta_i - \frac{1}{\beta}(1-e^{-\beta\eta_i})\right)w_0. \tag{2.7}$$

Here I_A denotes the *indicator function* of the set A. Since $Y_1, \cdots, Y_{i-1}$ are measurable with respect to $\mathscr{F}_{i-1}$ and are independent of η_i, (2.7) leads to

$$E(Y_i|Y_1,\cdots,Y_{i-1}) = E\left(\eta_i - \frac{1}{\beta}(1-e^{-\beta\eta_i})\right)w_0$$
$$= \left(\mu - \frac{1}{\beta}\left(1-\int_0^\infty e^{-\beta s}F_\mu(ds)\right)\right)w_0 = EY_i. \tag{2.8}$$

Thus, for every unit vector x,

$$X_i = \langle x, \mu^{-1/2}(Y_i - EY_i)\rangle \qquad (i \geqq 1), \tag{2.9}$$

is a sequence of martingale differences. The relations (2.5) also lead to

$$\begin{aligned}
&E(I_{\{\tau_{i-1}<s\leqq\tau_i\}}v^{(k)}(s)v^{(l)}(t)|\mathscr{F}_{i-1})\\
&= E(I_{\{\tau_{i-1}<s<t\leqq\tau_i\}}v^{(k)}(s)[c(t-s)(v^{(l)}(s)-w_0^{(l)})+w_0^{(l)}]|\mathscr{F}_{i-1})\\
&= I_{\{\tau_{i-1}<s<t\leqq\tau_i\}}\left\{\frac{c(t-s)}{2\beta}(1-c^2(s-\tau_{i-1}))D_{kl} + c(t-s)E(v^{(k)}(s)|\mathscr{F}_{i-1})\right.\\
&\qquad\left.\cdot E(v^{(l)}(s)|\mathscr{F}_{i-1}) + (1-c(t-s))w_0^{(l)}E(v^{(k)}(s)|\mathscr{F}_{i-1})\right\}\\
&= I_{\{\tau_{i-1}<s<t\leqq\tau_i\}}\left\{\frac{c(t-s)}{2\beta}(1-c^2(s-\tau_{i-1}))D_{kl} + c(t-s)(1-c(s-\tau_{i-1}))w_0^{(k)}\right.\\
&\qquad\left.\cdot(1-c(s-\tau_{i-1}))w_0^{(l)} + (1-c(t-s))w_0^{(l)}\cdot(1-c(s-\tau_{i-1}))w_0^{(k)}\right\}\\
&= I_{\{\tau_{i-1}<s<t\leqq\tau_i\}}\left\{\frac{c(t-s)}{2\beta}(1-c^2(s-\tau_{i-1}))D_{kl}\right.\\
&\qquad\left.+(1-c(s-\tau_{i-1}))(1-c(t-\tau_{i-1}))\cdot w_0^{(k)}w_0^{(l)}\right\} \qquad (s<t\leqq\tau_i).
\end{aligned} \tag{2.10}$$

From this on integration one obtains

$$E(Y_i^{(k)}Y_i^{(l)}|\mathscr{F}_{i-1}) = \frac{D_{kl}}{\beta^2}\left[\eta_i - \frac{2}{\beta}(1-e^{-\beta\eta_i}) + \frac{1}{2\beta}e^{-2\beta\eta_i}\right]$$
$$+ w_0^{(k)}w_0^{(l)}\left(\eta_i - \frac{1}{\beta}(1-e^{-\beta\eta_i})\right)^2. \tag{2.11}$$

Again, since $Y_1, \cdots, Y_{i-1}$ are measurable with respect to $\mathscr{F}_{i-1}$ and independent of η_i, $E(Y_i^{(k)}Y_i^{(l)}|Y_1, \cdots, Y_{i-1})$ is the expected value of the last expression in (2.11). From this fact and (2.8) it immediately follows that the dispersion matrix of the conditional distribution of Y_i (given $Y_1, \cdots, Y_{i-1}$) is the same as its unconditional dispersion matrix and that this common matrix is $\mu\tilde{D}$ (see (1.6)). Therefore,

$$E(X_i^2|Y_1,\cdots,Y_{i-1})=\sum_{k,l}\tilde{D}_{kl}x^{(k)}x^{(l)} \tag{2.12}$$
$$=\sum_{k,l}g(\delta)(D_1)_{kl}x^{(k)}x^{(l)}+\mu h(\delta)\sum_{k,l}(w_0'w_0)_{kl}x^{(k)}x^{(l)}.$$

Also,

$$X_i\equiv\mu^{-1/2}\langle x, Y_i-EY_i\rangle=\mu^{-1/2}\langle x, Y_i-E(Y_1|\mathscr{F}_{i-1})\rangle$$
$$+\mu^{-1/2}\langle x, E(Y_i|\mathscr{F}_{i-1})-EY_i\rangle, \tag{2.13}$$
$$X_i^4\leqq 2^3\mu^{-2}[\langle x, Y_i-E(Y_i|\mathscr{F}_{i-1})\rangle^4+\langle x, E(Y_i|\mathscr{F}_{i-1})-EY_i\rangle^4].$$

However,

$$\langle x, Y_i-E(Y_i|\mathscr{F}_{i-1})\rangle^4=(\tau_i-\tau_{i-1})^4\left[(\tau_i-\tau_{i-1})^{-1}\int_{\tau_{i-1}}^{\tau_i}\langle x, v(s)-E(v(s)|\mathscr{F}_{i-1})\rangle\,ds\right]^4$$
$$\leqq(\tau_i-\tau_{i-1})^4(\tau_i-\tau_{i-1})^{-1}\int_{\tau_{i-1}}^{\tau_i}\langle x, v(s)-E(v(s)|\mathscr{F}_{i-1})\rangle^4\,ds \tag{2.14}$$
$$\leqq\eta_i^3\int_{\tau_{i-1}}^{\tau_i}|v(s)-E(v(s)|\mathscr{F}_{i-1})|^4\,ds.$$

Conditionally given $\mathscr{F}_{i-1}$, $v(s)$ is Gaussian with mean $E(v(s)|\mathscr{F}_{i-1})$ and dispersion matrix $(2\beta)^{-1}(1-c^2(s-\tau_i))D$ for $\tau_{i-1}<s\leqq\tau_i$ (see (2.5)). Hence

$$E\langle x, Y_i-E(Y_i|\mathscr{F}_{i-1})\rangle^4\leqq E\left[\eta_i^3\int_{\tau_{i-1}}^{\tau_i}\frac{a}{\beta^2}\|D\|^2(1-c^2(s-\tau_{i-1}))^2\,ds\right]$$
$$\leqq a\|D_1\|^2\beta^2E\eta_i^4\leqq a'\|D_1\|^2\delta^2\mu^2, \tag{2.15}$$

where a, a' are absolute constants (i.e., not depending on the parameters δ, D_1, μ). Further, by (2.7),

$$E\langle x, E(Y_i|\mathscr{F}_{i-1})-EY_i\rangle^4=E\left\langle x,\left\{\eta_i-\frac{1}{\beta}(1-e^{-\beta\eta_i})\right\}w_0-EY_i\right\rangle^4\leqq b\mu^4, \tag{2.16}$$

where b does not depend on μ. Using (2.15), (2.16) in (2.13) one gets

$$EX_i^4\leqq 2^3(a'\|D_1\|^2\delta^2+b\mu^2)\qquad(i\geqq 1). \tag{2.17}$$

We shall now apply the functional central limit theorem of Drogin (1972, Thm. 1(a)) to $\{X_i:1\leqq i\leqq[\mu^{-2}]\}$, where $[y]$ is the integer part of y. The fact that for each μ (sufficiently small) we require a new probability space $(\Omega,\mathscr{A},P_\mu)$ to define a row of X_i's does not cause any difficulty, since the conditional second moment of X_i, given $Y_1,\cdots,Y_{i-1}$ (or given $X_1,\cdots,X_{i-1}$), is nonrandom (see (2.12)) and since we are interested only in weak convergence. To make the correspondence with Drogin's result explicit one may let $\mu=n^{-1/2}$, $v_m=m\sum_{k,l}\tilde{D}_{kl}x^{(k)}x^{(l)}$, and replace T_n by

$$T_\mu=\inf\left\{m:v_m\geqq\left[\frac{T}{\mu^2}\right]\right\}=\frac{1}{\gamma\mu^2}(1+O(\mu)), \tag{2.18}$$

where

$$\gamma=g(\delta)\sum_{k,l}(D_1)_{kl}x^{(k)}x^{(l)}. \tag{2.19}$$

The condition 2(a) in Drogin's theorem is verified using Schwarz and Chebyshev inequalities and (2.17):

$$\begin{aligned}\overline{\lim_{\mu\downarrow 0}}\,\mu^2\sum_{i=1}^{[1/\mu^2]} E_\mu(X_i^2 I_{\{X_i^2>\varepsilon/\mu^2\}}) &\leq \overline{\lim_{\mu\downarrow 0}}\,\mu^2\sum_{i=1}^{[1/\mu^2]}(E_\mu X_i^4)^{1/2}(P_\mu(X_i^2>\varepsilon/\mu^2))^{1/2}\\ &\leq \overline{\lim_{\mu\downarrow 0}}\,\mu^2\sum_{i=1}^{[1/\mu^2]}(E_\mu X_i^4)^{1/2}\cdot(E_\mu X_i^4)^{1/2}(\varepsilon/\mu^2)^{-1}=0,\end{aligned} \tag{2.20}$$

for every $\varepsilon>0$. Since $\tilde{D}\to g(\delta)D_1$ as $\mu\downarrow 0$, and since x is an arbitrary unit vector, the proof of Proposition 1 is complete.

In order to deduce theorem 1 from Proposition 1, write

$$X(t'/\mu)=\sum_{i=1}^{N(t'/\mu)} Y_i+\int_{\tau_{N(t'/\mu)}}^{t'/\mu} v(s)\,ds,$$

$$\begin{aligned}\mu^{1/2}(X(t'/\mu)-(t'/\mu)\alpha) &= \mu^{1/2}\sum_{i=1}^{N(t'/\mu)}(Y_i-\mu\alpha)\\ &\quad+\mu^{1/2}(N(t'/\mu)\mu-(t'/\mu))\alpha\\ &\quad+\mu^{1/2}\int_{\tau_{N(t'/\mu)}}^{t'/\mu} v(s)\,ds \qquad (0\leqq t'\leqq 1).\\ &= Z_1(t')+\mu^{1/2}Z_2(t')\alpha+Z_3(t'),\end{aligned} \tag{2.21}$$

say. By first conditioning with respect to $\mathscr{F}_{i-1}$ and then using a Chebyshev inequality involving the fourth moment to estimate $P_\mu(\mu^{1/2}\int_{\tau_{i-1}}^{\tau_i}\|v(s)\|\,ds>\varepsilon)$ one easily shows that the P_μ distribution of $Z_3(t')$, $0\leqq t'\leqq 1$, converges weakly (with respect to the uniform topology on $D[0,1]$ or $C[0,1]$) to the probability measure degenerate at the zero function, as $\mu\downarrow 0$. Next note that the P_μ distribution of $Z_2(\cdot)$ is the same as the P_1 distribution of

$$(M(t'/\mu^2)\mu-(t'/\mu)), \qquad 0\leqq t'\leqq 1, \tag{2.22}$$

where $M(\cdot)$ denotes the renewal process (the same as $N(\cdot)$) corresponding to independent interarrival times having the common distribution function F_1 (i.e., with $\mu=1$). By Theorem 17.3 in Billingsley (1968), the P_1 distribution of the stochastic process (2.22) converges weakly to a (nondegenerate) one-dimensional Brownian motion as $\mu\downarrow 0$. Hence the P_μ distribution of $\mu^{1/2}Z_2(\cdot)\alpha$ converges weakly to the probability measure degenerate at zero (function) as $\mu\downarrow 0$. It also follows from the convergence of the P_μ distribution of $Z_2(\cdot)$ that

$$P_\mu\Big(\sup_{0\leq t\leq 1}|N(t'/\mu)-t'/\mu^2|>\frac{1}{\mu^{1+\varepsilon}}\Big)\to 0 \quad \text{as} \quad \mu\downarrow 0, \tag{2.23}$$

for every $\varepsilon>0$ and, in particular, for $\varepsilon=\frac{1}{4}$. Combining this with Proposition 1 shows that the P_μ-distribution of $Z_1(\cdot)$ is asymptotically (as $\mu\downarrow 0$) the same as that of $\mu^{1/2}\sum_{i=1}^{[t'/\mu^2]}(Y_i-\mu\alpha)$, and that this latter distribution converges weakly to that of a Brownian motion with drift zero and diffusion matrix $g(\delta)D_1$.

Proof of Theorem 2. Part (a) (i.e., the Markovian property) follows from Theorem 1, p. 288, in Gihman and Skorohod (1972), although it may be deduced directly. The backward equation (1.20) follows from Theorem 4, p. 296, of the same monograph. One may also derive it by first deriving the backward equation for the velocity process, using the relation

$$
\begin{aligned}
g_1(t, v') &\equiv \int_{R^3} \phi(v) q(t, dv|v') \\
&= e^{-t/\mu} \int_{R^3} \phi(v) q_0(t, v|v')\, dv + e^{-t/\mu}(t/\mu) \\
&\cdot \int_{R^3} \phi(v) \left[\frac{1}{t} \int_{s=0}^{t} \left\{ \int_{R^3} q_0(s, u|v') E_0 q_0(t-s, v|\rho O u)\, du \right\} ds \right] dv \\
&+ O(t^2) \quad \text{as} \quad t \downarrow 0.
\end{aligned} \tag{2.24}
$$

In (2.24) ϕ is an arbitrary function on R^3 having continuous and bounded second and lower order derivatives, $q(t, dv|v')$ is the transition probability function of the velocity process, q_0 is the transition density of the Ornstein–Uhlenbeck process, and E_0 denotes expectation with respect to the distribution (Haar measure) of a random orthogonal matrix O. In deriving (2.24) one uses the following facts:

(i) given that $N(t) = 1$, the jump time is uniformly distributed in $[0, t]$;

(ii) given that this jump time is s, $v(s) = u$, and given O, the conditional probability density of $v(t)$ is $q_0(t-s, v|\rho O u)$;

(iii) the probability of two or more jumps in $[0, t]$ is $O(t^2)$ as $t \downarrow 0$. From (2.24) it is easy to check that the backward operator of the velocity process is $L_1 + B - \mu^{-1}$. This and a little semigroup theory provide an alternative derivation of (1.20). Q.E.D.

3. Conservation laws. The *formal adjoint* of the backward operator L is $L^* = L_2^* + B^* - \mu^{-1}$, where

$$
L_2^* \psi(v, y) = \frac{1}{2} \sum_{i,j=1}^{3} D_{ij} \frac{\partial^2 \psi}{\partial v^{(i)} \partial v^{(j)}} + \beta \sum_{i=1}^{3} [(v^{(i)} - u_0^{(i)} - g^{(i)}/\beta)\psi] - \sum_{i=1}^{3} v^{(i)} \frac{\partial \psi}{\partial y^{(i)}}, \tag{3.1}
$$

and

$$
B^* \psi(v, y) = \begin{cases} \mu^{-1} \rho^{-3} \int_{S^2} \psi(\rho^{-1}|v| a_1, y) H_1(da_1) & \text{if} \quad \rho > 0, \\ \mu^{-1} \left(\int_{R^3} \psi(a_1, y)\, da_1 \right) \delta_0(v) & \text{if} \quad \rho = 0. \end{cases} \tag{3.2}
$$

Here ψ is infinitely differentiable and has compact support, $\delta_0(\cdot)$ is the *Dirac delta function* with pole at zero, and H_1 is the uniform distribution on the sphere $S^2 = \{a_1 \in R^3 : |a_1| = 1\}$. The expression for L_2^* appearing in (3.1) is standard. To derive (3.2), let ϕ_1, ψ_1 be arbitrary functions on R^3 which are infinitely differentiable and have compact supports. Then, if $\rho > 0$,

$$
\begin{aligned}
\int_{R^3} (B\phi_1(v))\psi_1(v)\,dv &= \mu^{-1}\int_{R^3}\left(\int_{S^2}\phi_1(\rho|v|a_1)H_1(da_1)\right)\psi_1(v)\,dv \\
&= \mu^{-1}\int_{r=0}^{\infty} cr^2\left(\int_{S^2}\phi_1(\rho r a_1)H_1(da_1)\right) \\
&\qquad \cdot\left(\int_{S^2}\psi_1(ra_1')H_1(da_1')\right)dr \\
&= \mu^{-1}\rho^{-3}\int_{r'=r=0}^{\infty} cr'^2\left(\int_{S^2}\psi_1(\rho^{-1}r'a_1')H_1(da_1')\right) \qquad (3.3)\\
&\qquad \cdot\left(\int_{S^2}\phi_1(r'a_1)H_1(da_1)\right)dr' \\
&= \mu^{-1}\rho^{-3}\int_{R^3}\left(\int_{S^2}\psi_1(\rho^{-1}|v|a_1')H_1(da_1')\right)\phi_1(v)\,dv \\
&= \int_{R^3}\phi_1(v)B^*\psi_1(v)\,dv.
\end{aligned}
$$

If $\rho = 0$, then

$$
(3.4)\qquad \int_{R^3}(B\phi_1(v))\psi_1(v)\,dv = \mu^{-1}\phi_1(0)\int_{R^3}\psi_1(v)\,dv = \int_{R^3}\phi_1(v)B^*\psi_1(v)\,dv.
$$

The last integral is merely a formal way of writing the integral with respect to the Dirac measure.

Under the hypothesis of Theorem 2, one may show that (see Gihman and Skorohod (1972, relation (20), p. 297, and the relation below (25), p. 299))

$$
(3.5)\qquad \frac{\partial}{\partial t}\int_{R^3\times R^3}\psi(v,y)p(t,dv,dy|v',x') = \int_{R^3\times R^3}(L\psi(v,y))p(t,dv,dy|v',x'),
$$

for every ψ which is C^∞ and has compact support. Here p denotes the transition probability function of the $\{(v(t), X(t)) : t \geqq 0\}$ process. If p had a density π (i.e., $p(t, dv, dy|v', x') = \pi(t, v, y|v', x')\,dv\,dy$) which is continuously differentiable, once with respect to t, twice with respect to v, and once with respect to y, then one could use integration by parts to get (at least for $\rho > 0$)

$$
(3.6)\qquad \frac{\partial \pi}{\partial t} = L^*\pi,
$$

where π is treated as a function of t, v, y. While it is likely that this is the case for $\rho > 0$ the chances are even better for the *regularization*

$$
(3.7)\qquad \bar{p} = p * (\delta_{\{0\}} \times K_\varepsilon)
$$

where K_ε is a probability measure on R^3 (the 'position' space) having a density k_ε which is C^∞ and vanishes outside a ball of radius ε, and $\delta_{\{0\}}$ is the probability measure (in the 'velocity' space) degenerate at 0 ($\in R^3$), and $*$ denotes convolution of measures. For the rest of the section we *assume*, unless otherwise specified, that the regularized transition probability $\bar{p}$ has a density $\bar{\pi}(t, v, y|v', x')$ with respect to Lebesgue measure on $R^3 \times R^3$, and that $\bar{\pi}$ is continuously differentiable—at least once with respect to t, twice with respect to v, and once with respect to y. Since a measurement (on concentration of solute) may be viewed as a 'local average', $\bar{p}$ is an appropriate approximation of p if ε is small. For the computations which follow it will also be assumed that $\bar{\pi}$ and its derivatives are well behaved near infinity, i.e.,

(i) $|v|^3\bar{\pi}$ is integrable in v, and goes to zero as $|v|\to\infty$;

(ii) $|v|^2\partial\bar{\pi}/\partial v^{(i)}$, $1\leqq i\leqq 3$, are integrable in v and go to zero as $|v|\to\infty$;

(iii) $|v|^2\partial^2\bar{\pi}/\partial v^{(i)}\partial v^{(j)}$; $1\leqq i, j\leqq 3$, are integrable in v and go to zero as $|v|\to\infty$,

(iv) for every compact subset Δ of R^3 the functions $|v|^2 \sup\{\partial\bar{\pi}/\partial y^{(i)}: y\in\Delta\}$, are integrable in v;

(v) for every compact subset Γ of $(0,\infty)$ the function $|v|^2\sup\{\partial\bar{\pi}/\partial t: t\in\Gamma\}$ is integrable in v.

These conditions allow one to integrate by parts, neglecting the values at infinity, and to interchange orders of differentiation (with respect to t or y) and integration (with respect to v). The computations are otherwise straightforward and we shall omit details.

Since the coefficients in L and L^* depend only on the velocity coordinates, and not on the position coordinates (consequently convolution by $\delta_{\{0\}}\times K_\varepsilon$ commutes with L^*), it is simple to check that $\bar{\pi}$ (as a function of v and y) satisfies the *Fokker–Planck equation*:

$$\frac{\partial\bar{\pi}}{\partial t}=L^*\bar{\pi}. \tag{3.8}$$

This equation leads to important conservation laws. To state these we need some definitions. First, write

$$\theta(t,v,y)=\int_{R^3}\bar{\pi}(t,v,y\,|\,v',x')c_0(x')\,dx', \tag{3.9}$$

where $c_0(\cdot)$ is a nonnegative and nonzero C^∞ function on R^3 having compact support. The function $c_0(\cdot)$ will be referred to as the *initial concentration*. The *concentration* $c(t,y)$ at y and at time t is defined by

$$c(t,y)=\int_{R^3}\theta(t,v,y)\,dv. \tag{3.10}$$

The *volumetric flux density vector* $f(\cdot)=(f^{(1)}(\cdot), f^{(2)}(\cdot), f^{(3)}(\cdot))$ is defined by

$$f^{(j)}(t,y)=\int_{R^3}v^{(j)}\theta(t,v,y)\,dv \qquad (j=1,2,3). \tag{3.11}$$

Also write $u(\cdot)=(u^{(1)}(\cdot), u^{(2)}(\cdot), u^{(3)}(\cdot))$, where

$$u^{(j)}(t,y)=\begin{cases} f^{(j)}(t,y)/c(t,y) & \text{if } c(t,y)>0,\\ 0 & \text{if } c(t,y)=0, \ (j=1,2,3).\end{cases} \tag{3.12}$$

The *internal energy density* $d(t,y)$ is defined by

$$d(t,y)=\frac{1}{2}\int_{R^3}|v-u(t,y)|^2\theta(t,v,y)\,dv. \tag{3.13}$$

The *energy flow vector* $J(\cdot)\equiv(J^{(1)}(\cdot), J^{(2)}(\cdot), J^{(3)}(\cdot))$ is defined by

$$J^{(j)}(t,y)=\frac{1}{2}\int_{R^3}(v^{(j)}-u^{(j)}(t,y))|v-u(t,y)|^2\theta(t,v,y)\,dv \qquad (j=1,2,3). \tag{3.14}$$

Finally, define the *pressure tensor matrix* $((\rho_{ij}(\cdot)))$ by

$$(3.15)\quad \rho_{ij}(t, y) = \int_{R^3} (v^{(i)} - u^{(i)}(t, y))(v^{(j)} - u^{(j)}(t, y))\theta(t, v, y)\, dv, \qquad 1 \leqq i, j \leqq 3.$$

In view of (3.10), θ satisfies the Fokker–Planck equation

$$(3.16)\qquad \frac{\partial \theta}{\partial t} = L^*\theta.$$

Integrating both sides with respect to v one obtains the law of *mass conservation*:

$$(3.17)\qquad \frac{\partial c}{\partial t} + \sum_{j=1}^{3} \frac{\partial (u^{(j)} c)}{\partial y^{(j)}} = 0.$$

The equations for *momentum conservation* are obtained on differentiating both sides of (3.11) with respect to t:

$$(3.18)\quad \frac{\partial}{\partial t}(u^{(j)}c) = -\sum_{i=1}^{3} \frac{\partial}{\partial y^{(i)}}(\rho_{ij} + u^{(i)}u^{(j)}c) - (\mu^{-1} + \beta)u^{(j)}c + \beta w_0^{(j)}c, \qquad (j = 1, 2, 3).$$

Finally, differentiating both sides of (3.13) with respect to t and using (3.16) one obtains the *energy conservation law*

$$(3.19)\quad \begin{aligned} \frac{\partial}{\partial t} d(t, y) = {} & \frac{1}{2}\left(\sum_{i=1}^{3} D_{ii}\right) c + \mu^{-1}\frac{(1+\rho^2)}{2}|u|^2 c - \left(2\beta + \frac{1-\rho^2}{\mu}\right) d(t, y) \\ & - \sum_{i=1}^{3} \frac{\partial}{\partial y^{(i)}}(J^{(i)} + u^{(i)} d(t, y)) - \sum_{i=1}^{3}\sum_{k=1}^{3} \rho_{ik} \frac{\partial u^{(i)}}{\partial y^{(k)}}. \end{aligned}$$

For a discussion of the importance of the conservation laws for the dynamics of solute transport and for their derivation in the classical case of diffusion in pure liquids we refer to the book by DeGroot and Mazur (1962) (especially, pp. 188–190). If one takes $\mu^{-1} = 0$, $w_0 = 0$ and $D = d_0 I$, then our results reduce to the classical equations.

The concentration c and the other quantities above may be defined for p itself (and not for $\bar{p}$); in this case they have to be treated as generalized functions (or distributions); the equations (3.17)–(3.19) may then be established in the generalized sense; although this would eliminate the necessity to impose regularity assumptions (like those imposed on $\bar{p}$), the results are physically more meaningful when stated in the classical sense.

4. Miscellaneous comments. There is no doubt that one may extend Theorem 1 so as to apply to *nonhomogeneous* isotropic porous media under *nonconstant* convective fluxes. Although the additional technicalities involved in such an extension appear to be nontrivial, it is clear that one would use (2.1) locally, i.e., allow β, σ, μ, ρ to depend on x, but treat them as approximately constant within a macroscopically small volume. In the same vein one may extend the theory to apply to solute transport through *unsaturated* porous media. In this case β, σ will depend on the *concentration of the liquid* (even in a homogeneous medium) and, therefore, on t and x (see Bhattacharya et al. (1976)). Also, under the additional assumption that η_i's are 'locally exponential' (i.e., take the parameter μ^{-1} in the definition of the Poisson random measure to depend on x), Theorem 2 may be extended to show that $\{(v(t), X(t)) : t \geqq 0\}$ is Markovian in all the above cases. The proof of this extension may be based on the theory of the generalized Itô stochastic differential equations developed in Gihman and Skorohod (1972) (specifically, Theorem 1, p. 288, and Theorem 4, p. 296). This last extension may be carried through even for nonisotropic media.

Under the hypothesis of Theorem 2 one may attempt to derive Theorem 1 from Theorem 2. The natural route here would involve first showing that the velocity process is ergodic (thereby admitting a unique steady state), and then using a result such as the continuous time analogue of Theorem 21.1 in Billingsley (1968). However, even with the extra hypothesis, this procedure would not be simpler.

Finally, it may be shown by a fairly simple symmetry argument that the matrix D is diagonal (see Gupta et al. (1979)).

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16.2 "On the Taylor-Aris theory of solute transport in a capillary"

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ON THE TAYLOR-ARIS THEORY OF SOLUTE TRANSPORT IN A CAPILLARY*

R. N. BHATTACHARYA† AND VIJAY K. GUPTA‡

Abstract. A new simple derivation is given of G. I. Taylor's classic theory of solute transport in a straight capillary through which a liquid is flowing in a steady nonturbulent flow. The results derived are stronger, and an explicit representation is provided for the displacement of a solute molecule as the sum of a Brownian motion and the integral of an ergodic Markov process which is asymptotically a Brownian motion. Two curious identities involving zeros of the Bessel function of order one are obtained as a by-product.

In the classic work of Taylor (1953), as completed by Aris (1956), it was shown that when a solute in low concentration is injected in a liquid flowing through an infinite straight capillary of uniform cross-section with a steady convective velocity, then the concentration along the capillary (averaged over the cross-section) is asymptotically Gaussian.

Let the x-axis be taken to be a line inside the capillary parallel to its length; the cross-section E is the (y, z)-plane bounded by a smooth curve Γ. Let $C(\mathbf{x}, t)$ denote the solute concentration at the point $\mathbf{x}=(x, y, z)$ at time t. Taylor's starting equation is the *Fokker–Planck equation*

$$(1)\qquad \begin{aligned} &\frac{\partial C}{\partial t}=D_0\Delta C-U_0 f(y,z)\frac{\partial C}{\partial x} \quad \text{for } \mathbf{x}\in\mathbb{R}^1\times E^0, \quad t>0,\\ &\frac{\partial C}{\partial \nu}=0 \quad \text{for } \mathbf{x}\in\mathbb{R}^1\times\Gamma, \quad t>0.\end{aligned}$$

Here (i) D_0 is Einstein's molecular diffusion coefficient, (ii) Δ is the Laplacian, (iii) $(U_0 f(y, z), 0, 0)$ is the velocity field of the liquid, U_0 being the maximum velocity in the direction of flow, (iv) $\partial/\partial\nu$ denotes differentiation along the outward normal to the capillary boundary. Also E^0 denotes the interior of the cross-section E (so that $E=E^0\cup\Gamma$). The case explicitly dealt with by Taylor (1953) is that of a circular cross-section $E=\{y^2+z^2\leqq a\}$, in which case a linearized Navier–Stokes equation yields

$$(2)\qquad f(y,z)=1-\frac{y^2+z^2}{a^2}.$$

Aris (1956) extended the results to an arbitrary cross-section and to the case when the molecular diffusion coefficient is a smooth function of the transverse coordinates.

Aris (1956) in his treatment obtains asymptotic (i.e., for large t) expressions for moments of the average concentration $\bar{C}(x, t)$ (averaged over the cross-section) in order to establish its asymptotic Gaussian behavior. A different analytical derivation using perturbation techniques has been given by Fife and Nicholes (1975). Since the basis of (1) is Einstein's kinetic theory of diffusion (see Einstein (1905–1908), Nelson (1967)), it is more natural from a physical (or statistical-mechanical) point of view to look at the position process $\mathbf{X}(t)=(X(t), Y(t), Z(t))$ of a single solute molecule whose

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transition probability density function satisfies the *Kolmogorov forward equation* (1). The Taylor–Aris result is then mathematically equivalent to the asymptotic Gaussian nature of $X(t)$, with (half) the variance parameter giving the dispersion coefficient computed by them. Since the solute is in low concentration, the different solute molecules may be assumed to move independently, so that one may apply a law of large numbers to go from the asymptotic distribution of $X(t)$ to that of concentration in the x-direction. It also turns out that this approach is mathematically much simpler, at least from a probabilist's point of view.

In a series of remarks it is pointed out that this approach yields a stronger result than the Taylor–Aris result.

In the theorem below $\bar{v}$ denotes the average of f on E.

THEOREM. *Let* $\mathbf{X}(t)=(X(t), Y(t), Z(t))$ *be a Markov process having continuous sample paths and a transition probability density function satisfying Kolmogorov's forward equation* (1). *Then, as* $n\to\infty$, *the stochastic process* $\{X_n(t)=n^{-1/2}[X(nt)-\bar{v}U_0nt]; t\geqq 0\}$ *converges in distribution to a Brownian motion with zero drift and a positive variance parameter* σ^2. *In case the cross-section is circular, one has*

$$\bar{v}=\tfrac{1}{2},\qquad \sigma^2=2D_0+\frac{a^2U_0^2}{96D_0}. \tag{3}$$

Proof. Let $(Y(t),Z(t))$ be a reflecting two-dimensional Brownian motion on $E=E^0\cup\Gamma$, with zero drift and variance parameter $2D_0$. Let $B(t)$ be a standard one-dimensional Brownian motion independent of $\{(Y(t),Z(t)): t\geqq 0\}$ and a given random variable $X(0)$. Define $X(t)$ by

$$X(t)-X(0)=\sqrt{2D_0}B(t)+U_0\int_0^t f(Y(s),Z(s))\,ds. \tag{4}$$

Then $\mathbf{x}(t)=(X(t), Y(t), Z(t))$ is a Markov process satisfying the hypothesis of the theorem. Rewrite (4) as

$$X(t)-X(0)-\tfrac{1}{2}U_0t=\sqrt{2D_0}B(t)+U_0\int_0^t [f(Y(s),Z(s))-\tfrac{1}{2}]\,ds. \tag{5}$$

Now $(Y(t),Z(t))$ is an *ergodic Markov process* whose transition probability converges in (variation) norm exponentially fast to the uniform distribution on E (see, e.g., Bhattacharya and Majumdar (1980, Thm. 4.4(c))). Hence a general functional central limit theorem (FCLT) for ergodic Markov processes (Bhattacharya (1982)) yields an FCLT for the integral in (5). Since $\sqrt{2D_0}B(t)$ is independent of this integral, the desired FCLT follows. The variance parameter of the limiting Brownian motion is

$$\sigma^2=2D_0+2D_1, \tag{6}$$

where D_1 may be computed by the formula given in Bhattacharya (1982).

For the special case of a circular cross-section,

$$f(Y(s),Z(s))=1-R^2(s), \tag{7}$$

where $R(s)$ is the *radial process*

$$R(s)=\frac{1}{a}(Y^2(s)+Z^2(s))^{1/2}, \tag{8}$$

whose differential generator is

$$(9)\qquad A=\frac{D_0}{a^2}\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)\quad \text{for } 0<r<1,\qquad \left.\frac{d}{dr}\right|_{r=1}=0.$$

Thus one may apply the results in Bhattacharya (1982) to $h(r)=\frac{1}{2}-r^2$ (i.e., to the integrand in (5)) to compute D_1 as

$$(10)\qquad D_1=-\langle h,g\rangle U_0^2=\left(-\int_0^1 h(r)g(r)2r\,dr\right)U_0^2,$$

where $\langle\cdot,\cdot\rangle$ is the *inner product* on $L^2((0,1],2r\,dr)$, and g is a (any) solution of the equation

$$(11)\qquad Ag(r)=h(r)\quad \text{for } 0<r<1,\qquad g'(1)=0,$$

satisfying $\langle g,g\rangle=\int_0^1 g^2(r)2r\,dr<\infty$. Note that the invariant distribution of $R(s)$ is $2r\,dr$. It is elementary to show that

$$(12)\qquad g(r)=\frac{a^2}{4D_0}\left(\frac{r^2}{2}-\frac{r^4}{4}\right)+c,$$

where c is a constant of integration. Any value of c will suffice for (10), e.g., $c=0$. One then obtains from (10),

$$(13)\qquad D_1=\frac{a^2U_0^2}{192D_0}.\qquad \text{Q.E.D.}$$

Remark 1. Note that the theorem is proved for an arbitrary (initial) distribution of $\mathbf{X}(0)$, i.e., for an arbitrary initial concentration.

Remark 2. The theorem says that, when observed over nonoverlapping large time intervals, the displacements of a solute molecule in the x-direction are approximately independent and Gaussian. Such a functional result (FCLT) is stronger than a central limit theorem.

Remark 3. The representation (5) of $X(t)$ as the sum of a process which is asymptotically a Brownian motion and an independent Brownian motion implies that the *probability density function* of $n^{-1/2}[X(nt)-\bar{v}U_0nt]$ *exists, is continuous, and converges pointwise* (as $n\to\infty$) *to the Gaussian density function with mean zero and variance* $t\sigma^2$. It follows by *Scheffé's theorem* (Scheffé (1947)) *that the convergence is also in* L^1.

Remark 4. The differential operator defined by (9) is *self-adjoint* on $L^2((0,1]$, $2r\,dr)$ and has eigenvalues $-\lambda_n$ $(n=0,1,2,\cdots)$, where

$$(14)\qquad \lambda_0=0<\lambda_1<\lambda_2<\cdots,\qquad \lambda_n=\frac{D_0}{a^2}\beta_n^2,$$

β_n being the *nth zero of the Bessel function* J_1 *of first order* (see Courant and Hilbert (1953, Chap. V), or Duff and Naylor (1966, Chap. 8)). The corresponding (complete system of) normalized eigenfunctions are

$$(15)\qquad \psi_0\equiv 1,\qquad \psi_n=\frac{J_0(\beta_n r)}{[\int_0^1 J_0^2(\beta_n r)2r\,dr]^{1/2}},$$

where J_0 is the *Bessel function of order zero*. Since the integral in the denominator of ψ_n in (15) equals $J_0^2(\beta_n)$ (see Duff and Naylor (1966, p. 308)), one may rewrite (15) as

(16) $$\psi_0 \equiv 1, \qquad \psi_n = \frac{J_0(\beta_n r)}{|J_0(\beta_n)|} \qquad (n = 1, 2, \cdots).$$

Using (14) and (16) we give another computation of D_1 for the case of the circular cross-section. For this express h and g as

(17) $$h = \sum_{n=0}^{\infty} \langle h, \psi_n\rangle\psi_n = \sum_{n=1}^{\infty} \langle h, \psi_n\rangle\psi_n, \qquad g = -\sum_{n=1}^{\infty} \lambda_n^{-1}\langle h, \psi_n\rangle\psi_n.$$

Then, by (10),

(18) $$D_1 = -\langle h, g\rangle U_0^2 = \left(\sum_{n=1}^{\infty} \lambda_n^{-1}\langle h, \psi_n\rangle^2\right) U_0^2.$$

But

(19) $$\langle h, \psi_n\rangle = \int_0^1 (\tfrac{1}{2} - r^2) J_0(\beta_n r) 2r\, dr / |J_0(\beta_n)|.$$

Since (see Courant and Hilbert (1953, p. 484))

(20) $$J_0(\beta_n r) = \sum_{m=0}^{\infty} \frac{(-1)^m}{(m!)^2}\left(\frac{\beta_n r}{2}\right)^{2m},$$

it follows, on term by term integration of (19), that

(21) $$\langle h, \psi_n\rangle = \sum_{m=0}^{\infty} (-1)^m \frac{1}{m!(m+2)!}\left(\frac{\beta_n}{2}\right)^{2m} \Big/ |J_0(\beta_n)| = \frac{4}{\beta_n^2} J_2(\beta_n) \Big/ |J_0(\beta_n)|.$$

The last equality (J_2 is the *Bessel function of order two*) follows again from Courant and Hilbert (1953, p. 484). Hence

(22) $$\langle h, \psi_n\rangle^2 = \left(\frac{16}{\beta_n^4}\right)\frac{J_2^2(\beta_n)}{J_0^2(\beta_n)} = \frac{16}{\beta_n^4},$$

Since, $J_0(\beta_n) + J_2(\beta_n) = (2/\beta_n)J_1(\beta_n) = 0$ (Duff and Naylor (1966, p. 304)), $J_0^2(\beta_n) = J_2^2(\beta_n)$. Substituting (22) into (18) one gets,

(23) $$D_1 = \frac{16a^2 U_0^2}{D_0} \sum_{n=1}^{\infty} \frac{1}{\beta_n^6}.$$

By comparing with (13) we arrive at the curious result (which appears to be new)

(24) $$\sum_{n=1}^{\infty} \frac{1}{\beta_n^6} = \frac{1}{3072}.$$

By a formal manipulation, which we are unable to justify rigorously, one also gets

(25) $$-\sum_{n=1}^{\infty} \frac{1}{\beta_n^4 J_0(\beta_n)} = \frac{1}{96}.$$

A numerical check leaves little doubt about the validity of (25). The most comprehensive treatise on Bessel functions is Watson (1966).

Remark 5. The representation (5) or (4) is true for all times, and should lead to useful expressions for $\bar{C}(x, t)$ for small t, given any initial concentration. Although we have not been able to carry this out adequately, note that the moment generating function

$$\phi(t; r, \lambda) = E\left[\exp\left\{\lambda \int_0^t h(R(s))\,ds\right\}\middle| R(0) = r\right]$$

is, by the *Feynman–Kac formula*, the solution of

$$(26)\qquad \begin{aligned} &\frac{\partial \phi(t; r, \lambda)}{\partial t} = A\phi + \lambda h\phi \quad \text{for } t > 0, \quad 0 < r < 1, \\ &\left.\frac{\partial \phi}{\partial r}\right|_{r=1} = 0, \qquad \phi(0; \lambda, r) = 1 \quad \text{for } 0 < r \leqq 1. \end{aligned}$$

Remark 6. The method given here applies to arbitrary uniform cross-sections. Also, one may replace D_0 by any positive and continuous function $\phi(y, z)$ of the transverse coordinates. In general, assume that the velocity field is $(U_0 f(y, z), b_1(y, z), b_2(y, z))$, where b_1 and b_2 are continuously differentiable functions on E. The starting Fokker–Planck equation is then,

$$(27)\qquad \begin{aligned} &\frac{\partial C}{\partial t} = \Delta(\phi C) - U_0 f\frac{\partial C}{\partial x} - \frac{\partial}{\partial y}(b_1 C) - \frac{\partial}{\partial z}(b_2 C) \quad \text{for } \mathbf{x} \in R^1 \times E^0, \quad t > 0 \\ &\frac{\partial}{\partial \nu}(\phi C) - C(b \cdot \nu) = 0 \quad \text{for } \mathbf{x} \in R^1 \times \Gamma, \quad t > 0, \end{aligned}$$

where $b \cdot \nu = b_1\nu_1 + b_2\nu_2$ is the drift at the boundary in the direction of the unit normal (see Bhattacharya and Majumdar (1980, eq. (4.21))). Equation (1) is a special case of (27). Instead of (5), one now has

$$(28)\qquad X(t) - X(0) - U_0\bar{v} = \int_0^t \sqrt{2\phi(Y(s), Z(s))}\,dB(s) + U_0\int_0^t [f(Y(s), Z(s)) - \bar{v}]\,ds,$$

where $(Y(t), Z(t))$ is a two-dimensional diffusion on E whose transition probability density $q(t; y, z)$ satisfies the forward equation,

$$(29)\qquad \begin{aligned} &\frac{\partial q}{\partial t} = \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)(\phi q) - \frac{\partial}{\partial y}(b_1 q) - \frac{\partial}{\partial z}(b_2 q) \quad \text{on } E^0 \quad \text{for } t > 0, \\ &\frac{\partial}{\partial \nu}(\phi q) - q(b \cdot \nu) = 0 \quad \text{on } \Gamma \quad \text{for } t > 0. \end{aligned}$$

Let $\pi(y, z)\,dy\,dz$ denote the invariant distribution of the $(Y(t), Z(t))$ process, obtained by solving

$$(30)\qquad \begin{aligned} &\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)(\phi\pi) - \frac{\partial}{\partial y}(b_1\pi) - \frac{\partial}{\partial z}(b_2\pi) = 0 \quad \text{on } E^0, \\ &\frac{\partial}{\partial \nu}(\phi\pi) - \pi(b \cdot \nu) = 0 \quad \text{on } \Gamma. \end{aligned}$$

In general, π is *not a constant*. The constant $\bar{v}$ appearing in (28) is given by

$$\bar{v}=\int_E f(y,z)\pi(y,z)\,dy\,dz, \tag{31}$$

and $U_0\bar{v}$ is the "average" velocity in the x-direction. To show that the central limit theorem holds for $X(t)$, one may compute the characteristic function $\gamma_n(i\lambda;t)$ of $W_n(t)=n^{-1/2}[X(nt)-X(0)-nU_0\bar{v}t]$ using (28). First take the conditional expectation given the process $\{(Y(s),Z(s)): s\geqq 0\}$, and then take expectation of this conditional expectation. Since conditionally $W_n(t)$ is Gaussian with mean

$$U_0 n^{-1/2}\int_0^{nt}[f(Y(s),Z(s))-\bar{v}]\,ds$$

and variance

$$n^{-1}\int_0^{nt} 2\phi(Y(s),Z(s))\,ds,$$

one has

$$\gamma_n(i\lambda;t)=E(e^{i\lambda W_n(t)})$$

$$=E\exp\left\{i\lambda U_0 n^{-1/2}\int_0^{nt}[f(Y(s),Z(s))-\bar{v}]\,ds-\frac{\lambda^2}{2n}\int_0^{nt}2\phi(Y(s),Z(s))\,ds\right\}. \tag{32}$$

Applying the strong law of large numbers (i.e., the ergodic theorem) to the second term in the exponent and the central limit theorem to the first term, one gets

$$\lim_{n\to\infty}\gamma_n(i\lambda;t)=\exp\left\{-\frac{\lambda^2 t}{2}(2D_2+2\bar{\phi})\right\}, \tag{33}$$

where

$$\bar{\phi}=\int_E \phi(y,z)\pi(y,z)\,dy\,dz, \tag{34}$$

and

$$D_2=-\langle\langle f-\bar{v},g\rangle\rangle U_0^2. \tag{35}$$

Here the inner product $\langle\langle\cdot,\cdot\rangle\rangle$ is the one on the space $L^2(E,\pi\,dy\,dz)$, i.e.,

$$\langle\langle f-\bar{v},g\rangle\rangle=\int_E (f(y,z)-\bar{v})g(y,z)\pi(y,z)\,dy\,dz \tag{36}$$

with g a (any) solution in L^2 of

$$\phi\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)g+b_1\frac{\partial g}{\partial y}+b_2\frac{\partial g}{\partial z}=f-\bar{v}\quad\text{on } E^0, \tag{37}$$

and

$$\frac{\partial g}{\partial \nu}=0\quad\text{on }\Gamma. \tag{38}$$

Sometimes, as in the case of a circular cross-section, this may be simplified by separation of variables. In the more general case above the $X(t)$ process is asymptotically a

Brownian motion with drift $U_0\bar{v}$ and dispersion coefficient

$$\tfrac{1}{2}\sigma^2 = \bar{\phi} + D_2. \tag{39}$$

Notice that neither $\bar{v}$ nor $\bar{\phi}$ is, in general, an average with respect to the normalized Lebesgue measure on E. Aris (1956) considered the special case of a self-adjoint operator in (29). In this case the invariant distribution is the normalized Lebesgue measure on E. Finally, the above method easily extends to the case of a *nonscalar* 3×3 diffusion matrix of the form

$$\boldsymbol{\phi}(y,z) = \begin{pmatrix} \phi_{11}(y,z) & 0 & 0 \\ 0 & \phi_{22}(y,z) & \phi_{23}(y,z) \\ 0 & \phi_{23}(y,z) & \phi_{33}(y,z) \end{pmatrix}.$$

The appropriate Fokker–Planck equation along with the boundary condition for this case may be obtained from Bhattacharya and Majumdar (1980, pp. 32–33).

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16.3 "Asymptotics of solute dispersion in periodic porous media"

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ASYMPTOTICS OF SOLUTE DISPERSION IN PERIODIC POROUS MEDIA*

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Abstract. The concentration $C(\mathbf{x}, t)$ of a solute in a saturated porous medium is governed by a second-order parabolic equation $\partial C/\partial t = -U_0\mathbf{b}\cdot\nabla C + \frac{1}{2}\sum D_{ij}\partial^2 C/\partial x_i\,\partial x_j$. In the case that $\mathbf{b}$ is periodic and divergence free, and D_{ij} are constants and $((D_{ij}))$ positive definite, the concentration is asymptotically Gaussian for large times. This article analyzes the dependence of the dispersion matrix $\mathbf{K}$ of the limiting Gaussian distribution on the velocity parameter U_0 and the period "a." It is shown that each coefficient K_{ii} is asymptotically quadratic in aU_0 if $b_i - \bar{b}_i$ has a nonzero component in the null space of $\mathbf{b}\cdot\nabla$, and asymptotically constant in aU_0 if $b_i - \bar{b}_i$ belongs to the range of $\mathbf{b}\cdot\nabla$. It is shown in a more general context that $\mathbf{K}$ depends only on aU_0. An asymptotic expansion of the Cramer–Edgeworth type is derived for concentration refining the Gaussian approximation.

Key words. Markov process, large scale dispersion, eigenfunction expansion, singular perturbation, range, null space

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1. Introduction. Consider a nonreactive dilute solute injected into a porous medium saturated with a liquid under nonturbulent flow. Suppose the following parabolic equation governing solute concentration $C(\mathbf{x}, t)$ at position $\mathbf{x}$ at time t holds at a certain space-time scale:

$$\frac{\partial C}{\partial t}=\frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial^2}{\partial x_i\,\partial x_j}\left(D_{ij}\left(\frac{\mathbf{x}}{a}\right)C\right)-\sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left(U_0 b_i\left(\frac{\mathbf{x}}{a}\right)C\right),\qquad \mathbf{x}=(x_1, x_2, \cdots, x_n)\in\Re^n,\quad t>0. \tag{1.1}$$

In (1.1), $U_0\mathbf{b}(\mathbf{x}/a) = U_0(b_1(\mathbf{x}/a), b_2(\mathbf{x}/a), \cdots, b_n(\mathbf{x}/a))$ denotes the solute drift velocity vector, $D(\mathbf{x}/a) = ((D_{ij}(\mathbf{x}/a)))$ is a positive-definite symmetric matrix, and U_0, a are positive scalars. The parameters U_0 and a scale liquid velocity and spatial length, respectively. Although in the physical context $n=3$, for mathematical purposes we let n be arbitrary.

The solution $C(\mathbf{x}, t)$ of (1.1) is given by (Friedman (1975, pp. 139–144)),

$$C(\mathbf{x}, t)=\int_{\Re^n} h(\mathbf{z})p(t;\mathbf{z},\mathbf{x})\,d\mathbf{z}, \tag{1.2}$$

where h is the continuous, bounded, initial concentration, and $p(t;\mathbf{z},\mathbf{x})$ is the fundamental solution of (1.1). Conditions on the coefficients $b_i(\mathbf{x})$, $D_{ij}(\mathbf{x})$ that guarantee the uniqueness and necessary smoothness of the fundamental solution are assumed throughout. Now $p(t;\mathbf{z},\mathbf{x})$ is also the transition probability density function of the Markov process $\mathbf{X}(t)$ defined by Itô's stochastic differential equation

$$d\mathbf{X}(t)=U_0\mathbf{b}(\mathbf{X}(t)/a)\,dt+\boldsymbol{\sigma}(\mathbf{X}(t)/a)\,d\mathbf{B}(t),\qquad \mathbf{X}(0)=\mathbf{z}, \tag{1.3}$$

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where $\sigma(\mathbf{x})$ is the positive-definite matrix the square of which is $\mathbf{D}(\mathbf{x})$ and $\mathbf{B}(t) = (B_1(t), B_2(t), \cdots, B_n(t))$ is an n-dimensional standard Brownian motion process.

Analyzing the asymptotic behavior of $C(\mathbf{x}, t)$ for large t is equivalent to analyzing the asymptotic behavior of $\mathbf{X}(t)$ for large t. To be more specific, suppose that the stochastic process

$$(1.4) \qquad \mathbf{Z}_\varepsilon(t) \equiv \varepsilon[\mathbf{X}(t/\varepsilon^2) - \varepsilon^{-2} U_0 \bar{\mathbf{b}} t]$$

converges in distribution, as $\varepsilon \downarrow 0$, to a Brownian motion with zero mean and a dispersion matrix $\mathbf{K} = ((K_{ij}))$. Here $\bar{\mathbf{b}} = (\bar{b}_1, \cdots, \bar{b}_n)$ is a suitable constant vector interpreted as the *large scale average* of $\mathbf{b}(\mathbf{x})$. In other words, suppose that a *central limit theorem* (CLT) holds for $\mathbf{X}(t)$. Now the probability distribution of $\mathbf{Z}_\varepsilon(t)$ has the density (at $\mathbf{x}$) $\varepsilon^{-n} p(\varepsilon^{-2} t; \mathbf{z}, \varepsilon^{-1}\mathbf{x} + \varepsilon^{-2} t U_0 \bar{\mathbf{b}})$ if $\mathbf{X}(0) = \mathbf{z}$. Hence the CLT asserts that $\varepsilon^{-n} p(\varepsilon^{-2} t; \mathbf{z}, \varepsilon^{-1}\mathbf{x} + \varepsilon^{-2} t U_0 \bar{\mathbf{b}})\, d\mathbf{x}$ converges weakly, as $\varepsilon \downarrow 0$, to the Gaussian distribution:

$$(1.5) \qquad \phi(t, \mathbf{x})\, d\mathbf{x} = (2\pi t)^{-n/2} (\mathrm{Det}\, \mathbf{K})^{-1/2} \exp\left\{ -\frac{1}{2t} \sum_{i,j=1}^{n} K^{ij} x_i x_j \right\} d\mathbf{x}.$$

Here K^{ij} is the (i, j) element of the matrix $\mathbf{K}^{-1}$. Thus as $\varepsilon \downarrow 0$ we obtain

$$(1.6) \qquad \varepsilon^{-n} C(\varepsilon^{-1}\mathbf{x} + \varepsilon^{-2} t U_0 \bar{\mathbf{b}}, \varepsilon^{-2} t)\, d\mathbf{x} \to C_0 \phi(t, \mathbf{x})\, d\mathbf{x}$$

where C_0 is the total initial concentration.

From here on we will refer to $((D_{ij}))$ as the *small scale dispersion matrix* and $((K_{ij}))$ as the *large scale dispersion matrix.*

CLTs such as described above have been derived for periodic coefficients D_{ij}, b_i in Bensoussan, Lions, and Papanicolaou (1978) and Bhattacharya (1985). Under the assumption that the elliptic operator on the right-hand side of (1.1) is self-adjoint, Kozlov (1979), (1980), and Papanicolaou and Varadhan (1979) have proved such CLTs for the case where the coefficients are stationary, ergodic random fields. An extension to the nonself-adjoint case for almost periodic coefficients, when the large scale velocity $\bar{\mathbf{b}}$ is nonzero, is given in Bhattacharya and Ramasubramanian (1988). Papanicolaou and Pironeau (1981) also deal with a nonself-adjoint case when the coefficients constitute a general ergodic random field and $\bar{\mathbf{b}} = 0$.

Such problems arise in analyzing the movement of contaminants in saturated porous media such as aquifers as well as in laboratory columns. The dependence of $\mathbf{K}$ on U_0 has been studied experimentally in laboratory columns (see, e.g., Fried and Combarnous (1971)). The spatial scale parameter a is fixed in such experiments. In aquifers, on the other hand, the main interest from the point of view of long term prediction lies in the analysis of $\mathbf{K}$ as a function of the scale parameter a for a fixed velocity field, and therefore for a fixed U_0 (Gupta and Bhattacharya, (1986)). Field scale dispersions in aquifers have been analyzed for the ergodic random field case (when $\bar{b}$ is nonzero) in, e.g., Gelhar and Axness (1983), Winter, Newman, and Neuman (1984), and Dagan (1984). For certain classes of periodic coefficients, the dependence of $\mathbf{K}$ on a and U_0 has been analyzed in Gupta and Bhattacharya (1986) and Guven and Molz (1986). A more detailed survey of the hydrologic literature is given in Sposito, Jury, and Gupta (1986).

The dependence of $\mathbf{K}$ on U_0 has been treated in the literature separately from its dependence on a because of the physical contexts in which these arise. As we shall see in § 2, the roles of U_0 and a in this respect are interchangeable. Indeed $\mathbf{K}$ depends only on the product aU_0.

In § 3 we analyze the dependence of **K** on aU_0 for the class of periodic coefficients such that D_{ij}'s are constants and **b** has zero divergence. It is shown that for one broad class of periodic coefficients, the K_{ii}'s grow quadratically as $aU_0 \to \infty$, and that the K_{ii}'s approach asymptotic constancy for another class.

Section 4 provides a refinement of the Gaussian approximation (1.6) in the form of an asymptotic expansion in powers of ε. In probability theory such an expansion is called a *Cramer–Edgeworth expansion.* In the differential equations literature it is referred to as a *singular perturbation expansion.* For prediction of concentration $C(\mathbf{x}, t)$ in aquifers over time scales that are not very large, such expansions provide better approximations than the Gaussian. The importance of predictions over such time scales has been discussed, for example, by Guven and Molz (1986) and Dagan (1984).

2. Interchangeability of velocity and spatial scale parameters in K. Write,

$$\mathbf{K}(U_0, a) = \mathbf{K}, \qquad K_{ij}(U_0, a) = K_{ij}, \tag{2.1}$$

indicating the dependence of the large scale dispersion matrix **K** on the velocity and scale parameters U_0 and a.

PROPOSITION 2.1. *If the central limit theorem holds for the solution* $\mathbf{X}(t)$ *of* (1.3), *then* **K** *depends on* U_0 *and* a *only through their product* aU_0. *In particular,*

$$\mathbf{K}(U_0, a) = \mathbf{K}(a, U_0) = \mathbf{K}(aU_0, 1). \tag{2.2}$$

To prove this, express the solution of (1.3) as $\mathbf{X}(t; a, U_0)$ to indicate its dependence on a and U_0. Define the stochastic process

$$\mathbf{Y}(t; a, U_0) = a\mathbf{X}(t/a^2; 1, U_0). \tag{2.3}$$

Then $\mathbf{Y}(t; a, U_0)$ satisfies the Itô equation

$$\begin{aligned} d\mathbf{Y}(t; a, U_0) &= aU_0\mathbf{b}(\mathbf{X}(t/a^2; 1, U_0))\frac{dt}{a^2} + a\sigma(\mathbf{X}(t/a^2; 1, U_0))\, d\mathbf{B}(t/a^2) \\ &= \frac{U_0}{a}\mathbf{b}(\mathbf{Y}(t; a, U_0)/a)\, dt + \sigma(\mathbf{Y}(t; a, U_0)/a)\, d\bar{\mathbf{B}}(t), \end{aligned} \tag{2.4}$$

where $\bar{\mathbf{B}}(t)$ is defined by

$$d\bar{\mathbf{B}}(t) = a\, d\mathbf{B}(t/a^2), \qquad \bar{\mathbf{B}}(0) = \mathbf{B}(0) = 0. \tag{2.5}$$

Note that $\bar{\mathbf{B}}(t)$ is, like $\mathbf{B}(t)$, a standard n-dimensional Brownian motion. It now follows from (2.4) that $\mathbf{Y}(t; a, U_0)$ has the same distribution as $\mathbf{X}(t; a, U_0/a)$ (with the initial value $\mathbf{Y}(0; a, U_0) = a\mathbf{z}$). Hence

$$\lim_{t\to\infty} \frac{\operatorname{Var} \mathbf{Y}(t; a, U_0)}{t} = \lim_{t\to\infty} \frac{\operatorname{Var} \mathbf{X}(t; a, U_0/a)}{t} = \mathbf{K}(U_0/a, a), \tag{2.6}$$

where Var stands for the variance-covariance matrix. Now, from (2.3),

$$\begin{aligned} \lim_{t\to\infty} \frac{\operatorname{Var} \mathbf{Y}(t; a, U_0)}{t} &= \lim_{t\to\infty} a^2 \frac{\operatorname{Var} \mathbf{X}(t/a^2; 1, U_0)}{t} \\ &= \lim_{t\to\infty} \frac{\operatorname{Var} \mathbf{X}(t/a^2; 1, U_0)}{t/a^2} = \mathbf{K}(U_0, 1). \end{aligned} \tag{2.7}$$

Relations (2.6) and (2.7) yield,

$$\mathbf{K}(U_0/a, a) = \mathbf{K}(U_0, 1). \tag{2.8}$$

Write $\alpha = U_0/a$, $\beta = a$. Then (2.8) becomes

$$\mathbf{K}(\alpha, \beta) = \mathbf{K}(\alpha\beta, 1) \quad \text{for all } \alpha > 0, \quad \beta > 0. \tag{2.9}$$

This proves the proposition.

It may be remarked that in a periodic model a is simply the period (Gupta and Bhattacharya (1986)). In an ergodic random field model (see Gelhar and Axness (1983), Winter et al. (1984)), a may be taken to be the characteristic correlation length. Fried and Combarnous (1971) give an account of the fairly extensive laboratory experiments that have been done to study the effect of increase in velocity on dispersion in porous media. A broad mathematical justification of these experimentally observed relationships appears in Bhattacharya and Gupta (1983). In these studies the spatial scale is held fixed at the so-called *Darcy level*, while velocity is increased. On the other hand, dependence of dispersion on large spatial scales has been analyzed in field situations for various models of heterogeneous porous media. The above proposition shows that the two relationships are mathematically equivalent. For this reason, in the next section the spatial scale a is held fixed at $a = 1$, while the velocity parameter U_0 is allowed to vary.

3. An expansion of the large scale dispersion in the periodic model. In (1.1), take D_{ij}'s to be constants and b_i's continuously differentiable periodic functions satisfying the divergence condition

$$\operatorname{div} \mathbf{b} = 0. \tag{3.1}$$

In view of proposition (2.1), we take the period of b_i to be one in each coordinate without loss of generality. Let L denote the elliptic operator

$$Lg(\mathbf{x}) = Dg(\mathbf{x}) + U_0\mathbf{b}(\mathbf{x}) \cdot \nabla g(\mathbf{x}), \qquad \mathbf{x} \in \Re^n \tag{3.2}$$

where

$$D = \frac{1}{2} \sum D_{ij} \frac{\partial^2}{\partial x_i \, \partial x_j}. \tag{3.3}$$

Let $T = [0, 1]^n$. Define

$$\bar{b}_i = \int_T b_i(\mathbf{x}) \, d\mathbf{x}, \qquad i = 1, 2, \cdots, n, \tag{3.4}$$

and let g_i be a periodic function satisfying

$$Lg_i = b_i - \bar{b}_i. \tag{3.5}$$

Then it follows from Bhattacharya (1985) that the large scale dispersion coefficients are given by

$$K_{ij} = D_{ij} - U_0^2 \int_T g_i(\mathbf{x})(b_j(\mathbf{x}) - \bar{b}_j) \, d\mathbf{x} - U_0^2 \int_T g_j(\mathbf{x})(b_i(\mathbf{x}) - \bar{b}_i) \, d\mathbf{x}. \tag{3.6}$$

It is convenient to work with the following spaces of (equivalence classes of) complex-valued functions on T:

$$H^0 = \left\{ h: \int_T |h(\mathbf{x})|^2 \, d\mathbf{x} < \infty, \int_T \mathrm{h}(\mathbf{x}) \, d\mathbf{x} = 0, \right.$$

$$\left. \text{and } h \text{ satisfies periodic boundary conditions} \right\},$$

$$H^1 = \left\{ h \in H^0: \int_T |\nabla h(\mathbf{x})|^2 \, d\mathbf{x} < \infty \right\},$$

$$H^2=\left\{h\in H^1:\int_T\sum_{i,j=1}^n\left|\frac{\partial^2}{\partial x_i\,\partial x_j}h(\mathbf{x})\right|^2d\mathbf{x}<\infty\right\}.$$

Here, $|\cdot|$ denotes both absolute value and Euclidean norm. For convenience, we take the norm and inner product on H^1 to be

$$\|h\|_1^2=\int_T\sum_{i,j=1}^n D_{ij}\frac{\partial}{\partial x_i}h(\mathbf{x})\frac{\partial}{\partial x_j}\bar{h}(\mathbf{x})\,d\mathbf{x},\quad\text{and}$$

$$\langle h,w\rangle_1=\int_T\sum_{i,j=1}^n D_{ij}\frac{\partial}{\partial x_i}h(\mathbf{x})\frac{\partial}{\partial x_j}\bar{w}(\mathbf{x})\,d\mathbf{x}$$

for $h, w\in H^1$. This is allowed, since $((D_{ij}))$ is a real, positive-definite, symmetric matrix and

$$\int_T h(\mathbf{x})\,d\mathbf{x}=0$$

for $h\in H^1$.

For a given set f_i $(i=1,2,\cdots,n)$ in H^1 let g_i be the solutions in H^2 of

$$Lg_i=f_i. \tag{3.7}$$

Standard results in the theory of elliptic partial differential operators imply that (3.7) has a unique solution $g_i\in H^2$ for each $f_i\in H^1$.

Throughout we shall write

$$E_{ij}=E_{ij}(U_0)=-U_0^2\int_T g_i(\mathbf{x})f_j(\mathbf{x})\,d\mathbf{x}. \tag{3.8}$$

In this notation, $K_{ij}=D_{ij}+E_{ij}+E_{ji}$ with $f_i=b_i-\bar{b}_i$.

Note that the operator D is one to one on H^2 onto H^0. To obtain useful eigenfunction expansions we note that for $f\in H^0$ and $g\in H^2$, $Lg=f$ if and only if $[I+U_0H]g=D^{-1}f$, where $Hg(\mathbf{x})=D^{-1}\mathbf{b}(\mathbf{x})\cdot\nabla g(\mathbf{x})$. We can consider H as an operator from H^1 to itself; as such, it is compact and skew-symmetric. Then H has eigenfunctions $\{\phi_k\}_{k=1,2,\cdots}$ and corresponding eigenvalues $\{\sqrt{-1}\,\lambda_k\}_{k=1,2,\cdots}$ with the following properties:

(i) Each λ_k is real and $\lim_{k\to\infty}\lambda_k=0$.

(ii) $\{\phi_k\}_{k=1,2,\cdots}$ is a complete orthonormal set on $H^1\cap N^\perp$, where $N=\{h\in H^1: Hh=0\}$ is the null space of H in H^1 and $\perp$ denotes orthogonal complement.

(iii) Each $h\in H^1$ can be represented as

$$h=h_N+\sum_{k=1}^\infty \alpha_k\phi_k, \tag{3.9}$$

where $h_N\in N$ and for $k=1,2,\cdots$, $\alpha_k=\langle h,\phi_k\rangle_1$. Note that

$$\|h\|_1^2=\|h_N\|_1^2+\sum_{k=1}^\infty|\alpha_k|^2,\quad\text{and}$$

$$Hh=\sum_{k=1}^\infty\sqrt{-1}\,\lambda_k\alpha_k\phi_k.$$

Suppose that for $g\in H^2$ and $f\in H^0$, the representation (3.9) becomes

$$g=g_N+\sum_{k=1}^\infty\alpha_k\phi_k,\quad\text{and}$$

$$D^{-1}f=(D^{-1}f)_N+\sum_{k=1}^\infty\beta_k\phi_k.$$

Then $Lg=f$ if and only if $[I+U_0H]g=D^{-1}f$, i.e.,

$$g_N+\sum_{k=1}^{\infty}(1+\sqrt{-1}\,U_0\lambda_k)\alpha_k\phi_k=(D^{-1}f)_N+\sum_{k=1}^{\infty}\beta_k\phi_k,$$

i.e.,

$$g=L^{-1}f=(D^{-1}f)_N+\sum_{k=1}^{\infty}\frac{\beta_k}{1+\sqrt{-1}\,U_0\lambda_k}\phi_k. \tag{3.10}$$

Suppose that the given set of functions f_i is real valued and contained in H^0. If we have

$$D^{-1}f_i=(D^{-1}f_i)_N+\sum_{k=1}^{\infty}\beta_{ik}\phi_k$$

for each i, then (3.10) gives

$$g_i=L^{-1}f_i=(D^{-1}f_i)_N+\sum_{k=1}^{\infty}\frac{\beta_{ik}}{1+\sqrt{-1}\,U_0\lambda_k}\phi_k.$$

It follows that for general i and j

$$\begin{aligned}E_{ij}(U_0)&=-U_0^2\int_T g_i(\mathbf{x})DD^{-1}f_j(\mathbf{x})\,d\mathbf{x}=U_0^2\langle g_i, D^{-1}f_j\rangle_1\\&=U_0^2\left\{\langle(D^{-1}f_i)_N,(D^{-1}f_j)_N\rangle_1+\sum_{k=1}^{\infty}\frac{\beta_{ik}\bar{\beta}_{jk}}{1+\sqrt{-1}\,U_0\lambda_k}\right\}.\end{aligned} \tag{3.11}$$

If $i=j$, a sharper result can be obtained. We have

$$\begin{aligned}E_{ii}(U_0)&=-U_0^2\int_T g_i(\mathbf{x})D[I+U_0H]g_i(\mathbf{x})\,d\mathbf{x}\\&=U_0^2\{\|g_i\|_1^2+U_0\langle g_i, Hg_i\rangle_1\}.\end{aligned}$$

Since H is skewsymmetric on H^1 and g_i is real-valued, $\langle g_i, Hg_i\rangle_1=0$. Consequently,

$$E_{ii}(U_0)=U_0^2\left\{\|(D^{-1}f_i)_N\|_1^2+\sum_{k=1}^{\infty}\frac{|\beta_{ik}|^2}{1+U_0^2\lambda_k^2}\right\}. \tag{3.12}$$

It may not be apparent how to obtain (3.12) by taking $j=i$ in (3.11). The two formulas can be reconciled by noting the following:

(i) Since $((D_{ij}))$ and b_i are real, for each eigenfunction-eigenvalue pair ϕ_k, $\sqrt{-1}\,\lambda_k$ there is a complex conjugate pair $\phi_l=\bar{\phi}_k$, $\sqrt{-1}\,\lambda_l=-\sqrt{-1}\,\lambda_k$.

(ii) For such conjugate pairs,

$$\beta_{ik}=\langle f_i,\phi_k\rangle_1=\langle f_i,\bar{\phi}_l\rangle_1=\bar{\beta}_{il}$$

since f_i is real.

(iii) Then for such pairs,

$$\frac{|\beta_{ik}|^2}{1+\sqrt{-1}\,U_0\lambda_k}+\frac{|\beta_{il}|^2}{1+\sqrt{-1}\,U_0\lambda_l}=\frac{|\beta_{ik}|^2}{1+U_0^2\lambda_k^2}+\frac{|\beta_{il}|^2}{1+U_0^2\lambda_l^2}.$$

3.1. Applications and examples. Expressions (3.11) and (3.12) are our basic tools for analyzing the behavior of the E_{ij}'s and K_{ij}'s. In the following, we show how these expressions can be applied to the examples of Gupta and Bhattacharya (1986) as well as to new examples, and we give some results that illustrate how they can be used to obtain general statements.

It is obvious from (3.11) and (3.12) that $E_{ij}(U_0)=O(U_0^2)$ if $\langle (D^{-1}f_i)_N, (D^{-1}f_j)_N\rangle_1 \neq 0$ and $E_{ij}(U_0)=o(U_0^2)$ otherwise. In particular, $E_{ii}(U_0)=O(U_0^2)$ if $(D^{-1}f_i)_N \neq 0$ and $E_{ii}(U_0)=o(U_0^2)$ otherwise. We note that $N=\{h\in H^1: Hh=0\}$ is just the null space of $\mathbf{b}\cdot\nabla$ in H^1, i.e., the set of $h\in H^1$ such that $\mathbf{b}(\mathbf{x})\cdot\nabla h(\mathbf{x})=0$ almost everywhere in T. This is to say that N is the set of elements of H^1 that are constant along the *flow curves* determined by $\mathbf{b}$. By a flow curve, we mean a characteristic of the partial differential operator $\mathbf{b}\cdot\nabla$, i.e., a solution of the autonomous system $\dot{\mathbf{x}}=\mathbf{b}(\mathbf{x})$.

LEMMA 3.1. *Suppose that $f_i\in H^1$ is constant along each flow curve. Then either $f_i=0$, in which case $E_{ij}(U_0)=0$ for each j, or $E_{ii}(U_0)=O(U_0^2)$.*

Proof. We have that $f_i\in N$ and

$$\langle f_i, D^{-1}f_i\rangle_1 = -\int_T f_i(\mathbf{x})^2\,d\mathbf{x}.$$

It follows that if $f_i\neq 0$, then $(D^{-1}f_i)_N\neq 0$ and $E_{ii}(U_0)=O(U_0^2)$.

Example 3.2 (Gupta and Bhattacharya (1986)). Take $n=3$, and,

$$\mathbf{b}(\mathbf{x})=(1+\sin 2\pi x_3, \sin 2\pi x_3, 0), \qquad \mathbf{x}=(x_1,x_2,x_3).$$

Then it is simple to check that for $i=1,2$, $f_i=b_i-\bar{b}_i$ satisfies the hypothesis of Lemma 3.1 and E_{ii} and K_{ii} are $O(U_0^2)$. In fact, f_1 and f_2 depend only on x_3, and so $D^{-1}f_1$ and $D^{-1}f_2$ depend only on x_3. Then $D^{-1}f_1$ and $D^{-1}f_2$ are in N, and since

$$\langle D^{-1}f_1, D^{-1}f_2\rangle_1 = -\int_T \sin 2\pi x_3 D^{-1}\sin 2\pi x_3\,dx>0,$$

it follows that E_{12}, E_{21}, and K_{12} are $O(U_0^2)$.

As an operator on H^1, $\mathbf{b}\cdot\nabla$ has range

$$R=\{f\in H^0: f=\mathbf{b}\cdot\nabla h \text{ for some } h\in H^1\}$$

in H^0. This range R, as well as the null space N, can be helpful in determining the behavior of the E_{ij}'s and K_{ij}'s.

LEMMA 3.3. *Suppose that $f_i\in R$. Then*

$$\lim_{U_0\to\infty} E_{ii}(U_0)=\|h_i\|_1^2,$$

where h_i is the unique element of $H^1\cap N^\perp$ such that $f_i=\mathbf{b}\cdot\nabla h_i$. Also for $i\neq j$,

$$E_{ij}(U_0)=O(U_0)\simeq U_0\langle h_i, D^{-1}f_j\rangle_1, \quad \text{and} \tag{3.13}$$

$$E_{ji}(U_0)=O(U_0)\simeq -U_0\langle D^{-1}f_j, h_i\rangle_1, \tag{3.14}$$

for large U_0.

Remark. In (3.13) and (3.14), $\simeq$ means that after division by U_0, both sides approach the same limit as U_0 approaches infinity. In particular, if the inner products in (3.13) and (3.14) are zero, then $E_{ij}(U_0)$ and $E_{ji}(U_0)$ are $o(U_0)$.

Proof. It is clear that h_i exists, and we write

$$h_i=\sum_{k=1}^{\infty}\gamma_{ik}\phi_k.$$

Then

$$D^{-1}f_i=Hh_i=\sum_{k=1}^{\infty}\sqrt{-1}\,\lambda_k\gamma_{ik}\phi_k,$$

and (3.12) gives

$$E_{ii}(U_0) = U_0^2 \sum_{k=1}^{\infty} \frac{\lambda_k^2 |\gamma_{ik}|^2}{1 + U_0^2 \lambda_k^2}.$$

Thus

$$\lim_{U_0 \to \infty} E_{ii}(U_0) = \sum_{k=1}^{\infty} |\gamma_{ik}|^2 = \|h_i\|_1^2.$$

For $j \neq i$, we write

$$D^{-1} f_j = (D^{-1} f_j)_N + \sum_{k=1}^{\infty} \beta_{jk} \phi_k,$$

and (3.11) gives

$$E_{ij}(U_0) = U_0 \sum_{k=1}^{\infty} \frac{\sqrt{-1}\, U_0 \lambda_k \gamma_{ik} \bar{\beta}_{jk}}{1 + \sqrt{-1}\, U_0 \lambda_k}. \tag{3.15}$$

Then for large U_0,

$$E_{ij}(U_0) = O(U_0) \simeq U_0 \sum_{k=1}^{\infty} \gamma_{ik} \bar{\beta}_{jk} = U_0 \langle h_i, D^{-1} f_j \rangle_1.$$

Similarly,

$$\begin{aligned} E_{ji} &= -U_0 \sum_{k=1}^{\infty} \frac{\sqrt{-1}\, U_0 \lambda_k \beta_{jk} \bar{\gamma}_{ik}}{1 + \sqrt{-1}\, U_0 \lambda_k} = O(U_0) \\ &\simeq -U_0 \sum_{k=1}^{\infty} \beta_{jk} \bar{\gamma}_{ik} = -U_0 \langle D^{-1} f_j, h_i \rangle_1 \end{aligned} \tag{3.16}$$

for large U_0.

It is interesting to note the behavior of K_{ij} when $f_i \equiv b_i - \bar{b}_i$ belongs to R. From (3.15), (3.16), and an extension of the reasoning after (3.12), we obtain

$$E_{ij}(U_0) + E_{ji}(U_0) = 2U_0 \sum_{k=1}^{\infty} \frac{\sqrt{-1}\, U_0 \lambda_k}{1 + U_0^2 \lambda_k^2} \gamma_{ik} \bar{\beta}_{jk}. \tag{3.17}$$

Since the sum on the right-hand side of (3.17) approaches zero as U_0 grows large, K_{ij} is $o(U_0)$ for large U_0 when $f_i \in R$. More can be said if f_j as well as f_i is in R. Suppose $f_j \in R$ and

$$h_j = \sum_{k=1}^{\infty} \gamma_{jk} \phi_k$$

is the unique element of $H^1 \cap N^\perp$ such that $f_j = \mathbf{b} \cdot \nabla h_j$. Taking $\beta_{jk} = \sqrt{-1}\, \lambda_k \gamma_{jk}$ in (3.17) gives

$$E_{ij}(U_0) + E_{ji}(U_0) = 2 \sum_{k=1}^{\infty} \frac{U_0^2 \lambda_k^2}{1 + U_0^2 \lambda_k^2} \gamma_{ik} \bar{\gamma}_{jk},$$

and so

$$\begin{aligned} \lim_{U_0 \to \infty} K_{ij}(U_0) &= D_{ij} - \lim_{U_0 \to \infty} \{E_{ij}(U_0) + E_{ji}(U_0)\} \\ &= D_{ij} - 2\langle h_i, h_j \rangle_1. \end{aligned}$$

Unfortunately, we cannot characterize the range R without making restrictive assumptions about $\mathbf{b}$. We can imagine many applications in which one of the b_i's never vanishes on T, and so to be specific we assume for the remainder of this section that $b_1 > 0$ on T. This allows us to parameterize the flow curves in terms of x_1. Indeed, if we write $\mathbf{x} \in \mathfrak{R}^n$ as $\mathbf{x} = (x_1, \hat{\mathbf{x}})$ for $\hat{\mathbf{x}} = (x_2, \cdots, x_n) \in \mathfrak{R}^{n-1}$, then the flow curves are just the curves $(t, \hat{\mathbf{x}}(t))$, where $\hat{\mathbf{x}}(t)$ solves the nonautonomous system

$$\hat{\mathbf{x}}' = \hat{\mathbf{b}}(t, \hat{\mathbf{x}}) = \left(\frac{b_2(t, \hat{\mathbf{x}})}{b_1(t, \hat{\mathbf{x}})}, \cdots, \frac{b_n(t, \hat{\mathbf{x}})}{b_1(t, \hat{\mathbf{x}})}\right).$$

In fact, for each value of $\hat{\mathbf{x}}(0) \in \mathfrak{R}^{n-1}$, this system determines a unique curve $(t, \hat{\mathbf{x}}(t))$ in the strip $S = [0, 1] \times \mathfrak{R}^{n-1}$, which is defined for $0 \leqq t \leqq 1$; furthermore, each $\mathbf{x} \in T$ can be uniquely written as $\mathbf{x} = (x_1, \hat{\mathbf{x}}(x_1))$, a point on such a curve. (The periodicity assumption on $\mathbf{b}$ implies that $\hat{\mathbf{b}}$ is defined and bounded everywhere.) We identify functions on T satisfying periodic boundary conditions with periodic functions on S in the obvious way.

LEMMA 3.4. *Suppose $f \in C^1$ is a function on T that satisfies*

$$\int_0^1 \frac{f(t, \hat{\mathbf{x}}(t))}{b_1(t, \hat{\mathbf{x}}(t))}\, dt = 0, \tag{3.18}$$

for every flow curve $(t, \hat{\mathbf{x}}(t))$, $0 \leqq t \leqq 1$. Then $f \in R$.

Proof. For each $\mathbf{x} \in T$, we write uniquely $\mathbf{x} = (x_1, \hat{\mathbf{x}}(x_1))$ for a flow curve $(t, \hat{\mathbf{x}}(t))$ and define

$$h(\mathbf{x}) = \int_0^{x_1} \frac{f(t, \hat{\mathbf{x}}(t))}{b_1(t, \hat{\mathbf{x}}(t))}\, dt.$$

Since f and b_1 are C^1, so is h. Furthermore, for $\mathbf{x} \in T$,

$$\mathbf{b}(\mathbf{x}) \cdot \nabla h(\mathbf{x}) = b_1(\mathbf{x}) \frac{d}{dx_1} h(x_1, \hat{\mathbf{x}}(x_1)) = f(\mathbf{x}).$$

Clearly, $h(0, \hat{\mathbf{x}}) = 0$ for all $\hat{\mathbf{x}}$ and $h(x_1, \hat{\mathbf{x}})$ satisfies periodic boundary conditions in $\hat{\mathbf{x}}$ for $0 < x_1 < 1$. Also, (3.18) implies that $h(1, \hat{\mathbf{x}}) = 0$ for all $\hat{\mathbf{x}}$. Then $h \in H^1$ and $f \in R$.

COROLLARY 3.5. *Suppose that $f_i \in C^1$ and satisfies*

$$\int_0^1 \frac{f_i(t, \hat{\mathbf{x}}(t))}{b_1(t, \hat{\mathbf{x}}(t))}\, dt = 0$$

for every flow curve $(t, \hat{\mathbf{x}}(t))$, $0 \leqq t \leqq 1$. Then the conclusions of Lemma 3.3 hold.

Example 3.6 (Gupta and Bhattacharya (1986)). Take $n = 3$, and

$$\mathbf{b}(\mathbf{x}) = (\bar{b}_1, 1 + \sin 2\pi x_1, \sin 2\pi x_1).$$

Then $f_i = b_i - \bar{b}_i$, $i = 1, 2, 3$, satisfy the hypothesis of Lemma 3.4, and each E_{ii} and K_{ii} is $O(1)$. It follows from the remarks after the proof of Lemma 3.3 that each K_{ij} is $O(1)$.

In Example 3.2, each E_{ij} and K_{ij} is $O(U_0^2)$ for $i, j = 1, 2$; in Example 3.6, each E_{ij} and K_{ij} is $O(1)$. We give an additional example in which E_{22} and K_{22} are $O(U_0^2)$ and all other E_{ij}'s and K_{ij}'s are $O(1)$.

Example 3.7. Let $n = 3$, and $b_3(\mathbf{x}) = 2 + (\cos 2\pi x_1)(\cos 2\pi x_2)$, $b_1(x) = 2 + \sin 2\pi x_1$, $b_1(\mathbf{x}) = 0$. Then $E_{11} = 0$ and $K_{11} = D_{11}$. Also, clearly, $E_{12} = E_{13} = E_{21} = E_{31} = 0$ and $K_{13} = D_{13}$, $K_{12} = D_{12}$. Since $\mathbf{b} \cdot \nabla b_2 = 0$, E_{22} and K_{22} are $O(U_0^2)$ by Lemma 3.1. Now the coefficients of L do not involve x_3. Hence, the solution of $Lg_3(\mathbf{x}) = b_3(\mathbf{x}) - \bar{b}_3$ is of the form $g_3(\mathbf{x}) = g(x_1, x_2)$ where

$$\frac{1}{2} \sum_{i,j=1}^{2} D_{ij} \frac{\partial^2 g}{\partial x_i\, \partial x_j} + U_0(2 + \sin 2\pi x_1) \frac{\partial g}{\partial x_2} = (\cos 2\pi x_2)(\cos 2\pi x_1). \tag{3.19}$$

Since $b_2 > 0$, it follows from Lemma 3.4 (with $n = 2$) applied to the function f on the right-hand side of (3.19) that E_{33} is $O(1)$ and $K_{33} = D_{33} + O(1)$. A direct computation shows that $E_{23} = E_{32} = 0$ and $K_{23} = D_{23}$.

The above examples subtly reflect the influence of the geometry of the flow curves on the asymptotic behavior of the E_{ij}'s and K_{ij}'s. The tools developed here can be used to bring out this geometrical influence. In the remainder of this section, we illustrate how this can be done by making assumptions about the geometry of the flow curves and obtaining statements about the asymptotic behavior of the E_{ij}'s and K_{ij}'s. While these statements apply only to somewhat specialized situations, they and their proofs suggest promising directions for future work. They also show the type of asymptotic behavior that is possible in situations that come naturally to mind. Our first result is another corollary of Lemma 3.4.

COROLLARY 3.8. *Suppose that for some i, $2 \leqq i \leqq n$, every flow curve is periodic in the ith component, i.e., $x_i(0) = x_i(1)$ for every flow curve $(t, \hat{\mathbf{x}}(t)) = (t, x_2(t), \cdots, x_n(t))$, $0 \leqq t \leqq 1$. Then $\bar{b}_i = 0$ and the conclusions of Lemma 3.3 hold.*

Proof. We have

$$0 = x_i(1) - x_i(0) = \int_0^1 x_i'(t)\, dt = \int_0^1 b_i(t, \hat{\mathbf{x}}(t))/b_1(t, \hat{\mathbf{x}}(t))\, dt$$

for every flow curve $(t, \hat{\mathbf{x}}(t))$, $0 \leqq t \leqq 1$. It follows from Lemma 3.4 that $b_i \in R$, i.e., $b_i = \mathbf{b} \cdot \nabla h$ for some $h \in H^1$. Then

$$\bar{b}_i = \int_T \mathbf{b}(\mathbf{x}) \cdot \nabla h(\mathbf{x})\, d\mathbf{x} = 0,$$

which implies $f_i = b_i - \bar{b}_i = b_i \in R$.

The examples given previously have the property that each E_{ij} and K_{ij} is either $O(U_0^2)$ or $O(1)$. An important unresolved question is whether any other behavior is possible in general. We show now that under an additional restriction on the flow curves, i.e., on $\mathbf{b}$, each E_{ii} and K_{ii} must be either $O(U_0^2)$ or $O(1)$.

We assume not only that $b_1 > 0$ in T but also that the difference between any two flow curves is constant as x_1 varies. This is equivalent to assuming that for $i = 2, \cdots, n$, the ratio $b_i(\mathbf{x})/b_1(\mathbf{x})$ depends only on x_1. Under this assumption, the flow curves can be conveniently described as follows: Let $(t, \hat{\mathbf{x}}(t))$, $0 \leqq t \leqq 1$, be the flow curve passing through the origin, i.e., such that $\hat{\mathbf{x}}(0) = 0$; then every other flow curve can be written as $(t, \hat{\mathbf{x}}_0 + \hat{\mathbf{x}}(t))$, $0 \leqq t \leqq 1$, for an appropriate $\hat{\mathbf{x}}_0$.

PROPOSITION 3.9. *Under the present assumptions, b_1 is constant along each flow curve and either $b_1 \equiv \bar{b}_1$, in which case $E_{11}(U_0) = 0$, or $E_{11}(U_0) = O(U_0^2)$.*

Proof. We have that

$$\hat{\mathbf{x}}'(x_1) = (b_2(\mathbf{x})/b_1(\mathbf{x}), \cdots, b_n(\mathbf{x})/b_1(\mathbf{x})),$$

and so $\mathbf{b}(\mathbf{x}) = b_1(\mathbf{x})(1, \hat{\mathbf{x}}'(x_1))$. Then the assumption that $\nabla \cdot \mathbf{b}(\mathbf{x}) \equiv 0$ implies

$$(1, \hat{\mathbf{x}}'(x_1)) \cdot \nabla b_1(\mathbf{x}) = 0.$$

But this is to say that the directional derivative of b_1 along each flow curve is zero, and the proposition follows from Lemma 3.1.

THEOREM 3.10. *Under the present assumptions, either $E_{ii}(U_0) = O(U_0^2)$ or $f_i \in R$ and the conclusions of Lemma 3.3 hold.*

Proof. If $(D^{-1}f_i)_N \neq 0$, then $E_{ii}(U_0) = O(U_0^2)$. Suppose $(D^{-1}f_i)_N = 0$, i.e., that $\langle h, D^{-1}f_i \rangle_1 = 0$ for every $h \in N$. We show that $f_i \in R$.

Set $\hat{T}=\{\hat{\mathbf{x}}=(x_2,\cdots,x_n)\in\mathfrak{R}^{n-1}: -\frac{1}{2}\leqq x_i\leqq\frac{1}{2}, 2\leqq i\leqq n\}$, and denote by $\hat{\delta}$ the restriction of the Dirac delta distribution on $\mathfrak{R}^{n-1}$ to $\hat{T}$. Let $\{\hat{\psi}_k\}_{k=1,2,\cdots}$ be a sequence of C^∞ functions on $\hat{T}$ such that each $\hat{\psi}_k$ has support in the interior of $\hat{T}$ and

$$\lim_{k\to\infty}\hat{\psi}_k=\hat{\delta}$$

in the distributional sense. Extend $\hat{\delta}$ and each $\hat{\psi}_k$ to be periodic with period one in each variable over all $\mathfrak{R}^{n-1}$.

Let $(t,\hat{\mathbf{x}}_0+\hat{\mathbf{x}}(t))$, $0\leqq t\leqq 1$, be an arbitrary flow curve. For $\mathbf{x}=(x_1,\hat{\mathbf{x}})\in S$, define

$$\psi_k(\mathbf{x})=\hat{\psi}_k(\hat{\mathbf{x}}-\hat{\mathbf{x}}_0-\hat{\mathbf{x}}(x_1)),\qquad k=1,2,\cdots.$$

Each ψ_k is constant along every flow curve and so belongs to N. Also, for $\mathbf{x}=(x_1,\hat{\mathbf{x}})$,

$$\lim_{k\to\infty}\psi_k(\mathbf{x})=\hat{\delta}(\hat{\mathbf{x}}-\hat{\mathbf{x}}_0-\hat{\mathbf{x}}(x_1)) \tag{3.20}$$

in the sense of distributions on $\mathfrak{R}^{n-1}$. Then

$$\begin{aligned}0&=\lim_{k\to\infty}\langle\psi_k, D^{-1}f_i\rangle_1\\ &=\lim_{k\to\infty}-\int_T\psi_k(\mathbf{x})f_i(\mathbf{x})\,d\mathbf{x}\\ &=-\int_0^1 f_i(t,\hat{\mathbf{x}}_0+\hat{\mathbf{x}}(t))\,dt.\end{aligned} \tag{3.21}$$

The last equality follows from (3.20) by periodicity even when the flow curve is not contained in T. Since b_1 is constant along the flow curve by Proposition 3.9, (3.21) implies

$$\int_0^1\frac{f_i(t,\hat{\mathbf{x}}_0+\hat{\mathbf{x}}(t))}{b_1(t,\hat{\mathbf{x}}_0+\hat{\mathbf{x}}(t))}\,dt=0.$$

Since the flow curve is arbitrary, it follows from Corollary 3.5 that $f_i\in R$.

We offer a final example on which Corollary 3.8, Proposition 3.9, and Theorem 3.10 are applicable.

Example 3.11. Let ξ be any C^2 function on $\mathfrak{R}^1$ that is periodic with period one and such that $\xi(0)=\xi(1)=0$. We take $n=2$ and construct $\mathbf{b}:\mathfrak{R}^2\to\mathfrak{R}^2$ such that the flow curves in S are the curves

$$(t,x_2(t))=(t,x_2(0)+\xi(t)),\qquad 0\leqq t\leqq 1. \tag{3.22}$$

Let η be any C^1 function on $\mathfrak{R}^1$ that is periodic with period one and that is always positive. For $\mathbf{x}=(x_1,x_2)\in\mathfrak{R}^2$, set

$$b_1(\mathbf{x})=\eta(\xi(x_1)-x_2)\quad\text{and}\quad b_2(\mathbf{x})=\xi'(x_1)\eta(\xi(x_1)-x_2).$$

Then $\nabla\cdot\mathbf{b}(\mathbf{x})=0$ for $\mathbf{x}\in\mathfrak{R}^2$. Also $b_2(\mathbf{x})/b_1(\mathbf{x})=\xi'(x_1)$, and so the flow curves are given by (3.22). Note that every flow curve is periodic in the second component, i.e., $x_2(0)=x_2(1)$ for every flow curve. As a concrete example, take

$$b_1(\mathbf{x})=2+\sin(2\pi(\sin(2\pi x_1)-x_2)),\qquad b_2(\mathbf{x})=2\pi\cos(2\pi x_1)b_1(\mathbf{x}).$$

According to Theorem 3.10, each E_{ii} and K_{ii} is either $O(U_0^2)$ or $O(1)$. In fact, Proposition 3.9 implies that E_{11} and K_{11} are $O(U_0^2)$, and Corollary 3.8 implies that E_{22} and K_{22} are $O(1)$. It follows from the remarks after the proof of Lemma 3.3 that K_{12} is $o(U_0)$. With some effort, we can show that the inner products in (3.13) and (3.14) are zero, and so E_{12} and E_{21} are also $o(U_0)$.

Remark. Suppose the flow $Y(t, y)$ generated by $\mathbf{b} \cdot \nabla$ (i.e., $(d/dt)Y(t, y) = \mathbf{b}(Y)$, $Y(0, y) = y$) is *ergodic* on T, with the normalized Lebesgue measure as the invariant measure. This is true if and only if the null space N is $\{0\}$. Since $b_i(Y(t, \cdot)) - \bar{b}_i$ is then ergodic, we may expect a smaller value of E_{ii} and, therefore, of the dispersion $K_{ii} = D_{ii} + 2E_{ii}$. Lemma 3.3 shows that this expectation is justified. The precise mathematical connection between the topological dynamics of $\mathbf{b}$ and the asymptotic behavior of the effective dispersion $\mathbf{K}(U_0)$, as $U_0 \to \infty$, appears complicated.

4. An asymptotic expansion of concentration. Assume that $D_{ij}(\cdot)$ and $b_i(\cdot)$ are continuously differentiable and periodic (with period one in each coordinate), $((D_{ij}(\cdot)))$ positive definite. Write $\dot{X}(t) = (X_1(t)(\text{mod } 1), \cdots, X_n(t)(\text{mod } 1))$. Then $\dot{X}(t)$ is a Markov process on the torus $[0, 1]^n$. Let $\dot{p}(t; \dot{x}, \dot{y})$ denote the transition probability density of $\dot{X}(t)$ and $\pi(\dot{y})$ the corresponding *invariant probability density*: $\int \pi(\dot{x})\dot{p}(t; \dot{x}, \dot{y})\, d\dot{x} = \pi(\dot{y})$. If the probability density of $\mathbf{X}(0)$ is π (the entire probability mass being on $[0, 1]^n$), then for any $t > 0$ the sequences $Y_j \equiv \mathbf{X}(jt) - \mathbf{X}((j-1)t)$ and $(Y_j, \dot{X}(jt))$ $(j = 1, 2, \cdots)$ are stationary and ϕ-mixing with an exponentially decaying ϕ-mixing rate, the latter being also Markovian (see Bhattacharya (1985)). Also, Y_j has a density and finite moments of all orders. Hence Theorem (2.8) of Götze and Hipp (1983) applies (see Example (1.13) in that article), and we have an asymptotic expansion for the distribution of $[\mathbf{X}(Nt) - \mathbf{X}(0) - NtU_0\bar{\mathbf{b}}]/N^{1/2} = [\sum_{j=1}^{N}(Y_j - EY_j)]/N^{1/2}$. More precisely we have, for every positive integer s,

$$\text{(4.1)} \qquad \begin{aligned} &\text{Prob}\,((\mathbf{X}(Nt) - \mathbf{X}(0) - NtU_0\bar{\mathbf{b}})/N^{1/2} \in B) \\ &= \int_B \phi(t, \mathbf{x})\, d\mathbf{x} + \sum_{r=1}^{s} N^{-r/2} \int_B \psi_r(t, \mathbf{x})\, d\mathbf{x} + o(N^{-s/2}) \qquad (N \to \infty), \end{aligned}$$

uniformly over every class $\mathscr{B}$ of Borel sets B satisfying

$$\text{(4.2)} \qquad \sup_{B \in \mathscr{B}} \int_{(\partial B)^\delta} \phi(t, \mathbf{x})\, d\mathbf{x} = O(\delta^a) \qquad (\delta \downarrow 0),$$

for some $a > 0$, $(\partial B)^\delta$ being the δ-neighborhood of the boundary ∂B of B. Here $\phi(t, \mathbf{x})$ is the Gaussian density with mean zero and dispersion matrix $t\mathbf{K}$, $\mathbf{K}$ being the large scale dispersion. The functions $\psi_r(t, \mathbf{x})$ are polynomial multiples of $\phi(t, \mathbf{x})$. For the classical case of independent summands the details of the construction of such polynomials may be found in Bhattacharya and Ranga Rao (1976, § 7). For the present case the formalism is entirely analogous once the cumulants of the normalized sum $\sum_1^N (Y_j - EY_j)/N^{1/2}$ are expanded in powers of $N^{-1/2}$ (see Götze and Hipp (1983)). Note that (4.2) holds, e.g., for the class of all Borel measurable convex sets (see Bhattacharya and Ranga Rao (1976, p. 24)).

In the case the initial concentration is proportional to π, (4.1) may be expressed as (see (1.6)),

$$\text{(4.3)} \qquad \begin{aligned} &\int_B \varepsilon^{-n} C(\varepsilon^{-1}\mathbf{x} + \varepsilon^{-2}tU_0\bar{\mathbf{b}}, \varepsilon^{-2}t)\, d\mathbf{x} \\ &= C_0 \int_B \left[\phi(t, \mathbf{x}) + \sum_{r=1}^{s} \varepsilon^r \psi_r(t, \mathbf{x})\right] d\mathbf{x} + o(\varepsilon^s) \qquad (\varepsilon \downarrow 0), \end{aligned}$$

where C_0 is the total solute mass. On the other hand, if the initial concentration is arbitrary, say an integrable function or a point mass, the distribution of $\mathbf{X}(0)$ must be taken to be this concentration normalized. In this case Y_j is not stationary, but only asymptotically so, and the functions $\psi_r(t, \mathbf{x})$ must involve ε (or, $N^{-1/2}$) reflecting the nonstationarity of the moments, etc. Thus we have

$$\int_B \varepsilon^{-n} C(\varepsilon^{-1}\mathbf{x}+\varepsilon^{-2}tU_0\bar{\mathbf{b}}, \varepsilon^{-2}t)\, d\mathbf{x} = C_0 \int_B \left[\phi(t, \mathbf{x}) + \sum_{r=1}^{s} \varepsilon^r \psi_r(t, \mathbf{x}, \varepsilon)\right] d\mathbf{x} + o(\varepsilon^s) \qquad (\varepsilon \downarrow 0), \tag{4.4}$$

uniformly over $B \in \mathscr{B}$ satisfying (4.2). It is very likely that (4.4) holds uniformly over the class of *all* Borel sets, i.e., the expansion holds in $L^1(\mathfrak{R}^n, d\mathbf{x})$; however, a proof of this does not seem to be available.

The expansion (4.4) provides a better approximation to concentration than the Gaussian approximation ϕ. This improvement is particularly significant for relatively small times, i.e., in the so-called preasymptotic zone. By computing the first three moments of observed concentration, we may approximately calculate the expansion (4.4) for $s = 1$. The fourth- and higher-order cumulants only contribute to terms $O(\varepsilon^2)$.

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16.4 "Multiscale diffusion processes with periodic coefficients and an application to solute transport in porous media"

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MULTISCALE DIFFUSION PROCESSES WITH PERIODIC COEFFICIENTS AND AN APPLICATION TO SOLUTE TRANSPORT IN POROUS MEDIA[1]

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Consider diffusions on $\mathbb{R}^k$, $k > 1$, governed by the Itô equation $dX(t) = \{b(X(t)) + \beta(X(t)/a)\}\,dt + \sigma dB(t)$, where b, β are periodic with the same period and are divergence free, σ is nonsingular and a is a large integer. Two distinct Gaussian phases occur as time progresses. The initial phase is exhibited over times $1 \ll t \ll a^{2/3}$. Under a geometric condition on the velocity field β, the final Gaussian phase occurs for times $t \gg a^2(\log a)^2$, and the dispersion grows quadratically with a. Under a complementary condition, the final phase shows up at times $t \gg a^4(\log a)^2$, or $t \gg a^2 \log a$ under additional conditions, with no unbounded growth in dispersion as a function of scale. Examples show the existence of non-Gaussian intermediate phases. These probabilisitic results are applied to analyze a multiscale Fokker–Planck equation governing solute transport in periodic porous media. In case b, β are not divergence free, some insight is provided by the analysis of one-dimensional multiscale diffusions with periodic coefficients.

1. Introduction. In this article we consider phase changes with time for diffusions on $\mathbb{R}^k$ with multiple scale periodic drifts $b(x) + \beta(x/a)$,

$$X(t) = X(0) + \int_0^t \{b(X(s)) + \beta(X(s)/a)\}\,ds + \int_0^t \sigma(X(s))\,dB(s), \tag{1.1}$$

with $\sigma(\cdot)$ a nonsingular matrix-valued function, a being a large spatial scale parameter. Computations of these phase change and their time scales are carried out directly for some examples in Section 6, without requiring the machinery needed for the general case, and the reader may perhaps take a look at these first.

It may be shown that for times $t \ll a^{2/3}$ the large scale fluctuations may be ignored, that is, the function $\beta(x/a)$ in (1.1) may be replaced by the constant drift $\beta(X(0)/a)$. This holds generally, without the assumptions of periodicity of b, β (Theorem 2.1). As a consequence, if b is periodic and β is arbitrary Lipschitz, then for times $1 \ll t \ll a^{2/3}$ the process $X(t)$ is asymptotically a Brownian motion (Theorem 2.2). This *first phase* analysis is carried out in Section 2.

If $b(\cdot)$, $\beta(\cdot)$ are both periodic with the same period lattice, say $\mathbb{Z}^k$, $\sigma(\cdot) = \sigma$ is a constant matrix, and a is a positive integer, then, for a fixed a, $\dot{X}(t) := X(t) \bmod a$ is a diffusion on the *big torus* $\mathcal{T}_a := \{x \bmod a\colon x \in \mathbb{R}^k\}$, and a central

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limit theorem holds for $X(t)$ as $t \to \infty$ [Bensoussan, Lions and Papanicolaou (1978), Chapter 3; Bhattacharya (1985)]. For large a, that is, as $a \to \infty$, how large must t be for this approximation to take hold? This Gaussian law is referred to as the *final phase* in this article. Under the *divergence–free* condition $\operatorname{div} b(\cdot) = 0 = \operatorname{div} \beta(\cdot)$ (*incompressibility*), the Gaussian approximation for a set of k_1 coordinates $X_j(t)$, $1 \le j \le k_1$, holds at times $t \gg a^2(\log a)^2$ provided an appropriate geometric condition holds on $\beta(\cdot)$ (Theorem 5.2). Under a different geometric condition the time scales for this final phase of Gaussian approximation are $t \gg a^4(\log a)^4$ in Theorem 5.3 and $t \ge a^2 \log a$ in Theorem 5.4.

Two crucial ingredients for this final phase analysis are (1) the speed at which $\dot{X}(t)$ approaches the uniform (equilibrium) distribution on $\mathscr{T}_a$ (as $a \to \infty$), and (2) the asymptotic relation between a and the dispersion matrix of the limiting Gaussian in the final phase. By spectral methods analogous to those of Diaconis and Stroock (1991) and Fill (1991), the L^1-distance between the distributions of $\dot{X}(t)$, with arbitrary $\dot{X}(0)$, and the equilibrium distribution is bounded above by $ca^{k/2}\exp\{-c't/a^2\}$ for some positive constants c and c' (Theorem 4.5). For the analysis of final phase dispersion as a function of the scale parameter, it is convenient to look at the related process $Y(t) = X(a^2t)/a$. Then $\dot{Y}(t) := Y(t) \bmod 1$ is a diffusion on the unit torus $\mathscr{T}_1$ with generator $A_a := \mathscr{D} + a(b(a\cdot) + \beta(\cdot)) \cdot \nabla$, with $\mathscr{D} = (1/2)\sum_{j,j'} D_{jj'}\partial^2/(\partial x_j \partial x_{j'})$ ($((D_{jj'})) := \sigma\sigma'$) and $\nabla = \operatorname{grad}$. Since $b(a\cdot)$ is rapidly oscillating, one may approximate A_a by $\overline{A} := \mathscr{D} + a(\overline{b} + \beta(\cdot)) \cdot \nabla$, where $\overline{b} = (\overline{b}_1, \ldots, \overline{b}_k)$ is the mean of $b(\cdot)$ w.r.t. the uniform distribution on $\mathscr{T}_1$. According to the central limit theorem for $X(t)$, with a fixed, the asymptotic dispersion (or variance) per unit time of $Y_j(t)$ is given by $D_{jj} - 2\|g_j\|_1^2$, where g_j is the mean-zero solution of $A_a g_j(x) = b_j(ax) + \beta_j(x) - \overline{b}_j - \overline{\beta}_j$. Here $\|g_j\|_1$ is the norm in the complex Hilbert space $H^1 = \{h$ mean-zero, periodic: $|h|^2$ and $|\nabla h|^2$ integrable w.r.t. uniform distribution on $\mathscr{T}_1\}$ endowed with the inner product $\langle g, f\rangle_1 = \int_{[0,1)^k} (\nabla g(x))' D \nabla f(x)^- \, dx$, f^- being the complex conjugate of f. One may replace g_j by the solution h_j to $\overline{A} h_j = \beta_j - \overline{\beta}_j$. The last equation may be expressed as $(\mathscr{I} + a\mathscr{D}^{-1}(\overline{b} + \beta(\cdot)) \cdot \nabla\} h_j = \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$, or $(\mathscr{I} + a\overline{S}) h_j = \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$, with $\mathscr{I}$ as the identity operator, and $\overline{S} = \mathscr{D}^{-1}(\overline{b} + \beta(\cdot)) \cdot \nabla$. Since $\overline{S}$ is a skew-symmetric compact operator on H^1 (Proposition 3.2), one may now use the spectral decomposition of $\overline{S}$ to express h_j in an eigenfunction expansion, arriving at $\|h_j\|_1^2 \simeq \|g_j\|_1^2$. This gives an asymptotic relation between a and the dispersion of $X_j(t)$ as that of a^2 times that of $Y_j(t)$. The dominant term in this expansion of the dispersion is $2a^2\|(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\|_1^2$ where $f_{\underline{N}}$ is the projection of f in H^1 onto the null space $\underline{N}$ of $\overline{S}$. Thus, if $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} \neq 0$, the dispersion of $X_j(t)$ per unit time grows with a quadratically and is asymptotically bounded away from 0 and ∞ if $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} = 0$ (Theorems 3.7, 3.8).

The Gaussian approximations derived in this paper may be readily strengthened to their functional forms (see Remark 5.2.1). In other words, under appropriate scaling, the diffusion process $X(\cdot)$ in (1.1) has different Brownian motion approximations in the first and final phases.

Multiscale phenomena occur commonly in nature. The present study was motivated in part by the so-called *scale effect* in the dispersion of solute matter such as a chemical pollutant injected at a point in an underground water system, called an aquifer, saturated with water. It has been widely observed that for the solute concentration profile different Gaussian approximations with increasing dispersivity, or variance per unit time, hold at successively larger time scales [Fried and Combarnous (1971); Garabedian, LeBlanc, Gelhar and Colin (1991); Gelhar and Axness (1983); Guven and Molz (1986); LeBlanc, Garabedian, Hess, Gelhar, Quadri, Stollenwerk and Wood (1991); Sauty (1980); Sudicky (1986)]. The concentration $c(t, y)$ is governed at a local scale by a second-order linear parabolic (Fokker–Planck) equation with a drift term $v(\cdot)$ given by the velocity of water and diffusion coefficients which are of a somewhat larger order than the molecular diffusion coefficient of the solute. Since $v(\cdot)$ does not depend on time in a saturated aquifer under isothermal conditions, the root cause for the observed increase in dispersivity is the existence of multiscale heterogeneities in the medium [Bhattacharya and Gupta (1983) and Sposito, Jury and Gupta (1986)]. For the understanding of this it is enough to consider only two such scales of heterogeneity, reflected in the flow velocity as

$$v(y) = b(y) + \beta(y/a), \tag{1.2}$$

with a large. Here b and β are functions whose derivatives are of the same order, so that the derivatives of $\beta(\cdot/a)$ are small, namely, $O(1/a)$. Thus the fluctuations of $\beta(\cdot/a)$—the *large scale fluctuations*—are manifested only over large distances. Note that the solute concentration $c(t, y)$ corresponding to a unit local initial injection at x is simply the transition probability density $p(t; x, y)$ of a diffusion process $X(t)$ governed by the Itô equation (1.1).

It follows that the asymptotics of $t \to c(t, y)$ are given by the asymptotic distribution of $X(t)$. The proper way to look at this, when a is very large compared to the local scale, is to let $a \to \infty$ and let $t \to \infty$ at slower to higher rates relative to a. Initially, for a period of time $t \ll a^{2/3}$ (i.e., $t/a^{2/3} \to 0$), the fluctuations of $\beta(\cdot/a)$ may be ignored and $\beta(X(s)/a)$ may be replaced by its initial value $\beta(X(0)/a)$. Theorem 2.1 says that this new process, say $Y(\cdot)$, approximates the $X(\cdot)$ process up to such times t well in total variation distance. In particular, if $Y(\cdot)$ is asymptotically Gaussian, then so is $X(\cdot)$ for times $1 \ll t \ll a^{2/3}$. This holds, for example, if $b(\cdot)$ is periodic (Theorem 2.2).

The preceding analysis of dispersion of $X_j(t)$ as a function of the distance scale parameter a is formally the same as that for the dispersion of a diffusion $\hat{X}(t)$ with drift $a(\bar{b} + \beta(\cdot))$ [or $a\beta(\cdot)$, absorbing $\bar{b}$ in $\beta(\cdot)$] and diffusion matrix $D = \sigma\sigma'$. For the latter, one may regard $a = u_0$ as the *velocity parameter*. This enables one to study dispersion at a single scale as a function of u_0 (see Proposition 3.1). This latter analysis is also of importance in hydrology, and has been studied experimentally at the laboratory (or Darcy) scale extensively

[Fried and Combarnous (1971)]. This is discussed, along with the scale effect, in greater detail in Section 7.

Although the major emphasis in this article is on the case of divergence-free velocity fields, we also consider general one-dimensional multiscale diffusions with periodic coefficients. Here the speed of convergence to equilibrium may be either of the same order as in the divergence-free case ($k > 1$), or may be exponentially slow in a, requiring times $t \gg \exp\{ca\}$ to approach equilibrium (Theorems 4.6, 4.7, 4.9). The dispersion per unit time in the final phase is always asymptotically constant in a. In the time-reversible case this dispersion actually goes to zero exponentially fast with a. This study throws some light on the general *nondivergence-free case*.

It would be interesting and challenging to extend this study to the case of multiscale diffusions whose coefficients constitute an ergodic random field, or are almost periodic. For central limit theorems with such coefficients see Papanicolaou and Varadhan (1979), Kozlov (1979, 1980), Bhattacharya and Ramasubramanian (1988).

The present article provides a synthesis as well as an exposition of earlier work, often done in collaboration with Vijay Gupta, Homer Walker, and Friedrich Götze [Bhattacharya and Götze (1995); Bhattacharya and Gupta (1979, 1983); Bhattacharya, Gupta and Walker (1989)], although a number of results are either modified versions of earlier results or new. To facilitate exposition, detailed proofs are given for the most part. They also serve to remove some lacunae in Bhattacharya and Götze (1995).

A word on notation. The constants c, c' appearing in this article, with or without subscripts or superscripts, are all independent of the parameter a. The process $Y(\cdot)$ in Section 2 is different from the process $Y(\cdot)$ in Sections 3, 4, 5.

2. First phase of asymptotics. Consider a k-dimensional diffusion ($k \geq 1$) governed by the stochastic integral equation,

$$X(t) = X(0) + \int_0^t \{b(X(s)) + \beta(X(s)/a)\}\, ds + \int_0^t \sigma(X(s))\, dB(s), \quad t \geq 0. \tag{2.1}$$

Here $b(\cdot) \equiv (b_1(\cdot), \dots, b_k(\cdot))$, $\beta(\cdot) \equiv (\beta_1(\cdot), \dots, \beta_k(\cdot))$ are Lipschitzian functions on $\mathbb{R}^k$ to $\mathbb{R}^k$, $\sigma(\cdot)$ is a $(k \times k)$-matrix valued Lipschitzian function on $\mathbb{R}^k$, $B(\cdot)$ is a standard k-dimensional Brownian motion and the initial state $X(0)$ is independent of $B(\cdot)$. The *spatial scale parameter* a is assumed to be "large." One may think of $b(\cdot)$ as the drift velocity at the *local scale,* while $\beta(\cdot/a)$ is the *large scale* drift velocity. Since the vector field $x \to \beta(x/a)$ changes very slowly, the large scale fluctuations are manifested only at large distances and, therefore, not experienced by the process $X(\cdot)$ over an initial stretch of time. Over this time period one would then expect $X(\cdot)$ to behave like the process governed by the Itô equation

$$Y(t) = X(0) + \int_0^t \{b(Y(s)) + \beta(X(0)/a)\}\,ds + \int_0^t \sigma(Y(s))\,dB(s), \quad t \geq 0. \tag{2.2}$$

Note that the large-scale drift velocity $\beta(\cdot/a)$ in (2.1) is replaced by its initial value $\beta(X(0)/a)$ in (2.2). As an appropriate initial condition we will scale the initial state $X(0)$ as

$$X(0) = ax_0, \qquad x_0 \in \mathbb{R}^k. \tag{2.3}$$

This is merely to avoid the artificial importance of the origin that would arise from the assignment $X(0) = x_0$, since in the latter case $\beta(X(0)/a) \to \beta(0)$ as $a \to \infty$.

Our first result identifies the time period over which $Y(\cdot)$ is a good approximation to $X(\cdot)$. In order to state it, let $\mathscr{F}_t$ denote the Borel sigma-field of $\mathscr{C}[0, t]$—the set of all continuous functions on $[0, t]$ into $\mathbb{R}^k$, and let $P_{0,t}$ and $P_{1,t}$ denote the distributions of $Y_0^t := \{Y(s)\colon 0 \leq s \leq t\}$ and $X_0^t := \{X(s)\colon 0 \leq s \leq t\}$, respectively, on $\mathscr{F}_t$. The *total variation distance* between two measures μ and ν is denoted $\|\mu - \nu\|_{\mathrm{TV}}$.

THEOREM 2.1. *Assume that $b(\cdot)$ and its first-order derivatives are bounded, $\beta(\cdot)$ is bounded and has continuous and bounded derivatives of orders one and two, $\sigma(\cdot)$ is Lipschitzian, and the eigenvalues of $\sigma(\cdot)\sigma(\cdot)'$ are bounded away from zero and infinity.*

(a) *Then there exist constants c_i $(i = 1, 2, 3)$ which do not depend on "a" or t such that, uniformly for all x_0,*

$$\|P_{0,t} - P_{1,t}\|_{\mathrm{TV}} \leq c_1\frac{t^{3/2}}{a} + c_2\frac{t}{a} + c_3\frac{t^{3/2}}{a^2}. \tag{2.4}$$

(b) *If $b_j(x) \equiv 0$ and $\beta_j(x_0) = 0$ for $2 \leq j \leq k$, and*

$$\frac{\partial \beta_j(x)}{\partial x_1} \equiv 0 \quad \text{for } 1 \leq j \leq k, \tag{2.5}$$

then one may take $c_1 = 0$ in (2.4).

(c) *If, in addition to the hypothesis in* (b), *one has*

$$\left(\frac{\partial \beta_j}{\partial x_i}\right)(x_0) = 0 \quad \text{for } 1 \leq j \leq k, 2 \leq i \leq k, \tag{2.6}$$

then one may take $c_1 = c_2 = 0$ in (2.4).

Before proving the theorem we make a few remarks on the time scales under (a)–(c) for the validity of the approximation of $X(\cdot)$ by $Y(\cdot)$, and on the physical significance of the conditions (2.5), (2.6).

REMARK 2.1.1. Condition (2.5) means that the large-scale velocity does not depend on the first coordinate x_1. This condition is satisfied by the so-called *stratified media* (see Sections 6 and 7). The condition $b_j(x) \equiv 0$ for $2 \le j \le k$ of course means that there is no small scale velocity in directions other than that in the x_1-direction. The conditions $\beta_j(x_0) = 0$ $(2 \le j \le k)$ and $(\partial\beta_j/\partial x_i)(x_0) = 0$ $(1 \le j \le k,\ 2 \le i \le k)$ are specific requirements on the initial point.

REMARK 2.1.2. It follows from (2.4) that

$$\|P_{0,t} - P_{1,t}\|_{TV} \to 0 \quad \text{as } \frac{t^{3/2}}{a} \to 0, \tag{2.7}$$

that is, $Y(\cdot)$ is a good approximation of $X(\cdot)$ for times

$$t \ll a^{2/3} \quad \text{or for } \frac{t}{a^{2/3}} \text{ small.} \tag{2.8}$$

Under the additional assumptions in part (b) of Theorem 2.1,

$$\|P_{0,t} - P_{1,t}\|_{\text{TV}} \le c_2\frac{t}{a} + c_3\frac{t^{3/2}}{a^2} \to 0 \quad \text{as } \frac{t}{a} \to 0, \tag{2.9}$$

that is, $Y(\cdot)$ provides a good approximation to $X(\cdot)$ over a period of time

$$t \ll a. \tag{2.10}$$

Under the hypothesis of part (c),

$$\|P_{0,t} - P_{1,t}\|_{\text{TV}} \le c_3\frac{t^{3/2}}{a^2} \to 0 \quad \text{as } \frac{t}{a^{4/3}} \to 0, \tag{2.11}$$

that is, the initial phase of asymptotics governed by $Y(\cdot)$ holds over times satisfying

$$t \ll a^{4/3}. \tag{2.12}$$

Examples in Section 6 show that the estimates in Theorem 2.1 are, in general, optimal.

REMARK 2.1.3. The assumption that $\beta(\cdot)$ *is bounded* is only used in part (a) of Theorem 2.1. In the absence of this assumption, only the constants c_1', c_1'' in (2.4), (2.2) need to be changed to $c_1(1 + \|\beta(x_0)\|)$ and $c_1''(1 + \|\beta(x_0)\|)$, respectively.

PROOF OF THEOREM 2.1. By the Cameron–Martin–Girsanov theorem [see, e.g., Ikeda and Watanabe (1981), pages 176–181 or Friedman (1975), pages 164–169],

$$\|P_{0,t} - P_{1,t}\|_{\text{TV}} = E|\exp\{Z(t)\} - 1|, \tag{2.13}$$

where, with $Y(0) = X(0)$,

$$(2.14)\qquad \begin{aligned} Z(t) = \int_0^t \sigma^{-1}(Y(s))\{\beta(Y(s)/a) - \beta(Y(0)/a)\}\, dB(s) \\ - \tfrac{1}{2}\int_0^t \left|\sigma^{-1}(Y(s))\{\beta(Y(s)/a) - \beta(Y(0)/a)\}\right|^2 ds. \end{aligned}$$

By Itô's lemma [Ikeda and Watanabe (1981), pages 66 and 67, Bhattacharya and Waymire (1990), page 585],

$$(2.15)\qquad \begin{aligned} &\beta_j(Y(s)/a) - \beta_j(Y(0)/a) \\ &\quad = \int_0^s (L_0\beta_j(\cdot/a))(Y(s'))\, ds' \\ &\quad\quad + \int_0^s (\nabla(\beta_j(\cdot/a)))(Y(s'))\sigma(Y(s'))\, dB(s'), \qquad \nabla := \text{grad}, \end{aligned}$$

where, writing $D(x) := \sigma(x)\sigma'(x) = ((D_{ij}(x)))$,

$$(2.16)\qquad L_0 = \frac{1}{2}\sum_{i,i'} D_{ii'}(\cdot)\frac{\partial^2}{\partial x_i \partial x_{i'}} + \big(b(\cdot) + \beta(x_0)\big)\cdot\nabla.$$

Thus,

$$(2.17)\qquad \begin{aligned} \big(L_0(\beta_j(\cdot/a))\big)(Y(s')) = \frac{1}{2a^2}\sum_{i,i'} D_{ii'}(Y(s'))\left(\frac{\partial^2\beta_j(\cdot)}{\partial x_i\partial x_{i'}}\right)(Y(s')/a) \\ + \frac{1}{a}\big(b(Y(s')) + \beta(x_0)\big)\cdot\big(\nabla\beta_j(\cdot)\big)(Y(s')/a). \end{aligned}$$

Denoting the Reimann integral on the right side of (2.15) by $I_{1j}(s)$ and the stochastic integral by $I_{2j}(s)$, we have

$$(2.18)\qquad E\big(\beta_j(Y(s)/a) - \beta_j(Y(0)/a)\big)^2 \le 2EI_{1j}^2(s) + 2EI_{2j}^2(s).$$

Letting λ denote the infimum (over $x \in \mathbb{R}^k$) of the smallest eigenvalue of $D(x)$, one has

$$(2.19)\qquad \begin{aligned} E|Z(t)| \le \frac{1}{\sqrt{\lambda}}\left(\int_0^t \sum_{j=1}^k E\big(\beta_j(Y(s)/a) - \beta_j(Y(0)/a)\big)^2 ds\right)^{1/2} \\ + \frac{1}{2\lambda}\int_0^t \sum_{j=1}^k E\big(\beta_j(Y(s)/a) - \beta_j(Y(0)/a)\big)^2 ds. \end{aligned}$$

Also, denoting by $\|\cdot\|_\infty$ the supremum of the Euclidean norm of a real-, vector-, or matrix-valued function, one has

$$
\begin{aligned}
EI_{1j}^2(s) &\le s^2\left\{\frac{c_1'}{a^4}\,\|D(\cdot)\|_\infty^2 \left\|\left(\max_{i,i'}\left|\frac{\partial^2\beta_j(\cdot)}{\partial x_i \partial x_{i'}}\right|\right)\right\|_\infty^2 \right.\\
&\qquad\qquad \left. + \frac{2}{a^2}\left\|(b(\cdot)+\beta(x_0))\cdot(\nabla\beta_j)(\cdot/a)\right\|_\infty^2\right\},\\
EI_{2j}^2(s) &\le \frac{s}{a^2}\|D(\cdot)\|_\infty \|\nabla\beta_j(\cdot)\|_\infty^2,
\end{aligned} \tag{2.20}
$$

so that

$$
\begin{aligned}
\int_0^t &\sum_{j=1}^k (EI_{ij}^2(s) + EI_{2j}^2(s))\,ds\\
&\le \frac{t^3}{a^4}c_2'\|D(\cdot)\|_\infty^2\left[\sum_{j=1}^k \left\|\left(\max_{i,i'}\left|\frac{\partial^2\beta_j(\cdot)}{\partial x_i\partial x_{i'}}\right|\right)\right\|_\infty^2\right]\\
&\quad + \frac{2t^3}{3a^2}\sum_{j=1}^k \left\|(b(\cdot)+\beta(x_0))\cdot(\nabla\beta_j)(\cdot/a)\right\|_\infty^2\\
&\quad + \frac{t^2}{2a^2}\|D(\cdot)\|_\infty\left(\sum_{j=1}^k\|\nabla\beta_j(\cdot)\|_\infty^2\right).
\end{aligned} \tag{2.21}
$$

Using the last inequality in (2.19), we get

$$
\begin{aligned}
E|Z(t)| &\le \left(c_1''\frac{t^3}{a^2} + c_2''\frac{t^2}{a^2} + c_3''\frac{t^3}{a^4}\right)^{1/2}\frac{1}{\sqrt{\lambda}}\\
&\quad + \left(c_1''\frac{t^3}{a^2} + c_2''\frac{t^2}{a^2} + c_3''\frac{t^3}{a^4}\right)\frac{1}{2\lambda}.
\end{aligned} \tag{2.22}
$$

Here the constants c_i'' $(i = 1, 2, 3)$ do not depend on a, t or x_0. Next note that $\exp\{Z(t)\}$, $t \ge 0$, is a martingale and, in particular, $E\exp\{Z(t)\} = 1$, or

$$
\begin{aligned}
0 &= E(1-\exp\{Z(t)\}) = E(1-\exp\{Z(t)\})^+ - E(1-\exp\{Z(t)\})^-,\\
E|1-\exp\{Z(t)\}| &= 2E(1-\exp\{Z(t)\})^+ \le 2[E(|Z(t)|\wedge 1)].
\end{aligned} \tag{2.23}
$$

The last inequality follows from the relation $1 - e^x \le |x| \wedge 1$ for $x \le 0$. The desired result (2.4) is now a consequence of (2.22) and (2.23).

To prove part (b), note that the second term on the right of (2.21) now vanishes. It remains to prove part (c). Under the additional assumption (2.6), one may express $Y_i(\cdot)$, $2 \le i \le k$, as

$$
Y_i(t) = Y_i(0) + \int_0^t \sum_{r=1}^k \sigma_{ir}(Y(s))\,dB_r(s), \qquad 2 \le i \le k, \tag{2.24}
$$

so that the expected square of the stochastic integral in (2.15) may be estimated as

$$
\begin{aligned}
EI^2_{2j}(s) &= \frac{1}{a^2} E\left[\sum_{i=2}^{k} \int_0^s \left(\frac{\partial \beta_j}{\partial x_i}\right)\left(\frac{Y(s')}{a}\right) \sum_{r=1}^{k} \sigma_{ir}(Y(s'))\, dB_r(s')\right]^2 \\
&\le \frac{c_4''}{a^2} \int_0^s \sum_{i=2}^{k} E\left[\left(\frac{\partial \beta_j}{\partial x_i}\right)\left(\frac{Y(s')}{a}\right)\right]^2 ds'.
\end{aligned}
\tag{2.25}
$$

In view of (2.6), $(\partial \beta_j/\partial x_i)(Y(0)/a) \equiv (\partial \beta_j / \partial x_i)(x_0) = 0$ for $i \ge 2$. Thus

$$
\begin{aligned}
&E\left[\left(\frac{\partial \beta_j}{\partial x_i}\right)\left(\frac{Y(s')}{a}\right)\right]^2 \\
&\quad = E\left[\left(\frac{\partial \beta_j}{\partial x_i}\right)\left(\frac{Y(s')}{a}\right) - \left(\frac{\partial \beta_j}{\partial x_i}\right)\left(\frac{Y(0)}{a}\right)\right]^2 \\
&\quad = E\left[\left(\frac{Y(s')}{a} - \frac{Y(0)}{a}\right) \cdot \left(\nabla \frac{\partial \beta_j}{\partial x_i}\right)(\tilde{Y}/a)\right]^2 \\
&\qquad\qquad [\tilde{Y} \text{ lying in the line segment joining } Y(0) \text{ and } Y(s')] \\
&\quad = E\left[\frac{1}{a} \sum_{i'=1}^{k} (Y_{i'}(s') - Y_{i'}(0)) \frac{\partial^2 \beta_j(\cdot)}{\partial x_{i'} \partial x_i}(\tilde{Y}/a)\right]^2 \\
&\quad = \frac{1}{a^2} E\left[\sum_{i'=2}^{k} (Y_{i'}(s') - Y_{i'}(0)) \left(\frac{\partial}{\partial x_i} \frac{\partial \beta_j(\cdot)}{\partial x_{i'}}\right)(\tilde{Y}/a)\right]^2 \\
&\quad \le \frac{c_5''}{a^2} s' \quad \text{by (2.24).}
\end{aligned}
\tag{2.26}
$$

Use this and (2.25) to get

$$
\sum_{j=1}^{k} EI^2_{2j}(s) \le \frac{c_6''}{a^4} s^2. \tag{2.27}
$$

Using this estimate in place of the estimate of $EI^2_{2j}(s)$ in (2.20), the last term on the right side involving t^2/a^2 may be replaced by $c_7''\, t^3/a^4$. Since the second term on the right of (2.21) (involving t^3/a^2) vanishes, as for part (b), the proof of part (c) is complete. □

REMARK 2.1.4. The significance of Theorem 2.1 is that it identifies the time scale for a change in the behavior of $X(\cdot)$, and shows that, prior to this threshold, $X(\cdot)$ and $Y(\cdot)$ are close in total variation distance. This is especially important in those cases in which $Y(\cdot)$ has interesting analyzable behavior. For example, if $b(\cdot) \equiv 0$ and $\sigma(\cdot)$ is a constant matrix, then $Y(\cdot)$ is a Brownian motion, so that $X(\cdot)$ is approximately a Brownian motion for times $t \ll a^{\frac{2}{3}}$. More important, Theorem 2.2 below identifies a class of coefficients $b(\cdot)$ such that $Y(\cdot)$ is asymptotically a Brownian motion and, for $1 \ll t \ll a^{2/3}$, so is

$X(\cdot)$. One may also consider a class of (nonperiodic) coefficients $b(\cdot)$, $\beta(x_0)$, such that $Y(\cdot)$ is ergodic, that is, $Y(\cdot)$ has a unique invariant probability and is Harris recurrent.

For Theorem 2.2 below, assume $b(\cdot)$, $\sigma(\cdot)$ are periodic having the same period lattice. Since by an appropriate nonsingular linear transformation of $X(\cdot)$, the period lattice of the transformed coefficients becomes the standard lattice $\mathbb{Z}^k$, we will assume without loss of generality that $b(\cdot)$, $\sigma(\cdot)$ are periodic with period one in each coordinate, that is,

$$(2.28)\qquad b(x+r)=b(x),\qquad \sigma(x+r)=\sigma(x)\qquad \forall\, x\in\mathbb{R}^k,\, r\in\mathbb{Z}^k.$$

In this case the process $\dot{Y}(\cdot)$ defined by

$$(2.29)\qquad \dot{Y}(t):=Y(t)\bmod 1\equiv\big(Y_1(t)\bmod 1,\dots,Y_k(t)\bmod 1\big),$$

is a Markov process, a diffusion on the *unit torus*

$$\mathscr{T}_1:=\{x\bmod 1\colon x\in\mathbb{R}^k\}\equiv\{(x_1\bmod 1,\dots,x_k\bmod 1)\colon x=(x_1,\dots,x_k)\in\mathbb{R}^k\}$$

[see, e.g., Bhattacharya and Waymire (1990), page 518]. Given that the transition probability density of $Y(\cdot)$ [and, therefore, of $\dot{Y}(\cdot)$] is positive, it is simple to check that $\dot{Y}(\cdot)$ has a unique invariant probability $\pi(x)\,dx$ and that $\dot{Y}(\cdot)$ has an exponentially decaying phi-mixing rate. Also, as shown in Bensoussan, Lions and Papanicolaou [(1978), Chapter 3] and Bhattacharya (1985), $Y(\cdot)$ is asymptotically a Brownian motion, in the sense that the sequence of processes

$$(2.30)\qquad \frac{Y(nt)-Y(0)-nt(\bar{b}+\beta(x_0))}{\sqrt{n}},\qquad 0\le t\le 1$$

converges in distribution, as $n\to\infty$, to a Brownian motion with zero drift and dispersion matrix K. Here

$$(2.31)\qquad \begin{aligned}\bar{b}&=(\bar{b}_1,\bar{b}_2,\dots,\bar{b}_k),\\ \bar{b}_j&:=\int_{\mathscr{T}_1} b_j(x)\pi(x)\,dx,\qquad 1\le j\le k,\\ K&=\int_{\mathscr{T}_1}(\operatorname{grad}\psi(x)-I_k)D(x)(\operatorname{grad}\psi(x)-I_k)'\pi(x)\,dx,\end{aligned}$$

I_k being the $k\times k$ identity matrix and $\psi=(\psi_1,\psi_2,\dots,\psi_k)'$ being the unique mean-zero periodic solution of

$$(2.32)\qquad L_0\psi_j(x)=b_j(x)-\bar{b}_j,\qquad 1\le j\le k.$$

Recall that L_0 is the generator of $Y(\cdot)$ [see (2.16)], and therefore of $\dot{Y}(\cdot)$ when restricted to periodic functions. The existence and uniqueness of the solution of (2.32) follows from a general theorem for ergodic Markov processes [see Bhattacharya (1982)]. Indeed, the solution is given by (2.37) below. A proof of the convergence in distribution of (2.30) is sketched in the course of the proof of the theorem below. We will occasionally write $\to_{\mathscr{L}}$ to denote *convergence in law*, or in distribution.

The normal distribution on $\mathbb{R}^k$ having mean vector zero and dispersion matrix K will be denoted by Φ_K or $\mathscr{N}(0, K)$.

THEOREM 2.2. *Assume that $b(\cdot)$ is continuously differentiable, and $\sigma(\cdot)$ is Lipschitzian, and $b(\cdot)$ and $\sigma(\cdot)$ are periodic as shown in* (2.28). *Assume also that $\beta(\cdot)$ has continuous and bounded derivatives of orders one and two. Let the diffusion $X(\cdot)$ be as defined in* (2.1) *with initial value* (2.3). *Then, as $n \to \infty$, $a \to \infty$, such that*

$$\frac{n}{a^{2/3}} \to 0, \tag{2.33}$$

the process

$$\frac{X(nt) - X(0) - nt(\bar{b} + \beta(x_0))}{\sqrt{n}}, \qquad 0 \le t \le 1, \tag{2.34}$$

converges in distribution to a Brownian motion with zero drift and dispersion matrix K. In particular,

$$\frac{X(t) - X(0) - t(\bar{b} + \beta(x_0))}{\sqrt{t}} \to_{\mathscr{L}} \Phi_K \tag{2.35}$$

as $t \to \infty$, $a \to \infty$ such that

$$\frac{t}{a^{2/3}} \to 0. \tag{2.36}$$

PROOF. In view of Theorem 2.1(a) (also see Remark 2.1.3), it is enough to prove that the process (2.30) converges to a Brownian motion, as $n \to \infty$. Although the latter is proved in Bensoussan, Lions and Papanicolaou [(1978), Chapter 3] and Bhattacharya (1985), we will sketch the arguments here for completeness and for later use. First note that

$$\psi_j(\cdot) := -\int_0^\infty T_t(b_j(\cdot) - \bar{b}_j)\,dt \tag{2.37}$$

is well defined as an element of $\mathscr{L}^2(\mathscr{T}_1, \pi)$, where T_t is the transition operator

$$(T_t f)(y) := E\big[f(\dot{Y}(t)) \mid \dot{Y}(0) = y\big], \qquad f \in \mathscr{L}^2(\mathscr{T}_1, \pi). \tag{2.38}$$

Note that $T_t f \to \bar{f}$, exponentially fast as $t \to \infty$, in the $\mathscr{L}^2$-norm. By applying T_h to both sides of (2.37), one obtains $(T_h\psi_j - \psi_j)/h \to b_j - \bar{b}_j$ in $\mathscr{L}^2(\mathscr{T}_1, \pi)$. In other words, (2.32) holds. By Itô's lemma,

$$\begin{aligned} &\psi_j(\dot{Y}(t)) - \psi_j(\dot{Y}(0)) \\ &\quad = \int_0^t L_0\psi_j(\dot{Y}(s))\,ds + \int_0^t \operatorname{grad}\psi_j(\dot{Y}(s)) \cdot \sigma(\dot{Y}(s))\,dB(s) \\ &\quad = \int_0^t (b_j(\dot{Y}(s)) - \bar{b}_j)\,ds + \int_0^t \operatorname{grad}\psi_j(\dot{Y}(s)) \cdot \sigma(\dot{Y}(s))\,dB(s). \end{aligned} \tag{2.39}$$

Hence,

$$
\begin{aligned}
&Y(t) - Y(0) - t(\bar{b} + \beta(x_0)) \\
(2.40)\qquad &\equiv \int_0^t (b_j(\dot{Y}(s)) - \bar{b})\, ds + \int_0^t \sigma(\dot{Y}(s))\, dB(s) \\
&= \psi(\dot{Y}(t)) - \psi(\dot{Y}(0)) - \int_0^t (\operatorname{grad} \psi(\dot{Y}(s)) - I_k)\sigma(\dot{Y}(s))\, dB(s).
\end{aligned}
$$

On dividing both sides of (2.40) by $\sqrt{t}$ and letting $t \to \infty$, one shows that the asymptotic distribution of $t^{-1/2}(Y(t) - Y(0) - t\bar{b} - t\beta(x_0))$ is the same as that of

$$
(2.41)\qquad -\frac{1}{\sqrt{t}} \int_0^t (\operatorname{grad} \psi(\dot{Y}(s)) - I_k)\sigma(\dot{Y}(s))\, dB(s).
$$

But the integrand in (2.41) is stationary and ergodic. Thus if $\dot{Y}(0)$ has distribution π then, by the Billingsley–Ibragimov central limit theorem for martingales [Billingsley (1968), page 206], (2.41) converges in law to $\Phi_K \equiv \mathscr{N}(0, K)$. Since the transition probability density $\dot{p}(t; z, y)$ converges to $\pi(y)$ exponentially fast as $t \to \infty$, uniformly in z and y, the limit law of (2.41) under $\dot{Y}(0) = x_0$ is the same as under the initial distribution π. □

REMARK 2.2.1. Under the hypothesis of Theorem 2.2, a Berry–Esséen type bound may be derived for the process $Y(t)$ defined by (2.2), namely,

$$
(2.42)\qquad \sup_{C \in \mathscr{C}} \left| P\left(\frac{Y(t) - Y(0) - t(\bar{b} + \beta(x_0))}{\sqrt{t}} \in C \right) - \Phi_K(C) \right| \le \frac{c_4}{\sqrt{t}},
$$

where $\mathscr{C}$ is the class of all Borel measurable convex sets in $\mathbb{R}^k$ and c_4 is a positive constant which depends only on $b(\cdot)$, $\beta(\cdot)$ and $D(\cdot)$; in particular, c_4 is independent of a [see, e.g., Nagaev (1961) or Tikhomirov (1980)]. Combining (2.4) and (2.42), we get the following refinement of (2.35):

$$
\begin{aligned}
&\sup_{C \in \mathscr{C}} \left| P\left(\frac{X(t) - X(0) - t(\bar{b} + \beta(x_0))}{\sqrt{t}} \in C \right) - \Phi_K(C) \right| \\
(2.43)\qquad &\le c_1 \frac{t^{3/2}}{a} + c_2 \frac{t}{a} + c_3 \frac{t^{3/2}}{a^2} + \frac{c_4}{\sqrt{t}}.
\end{aligned}
$$

This goes to zero as $t \to \infty$ and $t/a^{2/3} \to 0$. Indeed, one may bound the right side by $c_5 \frac{t^{3/2}}{a} + \frac{c_4}{\sqrt{t}}$, if $t/a^{2/3} < 1$, $a > 1$. Assuming that this is the precise order of the error of normal approximation, the approximation by Φ_K improves as t ($\gg 1$) increases to an order such that $\frac{t^{3/2}}{a} = O(\frac{1}{\sqrt{t}})$, that is, $t = 0(a^{1/2})$ (a large), the minimum error being $O(a^{-1/4})$. After this time, this normal approximation worsens, and it breaks down for t of order $a^{2/3}$ or larger. Under the special assumptions in part (b) of Theorem 2.1, in addition to the assumptions of Theorem 2.2, one may use (2.9), instead of (2.4), to take $c_1 = 0$ in (2.43), so that the error may be bounded by $c_5(t/a) + (c_4/\sqrt{t})$, which has its smallest value $O(a^{-1/3})$ at a time $t = 0(a^{2/3})$. If, in addition, the assumption in part (c) of Theorem 2.1 holds, then one may take $c_1 = 0 = c_2$ in (2.43) to get an error bound $c_3(t^{2/3}/a^2) + c_4/\sqrt{t}$, which becomes minimum for $t = O(a)$, the minimum error being $O(a^{-1/2})$.

REMARK 2.2.2. Central limit theorems for a process such as $Y(\cdot)$ in (2.2) have been studied in the literature under assumptions other than periodicity of $b(\cdot)$, $\sigma(\cdot)$. For example, one may take $b(\cdot)$, $\sigma(\cdot)$ to be (i) almost periodic, or (ii) stationary ergodic random fields [see Papanicolaou and Varadhan (1979), Kozlov (1979, 1980) and Bhattacharya and Ramasubramanian (1988)]. If a is sufficiently large, so that these Gaussian approximations for $Y(t)$ hold for $1 \ll t \ll a^{2/3}$, then they hold for $X(t)$ over the same time scale.

3. Analysis of dispersion in the final phase: the divergence-free case. In this section we first analyze the functional dependence of the asymptotic dispersion of a diffusion with periodic coefficients on a large *velocity parameter* u_0. This is of importance in itself, and has been studied extensively in the hydrology literature [see, e.g., Fried and Combarnous (1971)]. More important for us is the fact (see Proposition 3.1 below) that the asymptotic dispersion matrix is the same function of the spatial parameter "a" in the absence of u_0, as it is of u_0 in the absence of "a." We will use this fact later in the section to analyse the dispersion in the final phase. Consider then the k-dimensional diffusion $\hat{X}(t)$ governed by the Itô equation,

$$\hat{X}(t) = \hat{X}(0) + u_0 \int_0^t \beta(\hat{X}(s))\, ds + \int_0^t \sigma(\hat{X}(s))\, dB(s), \tag{3.1}$$

where $\beta(\cdot)$ is continuously differentiable and periodic with period lattice $\mathbb{Z}^k$, $\sigma(\cdot)$ is a Lipschitzian matrix-valued periodic function of period one whose eigenvalues are bounded away from zero, $\hat{X}(0)$ is independent of the k-dimensional standard Brownian motion $B(\cdot)$, and u_0 is a "large" parameter scaling the velocity magnitude. We have seen in Section 2 that $(\hat{X}(t) - \hat{X}(0) - t\overline{\beta})/\sqrt{t}$ converges in distribution to a Gaussian $\mathscr{N}(0, K)$ with mean zero and dispersion matrix $K = K(u_0)$, say. On the other hand, one may consider the diffusion $\tilde{X}(\cdot)$ governed by

$$\tilde{X}(t) = \tilde{X}(0) + \int_0^t \beta(\tilde{X}(s)/a)\, ds + \int_0^t \sigma(\tilde{X}(s/a) d\tilde{B}(s), \tag{3.2}$$

with the same assumptions on $\beta(\cdot)$, $\sigma(\cdot)$ as above, $\tilde{B}(\cdot)$ a standard Brownian motion independent of $\tilde{X}(0)$, and a a "large" parameter scaling distance. Let $\tilde{K}(a)$ denote its asymptotic dispersion matrix as computed in Section 2.

PROPOSITION 3.1. *Under the above assumptions,* $K(\cdot) \equiv \tilde{K}(\cdot)$.

PROOF. Define the process

$$\hat{Y}(t) := u_0 \hat{X}(t/u_0^2), \qquad t \geq 0. \tag{3.3}$$

Then

$$d\hat{Y}(t) = \beta(\hat{Y}(t)/u_0)\,dt + \sigma(\hat{Y}(t)/u_0)\,d\overline{B}(t), \tag{3.4}$$

where $\overline{B}(t) := u_0 B(t/u_0^2)$ is again a k-dimensional standard Brownian motion. Thus, with $a = u_0$, $\hat{Y}(\cdot)$ and $\tilde{X}(\cdot)$ have the same law, if their initial states are the same. However, irrespective of initial states, the scaled processes converge weakly to the same Gaussian law. Finally, the asymptotic dispersion matrix of $\hat{Y}(\cdot)$ is the same as that of $\hat{X}(\cdot)$. For $\lim_{t\to\infty} \operatorname{var} \hat{Y}(t)/t = \lim_{t\to\infty} \operatorname{var} \hat{X}(t/u_0^2)/(t/u_0^2) = \lim_{t\to\infty} \operatorname{var} \hat{X}(t)/t = K(u_0)$. Therefore, $K(\cdot) \equiv \tilde{K}(\cdot)$. □

The analysis of the asymptotic dispersion of $\hat{X}(\cdot)$ [governed by (3.1)] will be carried out under the additional assumptions,

$$\operatorname{div} \beta(x) \equiv \sum_{j=1}^{k} \frac{\partial \beta_j(x)}{\partial x_j} = 0 \qquad \forall\, x \tag{3.5}$$

and

$$\sigma(x) \equiv \sigma, \tag{3.6}$$

where σ is a constant nonsingular $k \times k$ matrix. An extension to nonconstant σ is indicated later (see Remark 4.5.2). We will write $D = ((D_{jj'}))$ for $\sigma\sigma'$. The *divergence-free* condition (3.5) means that the medium through which the transport (of a solute, e.g.) is taking place is *incompressible*. The spectral method of this section does not extend to velocity fields which are not divergence free. The latter are treated in Section 5 by direct calculations for the case of dimension one.

Under the assumptions that $\beta(\cdot)$ is periodic with period lattice $\mathbb{Z}^k$, and (3.5), (3.6) hold, the diffusion $\dot{X}(t) := \hat{X}(t) \bmod 1$ on the torus $\mathcal{T}_1 := \{x \bmod 1\colon x \in \mathbb{R}^k\}$ has the normalized Lebesgue measure dx as the invariant distribution. To see this check that $L^*1 = 0$, where L^* is the *formal adjoint* of the generator L of $\dot{X}$,

$$\begin{aligned}
Lf(x) &= \frac{1}{2} \sum_{j,j'=1}^{k} D_{jj'} \frac{\partial^2 f(x)}{\partial x_j \partial x_{j'}} + u_0 \sum_{j=1}^{k} \beta_j(x) \frac{\partial f}{\partial x_j},\\
L^* f &= \frac{1}{2} \sum_{j,j'=1}^{k} \frac{\partial^2}{\partial x_j \partial x_{j'}} (D_{jj'} f(x)) - u_0 \sum_{j=1}^{k} \frac{\partial}{\partial x_j} (\beta_j(x) f(x))\\
&= \frac{1}{2} \sum_{j,j'=1}^{k} D_{jj'} \frac{\partial^2 f(x)}{\partial x_j \partial x_{j'}} - u_0 \sum_{j=1}^{k} \beta_j(x) \frac{\partial f(x)}{\partial x_j}.
\end{aligned} \tag{3.7}$$

The last equality follows from (3.5).

It follows from Section 2 [see (2.30)–(2.32)] that

$$\frac{\hat{X}(t) - \hat{X}(0) - u_0 t\overline{\beta}}{\sqrt{t}} \to_{\mathscr{L}} \Phi_K \quad \text{as } t \to \infty, \tag{3.8}$$

where $\overline{\beta} = (\overline{\beta}_1, \dots, \overline{\beta}_k)$, with $\overline{\beta}_j$ given by

$$\overline{\beta}_j = \int_{[0,1]^k} \beta_j(x)\,dx \tag{3.9}$$

and

$$\begin{aligned} K &= \int_{[0,1]^k} (\operatorname{grad}\psi(x) - I_k) D (\operatorname{grad}\psi(x) - I_k)'\,dx \\ &= ((K_{jj'})). \end{aligned} \tag{3.10}$$

Here $\psi(\cdot) = (\psi_1(\cdot), \dots, \psi_k(\cdot))$ is the unique mean-zero solution in the domain of L [in $\mathscr{L}^2(\mathscr{T}_1, dx)$],

$$L\psi_j(\cdot) = u_0(\beta_j(\cdot) - \overline{\beta}_j), \qquad 1 \le j \le k. \tag{3.11}$$

Further, one has

$$\begin{aligned} K_{jj'} &= E_{jj'} + D_{jj'}, \\ E_{jj'} &:= \int_{[0,1]^k} \operatorname{grad}\psi_j(x) \cdot D \operatorname{grad}\psi_{j'}(x)\,dx. \end{aligned} \tag{3.12}$$

This follows from (3.10) using periodic boundary conditions, namely,

$$\int_{[0,1]^k} \frac{\partial \psi_j(x)}{\partial x_r}\,dx = 0, \qquad 1 \le j, r \le k. \tag{3.13}$$

To analyze $E_{jj'}$ let us introduce the complex Hilbert space,

$$H^0 = \mathscr{L}^2(\mathscr{T}_1, dx) \cap 1^{\perp} = 1^{\perp}, \tag{3.14}$$

where dx denotes Lebesgue measure, or the uniform distribution on the unit torus $\mathscr{T}_1$, and $\mathscr{L}^2(\mathscr{T}_1, dx) \equiv \mathscr{L}^2$ is the space of complex-valued square integrable (w.r.t. dx) functions on $\mathscr{T}_1$. Here $1^{\perp}$ is the subspace of $\mathscr{L}^2$ orthogonal to constants, that is, the set of all mean-zero elements of $\mathscr{L}^2$. This identifies H^0 and its inner product as

$$\begin{aligned} H^0 &= \left\{ h \text{ periodic: } \int_{[0,1]^k} |h(x)|^2\,dx < \infty, \int_{[0,1]^k} h(x)\,dx = 0 \right\}, \\ \langle f, g\rangle_0 &:= \int_{[0,1]^k} f(x) g^{-}(x)\,dx. \end{aligned} \tag{3.15}$$

Here g^- is the *complex conjugate* of g. The spectral expansion of $E_{jj'}$ is carried out on the Hilbert space H^1 defined by

$$(3.16)\quad \begin{aligned} H^1 &= \left\{ h \in H^0 \colon \int_{[0,1]^k} |\nabla h|^2(x)\,dx < \infty \right\}, \qquad \nabla := \text{grad}, \\ \langle f, g\rangle_1 &:= \frac{1}{2}\sum_{j,j'=1}^{k} D_{jj'} \int_{[0,1]^k} \frac{\partial f}{\partial x_j}\frac{\partial g^-}{\partial x_{j'}}\,dx. \end{aligned}$$

Note that for all twice continuously differentiable periodic f and once continuously differentiable periodic g, integration by parts yields

$$(3.17)\quad \langle f, g\rangle_1 = -\langle \mathscr{D} f, g\rangle_0,$$

where

$$(3.18)\quad \mathscr{D} := \frac{1}{2}\sum_{j,j'=1}^{k} D_{jj'} \frac{\partial^2}{\partial x_j \partial x_{j'}}.$$

The *Sobolev space* H^1, given in (3.16), is the closure in the norm $\|f\|_1 := (\langle f, f\rangle_1)^{1/2}$ of the space of all twice continuously differentiable periodic functions in H^0, and the elements of H^1 are those elements of H^0 which have square integrable derivatives on $[0,1]^k$. Finally let H^2 be the subspace of H^1 having square integrable derivatives of order two. The operator $\mathscr{D}$ maps H^2 onto H^0 and is in fact invertible. Indeed, if $g \in H^2$ is such that $\mathscr{D} g = f$, then the *Fourier transforms* $\hat{g}$, $\hat{f}$ of g and f are related, on integration by parts, by

$$(3.19)\quad \begin{aligned} \hat{f}(r) &= \int_{[0,1]^k} f(x)\exp(-2\pi i r\cdot x)\,dx \\ &= \int_{[0,1]^k} (\mathscr{D} g)(x)\exp(-2\pi i r\cdot x)\,dx \\ &= \frac{1}{2}\sum_{j,j'=1}^{k} D_{jj'} \int_{[0,1]^k} \frac{\partial^2 g(x)}{\partial x_j \partial x_{j'}} \exp(-2\pi i r\cdot x)\,dx \\ &= \frac{1}{2}\sum_{j,j'=1}^{k} D_{jj'}(2\pi i r_j)(2\pi i r_{j'}) \int_{[0,1]^k} g(x)\exp(-2\pi i r\cdot x)\,dx \\ &= -2\pi^2\left(\sum_{j,j'=1}^{k} D_{jj'} r_j r_{j'}\right)\hat{g}(r), \qquad r \in \mathbb{Z}^k. \end{aligned}$$

Thus $\hat{g}$ is given by

$$(3.20)\quad \hat{g}(0) = 0, \qquad \hat{g}(r) = -\frac{1}{2\pi^2}\left(\sum_{j,j'=1}^{k} D_{jj'} r_j r_{j'}\right)^{-1} \hat{f}(r), \qquad r \in \mathbb{Z}^k\backslash\{0\}.$$

Note that

$$(3.21)\quad |\hat{g}(r)| \geq \frac{1}{2\alpha_2 \pi^2 |r|^2} |\hat{f}(r)|, \qquad r \in \mathbb{Z}^k\backslash\{0\},$$

where α_1 is the smallest eigenvalue of D and α_2 is the largest. We will show that the operator $\mathscr{D}^{-1}$: $H^0 \to H^1$ is *compact*. For this, let f_k ($k = 1, 2, \ldots$) be a bounded sequence in H^0, say $\|f_k\|_0 \le 1 \,\forall\, k$. Then there exists a subsequence $f_{k'}$ ($k = 1, 2, \ldots$) which converges weakly to some element f_0 of the unit ball of H^0. In particular,

$$\text{(3.22)}\qquad \begin{aligned} &\hat{f}_{k'}(r) \to \hat{f}_0(r) \quad \text{as } k' \to \infty \quad (r \in \mathbb{Z}^k \setminus \{0\}),\\ &\hat{f}_{k'}(0) = 0 = \hat{f}_0(0) \qquad \forall\, k'. \end{aligned}$$

Let

$$\text{(3.23)}\qquad g_k := \mathscr{D}^{-1} f_k, \qquad g_0 := \mathscr{D}^{-1} f_0.$$

We now show that $\|g_{k'} - g_0\|_1 \to 0$ as $k' \to \infty$. For this write [see (3.17)–(3.21)]

$$\begin{aligned} \|g_{k'} - g_0\|_1^2 &= -\langle \mathscr{D}(g_{k'} - g_0), g'_k - g_0\rangle_0 = -\langle f_{k'} - f_0, \mathscr{D}^{-1}(f_{k'} - f_0)\rangle_0\\ &= \frac{1}{2\pi^2} \sum_{r \ne 0} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 \frac{1}{\Sigma D_{jj'} r_j r_{j'}}\\ \text{(3.24)}\qquad &\le \frac{1}{2\alpha_1 \pi^2} \sum_{r \ne 0} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 \frac{1}{|r|^2}\\ &\le \frac{1}{2\alpha_1 \pi^2} \left\{ \sum_{|r| \le R} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 + \frac{1}{R^2} \sum_{|r| > R} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 \right\}\\ &\le \frac{1}{2\alpha_1 \pi^2} \left\{ \sum_{|r| \le R} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 + \frac{4}{R^2} \right\}, \end{aligned}$$

since $\|f_{k'}\|_0 \le 1$, $\|f_0\|_0 \le 1$. Given $\varepsilon > 0$, choose R_ε such that $(1/2\alpha_1\pi^2)((4/R^2)) < \varepsilon/2$ for $R \ge R_\varepsilon$. Now choose k'_ε large so that $\sum_{|r| \le R_\varepsilon} |\hat{f}_{k'}(r) - \hat{f}_0(r)|^2 < \varepsilon/2 \;\forall\, k' \ge k'_\varepsilon$. Then

$$\|g_{k'} - g_0\|_1^2 < \varepsilon \qquad \forall\, k' \ge k'_\varepsilon.$$

Thus $g_{k'} \to g_0$ in H^1, proving the compactness of $\mathscr{D}^{-1}$.

We may now express (3.11) as

$$\text{(3.25)}\qquad (\mathscr{D} + u_0 \beta(\cdot) \cdot \nabla)\psi_j(\cdot) = u_0(\beta_j(\cdot) - \overline{\beta}_j), \qquad 1 \le j \le k.$$

Rewrite (3.25) as

$$\text{(3.26)}\qquad (\mathscr{I} + u_0 S)\psi_j = u_0 \mathscr{D}^{-1}(\beta_j(\cdot) - \overline{\beta}_j), \qquad 1 \le j \le k,$$

where $\mathscr{I}$ is the *identity operator on* H^1, and S is the linear operator

$$\text{(3.27)}\qquad S = \mathscr{D}^{-1}\beta(\cdot) \cdot \nabla$$

acting on H^1. Note that, for $f, g \in H^1$,

$$
\begin{aligned}
\langle \mathscr{D}^{-1}\beta(\cdot)\cdot\nabla f, g\rangle_1 &= -\langle \beta(\cdot)\cdot\nabla f, g\rangle_0 \\
&= -\sum_{j=1}^{k}\int_{[0,1]^k}\beta_j(x)\frac{\partial f(x)}{\partial x_j}\,g^-(x)\,dx \\
&= \int_{[0,1]^k} f(x)\sum_{j=1}^{k}\frac{\partial}{\partial x_j}\big(\beta_j(x)g^-(x)\big)\,dx \\
&= \int_{[0,1]^k} f(x)\left\{g^-(x)(\operatorname{div}\beta)(x)+\sum_{j=1}^{k}\beta_j(x)\frac{\partial g^-(x)}{\partial x_j}\right\}dx \\
&= \int_{[0,1]^k} f(x)(\beta(\cdot)\cdot\nabla g)(x)\,dx = \langle f, \beta(\cdot)\cdot\nabla g\rangle_0 \\
&= -\langle \mathscr{D}^{-1}f, \beta(\cdot)\cdot\nabla g\rangle_1.
\end{aligned}
\tag{3.28}
$$

Thus S is skew symmetric. Noting that $\beta(\cdot)\cdot\nabla\colon H^1 \to H^0$ is bounded, while $\mathscr{D}^{-1}\colon H^0 \to H^1$ is compact, we have the following result [see Reed and Simon (1980), page 200].

PROPOSITION 3.2. *Let $\beta(\cdot)$ be continuously differentiable and periodic and* (3.5), (3.6) *hold. Then $S := \mathscr{D}^{-1}\beta(\cdot)\cdot\nabla$ is a skew symmetric compact operator on H^1 and, therefore, may be expressed as $S = iG$ where G is a compact and self–adjoint operator on H^1.*

Applying the spectral theorem for compact self-adjoint operators [see Reed and Simon (1980), page 203], it now follows that G has a sequence of nonzero eigenvalues $\lambda_n \to 0$ with corresponding eigenfunctions φ_n $(n \geq 1)$ such that $\{\varphi_n\colon n \geq 1\}$ form a complete orthonormal sequence for $N^\perp$, the subspace of H^1 orthogonal to the *null space* N of G or S. Hence one has the eigenfunction expansion,

$$
f = f_N + \sum_{n=1}^{\infty}\langle f, \varphi_n\rangle_1\varphi_n, \qquad f \in H^1, \tag{3.29}
$$

where f_N is the *orthogonal projection* of f onto N. Also,

$$
Sf = \sum_{n=1}^{\infty} i\lambda_n\langle f, \varphi_n\rangle_1\varphi_n, \qquad f \in H^1. \tag{3.30}
$$

Taking $f = \psi_j$ in (3.29), (3.30), one may now express the equation (3.26) in spectral form

$$
\begin{aligned}
(\psi_j)_N &= u_0\big(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\big)_N, \\
(1 + iu_0\lambda_n)\langle\psi_j, \varphi_n\rangle_1 &= u_0\langle\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j), \varphi_n\rangle_1, \qquad n \geq 1.
\end{aligned}
\tag{3.31}
$$

Hence,

$$
\langle\psi_j, \varphi_n\rangle_1 = \frac{u_0\beta_{jn}}{1 + iu_0\lambda_n}, \qquad \beta_{jn} := \langle\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j), \varphi_n\rangle_1, \qquad n \geq 1. \tag{3.32}
$$

Thus the components $E_{jj'}$ of the dispersion matrix $((K_{jj'}))$ arising from the heterogeneity of the medium of transport may be expressed as [see (3.12), (3.16)]

$$\begin{aligned} E_{jj'} &= 2\langle \psi_j, \psi_{j'} \rangle_1 \\ &= 2\langle (\psi_j)_N, (\psi_{j'})_N \rangle_1 + 2 \sum_{n=1}^{\infty} \langle \psi_j, \varphi_n \rangle_1 \overline{\langle \psi_{j'}, \varphi_n \rangle_1} \\ &= 2u_0^2 \langle (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N, (\mathscr{D}^{-1}(\beta_{j'} - \overline{\beta}_{j'}))_N \rangle_1 + 2 \sum_{n=1}^{\infty} \frac{u_0^2 \beta_{jn} \overline{\beta_{j'n}}}{1 + u_0^2 \lambda_n^2}. \end{aligned} \tag{3.33}$$

In particular,

$$E_{jj} = 2u_0^2 \left\{ \|(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N\|_1^2 + \sum_{n=1}^{\infty} \frac{|\beta_{jn}|^2}{1 + u_0^2 \lambda_n^2} \right\}, \qquad 1 \le j \le k. \tag{3.34}$$

THEOREM 3.3. *Suppose the assumptions in Proposition* 3.2 *hold.*

(a) *If* $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N \neq 0$, *then*

$$\lim_{u_0 \to \infty} \frac{K_{jj}}{u_0^2} = \lim_{u_0 \to \infty} \frac{E_{jj}}{u_0^2} = 2\|(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N\|_1^2 > 0. \tag{3.35}$$

(b) *If* $\beta_j - \overline{\beta}_j$ *belongs to the range of* $\beta(\cdot) \cdot \nabla$, *say*, $\beta(\cdot) \cdot \nabla h = \beta_j - \overline{\beta}_j$ *for some* $h \in H^1$, *then*

$$\lim_{u_0 \to \infty} K_{jj} = \lim_{u_0 \to \infty} E_{jj} + D_{jj} = 2\|h_0\|_1^2 + D_{jj}, \tag{3.36}$$

where h_0 *is the projection of* h *on* $N^{\perp}$ *or, equivalently,* h_0 *is the unique element in* $N^{\perp}$ *such that* $\beta(\cdot) \cdot \nabla h_0 = \beta_j - \overline{\beta}_j$.

PROOF. (a) If $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N \neq 0$, then (3.35) is an immediate consequence of (3.12) and (3.34).

(b) In this case, $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j) = \mathscr{D}^{-1}\beta(\cdot) \cdot \nabla h \equiv Sh$ belongs to the range of S and is, therefore, orthogonal to N. Writing

$$h = \sum_{n=1}^{\infty} \langle h, \varphi_n \rangle_1 \varphi_n + h_N, \qquad Sh = \sum_{n=1}^{\infty} i\lambda_n \langle h, \varphi_n \rangle_1 \varphi_n,$$

one has [see (3.32), (3.34)]

$$\begin{aligned} \beta_{jn} &= \langle \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j), \varphi_n \rangle_1 = \langle Sh, \varphi_n \rangle_1 = i\lambda_n \langle h, \varphi_n \rangle_1, \\ E_{jj} &= 2u_0^2 \sum_{n=1}^{\infty} \frac{\lambda_n^2 \langle h, \varphi_n \rangle_1^2}{1 + u_0^2 \lambda_n^2} \\ &\to 2 \sum_{n=1}^{\infty} \langle h, \varphi_n \rangle_1^2 = 2\|h_0\|_1^2. \end{aligned}$$

□

REMARK 3.3.1. Under the hypothesis of part (a) of Theorem 3.3, the dispersion coefficient $K_{jj} = E_{jj} + D_{jj}$ [see (3.12)] grows quadratically with u_0. Experimental studies have shown a similar growth pattern for solute dispersion in saturated porous media. See Fried and Combarnous (1971), and Figures 1 and 2 in Section 7.

Consider now the diffusion $\tilde{X}(t)$ governed by the Itô equation (3.2) involving a spatial scale parameter a. Then $\tilde{X}(t) \bmod a$ is a diffusion on the torus $\mathscr{T}_a := \{x \bmod a \colon x \in \mathbb{R}^k\}$ and therefore $\tilde{X}(t)$ is asymptotically Gaussian. Indeed, in view of Proposition 3.1, the matrix $((\tilde{K}_{jj'}))$ of dispersion coefficients of this asymptotic distribution is the same as that of $\hat{X}(t)$, namely, $((K_{jj'}))$ for $u_0 = a$. The following is then an immediate consequence of Theorem 3.3.

COROLLARY 3.4. *Suppose the hypothesis of Proposition 3.2 holds for the coefficients of the diffusion $\tilde{X}(t)$.*

(a) *If $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N \neq 0$, then*

$$\lim_{a\to\infty} \frac{\tilde{K}_{jj}}{a^2} = 2\|(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_N\|_1^2 > 0. \tag{3.37}$$

(b) *If $\beta_j - \overline{\beta}_j$ belongs to the range of $\beta(\cdot)\cdot\nabla$, $\beta_j - \overline{\beta}_j = \beta\cdot\nabla h$, then, with h_0 as the projection of h on $N^{\perp}$,*

$$\lim_{a\to\infty} \tilde{K}_{jj} = 2\|h_0\|_1^2 + D_{jj}. \tag{3.38}$$

We now turn to the multiscale process of interest, namely [see (2.1)],

$$X(t) = X(0) + \int_0^t \{b(X(s)) + \beta(X(s)/a)\}\, ds + \sigma B(t), \tag{3.39}$$

where it is assumed that

(3.40)(A1) $b(\cdot)$, $\beta(\cdot)$ are continuously differentiable, divergence free and periodic with period lattice $\mathbb{Z}^k$;
(3.40)(A2) σ is a constant $k\times k$ nonsingular matrix;
(3.40)(A3) a is a positive integer.

Then

$$\dot{X}(t) := X(t) \bmod a \equiv (X_1(t) \bmod a, \ldots, X_k(t) \bmod a) \tag{3.41}$$

is a diffusion on the torus $\mathscr{T}_a := \{x \bmod a \colon x \in \mathbb{R}^k\}$, whose unique invariant probability is the uniform distribution on $\mathscr{T}_a$. It is convenient to scale this process to bring it to the unit torus $\mathscr{T}_1 = \{x \bmod 1, x \in \mathbb{R}^k\}$. For this, define

$$Y(t) := \frac{X(a^2 t)}{a}, \qquad \dot{Y}(t) := Y(t) \bmod 1 \equiv \frac{\dot{X}(a^2 t)}{a}. \tag{3.42}$$

Note that apart from the scaling of distance, in which one unit of length in the Y-scale equals "a" units of length in the original X-scale, one unit of time for Y equals a^2 units of time for X. The process $Y(t)$ is governed by the Itô equation

$$Y(t) = Y(0) + \int_0^t a\{b(aY(s)) + \beta(Y(s))\}\,ds + \sigma\overline{B}(t), \tag{3.43}$$

where $\overline{B}(t) := B(a^2t)/a$ is a standard Brownian motion on $\mathbb{R}^k$. The infinitesimal generator of $\dot{Y}(t)$ is given by $A_a = \mathscr{D} + a(b(a\cdot) + \beta)\cdot\nabla$, that is,

$$A_a f(x) = \frac{1}{2}\sum_{j,\,j'=1}^{k} D_{jj'}\frac{\partial^2 f(x)}{\partial x_j \partial x_{j'}} + a(b(ax) + \beta(x))\cdot\nabla f(x) \tag{3.44}$$

for smooth functions which are periodic: $f(y+r) = f(y)$ for all $r \in \mathbb{Z}^k$, all $y \in \mathbb{R}^k$; that is, A_a acts on (a dense subspace of) $\mathscr{L}^2(\mathscr{T}_1, dx)$. Let g_j $(1 \le j \le k)$ be the unique solution in $1^\perp$ of

$$A_a g_j(x) = b_j(ax) + \beta_j(x) - \overline{b}_j - \overline{\beta}_j. \tag{3.45}$$

By Itô's lemma [see (2.40)], writing $g = (g_1, \dots, g_k)'$,

$$\begin{aligned} &Y(t) - Y(0) - at(\overline{b} + \overline{\beta}) \\ &\quad = g(\dot{Y}(t)) - g(\dot{Y}(0)) - \int_0^t a\{\operatorname{grad} g(\dot{Y}(s)) - I\}\sigma d\overline{B}(s) \\ &\qquad\qquad \left(\operatorname{grad} g(x) := \left(\left(\frac{\partial g_j(x)}{\partial x_{j'}}\right)\right)\right). \end{aligned} \tag{3.46}$$

Hence, for a fixed "a,"

$$\frac{Y(t) - Y(0) - at(\overline{b} + \overline{\beta})}{\sqrt{t}} \to_{\mathscr{L}} \Phi_K \quad \text{as } t \to \infty, \tag{3.47}$$

where

$$\begin{aligned} K_{jj'} &= E_{jj'} + D_{jj'}, \\ E_{jj'} &:= a^2(\langle g_j, g_{j'}\rangle_1 + \langle g_{j'}, g_j\rangle_1), \qquad 1 \le j,\ j' \le k. \end{aligned} \tag{3.48}$$

Since the function $x \to b(ax)$ is *rapidly oscillating* for large a, one may think of approximating A_a by $\overline{A} = \mathscr{D} + a(\overline{b} + \beta)\cdot\nabla$,

$$\overline{A}f(x) = \frac{1}{2}\sum_{j,\,j'=1}^{k} D_{jj'}\frac{\partial^2 f(x)}{\partial x_j \partial x_{j'}} + a(\overline{b} + \beta)\cdot\nabla f(x). \tag{3.49}$$

Correspondingly, define on H^1 the skew symmetric compact operators

$$S_a = \mathscr{D}^{-1}(b(a\cdot) + \beta)\cdot\nabla, \qquad \overline{S} = \mathscr{D}^{-1}(\overline{b} + \beta)\cdot\nabla. \tag{3.50}$$

Let $\underline{N}$ denote the *null space* of $\overline{S}$. We will denote by $f_{\underline{N}}$ the orthogonal projection of an element f of H^1 on $\underline{N}$. The following result provides preliminary estimates of the norms of the solution g_j of the equation (3.45) in H^0 and H^1.

LEMMA 3.5. *Under assumptions* (A1)–(A3) *in* (3.40) *one has*

$$\sup_a \|g_j\|_1^2 < \infty, \qquad \|g_j\|_0^2 \le \frac{1}{2\pi^2\alpha_1}\|g_j\|_1^2, \tag{3.51}$$

where α_1 *is the smallest eigenvalue of the diffusion matrix* $D = \sigma\sigma'$.

PROOF. The operators S_a, $\overline{S}$ are skew symmetric so that

$$\langle S_a f, f\rangle_1 = 0, \qquad \langle \overline{S} f, f\rangle_1 = 0 \qquad \forall f \in H^1. \tag{3.52}$$

Therefore,

$$\|(\mathscr{I} + aS_a)f\|_1^2 = \|f\|_1^2 + a^2\|S_a f\|_1^2 \ge \|f\|_1^2. \tag{3.53}$$

Rewrite the defining equation (3.45) for g_j as

$$(\mathscr{I} + aS_a)g_j = \mathscr{D}^{-1}[b_j(a\cdot) - \overline{b}_j + \beta_j(\cdot) - \overline{\beta}_j]. \tag{3.54}$$

It now follows from (3.53) [also see (3.17)] that

$$\begin{aligned}\|g_j\|_1^2 &\le \|\mathscr{D}^{-1}[b_j(a\cdot) - \overline{b}_j + \beta_j(\cdot) - \overline{\beta}_j]\|_1^2 \\ &= \langle b_j(a\cdot) - \overline{b}_j + \beta_j(\cdot) - \overline{\beta}_j, -\mathscr{D}^{-1}[b_j(a\cdot) - \overline{b}_j + \beta_j(\cdot) - \overline{\beta}_j]\rangle_0.\end{aligned} \tag{3.55}$$

Writing $r = (r_1, \ldots, r_k) \in \mathbb{Z}^k$, and using Parseval's relation and (3.20), one has for all $f \in H^0$,

$$\begin{aligned}\langle -\mathscr{D}^{-1}f, f\rangle_0 &= \sum_{r\in\mathbb{Z}^k\setminus\{\mathbf{0}\}} \Big(2\pi^2 \sum_{j,j'} D_{jj'}r_j r_{j'}\Big)^{-1} |\hat{f}(r)|^2 \\ &\le \sum_{r\in\mathbb{Z}^k\setminus\{\mathbf{0}\}} (2\pi^2\alpha_1|r|^2)^{-1}|\hat{f}(r)|^2 \\ &\le \frac{1}{2\pi^2\alpha_1}\|f\|_0^2.\end{aligned} \tag{3.56}$$

Therefore, (3.55) leads to the first inequality in (3.51). The second inequality in (3.51) follows from

$$\begin{aligned}\|f\|_1^2 &= \langle -\mathscr{D}f, f\rangle_0 = \textstyle\sum_{r\ne 0} 2\pi^2\Big(\sum_{j,j'} D_{jj'}r_j r_{j'}\Big)|\hat{f}(r)|^2 \\ &\ge \sum_{r\ne 0} 2\pi^2\alpha_1|r|^2|\hat{f}(r)|^2 \ge 2\pi^2\alpha_1 \sum_{r\ne 0}|\hat{f}(r)|^2 \\ &= 2\pi^2\alpha_1\|f\|_0^2 \qquad \forall f \in H^1.\end{aligned} \tag{3.57}$$

□

The next lemma enables one to estimate the error in replacing $b(a\cdot)$ by $\overline{b}$ in variance calculations.

LEMMA 3.6. *Suppose* $f \in H^0$ *and "a" is a positive integer.*

(a) *If $\mathscr{G}$ is a relatively compact subset of H^1 then*

$$\sup_{g\in\mathscr{G}}\left|\langle f(a\cdot), g\rangle_0\right| = o\left(\frac{1}{a}\right) \quad \text{as } a\to\infty, \tag{3.58}$$

(b) *If $\mathscr{G}$ is a relatively compact subset of H^0, then*

$$\sup_{g\in\mathscr{G}}\left|\langle f(a\cdot), g\rangle_0\right| = o(1) \quad \text{as } a\to\infty. \tag{3.59}$$

PROOF. Assume first that f is continuously differentiable of all orders up to at least $[k/2]+1 = k_0$, say. Then

$$\langle f(a\cdot), g\rangle_0 = \sum_{r\in\mathbb{Z}^k\setminus\{0\}} f(a\cdot)\hat{\ }(r)\hat{g}^-(r), \qquad r\in\mathbb{Z}^k\setminus\{0\}. \tag{3.60}$$

Now

$$\begin{aligned}\sum_{r\neq 0}|\hat{f}(r)| &= \sum_{r\neq 0}\frac{|r|^{k_0}|\hat{f}(r)|}{|r|^{k_0}}\\ &\le \left(\sum_{r\neq 0}|r|^{2k_0}|\hat{f}(r)|^2\right)^{1/2}\left(\sum_{r\neq 0}\frac{1}{|r|^{2k_0}}\right)^{1/2} < \infty.\end{aligned} \tag{3.61}$$

It follows that the Fourier series for f, namely $\sum_{r\neq 0}\hat{f}(r)\exp\{2\pi i r\cdot x\}$, converges uniformly to $f(x)$ so that

$$f(ax) = \sum_{r\neq 0}\hat{f}(r)\exp(2\pi i r\cdot ax) = \sum_{r\neq 0}\hat{f}(r)\exp(2\pi i a r\cdot x). \tag{3.62}$$

In particular,

$$f(a\cdot)^\wedge(r) = \begin{cases} 0, & \text{if } r\notin a\mathbb{Z}^k\setminus\{0\},\\ \hat{f}(r/a), & \text{if } r\in a\mathbb{Z}^k\setminus\{0\}.\end{cases} \tag{3.63}$$

Using this in (3.60) we get

$$\begin{aligned}\left|\langle f(a\cdot), g\rangle_0\right| &= \left|\sum_{r\in a\mathbb{Z}^k\setminus\{0\}}\hat{f}(r/a)\hat{g}^-(r)\right|\\ &\le \left(\sum_{r\in a\mathbb{Z}^k\setminus\{0\}}\left|\hat{f}(r/a)\right|^2\right)^{1/2}\left(\sum_{|r|\ge a}\left|\hat{g}(r)\right|^2\right)^{1/2}\\ &\le \|f_0\|\left(\sum_{|r|\ge a}\frac{1}{a^2}|r|^2|\hat{g}(r)|^2\right)^{1/2}\\ &\le \frac{\|f\|_0}{a}\left(\sum_{|r|\ge a}|r|^2|\hat{g}(r)|^2\right)^{1/2} \le c\|f\|_0\|g\|_1/a.\end{aligned} \tag{3.64}$$

To prove (3.58), note that if $\mathscr{G}$ is a relatively compact subset of H^1 then

$$\sup_{g\in\mathscr{G}}\Big(\sum_{|r|\geq a}|r|^2|\hat{g}(r)|^2\Big)^{1/2}\to 0 \quad \text{as } a\to\infty. \tag{3.65}$$

To prove part (b), use the first inequality in (3.64) to get

$$|\langle f(a\cdot), g\rangle_0| \leq \|f\|_0\Big(\sum_{|r|\geq a}|\hat{g}(r)|^2\Big)^{1/2}, \tag{3.66}$$

and note that the right side goes to zero as $a\to\infty$, uniformly for g belonging to a relatively compact subset of H^0.

Since the final estimates in (3.64), (3.66) involve only the H^0-norm of f, and the set of all infinitely differentiable functions in H^0 is dense in H^0, the proof of the lemma is complete. □

We are now ready to prove two of the main results of this section. The following technical condition will be made use of in the proof.

Consider the "approximation" of g_j provided by the solution h_j in H^1 to the equation

$$\begin{aligned}\overline{A}h_j &= \beta_j-\overline{\beta}_j \quad \text{or}\\ (\mathscr{I}+a\overline{S})h_j &= \mathscr{D}^{-1}(\beta_j-\overline{\beta}_j),\end{aligned} \tag{3.67}$$

and let $i\lambda_n$ be the eigenvalues of $\overline{S}$ corresponding to normalized eigenfunctions φ_n $(n\geq 1)$. We assume

(3.68)(A4)j (i) $\{g_j\colon a\geq 1\}$, $\{g_j^-\partial/\partial x_s(\mathscr{D}^{-1}(\beta_j-\overline{\beta}_j))_{\underline{N}}\colon a\geq 1\}$ $(1\leq s\leq k)$ are relatively compact subsets of H^1, and
(ii) $\{\varphi_n\partial g_j^-/\partial x_s\colon a\geq 1\}$ $(1\leq s\leq k,\ n\geq 1)$ are relatively compact in H^0.

See Remark 3.7.1 for some simpler conditions which guarantee (A4)j.

For the statement of the theorem below recall that $K_{jj'}=E_{jj'}+D_{jj'}$ are the elements of the dispersion matrix of the limiting Gaussian distribution of the scaled $Y(t)$ process (3.47) [see (3.48)].

THEOREM 3.7. *Assume* (A1)–(A3) *in* (3.40), *and* (A4)j *in* (3.67). *Then*

$$\lim_{a\to\infty}\frac{K_{jj}}{a^2}=2\,\|(\mathscr{D}^{-1}(\beta_j-\overline{\beta}_j))_{\underline{N}}\|_1^2. \tag{3.69}$$

PROOF. Since [see (3.48)]

$$K_{jj}=a^2E_{jj}+D_{jj}=2a^2\|g_j\|_1^2+D_{jj}, \tag{3.70}$$

it is enough to show that

$$\lim_{a\to\infty}\|g_j\|_1^2=\|(\mathscr{D}^{-1}(\beta_j-\overline{\beta}_j))_{\underline{N}}\|_1^2. \tag{3.71}$$

Now g_j solves (3.45) or (3.54). Hence [see (3.52) and Lemma 3.6],

$$\begin{aligned}\|g_j\|_1^2 &= \langle g_j, (\mathscr{I} + aS_a)g_j\rangle_1 = \langle g_j, \mathscr{D}^{-1}[b_j(a\cdot) - \overline{b}_j + \beta_j - \overline{\beta}_j]\rangle_1 \\ &= -\langle g_j, b_j(a\cdot) - \overline{b}_j + \beta_j - \overline{\beta}_j\rangle_0 \simeq -\langle g_j, \beta_j - \overline{\beta}_j\rangle_0 \\ &= \langle g_j, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1.\end{aligned} \tag{3.72}$$

Here $\simeq$ indicates that the difference between its two sides goes to zero as $a \to \infty$. As in the proof of Theorem 3.3(a), letting $i\lambda_n$ be the eigenvalues of $\overline{S}$ corresponding to eigenfunctions φ_n ($n \geq 1$), one may express the second equation in (3.67) as

$$\begin{aligned}&(h_j)_{\underline{N}} = (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}, \\ &\langle h_j, \varphi_n\rangle_1 = \frac{\beta_{jn}}{1 + ia\lambda_n}, \qquad \beta_{jn} := \langle \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j), \varphi_n\rangle_1, \qquad n \geq 1.\end{aligned} \tag{3.73}$$

Hence

$$\|h_j - (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\|_1^2 = \sum_{n=1}^{\infty} \frac{\beta_{jn}^2}{1 + a^2\lambda_n^2} \to 0 \quad \text{as } a \to \infty, \tag{3.74}$$

since the sum on the right is bounded above by $\sum_{n=1}^{\infty} \beta_{jn}^2 \leq \|\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\|_1^2$ for all a. Hence,

$$h_j \to (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} \quad \text{in } H^1\text{-norm, as } a \to \infty. \tag{3.75}$$

Now, using $(\mathscr{I} + aS_a)g_j = \mathscr{D}^{-1}[b_j(a\cdot) - \overline{b}_j + \beta_j - \overline{\beta}_j]$ and $(\mathscr{I} + a\overline{S})h_j = \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$, one gets

$$(\mathscr{I} + a\overline{S})(g_j - h_j) = \mathscr{D}^{-1}(b_j(a\cdot) - \overline{b}_j) - a\mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla g_j. \tag{3.76}$$

Therefore,

$$(g_j - h_j)_{\underline{N}} = (\mathscr{D}^{-1}(b_j(a\cdot) - \overline{b}_j))_{\underline{N}} - a(\mathscr{D}^{-1}[(b(a\cdot) - \overline{b}) \cdot \nabla g_j])_{\underline{N}} \tag{3.77}$$

and

$$\begin{aligned}\langle g_j - h_j, \varphi_n\rangle_1 &= \frac{1}{1+ia\lambda_n}\langle \mathscr{D}^{-1}(b_j(a\cdot) - \overline{b}_j), \varphi_n\rangle_1 \\ &\quad - \frac{a}{1 + ia\lambda_n}\langle \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla g_j, \varphi_n\rangle_1, \qquad n \geq 1.\end{aligned} \tag{3.78}$$

The first term on the right in (3.78) goes to zero by (3.58) or (3.59). To evaluate the second term, express the inner product as

$$\begin{aligned}\langle \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla g_j, \varphi_n\rangle_1 &= \langle -(b(a\cdot) - \overline{b}) \cdot \nabla g_j, \varphi_j\rangle_0 \\ &= -\sum_{s=1}^{k} \langle (b_s(a) - \overline{b}_s)\frac{\partial g_j}{\partial x_s}, \varphi_n\rangle_0 \\ &= -\sum_{s=1}^{k} \left\langle (b_s(a\cdot) - \overline{b}_s), \varphi_n \frac{\partial \overline{g_j}}{\partial x_s}\right\rangle_0 \to 0 \quad \text{as } a \to \infty,\end{aligned} \tag{3.79}$$

using the assumption that $\{\varphi_n \partial g_j^- / \partial x_s \colon a \geq 1\}$, $1 \leq s \leq k$, are relatively compact subsets of H^0 [see (A4)j and Lemma 3.6(b)]. Thus

$$\langle g_j - h_j, \varphi_n \rangle_1 \to 0 \quad \text{as } a \to \infty \ (n = 1, 2, \ldots). \tag{3.80}$$

Since $\{g_j - h_j \colon a = 1, 2, \ldots\}$ is relatively compact in H^1, (3.80) implies $(g_j - h_j)_{\underline{N}^-} \to 0$ weakly in H^1, that is, $(g_j)_{\underline{N}^\perp} \to 0$ weakly in H^1. Now use (3.72) to write

$$\begin{aligned} \|g_j\|_1^2 &\simeq \langle g_j, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1 \\ &= \langle g_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1 + \langle g_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}^-}\rangle_1 \\ &\simeq \langle g_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1 \\ &= \langle h_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1 + \langle g_j - h_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1 \\ &\simeq \|(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\|_1^2 + \langle (g_j - h_j)_{\underline{N}}, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1. \end{aligned} \tag{3.81}$$

Now, by (3.77) and Lemma 3.6,

$$\begin{aligned} &\langle (g_j - h_j)_{\underline{N}}, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1 \\ &\quad\simeq -a\langle (\mathscr{D}^{-1}[(b(a\cdot) - \overline{b}) \cdot \nabla g_j])_{\underline{N}}, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1 \\ &\quad= -a\langle \mathscr{D}^{-1}[(b(a\cdot) - \overline{b}) \cdot \nabla g_j], (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1 \\ &\quad= a\langle (b(a\cdot) - \overline{b}) \cdot \nabla g_j, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_0 \\ &\quad= a\sum_{s=1}^{k} \left\langle \frac{\partial}{\partial x_s}\{(b_s(a\cdot) - \overline{b}_s) g_j\}, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} \right\rangle_0 \\ &\quad= -a\sum_{s=1}^{k} \left\langle (b_s(a\cdot) - \overline{b}_s), g_j^- \frac{\partial}{\partial x_s}(\mathscr{D}^{-1}(\beta_j - \overline{\beta})_j))_{\underline{N}} \right\rangle_0 \to 0, \end{aligned} \tag{3.82}$$

since $\{g_j^-(\partial/\partial x_s)(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} \colon a \geq 1\}$, $1 \leq s \leq k$, are relatively compact subsets of H^1. Relations (3.81) and (3.82) imply (3.71). □

REMARK 3.7.1. Assumption (A4)j is probably redundant, in the presence of assumptions (A1)–(A3), for the proof of the theorem above. But we are unable to dispense with it.

A set of sufficient conditions for (A4)j to hold are

$$\sup_{a \geq 1} \sup_x |\nabla g_j(x)| < \infty, \quad \lim_{a \to \infty} \nabla g_j(x) \text{ exists a.e.} \tag{3.83}$$

and

(3.84) $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}$ have bounded first, and second-order derivatives.

Indeed, (3.83) guarantees that g_j converges in H^1 to some q, say. One may then use the inequality

$$\|uv\|_1^2 \le c'\left(\|u\|_1^2\|v\|_\infty^2 + \|u\|_0^2\left(\sum_{s'=1}^{k}\left\|\frac{\partial v}{\partial x_{s'}}\right\|_\infty^2\right)\right), \tag{3.85}$$

with $u = g_j - q$ and $v = \partial/\partial x_s(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}$. One also has the more symmetric inequality,

$$\|uv\|_1^2 \le c'\big(\|u\|_1^2\|v\|_\infty^2 + \|u_\infty\|^2\|v\|_1^2\big). \tag{3.86}$$

It may be noted in this connection that the inequality (3.86) corrects a careless error in Bhattacharya and Götze [(1995), relation (4.86)]. Finally, it may be noted that (3.83), (3.84) hold in the examples in Section 6.

The next result deals with the case

$$(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} = 0. \tag{3.87}$$

We will make use of the following assumption, in addition to (A1)–(A3):

(3.88)(A5)j There exists a twice continuously differentiable solution $p \in H^1$ of the equation

$$(\overline{b} + \beta)\cdot\nabla p = \beta_j - \overline{\beta}_j.$$

Note that (A5)j says that $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$ belongs to the *range of* $\overline{S}$, so that (3.87) holds.

THEOREM 3.8. *Assume* (A1)–(A3), (A5)j. *Then*

$$D_{jj} \le \liminf_{a\to\infty} K_{jj} \le \limsup_{a\to\infty} K_{jj} < \infty. \tag{3.89}$$

PROOF. In view of (3.48) [see (3.70)], it is enough to show that

$$\limsup_{a\to\infty} a^2\|g_j\|_1^2 < \infty. \tag{3.90}$$

Letting p be as in (3.88) one has, by the last inequality in (3.64),

$$\begin{aligned}\|g_j\|_1^2 &= \langle g_j, (\mathscr{I} + aS_a)g_j\rangle_1\\ &= \langle g_j, \mathscr{D}^{-1}(b_j(a\cdot) - \overline{b_j})\rangle_1 + \langle g_j, \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)\rangle_1\\ &\le \frac{c_1\|g_j\|_1\|b_j\|_0}{a} + \langle g_j, \overline{S}p\rangle_1.\end{aligned} \tag{3.91}$$

Now

$$
\begin{aligned}
\langle g_j, \overline{S}p\rangle_1 &= \langle g_j, S_a p\rangle_1 - \langle g_j, (S_a - \overline{S})p\rangle_1 \\
&= -\langle S_a g_j, p\rangle_1 - \langle g_j, \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla p\rangle_1 \\
&= -\frac{1}{a}\langle -g_j + \mathscr{D}^{-1}(b_j(a\cdot) - \overline{b}_j) + \mathscr{D}^{-1}(\beta_j - \overline{\beta}_j), p\rangle_1 \\
&\quad - \langle g_j, \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla p\rangle_1 \\
&= \frac{1}{a}\langle g_j, p\rangle_1 + \frac{1}{a}\langle b_j(a\cdot) - \overline{b}_j, p\rangle_0 \\
&\quad - \frac{1}{a}\langle \overline{S}p, p\rangle_1 - \langle g_j, \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla p\rangle_1 .
\end{aligned} \tag{3.92}
$$

Since $\langle \overline{S}p, p\rangle_1 = 0$, and $p \in H^1$, (3.91) and (3.92) lead to

$$
\|g_j\|_1^2 \le \frac{c_2\|g_j\|_1}{a} + \frac{c_3}{a^2} + \left|\langle g_j, \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla p\rangle_1\right|. \tag{3.93}
$$

By Lemma 3.6(a),

$$
\begin{aligned}
&\left|\langle g_j, \mathscr{D}^{-1}(b(a\cdot) - \overline{b}) \cdot \nabla p\rangle_1\right| \\
&\quad = \left|\left\langle g_j, \sum_{s=1}^{k} (b_s(a\cdot) - \overline{b}_s)\frac{\partial p}{\partial x_s}\right\rangle_0\right| \\
&\quad = \left|\sum_{s=1}^{k}\left\langle g_j \frac{\partial p^-}{\partial x_s}, b_s(a\cdot) - \overline{b}_s\right\rangle_0\right| \le c_4\|g_j\|_1/a.
\end{aligned} \tag{3.94}
$$

The last inequality follows from (3.58) using the fact that [see (3.85)]

$$
\begin{aligned}
\left\| g_j \tfrac{\partial p^-}{\partial x_s}\right\|_1^2 &\le c'\left\{\|g_j\|_1^2 \left\|\frac{\partial p^-}{\partial x_s}\right\|_\infty^2 + \|g_j\|_0^2 \sum_{s'=1}^{k}\left\|\frac{\partial^2 p^-}{\partial x_{s'}\partial x_s}\right\|_\infty^2\right\} \\
&\le c_5\|g_j\|_1^2.
\end{aligned} \tag{3.95}
$$

From (3.93), (3.94), one derives the relation

$$
a^2\|g_j\|_1^2 \le c_6 a\|g_j\|_1 + c_7, \tag{3.96}
$$

where c_6 and c_7 do not depend on "a." It is clear from (3.96) that $\{a\|g_j\|_1 \colon a = 1, 2, \ldots\}$ is a bounded sequence, that is, (3.90) holds. □

REMARK 3.8.1. The assumption of boundedness of derivatives of p in (A5)j is probably redundant. In any case, it is satisfied in Example 2 of Section 6.

4. Speed of convergence to equilibrium of diffusions on a big torus. A crucial element in the analysis of the asymptotic behavior of multiscale diffusions with periodic coefficients, such as $X(t)$ in (3.39), is the estimation of the total variation distance between the distribution at large times t of the corresponding diffusion $\dot{X}(\cdot) := X(\cdot) \bmod a$ on the big torus $\mathscr{T}_a = \{x \bmod a: x \in \mathbb{R}^k\}$ and its equilibrium distribution uniformly with respect to all initial states of $\dot{X}(\cdot)$. To derive such an estimate we first obtain an analogue of a result of Fill (1991) [also see Diaconis and Stroock (1991) for the time-reversible case], which holds for general Markov processes in continuous time.

Let $U(t)$, $t \geq 0$, be a Markov process on a measurable state space $(M, \mathscr{M})$, having a transition probability density $r(t; x, y)$ with respect to a sigma-finite measure ν. Suppose r admits a unique invariant probability $\pi(dx) = \pi(x)\nu(dx)$. Let $\mathscr{L}^2 = \mathscr{L}^2(M, \pi)$ be the real Hilbert space of square integrable (w.r.t. π) functions on M and T_t $(t > 0)$ the semigroup of transition operators on $\mathscr{L}^2$,

$$(T_t f)(x) = \int f(y) r(t; x, y)\nu(dy), \qquad f \in \mathscr{L}^2. \tag{4.1}$$

Define also the transition probability density $q(t; x, y)$ of the *time-reversed Markov process,* by

$$q(t; x, y) = r(t; y, x)\pi(y)/\pi(x) \tag{4.2}$$

if $\pi(x) > 0$ [and arbitrarily, measurably, if $\pi(x) = 0$]. Let $\tilde{T}_t$, $t > 0$, denote the corresponding transition semigroup,

$$(\tilde{T}_t g)(x) = \int g(y) q(t; x, y)\nu(dy), \qquad g \in \mathscr{L}^2. \tag{4.3}$$

It is simple to check that $\tilde{T}_t$ is the *adjoint* of T_t, that is,

$$\langle T_t f, g\rangle = \langle f, \tilde{T}_t g\rangle, \qquad f, g \in \mathscr{L}^2, \tag{4.4}$$

where $\langle\ ,\ \rangle$ is the *inner product* on $\mathscr{L}^2$. Let B and $\tilde{B}$ denote the infinitesimal generators of the semigroups T_t $(t > 0)$ and $\tilde{T}_t$ $(t > 0)$, respectively, and $\mathbf{D}_B$, $\mathbf{D}_{\tilde{B}}$ their domains. Let $1^{\perp}$ denote the subspace of $\mathscr{L}^2$ orthogonal to constants and write $\|\cdot\|$ for the *norm* in $\mathscr{L}^2$.

PROPOSITION 4.1. *Assume that $\mathbf{D}_{\tilde{B}}$ is dense in $\mathscr{L}^2$, and define*

$$\lambda = \inf\{\langle -\tilde{B}f, f\rangle: f \in 1^{\perp} \cap \mathbf{D}_{\tilde{B}}, \|f\| = 1\}. \tag{4.5}$$

Then if $U(0)$ has a probability density η w.r.t. ν, the density η_t of $U(t)$ satisfies

$$\int |\eta_t(y) - \pi(y)|\nu(dy) \leq e^{-\lambda t}\|\psi_0\|, \tag{4.6}$$

where ψ_0 is given by

$$\psi_0(y) = \frac{\eta(y) - \pi(y)}{\pi(y)} \quad a.e., w.r.t.\ \pi(dy). \tag{4.7}$$

PROOF. Without loss of generality, assume $\|\psi_0\| < \infty$, that is, $\psi_0 \in 1^{\perp}$. Now if $g \in 1^{\perp} \cap \mathbf{D}_{\tilde{B}}$, then $\tilde{T}_t g \in 1^{\perp} \cap \mathbf{D}_{\tilde{B}}$ $\forall\, t > 0$ so that, by (4.5),

$$\begin{aligned} \frac{d}{dt}\|\tilde{T}_t g\|^2 &= \frac{d}{dt}\langle \tilde{T}_t g, \tilde{T}_t g\rangle = 2\langle \tilde{T}_t g, \tilde{B}\tilde{T}_t g\rangle \\ &\leq -2\lambda\|\tilde{T}_t g\|^2, \end{aligned} \tag{4.8}$$

leading to

$$\|\tilde{T}_t g\|^2 \leq e^{-2\lambda t}\|g\|^2, \qquad g \in 1^{\perp} \cap \mathbf{D}_{\tilde{B}}. \tag{4.9}$$

Note that $1^{\perp} \cap \mathbf{D}_{\tilde{B}}$ is dense in $1^{\perp}$, since $\mathbf{D}_{\tilde{B}}$ is dense in $\mathscr{L}^2$. Hence (4.9) holds for all $g \in 1^{\perp}$. Now one may write

$$\begin{aligned} \tilde{T}_t\left(\frac{\eta}{\pi}\right)(y) &= \int \frac{\eta(x)}{\pi(x)}\, q(t; y, x)\nu(dx) \\ &= \int \frac{\eta(x)}{\pi(x)}\, r(t; x, y)\frac{\pi(x)}{\pi(y)}\, \nu(dx) = \frac{\eta_t(y)}{\pi(y)}, \end{aligned} \tag{4.10}$$

which implies $\tilde{T}_t\psi_0 = \eta_t/\pi - 1$. Therefore, by the Cauchy–Schwarz inequality and (4.9),

$$\begin{aligned} \int |\eta_t(y) - \pi(y)|\nu(dy) &= \int \left|\frac{\eta_t(y)}{\pi(y)} - 1\right| \pi(y)\nu(dy) \\ &= \int \left|\tilde{T}_t\psi_0(y)\right| \pi(y)\nu(dy) \\ &\leq \|\tilde{T}_t\psi_0\| \leq e^{-\lambda t}\|\psi_0\|. \end{aligned} \tag{4.11}$$

□

REMARK 4.1.1. If B is *self-adjoint*, that is, if $\tilde{B} = B$, λ defined in (4.5) is the *spectral gap* of B. Note that in this case the spectrum of B lies on the negative half of the real-axis (in the complex plane), with 0 as the simple eigenvalue corresponding to the eigenspace of constants in $\mathscr{L}^2(M, \pi)$. The point of the rest of the spectrum closest to 0 is $-\lambda$, if $\lambda > 0$. If B is not self-adjoint then, assuming that the symmetric operator $B + \tilde{B}$ is closed with a domain dense in $\mathscr{L}^2(M, \pi)$, the quantity λ in (4.5) is the spectral gap of $\frac{1}{2}(B+\tilde{B})$. For notational purposes, we will often write λ_B for λ in (4.5).

The following simple lemma shows the change in λ that occurs under a change in the time scale.

LEMMA 4.2. *Assume the hypothesis of Proposition* 4.1 *and consider the Markov process* $V(t) := U(ct)$, $t \geq 0$.

(a) *Then* $V(\cdot)$ *has invariant probability* π *and for its infinitesimal generator* B_c, *say, one has*

$$\lambda_{B_c} := \inf\{\langle -\tilde{B}_c f, f\rangle \colon \|f\| = 1, f \in 1^{\perp} \cap \mathbf{D}_{\tilde{B}_c}\} = c\lambda_B. \tag{4.12}$$

(b) *Also, if* $V(0)$ *has a probability density* η *w.r.t.* ν, *and* $V(t)$ *has the corresponding density* η_t, *then one has*

$$\int_M |\eta_t(y) - \pi(y)|\nu(dy) \le \exp(-c\lambda_B t)\|\psi_0\|, \tag{4.13}$$

where $\psi_0(y) = (\eta_0(y) - \pi(y))/\pi(y)$.

PROOF. Clearly, $V(\cdot)$ has the same invariant probability as $U(\cdot)$. Also, the infinitesimal generator of $V(\cdot)$ is $B_c = cB$ (with domain $\mathbf{D}_{B_c} = \mathbf{D}_B$), so that $\tilde{B}_c = c\tilde{B}$ and λ_{B_c} is given by

$$\inf\{\langle -c\tilde{B}f, f\rangle : \|f\| = 1, f \in 1^\perp \cap \mathbf{D}_{\tilde{B}}\} = c\lambda_B. \tag{4.14}$$

This proves part (a). Part (b) follows from (4.7). □

We now apply this lemma to the scaled diffusion $\dot{Y}$ on the unit torus and its generator A_a on $\mathscr{L}^2(\mathscr{T}_1, dx)$ [see (3.42), (3.44)]. Recall that, under the divergence-free assumption in (3.40), dx is the unique invariant probability of $\dot{Y}$. The adjoint operator $\tilde{A}_a$ is then easily seen to be

$$\begin{aligned}\tilde{A}_a &= \frac{1}{2}\sum_{j,j'=1}^{k} D_{jj'}\frac{\partial^2}{\partial x_j \partial x_{j'}} - a(b(a\cdot) + \beta)\cdot\nabla \\ &= \mathscr{D} - a(b(a\cdot) + \beta)\cdot\nabla.\end{aligned} \tag{4.15}$$

Denote by $\overline{\lambda}$ the infimum in (4.5) for the case $B = A_a$, $\tilde{B} = \tilde{A}_a$. That is, $\overline{\lambda}$ is the spectral gap of $\frac{1}{2}(\mathscr{D} + a(b(a\cdot) + \beta)\cdot\nabla) + \frac{1}{2}(\mathscr{D} - a(b(\cdot) + \beta)\cdot\nabla) = \mathscr{D}$ on $\mathscr{L}^2(\mathscr{T}_1, dx)$.

PROPOSITION 4.3. *Under assumptions* (A1)–(A3) *in* (3.40), *writing* α_1 *for the smallest eigenvalue of the matrix* $((D_{jj'}))$, *and* $\lambda_1 = \min\{D_{jj}: 1 \le j \le k\}$, *one has*

$$2\pi^2\alpha_1 \le \overline{\lambda} \le 2\pi^2\lambda_1. \tag{4.16}$$

PROOF. Denote by $\mathbf{D}$ the domain of $\mathscr{D}$ on $\mathscr{L}^2(\mathscr{T}_1, dx)$. As before, let $\hat{f}$ denote the Fourier transform of f on $\mathscr{L}^2(\mathscr{T}_1, dx)$. Then one has

$$\begin{aligned}\overline{\lambda} &= \inf\{-\langle f, \mathscr{D}f\rangle : \|f\| = 1, f \in 1^\perp \cap \mathbf{D}\} \\ &= \inf\left\{2\pi^2 \sum_{r\in\mathbb{Z}^k\setminus\{\mathbf{0}\}} |\hat{f}(r)|^2\left(\sum_{j,j'} D_{jj'}r_j r_{j'}\right)\right\} \\ &\ge 2\pi^2 \inf\left\{\sum_{r\in\mathbb{Z}^k\setminus\{\mathbf{0}\}} |\hat{f}(r)|^2 \alpha_1 |r|^2\right\} \ge 2\pi^2\alpha_1.\end{aligned} \tag{4.17}$$

On the other hand, letting $f(x) = \sqrt{2}\cos 2\pi x_j$, one gets $-\langle f, \mathscr{D}f\rangle = 2\pi^2 D_{jj}$. Hence $\overline{\lambda} \le 2\pi^2\lambda_1$. □

By using Lemma 4.2, one arrives at the following corollary of Proposition 4.3. To state it, assume (A1)–(A3). Let L denote the generator of the diffusion $\dot{X}(t)$ on the big torus $\mathscr{T}_a = \{x \bmod a: x \in \mathbb{R}^k\}$, and let m denote the normalized Lebesgue measure or the *uniform distribution* on $\mathscr{T}_a$. Note that m is the unique invariant probability of $\dot{X}$ and that $\frac{1}{2}(L+\tilde{L}) = \mathscr{D}$ on $\mathscr{L}^2(\mathscr{T}_a, m)$. Let $\mathbf{D}$ denote the domain of $\mathscr{D}$ in $\mathscr{L}^2(\mathscr{T}_a, m)$.

COROLLARY 4.4. *Assume* (A1)–(A3) *in* (3.40). *Then the quantity* $\lambda_L := \inf\{-\langle f, \tilde{L}f\rangle: \|f\| = 1,\ f \in 1^{\perp} \cap \mathbf{D}_{\tilde{L}}\}$ *satisfies*

$$2\pi^2 \frac{\alpha_1}{a^2} \le \lambda_L \le \frac{2\pi^2}{a^2}\lambda_1, \tag{4.18}$$

where α_1, λ_1 *are as in Proposition* 4.3.

PROOF. First note that $V(t) := \dot{X}(a^2 t)$, $t \ge 0$, has the generator $a^2 L$ on $\mathscr{L}^2(\mathscr{T}_a, m)$. The generator A_a of $\dot{Y}(t) = V(t)/a$ has the same spectrum on $\mathscr{L}^2(\mathscr{T}_1, dx)$ as that of $V(t)$ on $\mathscr{L}^2(\mathscr{T}_a, m)$. Therefore, $\overline{\lambda} = \lambda_{a^2L} \in [c_1, c_2]$, where c_1, c_2 are as in (4.16). On the other hand, by Lemma 4.2, $\lambda_{a^2L} = a^2\lambda_L$. Hence $\lambda_L = 1/a^2 \lambda_{a^2L} \in [c_1/a^2, c_2/a^2]$. □

One of the main results of this section may now be stated and proved.

THEOREM 4.5. *Assume* (A1)–(A3) *in* (3.40), *and let* $p_a(t; x, y)$ *denote the transition probability density of* $\dot{X}(t)$ *with respect to Lebesgue measure on* $[0, a)^k$. *Then there exists a positive constant* c_5 *independent of* a *such that*

$$\sup_x \int_{[0,a)^k} \left| p_a(t; x, y) - \frac{1}{a^k} \right| dy \le c_5 a^{k/2} \exp\{-2\pi^2 \alpha_1 t/a^2\}, \tag{4.19}$$

α_1 *being the smallest eigenvalue of the matrix* $((D_{jj'}))$.

PROOF. By Corollary 4.4 and Proposition 4.1 one has, for every initial density η of $\dot{X}$,

$$\int_{[0,a)^k} \left| \eta_t(y) - \frac{1}{a^k} \right| dy \le \exp\left(\frac{-2\pi^2 \alpha_1 t}{a^2} \right) \|\psi_0\|, \tag{4.20}$$

where $\psi_0(y) = (\eta(y) - a^{-k})/a^{-k}$, and η_t is the density of $\dot{X}(t)$. Now

$$\begin{aligned} \|\psi_0\|^2 &= a^{2k} \int_{[0,a)^k} (\eta^2(y) + a^{-2k} - 2a^{-k}\eta(y)) a^{-k}\, dy \\ &= a^k \int_{[0,a)^k} \eta^2(y) dy - 1 \\ &\le a^k \sup\{\eta(y): y \in [0, a)^k\}. \end{aligned} \tag{4.21}$$

Since $p_a(t; x, y)$ is the density of $\dot{X}(t)$, when $\dot{X}(0)$ has the degenerate distribution δ_x, we will apply (4.20), (4.21) to $\eta(y) = p_a(1; x, y)$ and with t replaced by $t-1$ to get

$$\begin{aligned}(4.22)\qquad &\int_{[0,a)^k}\left|p_a(t;x,y)-\frac{1}{a^k}\right|dy\\ &\leq \left(a^k\sup\left\{p_a(1;x,y): y\in[0,a)^k\right\}\right)^{1/2}\exp\left\{-2\pi^2\alpha_1(t-1)/a^2\right\}.\end{aligned}$$

To estimate the supremum on the right side we apply a result of Aronson (1967), which implies that the transition probability density $f(1;x,y)$ of the process $X(t)$ satisfies

$$(4.23)\qquad f(1;x,y)\leq c'\exp\{-c|x-y|^2\},\qquad x,y\in\mathbb{R}^k,$$

where c and c' are positive constants not depending on a. Now

$$\begin{aligned}(4.24)\qquad p_a(1;x,y) &= \sum_{r\in\mathbb{Z}^k} f(1;x,y+ar),\qquad x,y\in[0,a)^k\\ &\leq c'\sum_{r\in\mathbb{Z}^k}\exp\{-c|x-y-ar|^2\}\leq c'',\end{aligned}$$

where c'' does not depend on a. Therefore, (4.22) and (4.24) lead to (4.19). □

REMARK 4.5.1. It follows from the above proof that the transition density $q_a(t;x,y)$, say, of $\dot{Y}(t)$ satisfies the inequality

$$(4.19)'\qquad \sup_x\int_{[0,1)^k}|q_a(t;x,y)-1|\,dy\leq c_5a^{k/2}\exp\{-2\pi^2\alpha_1 t\}.$$

REMARK 4.5.2. One may extend Theorem 4.5 by relaxing the assumptions (A1)–(A3) to the case of diffusions $X(t)$ with generators of the form

$$(4.25)\qquad L=\frac{1}{2}\sum_{j,j'=1}^{k}\frac{\partial}{\partial x_j}(D_{jj'}(x))\frac{\partial}{\partial x_{j'}}+\sum_{j=1}^{k}\{b_j(x)+\beta_j(x/a)\}\frac{\partial}{\partial x_j},$$

where the assumptions (A1), (A3) hold for b_j, β_j and a, but (A2) is replaced by

(A2)′ $((D_{jj'}(x)))$ is a (positive definite)-matrix valued continuously differentiable periodic function with period lattice $\mathbb{Z}^k$.

In this case the diffusion $\dot{X}(t)=X(t)\bmod a$ on the big torus $\mathscr{T}_a$ has again as its unique invariant probability the normalized Lebesgue measure $m=a^{-k}\,dx$, whose generator on $\mathscr{L}^2(\mathscr{T}_a,m)$ is L-restricted to periodic functions. Also, $\frac{1}{2}(L+\tilde{L})=\mathscr{D}_1:=\frac{1}{2}\sum_{j,j'}(\partial/\partial x_j)\,(D_{jj'}(x))\,(\partial/\partial x_{j'})$ is self-adjoint on $\mathscr{L}^2(\mathscr{T}_a,m)$ and has a spectral gap $O(1/a^2)$. This last statement is a consequence of the fact that for the generator A_a of $\dot{Y}(t):=\dot{X}(a^2t)/a$ one has $\frac{1}{2}(A_a+\tilde{A}_a)=\mathscr{D}_1$ on $\mathscr{L}^2(\mathscr{T}_1,dx)$, and the latter has a spectral gap independent of a. Thus under the hypotheses (A1), (A2)′, (A3) the transition probability density $p_a(t;x,y)$ of $\dot{X}(t)$ satisfies (4.19).

We next turn to a special class of diffusions with periodic diffusion coefficients whose drift terms are *not divergence free*. This is the class of one-dimensional multiscale diffusions with periodic coefficients. But, first, some general facts concerning diffusions on the *unit circle* $S^1 = \{x \bmod 1 : x \in \mathbb{R}^1\}$ are needed. For detailed derivations see Bhattacharya, Denker and Goswami (1999). Consider the one-dimensional Itô equation

$$Z(t) = Z(0) + \int_0^t \mu(Z(s))\,ds + \int_0^t \sigma(Z(s))\,dB(s), \tag{4.26}$$

where $\mu(\cdot)$, $\sigma(\cdot)$ are continuously differentiable periodic functions with period one, $\sigma^2(x) > 0\ \forall\, x$, $B(t)$ is a standard one-dimensional Brownian motion independent of $Z(0)$. The diffusion $\dot{Z}(t) := Z(t) \bmod 1$ on S^1 has a unique invariant probability with density π given by

$$\pi(x) = d\exp(I(0,x))/\sigma^2(x), \qquad I(0,x) := \int_0^x \frac{2\mu(y)}{\sigma^2(y)}\,dy, \tag{4.27}$$

provided one has

$$\int_0^1 \frac{\mu(y)}{\sigma^2(y)}\,dy = 0. \tag{4.28}$$

If (4.28) does not hold, then

$$\begin{aligned}\pi(x) = \frac{d'\exp(I(0,x))}{\sigma^2(x)}\bigg\{&\frac{\exp(I(0,1))}{\exp(I(0,1))-1}\int_0^1 \exp(-I(0,y))\,dy \\ &- \int_0^x \exp(-I(0,y))\,dy\bigg\}.\end{aligned} \tag{4.29}$$

The constant d in (4.27) is the normalizing constant, as is the constant d' in (4.29). The infinitesimal generator A of $\dot{Z}(t)$ on $\mathscr{L}^2(S^1,\pi)$ is $\frac{1}{2}\sigma^2(x)(d^2/dx^2) + \mu(x)(d/dx)$ acting on periodic functions. One can show that A is *self-adjoint*, that is, $A = \tilde{A}$, if and only if (4.28) holds. Write $\tilde{A}$ for the adjoint of A. Then, irrespective of whether A is self-adjoint or not, one can show on direct integration, using integration by parts and periodic boundary conditions [see Bhattacharya, Denker and Goswami (1999)] that

$$\begin{aligned}\langle -f, \tilde{A}f\rangle &= \frac{1}{2}\|\sigma(\cdot)f'\|^2 \qquad \forall\, f \in \mathbf{D}_{\tilde{A}}, \\ \lambda_A &:= \inf\Big\{-\langle f, \tilde{A}f\rangle : \|f\| = 1,\ f \in 1^\perp \cap \mathbf{D}_{\tilde{A}}\Big\} \\ &\ge \frac{1}{2M},\end{aligned} \tag{4.30}$$

where

$$\begin{aligned}M &:= \sup\Big\{\big(\sigma^2(y)\pi(y)\big)^{-1}\int_y^1 x\pi(x)\,dx : 0 \le y < 1\Big\} \\ &\le \Big(\min_y \sigma^2(y)\pi(y)\Big)^{-1}\Big(\max_y \pi(y)\Big)\Big/2.\end{aligned} \tag{4.31}$$

Now consider a general multiscale one-dimensional diffusion with periodic coefficients,

$$
\begin{aligned}
X(t) &= X(0) + \int_0^t \{b(X(s)) + \beta(X(s)/a)\}\,ds \\
&\qquad + \int_0^t \sigma(X(s))\,dB(s), \\
X(0) &= ax_0.
\end{aligned} \tag{4.32}
$$

Assume

(4.33)(B1) $b(\cdot)$, $\beta(\cdot)$, $\sigma(\cdot)$ are continuously differentiable and periodic with period one,

(4.33)(B2) $\sigma(x)$ does not vanish for any x,

(4.33)(B3) "a" *is a positive integer.*

Also, without any essential loss of generality, assume

(4.34)(B4) $\int_0^1 (b(x)/\sigma^2(x))\,dx = 0,$

by adding a constant to $\beta(\cdot)$ if necessary. As before, $\dot{X}(t) := X(t) \bmod a$ is a diffusion on the *big circle* $S_a^1 := \{x \bmod a\colon x \in \mathbb{R}^1\}$, which we identify with $[0, a)$ for purposes of integration. Let $\tilde{\pi}_a$ denote the unique invariant probability density of $\dot{X}(t)$. The infinitesimal generator of $\dot{X}(t)$ on $\mathscr{L}^2(S_a^1, \tilde{\pi}_a)$ is

$$
L = \frac{1}{2}\sigma^2(x)\frac{d^2}{dx^2} + \{b(x) + \beta(x/a)\}\frac{d}{dx} \tag{4.35}
$$

acting on periodic functions. The diffusion $Y(t) := X(a^2t)/a$ is governed by the Itô equation

$$
\begin{aligned}
Y(t) &= Y(0) + \int_0^t a\{b(aY(s)) + \beta(Y(s))\}\,ds + \int_0^t \sigma(aY(s))\,d\overline{B}(s), \\
Y(0) &= x_0,
\end{aligned} \tag{4.36}
$$

where $\overline{B}(t) := B(a^2t)/a$ is a standard Brownian motion. Also, $\dot{Y}(t) := Y(t) \bmod 1$ is a diffusion on the unit circle S^1 having the invariant probability density π_a related to the invariant density of $\dot{X}(t)$ by $\pi_a(y) = a\tilde{\pi}_a(ay)$. Note that the generator of $\dot{Y}(t)$ is given by

$$
A_a = \frac{1}{2}\sigma^2(ax)\frac{d^2}{dx^2} + a\{b(ax) + \beta(x)\}\frac{d}{dx}. \tag{4.37}
$$

Assume now that $\beta(\cdot)$ is bounded away from zero. Then, in the presence of (B4) in (4.34), the relation (4.28) does not hold for the drift of $\dot{Y}(t)$. Hence in this case the invariant density π_a is given by (4.29) with

$$
I(0, x) = a\int_0^x \frac{b(ay)}{\sigma^2(ay)}\,dy + a\int_0^x \frac{\beta(y)}{\sigma^2(ay)}\,dy, \tag{4.38}
$$

and the generator A_a is not self-adjoint. In order to estimate λ_{A_a} using (4.30), (4.31), assume $\beta(x) > 0\ \forall x$. [The case $\beta(x) < 0\ \forall\ x$ is entirely analogous.] Write

$$d_1 = \min_y \sigma^2(y), \qquad d_2 = \max_y \sigma^2(y), \qquad \delta = \int_0^1 |b(y)|\,dy,$$
$$\beta_* = \min_y \beta(y), \qquad \beta^* = \max_y \beta(y). \tag{4.39}$$

By direct calculation one may now show [Bhattacharya, Denker and Goswami (1999)]

$$\begin{aligned}
&\left(\frac{d_1}{2a\beta^*}\right)\exp(-4\delta/d_1)\left(1-\exp\left(\frac{-2a\beta^*}{d_1}\right)\right)\\
&\quad\le \frac{\sigma^2(ax)\pi_a(x)}{d'}\\
&\quad\le \left(\frac{d_2}{2a\beta_*}\right)\left[\exp\left((2\delta/d_1)+\left(1+\frac{d_2}{2a\beta_*}\right)\exp(4\delta/d_1)\right].
\end{aligned}\tag{4.40}$$

From (4.40), (4.30), (4.31), one arrives at

$$\lambda_{A_a} \ge d_1 \frac{\min_y \pi_a(y)}{\max_y \pi_a(y)} \ge c_6 > 0,$$

where c_6 is independent of "a." To get an upper bound, let $f(x) = \sin 2\pi x - \int \sin 2\pi(y)\pi_a(y)\,dy$ to get [see (4.30)] $\langle -f, \tilde{A}f\rangle = \langle -f, Af\rangle = \frac{1}{2}\sigma^2\|f'\|^2 \le c_6'\|f\|^2$ for some c_6' independent of a. Thus one obtains

$$c_6 \le \lambda_{A_a} \le c_6'. \tag{4.41}$$

For the generator L of $\dot{X}(t)$ one then has, by the same argument as given in the proof of Corollary 4.4,

$$\frac{c_6}{a^2} \le \lambda_L \le \frac{c_6'}{a^2}. \tag{4.42}$$

Using this together with the Aronson estimate (4.23), and the relation (4.24), as in the proof of Theorem 4.5, one arrives at the following result.

THEOREM 4.6. *Assume* (B1)–(B4) *in* (4.33), (4.34). *In addition, assume* $\beta(x) > 0$ *for all* x. *Then*:

(a) (4.42) *holds, and*

(b) *The* L^1*-distance between the transition probability density* $p_a(t; x, y)$ *of* $\dot{X}(t)$ *and its invariant density* $\tilde{\pi}_a(y)$ *is estimated by*

$$\sup_x \int_{[0,a)} \left|p_a(t;x,y) - \tilde{\pi}_a(y)\right| dy \le c_7 a^{1/2}\exp\{-c_7' t/a^2\}, \tag{4.43}$$

where c_7 *and* c_7' *are positive constants independent of* a.

The next result concerns the self-adjoint case. For this we assume that the diffusion coefficient $\sigma^2(\cdot)$ is a (positive) *constant* $\sigma^2 > 0$, so that (B4) in (4.34) becomes

$$(4.44)(\mathrm{B4})' \quad \int_0^1 b(x)\,dx = 0.$$

The generator A_a of $\dot{Y}(t)$ is then self-adjoint if and only if

$$(4.45)(\mathrm{B5}) \quad \int_0^1 \beta(x)\,dx = 0.$$

As stated earlier, the invariant probability density π_a of $\dot{Y}(t)$ in this case is given by (4.27), with $I(0,x) = 2a/\sigma^2\{\int_0^x b(ay)\,dy + \int_0^x \beta(y)\,dy\}$. A fairly straightforward calculation [see Bhattacharya, Denker and Goswami (1999)] yields

$$(4.46) \qquad \begin{aligned} \frac{\exp(-2\delta/\sigma^2)}{d}\pi_a(x) &\le \exp\left(\frac{2a\theta^*}{\sigma^2}\right), \\ \exp\left(\frac{2\delta/\sigma^2)}{d}\right)\pi_a(x) &\ge \exp\left(\frac{2a\theta_*}{\sigma^2}\right), \end{aligned}$$

where $\delta = \int_0^1 |b(x)|\,dx$ and

$$(4.47) \qquad \theta_* = \min_x \int_0^x \beta(y)\,dy, \qquad \theta^* = \max_x \int_0^x \beta(y)\,dy.$$

From (4.46) one gets

$$(4.48) \qquad \frac{\max_x \pi_a(x)}{\min_x \pi_a(x)} \le \exp\left(\frac{4\delta}{\sigma^2}\right)\exp\Big(2a(\theta^* - \theta_*)/\sigma^2\Big).$$

Using this in (4.30) one obtains

$$(4.49) \qquad \lambda_{A_a} \ge \left(\sigma^2 \exp\left(\frac{-4\delta}{\sigma^2}\right)\right)\exp\left(\frac{-2a(\theta^* - \theta_*)}{\sigma^2}\right),$$

so that the spectral gap λ_L of the generator L of the diffusion $\dot{X}(t)$ on the big circle $S_a^1 = \{x \bmod a \colon x \in \mathbb{R}^1\}$ is estimated by

$$(4.50) \qquad \lambda_L = \frac{1}{a^2}\lambda_{A_a} \ge \left(\sigma^2\exp\left(\frac{-4\delta}{\sigma^2}\right)\right)\frac{1}{a^2}\exp(\frac{-2a(\theta^*-\theta_*)}{\sigma^2}\bigg).$$

Proceeding as in the proof of Theorem 4.5, or Theorem 4.6, one arrives at the following estimate of the speed of convergence to equilibrium in this case.

THEOREM 4.7. *In the self-adjoint case* (B4)$'$, (B5) *with constant* $\sigma^2 > 0$, *the* L^1*-distance between the transition probability density of* $\dot{X}(t)$ *and its equilibrium density* $\tilde{\pi}_a$ *is estimated by*

$$(4.51) \qquad \begin{aligned} &\sup_x \int_{[0,a)} |p_a(t;x,y) - \tilde{\pi}_a(y)|\,dy \\ &\quad \le c_8 a^{1/2}\exp\{c_9 a/2\}\exp\{-(c_8'/a^2)\exp(-c_9 a)t\} \end{aligned}$$

where c_8, c_8' $c_9 \equiv 2(\theta^* - \theta_*)/\sigma^2$ *are positive constants independent of* "a."

REMARK 4.7.1. The speed of convergence to equilibrium as estimated in Theorem 4.7 is exceedingly slow and, going by it, the process may take times $t \gg (a^2 \log a) \exp\{c_9 a\}$ to be close to equilibrium. This is in contrast to the nonself-adjoint case considered in Theorem 4.6, where for times $t \gg a^2 \log a$, the process is near equilibrium. The estimate (4.51) concerns the "worst case" scenario such as holds under the hypothesis of part (b) of Theorem 4.9 below. On the other hand, under the hypothesis of part (a) of Theorem 4.9, the speed of convergence is shown to be as fast as in the case of Theorem 4.6.

An important difference in the asymptotic behavior between the two classes of diffusions considered in Theorems 4.6 and 4.7 is provided by the following result.

PROPOSITION 4.8. (a) *Under the hypothesis of Theorem* 4.6, *the invariant probability density* π_a *of the diffusion* $\dot{Y}(t) = \dot{X}(a^2 t)/a$ *on* S^1 *is bounded away from zero uniformly in* a.

(*b*) *Assume the hypothesis of Theorem* 4.7. *If the "potential function"* $\psi(x) := \int_0^x \beta(y)\,dy$ *has its maximum attained at a single point* x^*, *then the invariant probability* $\pi_a(x)\,dx$ *converges weakly to the point mass* δ_{x^*} *as* $a \to \infty$. *More generally, if the maximum of* ψ *is attained at a finite number of points, then all weak limit points of* $\pi_a(x)\,dx$ *have support contained in this finite set.*

PROOF. Part (a) follows from the estimate $\min_y \pi_a(y)/\max_y \pi_a(y) \geq c_6/d_1$ [see (4.41)]. To prove part (b), let $x_1, x_2, \dots, x_m$ be the distinct points in $[0, 1)$ where the maximum of ψ is attained. Since $|a \int_0^x b(ay)\,dy| = |\int_0^{ax} b(y)\,dy| = |\int_{[ax]}^{ax} b(y)\,dy| \leq \delta \equiv \int_0^1 |b(y)|\,dy$ [in view of (4.44)], it is simple to check that $\pi_a(x)/\max_y \pi_a(y) \to 0$ if $x \notin \{x_1, x_2, \dots, x_m\}$. It follows that for any $\varepsilon > 0$, however small, the π_a-probability of the ε–neighborhood of the finite set $\{x_1, x_2, \dots, x_m\}$ goes to one as $a \to \infty$. □

The next result provides a dichotomy of the class of time-reversible diffusions on the big circle into (1) those for which the speed of convergence to equilibrium is the same as in the nonself-adjoint case considered in Theorem 4.6 and (2) those for which the convergence is exceedingly slow, requiring times $t \gg e^{ca}$. For this we need a result of Holley, Kusuoka and Stroock (1989) specialized to the circle. Consider the self-adjoint case with $b(\cdot) \equiv 0$, that is,

$$A_a = \frac{1}{2}\sigma^2 \frac{d^2}{dy^2} + a\beta(y)\frac{d}{dy}, \qquad \int_0^1 \beta(y)\,dy = 0. \tag{4.52}$$

In this case, according to Theorem 1.14 in Holley, Kusuoka and Stroock (1989), there exist constants $c^{(1)} > 0$, $c^{(2)} \geq 0$, independent of a, such that

$$c^{(1)} a^{-2} \exp\{-c^{(2)} a\} \leq \lambda_{A_a} \leq c^{(1)} a^6 \exp\{-c^{(2)} a\}. \tag{4.53}$$

The constant $c^{(2)}$ is computed as follows. Let $U(x) = (\theta^* - \psi(x))/\sigma^2$, where θ^* is given by (4.47) and $\psi(x) = \int_0^x \beta(y)\,dy$. For any given pair of points x, y in S^1 and a continuous curve γ joining x and y, let $H_\gamma(x, y)$ denote the maximum value of U on (the image of) γ. Define $H(x, y)$ to be the infimum over all such γ. Then

$$c^{(2)} = \sup_{x,y}\{H(x, y) - U(x) - U(y)\}. \tag{4.54}$$

THEOREM 4.9. *Consider the self-adjoint case* (B4)′, (B5) *with* $\sigma^2 > 0$, *and assume that the number of zeros of* β *on* $[0, 1)$ *is finite.*

(a) *If* $\psi(x) \equiv \int_0^x \beta(y)\,dy$ *has a unique maximum, then there exists a positive constant* $c^{(3)}$ *independent of* a *such that*

$$\lambda_L \geq \frac{c^{(3)}}{a^2}. \tag{4.55}$$

(b) *If* ψ *has more than one maximum then there exist positive constants* $c^{(2)}$, $c^{(4)}$, $c^{(5)}$ *independent of* a, *with* $c^{(2)}$ *as in* (4.54), *such that*

$$c^{(4)}a^{-5}\exp\{-c^{(2)}a\} \leq \lambda_L \leq c^{(5)}a^4\exp\{-c^{(2)}a\}. \tag{4.56}$$

PROOF. (a) Consider the generator A_a of $\dot{Y}(t)$ on $\mathscr{L}^2(S^1, \pi_a)$. Let π denote the probability density on $[0, 1]$ given by

$$\pi(x) = d'\exp\left\{\frac{2a}{\sigma^2}\psi(x)\right\}, \qquad 0 \leq x \leq 1, \tag{4.57}$$

d' being the normalizing constant. Since $|\int_0^x ab(ay)\,dy| \leq \delta \equiv \int_0^1 |b(y)|\,dy$ [see (4.44)] one has

$$\pi_a(x) \leq \exp(4\delta/\sigma^2)\pi(x), \qquad x \in [0, 1]. \tag{4.58}$$

Now let $f \in \mathbf{D}_{\tilde{A}_a} \cap 1^{\perp}$. Then, writing $c_{11} = \exp(8\delta/\sigma^2)$,

$$\begin{aligned}
\|f\|^2 &= \tfrac{1}{2}\int_0^1\int_0^1 (f(x) - f(y))^2\pi_a(x)\pi_a(y)\,dx\,dy \\
&\leq \tfrac{1}{2}c_{11}\int_0^1\int_0^1 (f(x) - f(y))^2\pi(x)\pi(y)\,dx\,dy \\
&= \tfrac{1}{2}c_{11}\left(\iint_{\{x<y\}} + \iint_{\{y<x\}}\right)(f(x) - f(y))^2\pi(x)\pi(y)\,dx\,dy \\
&= c_{11}\iint_{\{x<y\}} (f(x) - f(y))^2\pi(x)\pi(y)\,dx\,dy \qquad (4.59)\\
&= c_{11}\int_0^1\int_0^y (f(x) - f(y))^2\pi(x)\pi(y)\,dx\,dy \\
&= c_{11}\int_0^1\int_0^y \left(\int_x^y f'(z)\,dz\right)^2\pi(x)\pi(y)\,dx\,dy
\end{aligned}$$

$$\leq c_{11}\int_0^1\int_0^y (y-x)\left\{\int_x^y (f'(z))^2\,dz\right\}\pi(x)\pi(y)\,dx\,dy$$

$$= c_{11}\int_0^1 (f'(z))^2\left[\int_z^1\left\{\int_0^z (y-x)\pi(x)\,dx\right\}\pi(y)\,dy\right]dz.$$

By translation, if necessary, we may assume that the minimum of ψ is at 0, and the maximum is at x^*. Then $\psi(x)$ increases from $x = 0$ to $x = x^*$ and decreases from $x = x^*$ to $x = 1$. One thus has, for $z \leq x^*$,

$$\begin{aligned}(4.60)\qquad &\int_z^1\left\{\int_0^z (y-x)\pi(x)\,dx\right\}\pi(y)\,dy\\ &\leq \int_z^1\left\{\int_0^z (y-x)\pi(z)\,dx\right\}\pi(y)\,dy\\ &= \pi(z)\int_z^1\left\{\int_0^z (y-x)\,dx\right\}\pi(y)\,dy\\ &= \pi(z)\int_z^1\left(yz-\frac{z^2}{2}\right)\pi(y)\,dy\\ &\leq \pi(z)z.\end{aligned}$$

For $z > x^*$,

$$\begin{aligned}(4.61)\qquad &\int_z^1\left\{\int_0^z (y-x)\pi(x)\,dx\right\}\pi(y)\,dy\\ &= \int_0^z\left\{\int_z^1 (y-x)\pi(y)\,dy\right\}\pi(x)\,dx\\ &\leq \int_0^z\left\{\int_z^1 (y-x)\pi(z)\,dy\right\}\pi(x)\,dx\\ &= \pi(z)\int_0^z\left\{\frac{1-z^2}{2}-x(1-z)\right\}\pi(x)\,dx \leq \pi(z)\left(\frac{1-z^2}{2}\right).\end{aligned}$$

Using (4.60), (4.61) in (4.59) we get [see (4.30)]

$$\|f\|^2 \leq c_{11}\int_0^1 (f'(z))^2\pi(z)\,dz = \frac{c_{11}}{\sigma^2}\langle -f, \tilde{A}f\rangle, \tag{4.62}$$

so that $\lambda_{A_a} \geq \sigma^2/c_{11}$ and, as a consequence, the spectral gap λ_L of the generator L of $\dot{X}(t)$ satisfies

$$L = \frac{1}{a^2}\lambda_{A_a} \geq \frac{c_{12}}{a^2}, \tag{4.63}$$

where $c_{12} \equiv \sigma^2/c_{11}$ does not depend on a.

For part (b), first make the additional assumption $b(\cdot) \equiv 0$. Let x be a point where ψ attains its absolute maximum value θ^* and let y be another maximum of ψ. Then $U(x) = 0$ and y is a minimum of U, $U(y) \geq 0$. Every continuous curve γ joining x and y contains (in its range) a maximum of U, that is, $H_\gamma(x, y) \geq U(z) - U(x) - U(y) \equiv U(z) - U(y) > 0$, where $U(z) = \min\{U(z_1), U(z_2)\}$, and z_1, z_2 are the two points on the two arcs joining x and y at which U attains its maximum values. Hence $c^{(2)}$ defined by (4.54) is positive, and (4.56) is just (4.53) in this case. For the general case under (b), one shows, as in part (a) above, that the ratio of the invariant density to that with $b(\cdot) \equiv 0$ is bounded away from zero and infinity. Hence, using (4.30), one derives (4.53) with $c^{(1)}$ replaced by a smaller constant $c^{(4)}$ on the left and by a larger constant $c^{(5)}$ on the right. Since $\lambda_L = \lambda_{A_a}/a^2$, (4.56) follows. □

Using Lemma 4.2 and an estimate of Aronson (1967), exactly as in the proof of Theorem 4.6, we derive the following theorem.

THEOREM 4.10. *In addition to the hypothesis of Theorem 4.7, assume that the potential function $\psi(x) = \int_0^x \beta(y)\,dy$ on $[0, 1)$ has a unique maximum and a unique minimum. Then*

$$\sup_x \int_{[0,a)} \left|p_a(t; x, y) - \tilde{\pi}_a(y)\right| dy \leq c_{10} a^{1/2} \exp(-c'_{10} t/a^2), \tag{4.64}$$

where c_{10} and c'_{10} are independent of a.

EXAMPLE 4.10.1. Let $b(\cdot)$ be arbitrary (periodic and differentiable) satisfying $\int_0^1 b(y)\,dy = 0$. Let $\beta(x) = \pi \cos \pi x$, so that $\psi(x) = \sin \pi x$. Then, on the unit circle, the *flow* $dx(t)/dt = \beta(x(t))$ has one *stable equilibrium* $x = \frac{1}{2}$, where ψ is maximum, and one *unstable equilibrium* $x = 0$, where ψ is minimum. Thus Theorem 4.9 applies. One may expect a *relatively fast convergence* to equilibrium here for $\dot{Y}(t)$, since from every initial point $x \neq 0$ the flow approaches the stable equilibrium fast.

EXAMPLE 4.10.2. Let $b(\cdot)$ be arbitrary, as above, and $\beta(x) = 4\pi \cos 4\pi x$. Then $\psi(x) = \sin 4\pi x$ attains its maximum value at $x = \frac{1}{8}$ and $x = \frac{5}{8}$; these are the stable equilibria of the flow $dx(t)/dt = \beta(x(t))$. The minimum value of $\psi(x)$ is attained at $x = \frac{3}{8}$ and $x = \frac{7}{8}$; these are the unstable equilibria of the flow. In this case one would expect a relatively slow convergence to equilibrium of $\dot{Y}(t)$ starting from any point x, and Theorem 4.9(b) applies. The spectral gap in this case is exponentially small, namely, $O(e^{-\alpha a})$, for some $\alpha > 0$ which does not depend on a, and a slow convergence to equilibrium such as provided for by Theorem 4.7 results.

5. Final phase of asymptotics.

5.1. *The divergence-free case.* Consider again the multiscale diffusion on $\mathbb{R}^k$ with periodic coefficients as given in (3.39), namely,

$$X(t) = X(0) + \int_0^t \left\{b(X(s)) + \beta(X(s)/a)\right\} ds + \sigma B(t), \tag{5.1}$$

and its scaled version $Y(t) = X(a^2t)/a$ satisfying the Itô equation (4.36). Recall the diffusion $\dot{X}(t) = X(t) \bmod a$ on the big torus $\mathscr{T}_a$ and the diffusion $\dot{Y}(t) = Y(t) \bmod 1$ on the unit torus $\mathscr{T}_1$. We first derive a simple consequence of Theorem 4.5. To state it, write E_x for expectation under $\dot{X}(0) = x$ or $\dot{Y}(0) = x$, as the case may be, and E as the expectation under equilibrium, that is, the invariant distribution. Also, "cov_x" denotes covariance under $\dot{X}(0) = x$ [or $\dot{Y}(0) = x$], while "cov" denotes covariance under equilibrium. As before, $\|f\|_\infty$ denotes the supremum of $|f(x)|$ over all x for some measurable real-valued function f. The constants c_i c_i' below are positive and independent of a.

PROPOSITION 5.1. *Assume* (A1)–(A3) *in* (3.40). *There exist positive constants* c_i, c_i' $(i = 13, 14)$ *not depending on "a" such that for all bounded measurable* f, g *on* $\mathscr{T}_a$, *one has*

$$\begin{aligned} &\big|E_x f(\dot{X}(t)) - Ef(\dot{X}(t))\big| \\ &\qquad \le c_{13}a^{k/2}\|f\|_\infty \exp\{-c_{13}'t/a^2\}, \qquad t \ge 0, \\ &\big|\text{cov}_x\{f(\dot{X}(s)), g(\dot{X}(t))\}\big| \\ &\qquad \le c_{14}a^{k/2}\|f\|_\infty\|g\|_\infty \exp\{-c_{13}'(t-s)/a^2\}, \qquad 0 \le s \le t. \end{aligned} \tag{5.2}$$

Similarly, for all bounded measurable f, g *on* $\mathscr{T}_1$, *one has*

$$\begin{aligned} &\big|E_y f(\dot{Y}(t)) - Ef(\dot{Y}(t))\big| \\ &\qquad \le c_{13}a^{k/2}\|f\|_\infty \exp\{-c_{13}'t\}, \qquad t \ge 0, \\ &\big|\text{cov}_y\{f(\dot{Y}(s)), g(\dot{Y}(t))\}\big| \\ &\qquad \le c_{14}a^{k/2}\|f\|_\infty\|g\|_\infty \exp\{-c_{13}'(t-s)\}, \qquad 0 \le s \le t. \end{aligned} \tag{5.3}$$

PROOF. The first relation in (5.2) is an immediate consequence of Theorem 4.5 with $c_{13} = c_5$ and $c_{13}' = 2\pi^2\alpha_1$. For the second relation, use conditioning given $\sigma\{\dot{X}(u) \colon 0 \le u \le s\}$ to write

$$\begin{aligned} \text{cov}_x\{f(\dot{X}(s)), g(\dot{X}(t))\} = E_x\big[\{f(\dot{X}(s)) - E_x f(\dot{X}(s))\} \\ \times \{E_z g(\dot{X}(t-s))_{z=\dot{X}(s)} - E_x g(\dot{X}(t))\}\big]. \end{aligned} \tag{5.4}$$

Applying the first inequality in (5.2) to the second factor in (5.4), one gets the second relation in (5.2). Relations (5.3) follow from those in (5.2), noting that, for functions f, g on $\mathscr{T}_1$, $f(\dot{Y}(t)) = f(\dot{X}(a^2t)/a)$, $g(\dot{Y}(t)) = g(\dot{X}(a^2t)/a)$ so that (5.2) may be applied to functions $x \to f(x/a)$, $g(x/a)$ with times a^2t, a^2s in place of t, s. □

An immediate consequence of (5.2) and (5.3) is

$$
\begin{aligned}
&\left|\operatorname{cov}\{f(\dot{X}(s)), g(\dot{X}(t))\}\right| \\
&\qquad \le c'_{14} a^{k/2} \|f\|_\infty \|g\|_\infty \exp\{-c'_{13}(t-s)/a^2\}, \\
&\left|\operatorname{cov}\{f(\dot{Y}(s)), g(\dot{Y}(t))\}\right| \\
&\qquad \le c'_{14} a^{k/2} \|f\|_\infty \|g\|_\infty \exp\{-c'_{13}(t-s)\}, \qquad 0 \le s \le t.
\end{aligned} \tag{5.5}
$$

For this, simply replace cov_x, E_x in (5.4) by cov and E, respectively.

We are now ready to prove one of the main results of this article. Below, $\to_{\mathscr{L}}$ denotes convergence in law or distribution.

THEOREM 5.2. *Assume* (A1)–(A3) *in* (3.40). *Also assume that* (A4)j *in* (3.68) *holds for* $1 \le j \le k_1$ *for some* $k_1 \le k$. *If, in addition, the assumption*

(5.6)(A6) $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}$, $1 \le j \le k_1$, *are linearly independent elements of* H^1, *holds, then for* $t \gg a^2(\log a)^2$, *that is, as*

$$a \to \infty, \qquad \frac{t}{a^2(\log a)^2} \to \infty, \tag{5.7}$$

one has

$$\left\{\frac{1}{a\sqrt{t}}(X_j(t) - X_j(0) - t(\overline{b}_j + \overline{\beta}_j)) \colon 1 \le j \le k_1\right\} \to_{\mathscr{L}} \mathscr{N}(0, \Sigma_1), \tag{5.8}$$

no matter what the initial state $X(0)$ *may be. Here* $\Sigma_1 = ((\overline{\sigma}_{ij}))$ *is given by*

$$\overline{\sigma}_{ij} = 2\langle(\mathscr{D}^{-1}(\beta_i - \overline{\beta}_i))_{\underline{N}}, (\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}}\rangle_1, \qquad 1 \le i, j \le k_1. \tag{5.9}$$

PROOF. One needs to prove that an arbitrary non-zero linear combination of the random variables in (5.8), with coefficients ξ_j, say, converges in distribution to a normal law $\mathscr{N}(0, \gamma)$ where $\gamma = \sum_{i,j=1}^{k_1} \overline{\sigma}_{ij}\xi_i\xi_j$. To avoid a somewhat messy notation, we will prove the result for the case $\xi_j = 1$, $\xi_i = 0$ for $i \ne j$. The proof in the general case is entirely analogous. We will prove that for times t satisfying (5.7),

$$\frac{1}{a\sqrt{t}}\big(X_j(t) - X_j(0) - t(\overline{b}_j + \overline{\beta}_j)\big) \to_{\mathscr{L}} \mathscr{N}(0, \overline{\sigma}_{jj}), \tag{5.10}$$

under the assumptions (A1)–(A4) and $(\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j))_{\underline{N}} \ne 0$. This assertion is equivalent to

$$\frac{1}{a\sqrt{t}}\big(Y_j(t) - Y_j(0) - at(\overline{b}_j + \overline{\beta}_j)\big) \to_{\mathscr{L}} \mathscr{N}(0, \overline{\sigma}_{jj}), \tag{5.11}$$

under the same assumptions, but for times $t \gg (\log a)^2$, that is,

$$a \to \infty, \qquad \frac{t}{(\log a)^2} \to \infty. \tag{5.12}$$

Recalling that the left side of (5.11) equals [see (3.43)]

$$\frac{1}{\sqrt{t}}\int_0^t \{b_j(a\dot{Y}(s)) + \beta_j(\dot{Y}(s)) - \overline{b}_j - \overline{\beta}_j\}\, ds + \frac{(\sigma\overline{B}(t))_j}{a\sqrt{t}}, \tag{5.13}$$

where $(\sigma\overline{B}(t))_j$ is the jth component of the vector $\sigma\overline{B}(t)$, (5.11) is equivalent to

$$\frac{1}{\sqrt{t}}\int_0^t \{b_j(a\dot{Y}(s)) + \beta_j(\dot{Y}(s)) - \overline{b}_j - \overline{\beta}_j\} ds \to_{\mathscr{L}} \mathscr{N}(0, \overline{\sigma}_{jj}). \tag{5.14}$$

By Itô's lemma, the left side of (5.14) equals [see (3.45), (3.46)]

$$\frac{1}{\sqrt{t}}\left\{g_j(\dot{Y}(t)) - g_j(\dot{Y}(0))\right\} - \frac{1}{\sqrt{t}}\int_0^t \operatorname{grad} g_j(\dot{Y}(s))\sigma\, d\overline{B}(s). \tag{5.15}$$

Therefore, one has

$$\begin{aligned} &\frac{1}{\sqrt{t}}\int_0^t \{b_j(a\dot{Y}(s)) + \beta_j(\dot{Y}(s)) - \overline{b}_j - \overline{\beta}_j\}\, ds \\ &\qquad - \frac{1}{\sqrt{t}}\{g_j(\dot{Y}(t)) - g_j(\dot{Y}(0))\} \\ &\qquad = -\frac{1}{\sqrt{t}}\int_0^t \operatorname{grad} g_j(\dot{Y}(s))\sigma\, d\overline{B}(s). \end{aligned} \tag{5.16}$$

Assume first that $\dot{Y}(0)$ has the *uniform* (equilibrium) *distribution*. Then, by Lemma 3.5,

$$E\left(\frac{1}{\sqrt{t}}\{g_j(\dot{Y}(t)) - g_j(\dot{Y}(0))\}\right)^2 \le \frac{2}{t}\|g_j\|_0^2 \to 0 \quad \text{as } t \to \infty. \tag{5.17}$$

Letting $t = \varphi(a) \gg (\log a)^2$, $\varphi(a)$ integral, one may express the left side of (5.14) as

$$\begin{aligned} &\sum_{r=1}^{\varphi(a)} V_r, \\ &V_r := \frac{1}{\sqrt{\varphi(a)}}\int_{r-1}^{r} \{b_j(a\dot{Y}(s)) + \beta_j(\dot{Y}(s)) - \overline{b}_j - \overline{\beta}_j\}\, ds \ (1 \le r \le \varphi(a)). \end{aligned} \tag{5.18}$$

In view of (5.16), (5.17) and Theorem 3.7, one has

$$EV_r = 0, \quad E\left(\sum_{r=1}^{\varphi(a)} V_r\right)^2 \to \overline{\sigma}_{jj} \qquad \text{as } a \to \infty. \tag{5.19}$$

We will prove the asymptotic normality of $\sum_{r=1}^{\varphi(a)} V_r$ by representing it approximately as the sum of a number of nearly independent block sums. For this purpose, define

$$\begin{aligned} &\delta \equiv \delta(a) := \varphi(a)/(\log a)^2, \qquad \eta \equiv \eta(a) := [\delta^{1/8}\log a], \\ &\psi \equiv \psi(a) := [\delta^{3/8}\log a], \qquad m \equiv m(a) := \left[\frac{\varphi(a)}{\eta + \psi}\right], \end{aligned} \tag{5.20}$$

where $[z]$ denotes the integer part of z. Consider the "big" block sums

$$(5.21)\quad Z_1 = \sum_{r=1}^{\psi(a)} V_r, \qquad Z_2 = \sum_{r=1}^{\psi(a)} V_{r+\psi+\eta}, \ldots, \qquad Z_m = \sum_{r=1}^{\psi(a)} V_{r+(m-1)(\psi+\eta)}$$

and the "little" block sums

$$(5.22)\quad \begin{aligned} \xi_1 &= \sum_{r=1}^{\eta(a)} V_{r+\psi}, \\ \xi_2 &= \sum_{r=1}^{\eta(a)} V_{r+2\psi+\eta}, \ldots, \xi_m = \sum_{r=1}^{\eta(a)} V_{r+m(\psi+\eta)-\eta}. \end{aligned}$$

Then

$$(5.23)\quad \sum_{r=1}^{\varphi(a)} V_r \simeq \sum_{r=1}^{m(a)} Z_r + \sum_{r=1}^{m(a)} \xi_r.$$

To verify this, note that the right side of (5.23) is missing at most $\psi + \eta$ terms V_r from the left. By applying the convergence in (5.19), but with $\psi + \eta$ in place of φ, it follows that the expected value of the squared sum of the missing terms is no more than $O((\psi + \eta)/\varphi(a)) \to 0$. Next, by a similar argument,

$$(5.24)\quad E\xi_r^2 \le c_{15}\eta/\varphi(a), \qquad \sum_{r=1}^{m} E\xi_r^2 \le c'_{15} m\eta/\varphi(a) \to 0.$$

Also, for $r' \ge 1$,

$$(5.25)\quad \begin{aligned} E\xi_r\xi_{r+r'} &= \sum_{i=1}^{\eta}\sum_{i'=1}^{\eta} E\bigl(V_{i+\psi}V_{i'+(r'+1)(\psi+\eta)-\eta}\bigr) \\ &= \frac{1}{\varphi(a)} \sum_{i,\,i'=1}^{\eta} \int_0^1 \langle h, T_{i'-i-1+r'(\psi+\eta)+s} f\rangle\, ds, \end{aligned}$$

where $h(y) := b_j(ay) + \beta_j(y) - \overline{b}_j - \overline{\beta}_j$, $f(y) = E_y \int_0^1 h(\dot{Y}(s))\, ds$, and T_u is the transition operator of $\dot{Y}$ $(u \ge 0)$. By Proposition 5.1, the integral on the right in (5.25) is bounded in magnitude by $c_{16}\|h\|_\infty^2 a^{k/2} \exp\{-c'_{13} r'\psi\}$, so that

$$(5.26)\quad \begin{aligned} |E\xi_r\xi_{r+r'}| &\le c'_{16} \frac{\eta^2 a^{k/2}}{\varphi(a)} \exp\{-c'_{13} r'\psi\}, \\ \sum_{r=1}^{m}\sum_{r'=1}^{m-r} |E\xi_r\xi_{r+r'}| &\le c_{17} \frac{m\eta^2 a^{k/2}}{\varphi(a)} \exp\{-c'_{13}\psi\} \to 0 \quad \text{as } a \to \infty. \end{aligned}$$

Thus $E(\sum_{r=1}^m \xi_r)^2 \to 0$ as $a \to \infty$, and we get from (5.23) the relation

$$(5.27)\quad \sum_{r=1}^{\varphi(a)} V_r \simeq \sum_{r=1}^{m} Z_r.$$

We next show that the characteristic function of the right side of (5.27) is asymptotically the same as that of the sum of m i.i.d. random variables, each having the same distribution as Z_1. For this write, for any fixed $\xi \in \mathbb{R}^1$, $f(y) := E[\exp\{i\xi Z_1\} \mid \dot{Y}(0) = y]$, to derive the following approximation using Proposition 5.1:

$$
\begin{aligned}
&\left|E\left(\exp\left\{i\xi \sum_{r=1}^{m} Z_r\right\}\right)\right. \\
&\qquad \left. - E\left(\exp\left\{i\xi \sum_{r=1}^{m-1} Z_r\right\}\right)E\left(\exp\{i\xi Z_m\}\right)\right| \\
&\quad = \left|E\left[\exp\left\{i\xi \sum_{r=1}^{m-1} Z_r\right\}\left(T_\eta f(\dot{Y}(r')) - \overline{f}\right)\right]\right| \\
&\qquad \times \left(r' := (m-1)(\psi + \eta) - \eta\right) \\
&\quad \le c_{18} a^{k/2} \exp\{-c'_{13}\eta\}.
\end{aligned} \tag{5.28}
$$

Telescoping this process one arrives at

$$
\begin{aligned}
&\left|E\left(\exp\left\{i\xi \sum_{r=1}^{m} Z_r\right\}\right) - \prod_{r=1}^{m} E\left(\exp\{i\xi Z_r\}\right)\right| \\
&\qquad \le c_{18} m a^{k/2} \exp\{-c'_{13}\eta\} \to 0 \quad \text{as } a \to \infty.
\end{aligned} \tag{5.29}
$$

We will now verify Lindeberg's condition for the sum $m = m(a)$ i.i.d. random variables Z_r. Note that, for each $\varepsilon > 0$,

$$
\sum_{r=1}^{m} E\left(Z_r^2 \mathbb{1}_{\{|Z_r| > \varepsilon\}}\right) = m E Z_1^2 \mathbb{1}_{\{|Z_1| > \varepsilon\}} = 0 \tag{5.30}
$$

for all sufficiently large a, since $|Z_1| \le c\psi/\sqrt{\varphi(a)} \to 0$ as $a \to \infty$. This proves (5.11) under the invariant initial distribution [of $\dot{Y}(0)$].

It remains to consider the case of an arbitrary initial distribution [of $\dot{Y}(0)$]. Let $t = \varphi(a) \gg (\log a)^2$, $s = \psi(a) = \delta^{3/8} \log a$ as in (5.20). Write

$$
\begin{aligned}
\frac{Y_j(t) - t(\overline{b}_j + \overline{\beta}_j)}{a\sqrt{t}} &= \frac{Y_j(s) - s(\overline{b}_j + \overline{\beta}_j)}{a\sqrt{t}} \\
&\qquad + \frac{Y_j(t) - Y_j(s) - (t-s)(\overline{b}_j + \overline{\beta}_j)}{a\sqrt{t}}.
\end{aligned} \tag{5.31}
$$

Using the integral representation of $Y(\cdot)$ [see (3.43), (5.13)], it follows that

$$
E\left(\frac{Y_j(s) - s(\overline{b}_j + \overline{\beta}_j)}{a\sqrt{t}}\right)^2 \le \frac{c_{19} s^2}{t} \to 0 \quad \text{as } a \to \infty. \tag{5.32}
$$

Now the conditional distribution of $Y(t) - Y(s)$, given $\{Y(u)\colon 0 \le u \le s\}$, depends only on $\dot{Y}(s)$ and is, in fact, the same as the distribution of $Y(t-s) - z$ with an initial state $z = \dot{Y}(s)$. Therefore, by Theorem 4.5 and Proposition 4.3

(see Remark 4.5.1), the total variation distance between the distribution of $Y(t) - Y(s)$ under an arbitrary $\dot{Y}(0)$ and that under a uniformly distributed $\dot{Y}(0)$ goes to zero as $a \to \infty$. Using this fact and (5.32) in (5.31), it follows that the left side of (5.31) converges in law to $\mathscr{N}(0, \overline{\sigma}_{jj})$ as $a \to \infty$, no matter what the initial distribution may be. □

REMARK 5.2.1. Theorem 5.2 may be strengthened to the following functional form under the given hypothesis: *for any given sequence of integers* $\varphi(a)$ *such that*

$$\frac{\varphi(a)}{a^2(\log a)^2} \to \infty \quad \textit{as } a \to \infty,$$

one has

$$\frac{1}{a\sqrt{\varphi(a)}}\left\{X_j(\varphi(a)t) - X_j(0) - \varphi(a)t(\overline{b}_j + \overline{\beta}_j)\colon 1 \le j \le k_1\right\}_{t\ge 0}$$

$$\to_{\mathscr{L}} \{W(t)\}_{t\ge 0} \quad \textit{as } a \to \infty,$$

where $\{W(t)\}_{t\ge 0}$ *is a Brownian motion on* $\mathscr{C}([0,\infty) \to \mathbb{R}^k)$ *having the dispersion coefficients* (5.9). To prove this, one first uses the negligibility of ξ_r's to reduce the problem to that of the asymptotic distribution of the polygonal process corresponding to the partial sums of Z_r $(r \ge 1)$. We then show that the total variation distance between the distribution of $(Z_1, Z_2, \dots, Z_m)$ under equilibrium and the product measure G_a^m, where G_a is the distribution of Z_1, goes to zero as $m \to \infty$. To establish the latter, consider a real-valued bounded measurable function f on $\mathbb{R}^m$ and show, by using the Markov property, Proposition 5.1, and telescoping [as in (5.28), (5.29)], that

$$\left|Ef(Z_1, Z_2, \dots, Z_m) - \int f\,dG_a^m\right| \le c'_{18} m \|f\|_\infty a^{k/2} \exp\{-c'_{13}\eta\}.$$

Hence the proof of the functional limit theorem stated above boils down to that for triangular arrays of i.i.d. summands, making use of Lindeberg's condition (5.30) [Billingsley (1968), page 77]. The argument when $\dot{X}(0)$ or $\dot{Y}(0)$ is not in equilibrium remains the same as given at the end of the proof of Theorem 5.2.

The next result complements Theorem 5.2 by analyzing the case where $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$ belongs to the range of $\overline{S} = \mathscr{D}^{-1}(\overline{b} + \beta) \cdot \nabla$ for certain j's. Dramatic differences in the growth of dispersion in the two cases (see Theorems 3.7, 3.8) lead to significantly different scalings in Theorems 5.2 and 5.3.

For the statement of the following theorem, recall that $K = ((K_{jj'}))$ where $K_{jj'} = 2a^2\langle g_j, g_{j'}\rangle_1 + D_{jj'}$ [see (3.48)]. For a set of k_2 coordinates, $1 \le j \le k_2$, let K_2 denote the $k_2 \times k_2$ submatrix of K comprising elements belonging to the first k_2 rows and to the first k_2 columns of K. Also write I_{k_2} for the $k_2 \times k_2$ identity matrix.

THEOREM 5.3. *In addition to* (A1)–(A3) *in* (3.40), *assume that* (A5)j *in* (3.88) *holds for* $1 \le j \le k_2$ *and that the functions* p_j *in* H^1 *satisfying*

$(\overline{b}+\beta)\cdot\nabla p_j = \beta_j - \overline{\beta}_j$, $1 \le j \le k_2$, *are linearly independent. Then for* $t \gg a^4(\log a)^2$ *one has*

$$\frac{1}{\sqrt{t}} K_2^{-1/2}(\{X_j(t) - X_j(0) - t(\overline{b}_j + \overline{\beta}_j)\}_{1\le j\le k_2}) \to_{\mathscr{L}} \mathscr{N}(0, I_{k_2}) \tag{5.33}$$

as $a \to \infty$, *whatever be the initial distribution.*

PROOF. As in the proof of Theorem 5.2, we will prove that for $t \gg a^4(\log a)^2$ one has

$$\frac{1}{\sqrt{t K_{jj}}}(X_j(t) - X_j(0) - t(\overline{b}_j + \overline{\beta}_j)) \to_{\mathscr{L}} \mathscr{N}(0,1), \qquad 1 \le j \le k_2, \tag{5.34}$$

as $a \to \infty$. The proof for an arbitrary linear combination of X'_js $(1 \le j \le k_2)$ is analogous.

First assume $\dot{X}(0)$ has the uniform (equilibrium) distribution. Let w_j be the solution in H^1 of the equation

$$Lw_j = b_j + \beta_j(\cdot/a) - \overline{b}_j - \overline{\beta}_j, \tag{5.35}$$

where L is the generator of $\dot{X}(t)$ on $\mathscr{L}^2(\mathscr{T}_a, a^{-k}dx)$. Then $w_j(x) = a^2 g_j(x/a)$, g_j being as in (3.45). By Itô's lemma, with $t = \varphi(a) \gg a^4(\log a)^2$, $\varphi(a)$ integral,

$$\begin{aligned}
&\frac{1}{\sqrt{tK_{jj}}}(X_j(t) - X_j(0) - t(\overline{b}_j + \overline{\beta}_j)) \\
&\quad = \frac{1}{\sqrt{tK_{jj}}}\Big[w_j(\dot{X}(t)) - w_j(\dot{X}(0)) \\
&\qquad\qquad - \int_0^t \operatorname{grad} w_j(\dot{X}(s))\sigma\, dB(s) + (\sigma B(t))_j\Big] \\
&\quad = \sum_{r=1}^{\varphi(a)} V_r,
\end{aligned} \tag{5.36}$$

$$\begin{aligned}
V_r := \frac{1}{\sqrt{\varphi(a)K_{jj}}}\Big[\int_{r-1}^{r}\Big\{b_j(\dot{X}(s)) + \beta_j(\dot{X}(s)/a) - \overline{b}_j - \overline{\beta}_j\Big\}\, ds \\
+ \big(\sigma B(r) - \sigma B(r-1)\big)_j\Big].
\end{aligned}$$

Since $Ew_j^2(\dot{X}(t)) = Ew_j^2(\dot{X}(0)) = a^4 E g_j^2(\dot{Y}(0)) \le c_{20}a^2$ by Theorem 3.8 (also see Lemma 3.5), one has

$$E\Big(\frac{1}{\sqrt{tK_{jj}}}(w_j(\dot{X}(t)) - w_j(\dot{X}(0)))\Big)^2 \to 0 \quad \text{as } a \to \infty. \tag{5.37}$$

Therefore,

$$
\begin{aligned}
&\operatorname{var}\Bigl(\sum_{r=1}^{\varphi(a)} V_r\Bigr)\\
&\equiv E\Bigl(\sum_{r=1}^{\varphi(a)} V_r\Bigr)^2 \qquad (5.38)\\
&\to \lim_{a\to\infty} \operatorname{var}\biggl(\frac{1}{\sqrt{tK_{jj}}}\biggl\{\int_0^t \operatorname{grad} w_j(\dot{X}(s))\sigma B(s) + (\sigma B(t))_j\biggr\}\biggr) = 1.
\end{aligned}
$$

Indeed, the variance on the right is exactly 1. We will now prove the asymptotic normality of $\sum_{r=1}^{\varphi(a)} V_r$ by representing it approximately as the sum of a number of nearly independent block sums. For this purpose, define

$$
\begin{aligned}
&\delta = \varphi(a)/(a^4(\log a)^2), \qquad \eta = \bigl[\delta^{1/8}a^2\log a\bigr],\\
&\psi = \bigl[\delta^{3/8}a^2\log a\bigr], \qquad m = \biggl[\frac{\varphi(a)}{\eta+\psi}\biggr].
\end{aligned}
\tag{5.39}
$$

Define the "big" and "little" block sums as in (5.21), (5.22), respectively, but with V_r as in (5.36). The rest of the proof that $\sum_{r=1}^{\varphi(a)} V_r \to_{\mathscr{L}} \mathscr{N}(0,1)$ is entirely analogous to the corresponding proof for Theorem 5.2. The only changes are in replacing ψ by ψ/a^2 and η by η/a^2 in the exponents in (5.26), and (5.28), (5.29) respectively. The reason for this adjustment is that we are directly considering the $X(\cdot)$ process, and not its scaled version $Y(\cdot)$. To check that the Lindeberg condition holds, as $a \to \infty$, for the sum of m i.i.d. random variables each having the same distribution as Z_1, write

$$
\begin{aligned}
U_1 &= \int_0^{\psi}\Bigl\{b_j(\dot{X}(s)/a) + \beta_j(\dot{X}(s)/a) - \bar{b}_j - \bar{\beta}_j\Bigr\}\,ds,\\
U_1' &= \Bigl(\int_0^{\psi}\sigma\,dB(s)\Bigr)_j.
\end{aligned}
\tag{5.40}
$$

Then $Z_1^2 \le (2/\varphi(a))(U_1^2 + U_1'^2)$, so that

$$
\begin{aligned}
mE\bigl(Z_1^2\,\mathbb{1}_{\{|Z_1|>\varepsilon\}}\bigr) &\le \frac{2m}{\varphi(a)}E\bigl(U_1^2\,\mathbb{1}_{\{|U_1|>(\varepsilon/2)\sqrt{\varphi(a)}\}}\bigr)\\
&\quad+\frac{2m}{\varphi(a)}E\Bigl(U_1'^2\,\mathbb{1}_{\{|U_1'|>(\varepsilon/2)\sqrt{\varphi(a)}\}}\Bigr)\\
&\quad+\frac{2m}{\varphi(a)}E\Bigl(U_1^2\,\mathbb{1}_{\{|U_1'|>(\varepsilon/2)\sqrt{\varphi(a)}\}}\Bigr)\\
&\quad+\frac{2m}{\varphi(a)}E\Bigl(U_1'^2\,\mathbb{1}_{\{|U_1|>\varepsilon/2\sqrt{\varphi(a)}\}}\Bigr).
\end{aligned}
\tag{5.41}
$$

Since $|U_1| \le c\psi \le (\varepsilon/2)\sqrt{\varphi(a)}$ for all sufficiently large a, the first and last terms on the right side of (5.41) vanish for large a. Also, the second term is estimated by

$$(5.42)\qquad \begin{aligned} &\frac{2m}{\varphi(a)}E\Big(U_1'^2\,\mathbb{1}_{\{|U_1'|>(\varepsilon/2)\sqrt{\varphi(a)}\}}\Big)\\ &\quad\le \frac{2m}{\varphi(a)}(EU_1'^4)^{1/2}\Big(P\Big(|U_1'|>\frac{\varepsilon}{2}\sqrt{\varphi(a)}\Big)\Big)^{1/2}\\ &\quad\le \frac{2m}{\varphi(a)}(c_{21}\psi)\big(EU_1'^2/\varepsilon^2\varphi(a)\big)^{1/2}\le c_{21}'\frac{m\psi^{3/2}}{\varepsilon\varphi^{3/2}(a)}\to 0\end{aligned}$$

as $a\to\infty$. Finally, the third term on the right side of (5.41) is estimated by

$$(5.43)\qquad c_{22}\frac{m}{\varphi(a)}\psi^2P\Big(|U_1'|>\frac{\varepsilon}{2}\sqrt{\varphi(a)}\Big)^{1/2}\le c_{22}'\frac{m\psi^2}{\varphi(a)}\exp\Big\{-c_{23}\varepsilon^2\frac{\varphi}{\psi}\Big\}\to 0$$

as $a\to\infty$. We have used an exponential bound for the tail probability of a Gaussian random variable for the last inequality. This completes the proof when $\dot{X}(0)$ has the uniform distribution on $\mathscr{T}_a$.

The proof of (5.34) under an arbitrary (initial) distribution of $\dot{X}(0)$ is analogous to that given for Theorem 5.2. Once again one takes $t=\varphi(a)$, $s=\psi(a)$ as in (5.39) and makes use of Theorem 4.5 and the fact that $s^2/t\to 0$ as $a\to\infty$. □

REMARK 5.3.1. An example in the next section shows that the time scale for large scale asymptotics in Theorem 5.2 cannot be smaller than $t\gg a^2$ in general. The time scale $t\gg a^4(\log a)^2$ in Theorem 5.3, however, seems too large. To understand the nature of technical difficulty encountered in trying to bring down the scale, one may attempt a "more straightforward" martingale CLT using the first equality in (5.36). Leaving aside the term $R:=(tK_{jj})^{-1/2}[w_j(\dot{X}(t))-w_j(\dot{X}(0))]$, one needs to show that the CLT applies to the term M, say, involving the stochastic integral [including $(\sigma B(t))_j$]. The proof of the conditional Lindeberg condition [see, e.g., Bhattacharya and Waymire (1990), page 508] requires an estimate of the growth of the stochastic integrand grad w_j beyond its second moment. Even under equilibrium, we are unable to obtain a precise estimate of this growth. Note that grad $w_j(x)=a(\text{grad}\, g_j)(x/a)$. Thus under equilibrium $\|w^2\|_1^2\equiv a^2\|g_j\|_1^2$ is bounded by Theorem 3.8. If one could show that grad w_j is bounded in *sup norm* (not just in L^2) then, at least under equilibrium, the martingale term M is asymptotically normal for $t\gg a^2$. Similarly, under equilibrium, the L^2-norm of $w_j(x)\equiv a^2g_j(x/a)$ is of the order $O(a^2)$, so that $R\to 0$ in probability for $t\gg a^2$. However, a direct estimate of the sup norm of w_j using the identity $w_j(x)=-\int_0^\infty T_s(b_j(\cdot)+\beta_j(\cdot/a)-\overline{b}_j-\overline{\beta}_j)(x)\,ds$ (with T_s as the transition operator of $\dot{X}$), yields a value of order larger than $a^2\log a$, if one applies the rate of decay of the integrand given by (5.2). Thus, if $\dot{X}(0)$ is an arbitrary state, then to show $R\to 0$ in probability using this last estimate, we need $\sqrt{t}\gg a^2\log a$. If one could show that ag_j and a grad g_j are *bounded in sup norm*, then the above arguments would lead to an improvement of the time scale in Theorem 5.3 to $t \gg a^2 \log a$. It is worthwhile to write this out as a theorem.

THEOREM 5.4. *If, in addition to the hypothesis in Theorem* 5.3, *one assumes that the functions* ag_j *and* a grad g_j $(1 \le j \le k_2)$ *are bounded in* sup norm, *then* (5.33) *holds for* $t \gg a^2 \log a$.

REMARK 5.4.1. Functional versions of Theorems 5.3 and 5.4 may be derived by arguments analogous to those given under Remark 5.2.1.

5.2. *Final phase of asymptotics for vector fields which are not divergence free—the one-dimensional case.* Since the general case of multiscale diffusions with periodic nondivergence-free vector fields is intractable, we will consider only one-dimensional diffusions. This will provide some insight into the nature and diversity of phenomena in the general case. Let $X(\cdot)$ be a one-dimensional diffusion governed by the Itô equation (2.1) whose coefficients satisfy the assumptions (B1)–(B3) in (4.33). Following the treatment of these processes given in the last part of Section 4, we will consider the nonself-adjoint and the self-adjoint cases separately. Once again, without any essential loss of generality, we will assume that (B4) in (4.34) also holds, that is, $\int_0^1 (b(x)/\sigma^2(x))\,dx = 0$. Using the notation in Section 4, let $\tilde{\pi}_a$ and π_a denote the invariant probability densities of $\dot{X}(t) \equiv X(t) \bmod a$, and $\dot{Y}(t) \equiv Y(t) \bmod 1$ $(Y(t) := X(a^2 t)/a)$, respectively. Write

$$\overline{b} = \int_0^a b(x)\tilde{\pi}_a(x)\,dx, \qquad \overline{\beta} = \int_0^a \beta(x/a)\tilde{\pi}_a(x)\,dx. \tag{5.44}$$

Note that unlike the case where $\tilde{\pi}_a$ and π_a are uniform densities, in general $\overline{\beta} \ne \int_0^a \beta(x)\tilde{\pi}_a(x)\,dx$. Let L be the generator of $\dot{X}(t)$, as given by (4.35), and let h be the unique mean-zero solution in $L^2(S_a^1, \tilde{\pi}_a)$ of

$$Lh(x) = b(x) + \beta(x/a) - \overline{b} - \overline{\beta}. \tag{5.45}$$

Define

$$\theta^2 = \int_0^a \sigma^2(x)(h'(x) - 1)^2 \tilde{\pi}_a(x)\,dx. \tag{5.46}$$

Note that, by Itô's lemma,

$$\begin{aligned} X(t) - X(0) - t(\overline{b} + \overline{\beta}) &= h(\dot{X}(t)) - h(\dot{X}(0)) \\ &\quad + \int_0^t \sigma(\dot{X}(s))\{1 - h'(\dot{X}(s))\}\,dB(s), \end{aligned} \tag{5.47}$$

so that, for a fixed a, θ^2 is the variance of the asymptotic normal distribution of $t^{-1/2}(X(t) - X(0) - t(\overline{b} + \overline{\beta}))$. The proof of the following theorem is based on Theorem 4.6 and a direct computation of h and is given in detail in Bhattacharya, Denker and Goswami (1999).

THEOREM 5.5. *In addition to* (B1)–(B4) *in* (4.33), (4.34), *assume that* $\beta(\cdot)$ *is bounded away from zero. Then for* $t \gg a^2 \log a$ *one has, for all* $X(0)$,

$$\frac{X(t) - X(0) - t(\overline{b} + \overline{\beta})}{\theta\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}(0, 1) \quad \text{as } a \to \infty. \tag{5.48}$$

Here $\theta = \theta(a)$ *is bounded away from zero and infinity.*

Note that the time scale as well as the growth in dispersion here are comparable to those in Theorem 5.3. The next theorem is dramatically different in these respects. For the case $\int_0^1 \beta(y)\,dy = 0$, write

$$\theta^* = \max_x \int_0^x \beta(y)\,dy, \qquad \theta_* = \min_x \int_0^x \beta(y)\,dy. \tag{5.49}$$

THEOREM 5.6. *In addition to* (B1)–(B4) *in* (4.33), (4.34), *assume that* $\sigma(\cdot)$ *is a constant,* $\beta(\cdot)$ *is nonconstant and* $\int_0^1 \beta(y)dy = 0$.

(a) *Then* $\theta = \theta(a)$ *defined by* (5.46) *goes to zero exponentially fast as* $a \to \infty$.

(b) *If* $t \gg a^2 \exp\{(18a/\sigma^2(\theta^* - \theta_*)\}$, *one has, for arbitrary initial states* $X(0) = ax_0$,

$$\frac{X(t) - ax_0}{\sigma a \theta\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}(0, 1) \quad \text{as } a \to \infty. \tag{5.50}$$

(c) *If* $t \ll a^{-4} \exp\{(2a/\sigma^2)(\theta^* - \theta_*)\}$ *then* (5.50) *does not hold, unless* $X(t) - ax_0 \to 0$ *in probability.*

Part (a) follows from a direct computation of θ in this case, while part (b) uses this computation of θ and Theorem 4.7 [see Bhattacharya, Denker and Goswami (1999) for details]. For part (c), one shows that, for the given range of t, $a\theta\sqrt{t} \to 0$ [Bhattacharya, Denkar and Goswami (1999)]. Therefore, if (5.50) is to hold, $(X(t) - ax)/ax$ must go to zero in probability.

REMARK 5.6.1. With regard to the centering in (5.50), it may be shown that $\overline{b} + \overline{\beta} = 0$ for all a.

REMARK 5.6.2. Part (a) of Theorem 5.6 shows that the asymptotic variance parameter or dispersion per unit time goes to zero exponentially fast, in dramatic contrast to the divergence-free case (Theorems 5.2, 5.3) and the one-dimensional nonself-adjoint case (Theorem 5.5). A heuristic explanation is that the invariant probability π_a either converges to a point mass or at least gets confined to a small set in the limit, as $a \to \infty$.

REMARK 5.6.3. The exponentially large time needed for the final Gaussian phase to take hold, as indicated in parts (b), (c) of Theorem 5.6, is not really due to the slow convergence to equilibrium as estimated in Theorem 4.7 for the "worst case scenario." Note that Theorem 5.6 holds under the hypothesis of Theorem 4.9 where relatively speedy convergence to equilibrium takes place.

REMARK 5.6.4. Consider the possibility of $X(t) - ax_0$ converging to 0 in probability as indicated in part (c) of Theorem 5.6. For the scaled version of $X(t)$, namely, the $Y(t)$ process, this means $Y(t) \to x_0$ as $a \to \infty$, $t \to \infty$, but $t \ll a^{-6} \exp\{(2a/\sigma^2)(\theta^* - \theta_*)\}$. Under the hypothesis of Theorem 5.6, this is impossible unless $\psi(x) = \int_0^x \beta(y)\,dy$ has a maximum at x_0. To show this, consider x_0 where ψ does not have a maximum. By using standard formulas [see, e.g., Bhattacharya and Waymire (1990), page 422, equation (10.12)], it is not difficult to check that if $x_1 < x_0 < x_2$ are such that ψ does not have a maximum in $[x_1, x_2]$, then the exit time τ of $Y(\cdot)$ from (x_1, x_2) has an expected value $E_y\tau$ which satisfies $\sup\{E_y\tau\colon y \in [x_1, x_2], a \geq 1\} < \infty$.

REMARK 5.6.5. Although Theorems 5.5, 5.6 address the case of one-dimensional multiscale diffusions with periodic coefficients, they point to a range of diverse behavior in the final phase for the general multidimensional nondivergence-free case. Theorems 4.7, 4.10 similarly indicate widely different time scales for approach to equilibrium on the big torus for the latter case. For example, if the invariant density π_a of the scaled diffusion $\dot{Y}(t) = \dot{X}(a^2t)/a$ on $\mathscr{T}_1$ converges to a point mass as $a \to \infty$, one would expect the dispersion (per unit time) in the final phase to decay as $a \to \infty$ and the time scale for the final Gaussian approximation to be very large. This ought to be true, for example, in the case that the diffusion matrix is $\sigma^2 I_k$ (σ^2 a positive constant) and $b(x) = \operatorname{grad}\psi_1(x)$, $\beta(x) = \operatorname{grad}\psi_2(x)$, where (1) the "potential" functions ψ_1 and ψ_2 are periodic with period lattice $\mathbb{Z}^k$, (2) $\psi_1(\mathbf{n}) = 0 = \psi_2(\mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^k$ and (3) on $[0,1)^k$, ψ_2 has a unique maximum at x^*. In this case, the invariant probability $d(a)\exp\{(2/\sigma^2)(\psi_1(ay) + a\psi_2(y))\}\,dy$ of $\dot{Y}(t)$ converges to the point mass $\delta_{x^*}(dy)$ as $a \to \infty$; one would expect for this case an analog of Theorem 5.6 to hold.

6. Examples. In this section we provide two examples to illustrate the theory presented in Sections 2–5. Example 6.1 satisfies the hypotheses of Theorems 4.5 and 5.2, while Example 6.2 satisfies the hypotheses of Theorems 4.5 and 5.4.

EXAMPLE 6.1. Consider the diffusion on $\mathbb{R}^2$ defined by

$$\begin{aligned} dX_1(t) &= \{c_0 + c_1\sin(2\pi(X_2(t)) + c_2\cos(2\pi X_2(t)/a)\}\,dt + dB_1(t),\\ dX_2(t) &= dB_2(t), \qquad X(0) = ax = (ax_1, ax_2). \end{aligned} \tag{6.1}$$

Assume c_1, c_2 are nonzero and

$$\sin(2\pi x_2) = 0. \tag{6.2}$$

Table 1 shows the phase changes that occur along with their time scales. Here $\mathscr{L}(U)$ denotes the law, or distribution of a random variable U. The sign $\pm$ in (ii) is $+$ or $-$ according as $\cos 2\pi x_2 = -1$ or $+1$.

Table 1 is a modification of one derived in Bhattacharya and Götze (1995) under the initial condition $X(0) = x = (x_1, x_2)$. The latter initial condition implies $X(0)/a \to 0$ as $a \to \infty$, thereby essentially requiring that the process start at the origin. This issue becomes more important in the case (6.2) fails, as we show in a modification of Table 1 in Remark 6.1.1 below. The first row in the table is a consequence of Theorem 2.1(c), and Theorem 2.2. An alternative derivation may be given along the lines of case (i) of Example 6.2 below. To derive the second row, write

$$\begin{aligned}(6.3)\qquad &\frac{X_1(t)-X_1(0)-t(c_0+c_2\cos 2\pi x_2)}{t^2/a^2}\\ &= \frac{c_1}{t^2/a^2}\int_0^t \sin(2\pi(ax_2+B_2(s)))\,ds\\ &\quad+\frac{c_2}{t^2/a^2}\int_0^t\left\{\cos\left(2\pi\left(x_2+\frac{B_2(s)}{a}\right)\right)-\cos 2\pi x_2\right\}ds+\frac{B_1(t)}{t^2/a^2}.\end{aligned}$$

Note that $a^{4/3} \ll t \Leftrightarrow t^2/a^2 \gg t^{1/2}$. Therefore, $B_1(t)/(t^2/a^2) \to 0$ in probability. Now use Itô's lemma to get

$$\begin{aligned}(6.4)\qquad &\int_0^t \sin(2\pi(ax_2+B_2(s)))\,ds\\ &= -\frac{1}{2\pi^2}\{\sin(2\pi(ax_2+B_2(t)))-\sin 2\pi a x_2\}\\ &\quad+\frac{1}{\pi}\int_0^t \cos(2\pi(ax_2+B_2(s)))\,dB_2(s).\end{aligned}$$

From this it is clear that the first term on the right in (6.3) goes to zero. It remains to show that the middle term on the right in (6.3) has the asymptotic distribution $\mathscr{L}(\pm 2c_2\pi^2\int_0^1 B_2^2(s)\,ds)$. By a Taylor expansion,

$$\begin{aligned}(6.5)\qquad &\cos\left(2\pi\left(x_2+\frac{B_2(s)}{a}\right)\right)-\cos 2\pi x_2\\ &= -\frac{2\pi B_2(s)}{a}\sin 2\pi x_2-\frac{4\pi^2}{2a^2}B_2^2(s)\cos 2\pi x_2+\frac{8\pi^3}{6a^3}B_2^3(s)\theta,\end{aligned}$$

TABLE 1
Phase changes in Example 6.1

Time scale	**Asymptotic law**
(1) $1 \ll t \ll a^{4/3}$	$\dfrac{X_1(t)-X_1(0)-t(c_0+c_2\cos 2\pi x_2)}{\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}(0, 1+c_1^2/2\pi^2)$
(2) $a^{4/3} \ll t \ll a^2$	$\dfrac{X_1(t)-X_1(0)-t(c_0+c_2\cos 2\pi x_2)}{t^2/a^2} \to_{\mathscr{L}} \mathscr{L}\left(\pm 2c_2\pi^2\int_0^1 B_2^2(s)\,ds\right)$
(3) $t/a^2 \to r > 0$	$\dfrac{X_1(t)-X_1(0)-tc_0}{t} \to_{\mathscr{L}} \mathscr{L}\left(\dfrac{c_2}{r}\int_0^r \cos(2\pi(x_2+B_2(s)))\,ds\right)$
(4) $t \gg a^2$	$\dfrac{X_1(t)-X_1(0)-tc_0}{a\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}(0, c_2^2/2\pi^2)$

where θ is a random variable, $|\theta| \le 1$. The first term on the right is zero by assumption (6.2). Also, $E|B_2^3(s)| \le cs^{3/2}$, so that

$$\frac{c_2}{t^2/a^2}\left|\int_0^t \frac{8\pi^3}{6a^3} B_2^3(s)\theta\, ds\right| \le \frac{c'}{t^2 a} t^{5/2} = \frac{c' t^{1/2}}{a} \to 0, \tag{6.6}$$

since $t \ll a^2$. Thus the middle term on the right in (6.3) has the same asymptotic distribution as

$$\begin{aligned} &\frac{c_2}{t^2/a^2}\int_0^t -\frac{4\pi^2}{2a^2} B_2^2(s)\cos 2\pi x_2\, ds \\ &\quad = -\frac{2\pi^2 c_2 \cos 2\pi x_2}{t^2}\int_0^t B_2^2(s)\, ds =_{\mathscr{L}} -2\pi^2 c_2 \cos 2\pi x_2 \int_0^1 B_2^2(s)\, ds. \end{aligned} \tag{6.7}$$

For the last equality in law we use the fact that, for every $t > 0$, the distributions of the processes $\{\sqrt{t}\, B_2(s/t)\colon s \ge 0\}$ and $\{B_2(s)\colon s \ge 0\}$ are the same. To derive the third row in the table use the representation with a denominator t, instead of t^2/a^2, and omit the centering term $c_2 \cos 2\pi x_2$ from both sides, to get the desired asymptotic distribution the same as that of

$$\begin{aligned} &\frac{c_2}{t}\int_0^t \cos\left(2\pi\left(x_2 + \frac{B_2(s)}{a}\right)\right) ds \\ &\quad =_{\mathscr{L}} \frac{c_2}{t}\int_0^t \cos(2\pi(x_2 + B_2(s/a^2)))\, ds \\ &\quad = \frac{c_2}{t/a^2}\int_0^{t/a^2} \cos(2\pi(x_2 + B_2(s))\, ds \\ &\quad \to \frac{c_2}{r}\int_0^r \cos(2\pi(x_2 + B_2(s)))\, ds. \end{aligned} \tag{6.8}$$

The final phase (iv) in Table 1 follows from Theorem 5.2 for time scales $t \gg a^2(\log a)^2$. By explicit computation we now show that it holds for times $t \gg a^2$. As above, since $a\sqrt{t} \gg \sqrt{t}$, one only needs to evaluate the asymptotic distribution of

$$\frac{c_2}{a\sqrt{t}}\int_0^t \cos\left(2\pi\left(x_2 + \frac{B_2(s)}{a}\right)\right) ds. \tag{6.9}$$

Since the function $f(y) = -(c_2 a^2/2\pi^2)\cos(2\pi(x_2 + \frac{y}{a}))$ satisfies $\frac{1}{2}f''(y) = c_2\cos(2\pi(x_2 + y/a))$, Itô's lemma shows that (6.9) equals

$$\begin{aligned} &\frac{1}{a\sqrt{t}}\left(-\frac{c_2 a^2}{2\pi^2}\right)\left\{\cos\left(2\pi\left(x_2 + \frac{B_2(t)}{a}\right)\right) - \cos 2\pi x_2\right\} \\ &\quad - \frac{1}{a\sqrt{t}}\int_0^t \frac{c_2 a}{\pi}\sin\left(2\pi\left(x_2 + \frac{B_2(s)}{a}\right)\right) dB_2(s) \\ &\quad \simeq -\frac{c_2}{\pi\sqrt{t}}\int_0^t \sin\left(2\pi\left(x_2 + \frac{B_2(s)}{a}\right)\right) dB_2(s) = I(t), \end{aligned} \tag{6.10}$$

say. To show that the last expression is asymptotically normal, note that its quadratic variation is

$$
\begin{aligned}
Q(t) &:= \left(\frac{c_2^2}{\pi^2}\right)\frac{1}{t}\int_0^t \sin^2\!\left(2\pi\left(x_2+\frac{B_2(s)}{a}\right)\right)ds \\
&=_{\mathscr{L}} \left(\frac{c_2^2}{\pi^2}\right)\frac{1}{t}\int_0^t \sin^2\!\left(2\pi\left(x_2+B_2\left(\frac{s}{a^2}\right)\right)\right)ds \\
&= \frac{c_2^2}{\pi^2}\frac{1}{t/a^2}\int_0^{t/a^2} \sin^2(2\pi(x_2+B_2(u)))\,du \\
&\to \frac{c_2^2}{\pi^2}\int_0^1 \sin^2(2\pi y)\,dy = \frac{c_2^2}{2\pi^2} \quad \text{a.s.},
\end{aligned} \tag{6.11}
$$

since $t/a^2 \to \infty$, and the process $U(t) := (x_2 + B_2(t)) \bmod 1$ is a positive recurrent Markov process on $S^1 = \{x \bmod 1\colon x \in \mathbb{R}\}$ having the uniform distribution as its invariant probability. One may now check that the martingale central limit theorem [see, e.g., Bhattacharya and Waymire (1990), page 508] holds for the last expression $I(t)$ in (6.10), with the asymptotic variance $c_2^2/2\pi^2$. An alternative derivation may be given by noting that $E\exp\{i\xi I(t)+\xi^2/2Q(t)\} = 1\ \forall\,\xi$ and $\forall\,t$. By (6.11), $Q(t) \to c_2^2/2\pi^2$ a.s., as $a \to \infty$, $t \gg a^2$. Since $|Q(t)| \le c_2^2/\pi^2$ for all t and a, one may now easily show that $E\exp\{i\xi I(t)\} \to \exp\{-\xi^2/2\sigma^2\}$ with $\sigma^2 = c_2^2/2\pi^2$.

REMARK 6.1.1. The above example shows that the time scale for the first phase of asymptotics derived in Theorem 2.1(c), Theorem 2.2, is exact, namely, $1 \ll t \ll a^{4/3}$. Indeed, with an additional calculation one may show that if $a \to \infty$, $t/a^{4/3} \to r > 0$, then

$$
\begin{aligned}
&\frac{X_1(t) - X_1(0) - t(c_0 + c_2\cos 2\pi x_2)}{\sqrt{t}} \\
&\qquad - \frac{c_2\int_0^t\{\cos(2\pi(x_2+(B_2(s)/a))) - \cos 2\pi x_2\}\,ds}{\sqrt{t}} \\
&\qquad \to_{\mathscr{L}} \mathscr{N}\left(0, 1+\frac{c_1^2}{2\pi^2}\right).
\end{aligned} \tag{6.12}
$$

Now, by (6.5), and (6.6), (6.7) (with t^2/a^2 replaced by $\sqrt{t}$), one shows that

$$
\begin{aligned}
&-\frac{c_2}{\sqrt{t}}\int_0^t\left\{\cos\left(2\pi\left(x_2+\frac{B_2(s)}{a}\right)\right) - \cos 2\pi x_2\right\}ds \\
&\qquad \to_{\mathscr{L}} \mathscr{L}\left(2\pi^2 c_2 r^{3/2}(\cos 2\pi x_2)\int_0^1 B_2^2(u)\,du\right).
\end{aligned} \tag{6.13}
$$

The limiting law in (6.13) is that of a strictly positive or a strictly negative random variable (depending on whether $c_2\cos 2\pi x_2$ is positive or negative). From this it follows that for $t/a^{4/3} \to r > 0$, the asymptotic law in Table 1(1) does not hold.

REMARK 6.1.2. If in Example 6.1 we drop the assumption (6.2), and instead assume

$$\sin 2\pi x_2 \neq 0, \tag{6.14}$$

then the hypothesis of part (b) of Theorem 2.1 is satisfied, but not that of part (c). Therefore, the time scale for case (1) is $1 \ll t \ll a$. The arguments for cases (3) and (4) remain unchanged. Case (2), however, changes drastically. For $a \ll t \ll a^2$ one has, using (6.3) with t^2/a^2 replaced by $t^{3/2}/a$, and noting that $t^{3/2}/a \gg t^{1/2}$,

$$\begin{aligned} &\frac{X_1(t) - X_1(0) - t(c_0 + c_2 \cos 2\pi x_2)}{t^{3/2}/a} \\ &\simeq \frac{c_2}{t^{3/2}/a} \int_0^t \left\{ \cos\left(2\pi\left(x_2 + \frac{B_2(s)}{a}\right)\right) - \cos 2\pi x_2 \right\} ds \\ &= \frac{c_2}{t^{3/2}/a} \int_0^t (-\sin 2\pi x_2) \frac{2\pi B_2(s)}{a} \, ds \\ &\quad + O\left(\frac{a}{t^{3/2}} \int_0^t \frac{B_2^2(s)}{a^2} \, ds\right) \\ &\simeq -\frac{2\pi c_2 \sin 2\pi x_2}{t^{3/2}} \int_0^t B_2(s) \, ds, \end{aligned} \tag{6.15}$$

since the expected value of the magnitude of the O-term is $O(1/at^{3/2}t^2) = O(t^{1/2}/a) \to 0$ for $t \ll a^2$. Now the last expression in (6.15) has the same distribution as

$$-2\pi c_2 \sin 2\pi x_2 \int_0^1 B_2(s) \, ds, \tag{6.16}$$

which is $\mathscr{N}(0, (4\pi^2 c_2^2/3) \sin^2 2\pi x_2)$. Thus, under (6.14), the first two rows of Table 1 change to

Time scale	**Asymptotic law**
(1)′ $1 \ll t \ll a$	$\dfrac{X_1(t) - X_1(0) - t(c_0 + c_2 \cos 2\pi x_2)}{\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}\left(0, 1 + \dfrac{c_1^2}{2\pi^2}\right)$
(2)′ $a \ll t \ll a^2$	$\dfrac{X_1(t) - X_1(0) - t(c_0 + c_2 \cos 2\pi x_2)}{t^{3/2}/a} \to_{\mathscr{L}} \mathscr{N}\left(0, \dfrac{4\pi^2 c_2^2}{3} \sin^2 2\pi x_2\right)$

Once again, if $a \to \infty$, $t/a \to r > 0$, then the asymptotic law in (1)′ cannot hold. To see this note that in the integral representation of $t^{-1/2}(X_1(t) - X_1(0) - t(c_0 + c_2 \cos 2\pi x_2))$ [see (6.3)], $t^{-1/2} \int_0^t c_1 \sin 2\pi(ax_2 + B_2(s)) \, ds + t^{-1/2} \cdot$

$B_1(t)$ converges in law to $\mathscr{N}(0, 1 + c_1^2/2\pi^2)$, as in (1)′. However, here the middle term $t^{-1/2}\int_0^t c_2\{\cos(2\pi(x_2 + B_2(s)/a)) - \cos 2\pi x_2\}\,ds$ converges in law to $-r(2\pi c_2 \sin 2\pi x_2)\int_0^1 B_2(u)\,du = rZ_2$, say, by essentially the same argument as given for (2)′ above [see (6.15), (6.16)]. Thus if the asymptotic law in (1)′ is to hold for $t/a \to r > 0$ $(a \to \infty)$, then one would have in the limit $Z_1 + rZ_2 =_{\mathscr{L}} Z_1$, where Z_1 and Z_2 are nondegenerate normal. This can not hold if r is sufficiently large. Therefore, the time scale given in Theorem 2.1(b) cannot be improved upon in general. The preciseness of the time scale $t \ll a^{2/3}$ in part (a) of Theorem 2.1 will be shown in Remark 6.2.1 below.

REMARK 6.1.3. The time scale for the final phase in Example 6.1 is $t \gg a^2$, whereas Theorem 5.2 gives a time scale $t \gg a^2(\log a)^2$ in the general case. We do not know if, in general, the logarithmic factor can be dropped altogether. Recall that our estimation for the time scale to equilibrium on the big torus is already $t \gg a^2 \log a$ (Theorem 4.5).

EXAMPLE 6.2. Consider the same equation for $X_1(t)$ as in Example 6.1 [see (6.1)], but for $X_2(t)$ take a Brownian motion with a *nonzero drift* δ,

$$dX_2(t) = \delta\,dt + dB_2(t). \tag{6.17}$$

The initial condition is as in (6.1), namely, $X(0) = ax = (ax_1, ax_2)$, but we assume $\sin 2\pi x_2 \neq 0$ [i.e., (6.14)]. With this seemingly minor change, the asymptotic behavior and time scales are dramatically different at larger scales, as shown in Table 2.

Case (1) follows from Theorem 2.1(a) and Theorem 2.2, or one can directly use the integral representation (6.3), but with a different denominator, namely,

TABLE 2
Phase changes in Example 6.2

Time scale	Asymptotic law
(1) $1 \ll t \ll a^{2/3}$	$\dfrac{X_1(t) - X_1(0) - t(c_0 + c_2\cos 2\pi x_2)}{\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}\left(0, 1 + \dfrac{c_1^2}{2(\delta^2 + \pi^2)}\right)$
(2) $\dfrac{t}{a^{2/3}} \to r > 0$	$\dfrac{X_1(t) - X_1(0) - t(c_0 + c_2\cos 2\pi x_2)}{\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}\left(-c_2\delta r^{3/2}\pi \sin 2\pi x_2,\ 1 + \dfrac{c_1^2}{2(\delta^2 + \pi^2)}\right)$
(3) $t \gg a^2$	$\dfrac{X_1(t) - X_1(0) - tc_0}{\sqrt{t}} \to_{\mathscr{L}} \mathscr{N}\left(0, 1 + \dfrac{c_1^2}{2(\pi^2 + \delta^2)} + \dfrac{c_2^2}{2\delta^2}\right)$

$t^{1/2}$ (instead of t^2/a^2),

$$\begin{aligned}
&\frac{X_1(t) - X_1(0) - t(c_0 + c_2 \cos 2\pi x_2)}{\sqrt{t}} \\
(6.18)\qquad &= \frac{c_1}{\sqrt{t}} \int_0^t \sin 2\pi(ax_2 + s\delta + B_2(s))\, ds \\
&\quad + \frac{c_2}{\sqrt{t}} \int_0^t \left\{ \cos\left(2\pi\left(x_2 + \frac{s\delta}{a} + \frac{B_2(s)}{a}\right)\right) - \cos 2\pi x_2 \right\} ds + \frac{B_1(t)}{\sqrt{t}}.
\end{aligned}$$

Now $\sin 2\pi(ax_2 + s\delta + B_2(s)) = \sin 2\pi Z(s)$, where $Z(s) = X_2(s) \bmod 1$ is the Brownian motion on the unit circle with a drift. Since the distribution of $Z(s)$ approaches equilibrium (uniform distribution) exponentially fast in total variation distance, uniformly with respect to the initial state, it follows from a central limit theorem for Markov processes [see Bhattacharya (1982)] that the first term on the right in (6.18) converges in distribution to $\mathscr{N}(0, \sigma^2)$ where

$$(6.19)\qquad \sigma^2 = -2 \int_{[0,1)} f(y) u(y)\, dy, \qquad f(y) = c_1 \sin 2\pi y,$$

$u(y)$ being the mean zero solution of

$$(6.20)\qquad \tfrac{1}{2} u''(y) + \delta u'(y) = f(y).$$

A direct computation shows

$$(6.21)\qquad u(y) = -\frac{c_1 \delta}{\pi^2 + \delta^2} \left\{ \frac{\cos 2\pi y}{2\pi} + \frac{1}{2\delta} \sin 2\pi y \right\},$$

leading to

$$(6.22)\qquad \sigma^2 = \frac{2c_1^2 \delta}{\pi^2 + \delta^2} \left(\frac{1}{2\delta}\right) \int_{[0,1)} \sin^2 2\pi y\, dy = \frac{c_1^2}{2(\pi^2 + \delta^2)}.$$

The third term on the right in (6.18) is independent of the first, and its distribution is $\mathscr{N}(0, 1)$. Thus the sum of the first and third terms converges in distribution to $\mathscr{N}(0, 1 + c_1^2/2(\pi^2 + \delta^2))$ as $t \to \infty$ (uniformly w.r.t. a). If, in addition $a \to \infty$, $t/a^{2/3} \to r > 0$ then, using a Taylor expansion such as in (6.5), the middle term on the right in (6.18) may be expressed as

$$(6.23)\quad \frac{2\pi c_2}{\sqrt{t}} \int_0^t (-\sin 2\pi x_2)\left(\frac{B_2(s)}{a} + \frac{s\delta}{a}\right) ds + O\left(\frac{1}{\sqrt{t}} \int_0^t \left(\frac{B_2(s) + s\delta}{a}\right)^2 ds\right)$$

The expected value of the O-term is of the order $O(t^3/\sqrt{t}\, a^2) = O(t^{5/2}/a^2) \to 0$, since $t^{5/2} = O(a^{5/3})$. Since $E|B_2(s)| = c' s^{1/2}$, the dominant contribution in the first term in (6.23) comes from

$$\begin{aligned}
\frac{2\pi c_2}{\sqrt{t}}(-\sin 2\pi x_2) \frac{\delta}{a} \int_0^t s\, ds &= -\frac{2\pi c_2 \delta \sin 2\pi x_2}{\sqrt{t}\, a} \frac{t^2}{2} \\
&= (-c_2 \pi \delta \sin 2\pi x_2) \frac{t^{3/2}}{a} \to (-c_2 \pi \delta \sin 2\pi x_2) r^{3/2}.
\end{aligned}$$

Thus (2) is established. In particular, this shows, along with Example 6.1, that the time scales in Theorems 2.1, 2.2 are in general precise.

To derive case (3) in Table 2, we will use Itô's lemma to write

$$\frac{X_1(t)-X_1(0)-tc_0}{\sqrt{t}} = \frac{w_1(X_2(t))-w_1(X_2(0))}{\sqrt{t}} - \frac{1}{\sqrt{t}}\int_0^t w_1'(X_2(s))\,dB_2(s) + \frac{1}{\sqrt{t}}B_1(t), \tag{6.24}$$

where w_1 is a periodic solution of

$$\tfrac{1}{2}w_1''(y) + \delta w_1'(y) = c_1 \sin 2\pi y + c_2 \cos(2\pi y/a). \tag{6.25}$$

By direct computation, w_1 is given by [apart from an additive constant which does not affect the right side of (6.24)]

$$w_1(y) = -\frac{c_1\delta}{\pi^2+\delta^2}\left\{\frac{\cos 2\pi y}{2\pi} + \frac{\sin 2\pi y}{2\delta}\right\} + \frac{c_2\delta a^3}{\delta^2 a^2+\pi^2}\left\{\frac{\sin(2\pi y/a)}{2\pi} - \frac{\cos(2\pi y/a)}{2\delta a}\right\}. \tag{6.26}$$

Note that w_1 is $O(a)$. Therefore, if $t \gg a^2$, the first term on the right side in (6.24) goes to zero a.s. The integrand in the stochastic integral term is

$$w_1'(y) = \frac{c_1\delta}{\pi^2+\delta^2}\left\{\sin 2\pi y - \frac{\pi\cos 2\pi y}{\delta}\right\} + \frac{c_2\delta a^2}{\delta^2 a^2+\pi^2}\left\{\cos\left(\frac{2\pi y}{a}\right) + \frac{\pi\sin(2\pi y/a)}{\delta a}\right\}. \tag{6.27}$$

Neglecting the $O(1/a)$ term whose contribution in the stochastic integral obviously goes to zero in probability, one may then write

$$\frac{X_1(t)-X_1(0)-tc_0}{\sqrt{t}} \simeq -\frac{1}{\sqrt{t}}\int_0^t \left\{I_1(X_2(s)) + I_2(X_2(s))\right\} dB_2(s) + \frac{B_1(t)}{\sqrt{t}}, \tag{6.28}$$

where

$$I_1(y) = \frac{c_1\delta}{\pi^2+\delta^2}\left\{\sin 2\pi y - \frac{\pi\cos 2\pi y}{\delta}\right\}, \qquad I_2(y) = \frac{c_2\delta a^2}{\delta^2 a^2+\pi^2}\cos\left(\frac{2\pi y}{a}\right). \tag{6.29}$$

The stochastic integral in (6.28) is a martingale and its quadratic variation (divided by t) is

$$\frac{1}{t}\int_0^t I_1^2(X_2(s))ds + \frac{1}{t}\int_0^t I_2^2(X_2(s))\,ds + \frac{2}{t}\int_0^t I_1(X_2(s))I_2(X_2(s))\,ds. \tag{6.30}$$

As argued for case (1), $I_1(X_2(s)) = I_1(Z(s))$ ($Z(s) := X_2(s) \bmod 1$), when $Z(s)$ is a Brownian motion on the unit circle with a constant drift δ, which approaches equilibrium exponentially fast in t,

$$\begin{aligned}\frac{1}{t}\int_0^t I_1^2(X_2(s))\,ds \to \int_{[0,1)} I_1^2(y)\,dy &= \frac{c_1^2\delta^2}{(\pi^2+\delta^2)^2}\left\{\frac{1}{2}+\frac{\pi^2}{2\delta^2}\right\}\\ &= \frac{c_1^2}{2(\pi^2+\delta^2)} \quad \text{as } t\to\infty.\end{aligned} \tag{6.31}$$

For the second term in (6.30), write

$$\begin{aligned}\frac{1}{t}\int_0^t I_2^2(X_2(s))\,ds &\simeq \left(\frac{c_2}{\delta}\right)^2\frac{1}{t}\int_0^t \cos^2 2\pi\left(\frac{B_2(s)}{a}+\frac{s\delta}{a}+x_2\right)ds\\ &=_{\mathscr{L}} \left(\frac{c_2}{\delta}\right)^2\frac{1}{t}\int_0^t \cos^2 2\pi\left(B_2(s/a^2)+\frac{s\delta}{a}+x_2\right)ds\\ &= \left(\frac{c_2}{\delta}\right)^2\frac{1}{t/a^2}\int_0^{t/a^2} \cos^2 2\pi\big(B_2(s')+as'\delta+x_2\big)\,ds'.\end{aligned} \tag{6.32}$$

Once again one may replace $B_2(s')+as'\delta+x_2$ by its value mod 1 and use the fact that the latter is a Brownian motion on the unit circle with a drift $a\delta$. This Brownian motion on the circle approaches equilibrium as $s'\to\infty$, uniformly w.r.t. the drift $a\delta$ since the Brownian motion on the unit circle *without drift* approaches equilibrium (exponentially fast in total variation distance) *uniformly* with respect to the initial state. Thus, as $t/a^2\to\infty$,

$$\frac{1}{t}\int_0^t I_2^2(X_2(s))\,ds \to \frac{c_2^2}{2\delta^2} \quad \text{in probability.} \tag{6.33}$$

We now show that the product term in (6.30) goes to zero in probability. For this note that

$$\begin{aligned}&\frac{1}{t}\int_0^t \sin 2\pi\big(B_2(s)+s\delta+ax_2\big)\cos 2\pi\left(\frac{B_2(s)}{a}+\frac{s\delta}{a}+x_2\right)ds\\ &\quad=_{\mathscr{L}} \frac{1}{t/a^2}\int_0^{t/a^2} \sin 2\pi(aB_2(s)+a^2 s\delta+ax_2)\\ &\qquad\qquad \times \cos 2\pi(B_2(s)+as\delta+x_2)\,ds\\ &\quad= \frac{1}{t/a^2}\int_0^{t/a^2} \sin 2\pi(aZ_2(s))\cos 2\pi(Z_2(s))\,ds,\end{aligned} \tag{6.34}$$

where $Z_2(s) = (B_2(s)+sa\delta+x_2) \bmod 1$. Since, as argued earlier, $Z(s) := (B_2(s)+y) \bmod 1$ approaches equilibrium (exponentially fast in total variation distance) uniformly w.r.t. y, as $s\to\infty$, the last expression in (6.34) is asymptotically the same in distribution as

$$\frac{1}{t/a^2}\int_0^{t/a^2} \sin 2\pi(aZ(s))\sin 2\pi Z(s)\,ds, \tag{6.35}$$

where $\{Z(s): s \geq 0\}$ is the stationary standard Brownian motion on the unit circle. One may rewrite (6.35) as

$$\frac{1}{2t/a^2}\int_0^{t/a^2}\{\sin(2\pi(a+1)Z(s))+\sin(2\pi(a-1)Z(s))\}\,ds. \tag{6.36}$$

Now, uniformly for all $a = 1, 2, \dots,$

$$E\biggl(\frac{1}{A}\int_0^A \sin(2\pi(a+1)Z(s))\,ds\biggr)^2 \to 0 \quad \text{as } A \to \infty. \tag{6.37}$$

To see this, note that $Z(s)$ is exponentially φ-mixing, and $z \to \sin(2\pi(a+1)z)$ is uniformly bounded. Hence the covariance $E\sin(2\pi(a+1)Z(s))\sin(2\pi(a+1)Z(s'))\to 0$ exponentially fast, uniformly in a, as $|s-s'| \to \infty$. One may replace $a+1$ in (6.37) by $a-1$ and thus show that (6.36) goes to zero in mean square as $t/a^2 \to \infty$. It follows that (6.34) $\to 0$ in mean square. The same proof applies to the other term in $I_1(X_2(s))I_2(X_2(s))$ involving $\cos 2\pi(X_2(s))$ $\cos 2\pi(X_2(s)/a)$ [see (6.29)]. Thus the average quadratic variation (6.30) converges in probability to $c_1^2/2(\pi^2+\delta^2)+c_2^2/\delta^2$ [see (6.31), (6.33)]. One may now easily apply the martingale central limit theorem to the stochastic integral term in (6.28), verifying the Lindeberg-type condition using the fact that $|I_1(y)+I_2(y)|$ is bounded (uniformly in a) [see Bhattacharya and Waymire (1990), page 508]. Alternatively, one may also show that the characteristic function of $t^{-\frac{1}{2}}\int_0^t I(X_2(s))\,dB_2(s)$ converges to that of the appropriate Gaussian, by using the exponential martingale property, as in the proof of case (4) of Example 6.1.

REMARK 6.2.1. To show that the time scale $t \gg a^2$ for the final phase in Example 6.2 is precise, let $a \to \infty$, $t/a^2 \to r > 0$. Then, if r is sufficiently large, there exists a positive constant c (independent of a, t and r) such that $E(t^{-1/2}(w_1(X_2(t)) - w_1(X_2(0)))^2 \geq cr$ [see (6.26)]. On the other hand, the mean square of the sum of the two remaining terms on the right side of (6.24) is bounded by an absolute constant c'. Therefore, the first term will be dominant for large r. This shows that (3) in Table 2 does not hold if the time scale is extended to include $t = O(a^2)$.

REMARK 6.2.2. The hypothesis of Theorem 5.4 is satisfied by Example 6.2, with $k_2 = 1$.

REMARK 6.2.3. The Gaussian convergences in Examples 6.1 and 6.2 may be strengthened to their functional versions (i.e., convergence to Brownian motions) by standard results such as given in Theorem 7.1.4 in Ethier and Kurtz (1986) [also see Hall and Heyde (1980), page 99]. The non-Guassian convergences in these examples may also be expressed in functional forms.

7. An application to solute transport in porous media. Suppose a chemical pollutant, or some solute, is injected at a point in a saturated aquifer —an underground water system. How will it spread over large times? There is a vast engineering literature on this subject [see Adams and Gelhar (1992); Bhattacharya and Gupta (1983); Cushman (1990); Dagan (1984); Fried and Combarnous (1971); Garabedian, LeBlanc, Gelhar and Celia (1991); Gelhar and Axness (1983); Gupta and Bhattacharya (1986); Guven and Molz (1986); LeBlanc, Garabedian, Hess, Gelhard, Quadri, Stollenwerk and Wood (1991); Sauty (1980); Sposito, Jury and Gupta (1986); Sudicky (1986)]. It is generally accepted [Fried and Combarnous (1971)], and laboratory scale experiments have confirmed it, that the solute concentration $c(t, y)$ at y at time t at a local scale, say the laboratory scale, satisfies a Fokker–Planck equation,

$$\frac{\partial c}{\partial t} = \frac{1}{2} \sum_{j, j'=1}^{3} \frac{\partial^2}{\partial y_j \partial y_{j'}} (D_{jj'} c) - \sum_{j=1}^{3} \frac{\partial}{\partial y_j} (v_j(y) c), \tag{7.1}$$

with $v(y) = (v_1(y), v_2(y), v_3(y))$ representing the velocity of water at y, and satisfying the *incompressibility* condition

$$\operatorname{div} v(y) = 0 \quad \forall\, y. \tag{7.2}$$

The positive definite symmetric matrix $((D_{jj'}))$ may represent something akin to Einstein's molecular diffusion $\sigma^2 I_3$ at a scale somewhat larger than the hydrodynamical scale [see, e.g., Bhattacharya and Gupta (1979), where this is erroneously called the "Darcy scale"], or an enhanced dispersion due to heterogeneities in the porous medium at the laboratory, or the so-called Darcy scale [Fried and Combarnous (1971)]. A commonly used experimental methodology is to fit Gaussians to the concentration $c(t, y)$ as a function of y, for successively larger scales of t. One may think of this as different Brownian motion approximations at different scales of time. It has been widely observed that the diagonal dispersion coefficients, or variances per unit time, increase steadily with the time scale, especially in the direction of flow. This phenomenon has been called the *scale effect* in dispersion. A different kind of study has focussed on the increase in dispersion at the laboratory-, or Darcy-, scale with the increase in the velocity magnitude of the flow [Fried and Combarnous (1971)].

As is well known [see, e.g., Friedman (1975), pages 144–150, or Bhattacharya and Waymire (1990), pages 377–380], the solution to (7.1) with a point initial input c_0 at x is given by the function $(t, y) \to c_0 p(t; x, y)$, where $p(t; x, y)$ is the transition probability density of a diffusion $X(t)$ with drift velocity v and diffusion coefficients $D_{jj'}$. In general, for an arbitrary compactly supported and continuous initial concentration $c_0(x)$, the solution to (7.1) is

$$c(t, y) = \int c_0(x) p(t; x, y)\, dx. \tag{7.3}$$

It follows that the asymptotic behavior of $c(t, y)$ for large t is given by the asymptotic distribution of $X(t)$. The present article provides these asymptotics assuming v to be periodic. For the physical problem at hand, the initial concentration is always taken to be *localized* at a point.

To study the *effect of velocity* on dispersion, let $v = u_0 \beta$ where u_0 is a scalar and β is periodic. It is shown in Section 3 that $X(t)$ is asymptotically Gaussian for large t [and therefore so is $c(t, \cdot)$], but with two extreme behaviors of *dispersivity* (i.e., asymptotic variance per unit time) depending on the nature of the flow velocity. If $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j)$ has a nonzero component in the *null space* N of $S = \mathscr{D}^{-1}\beta\nabla$ in H^1, then the dispersivity of $X_j(t)$ grows quadratically with u_0 [Theorem 3.3(a)]. In the complementary case, $\mathscr{D}^{-1}(\beta_j - \overline{\beta_j})$ belong to the closure $\overline{\mathscr{R}}$ of the *range* $\mathscr{R}$ of S, since $H^1 = N \ominus \overline{\mathscr{R}}$. If $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j) \in \mathscr{R}$, then the dispersivity of $X_j(t)$ grows from D_{jj} to a larger constant value, as u_0 increases [Theorem 3.3(b)]. The boundary case, where $\mathscr{D}^{-1}(\beta_j - \overline{\beta}_j) \in \overline{\mathscr{R}} \backslash \mathscr{R}$, seems difficult to analyze. For two-dimensional flows (i.e., $k = 2$), more information on this may be found in Fannjiang and Papanicolaou (1994). Figures 1 and 2 represent observed functional relationships between velocity and dispersivity in certain laboratory experiments as presented by Fried and Combarnous (1971).

We now turn to the *scale effect* in dispersion. As pointed out in Bhattacharya and Gupta (1983), different Gaussian approximations accompanied with in-

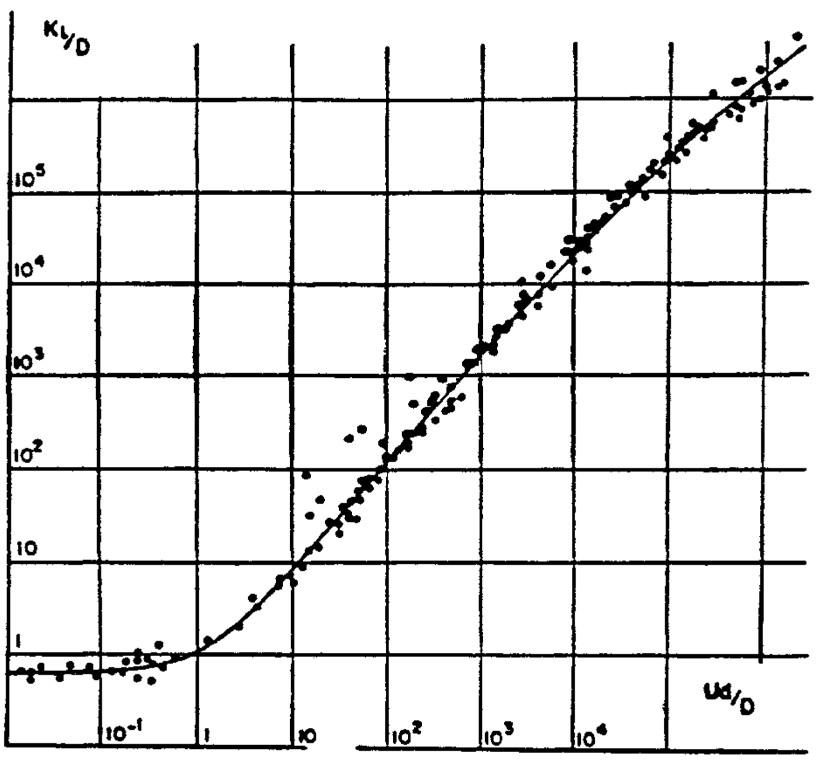

FIG. 1. *Laboratory experiments showing the growth in the dispersion coefficient K_L in the direction of flow with the velocity U. In order to make the coordinates dimensionaless, K_L/D is plotted against the Peclet number Ud/D, where D is the molecular diffusion coefficient and d is the diameter of a typical gain of the porous medium. Taken from Fried and Combarnous* (1971).

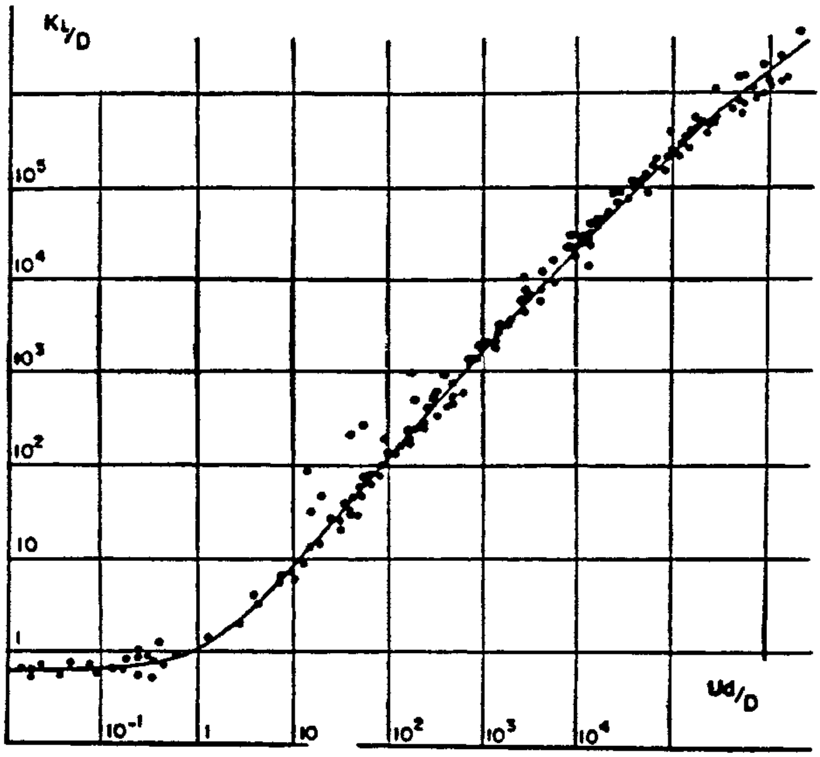

FIG. 2. *Laboratory experiments for the growth in the dispersion coefficient K_T in a direction transverse to the flow. The dotted line represents a fitted curve for K_L/D in the same experiment. Taken from Fried and Combarnous* (1971).

crease in dispersivity at successively larger time scales can only occur in a medium (aquifer) with new heterogeneities appearing at higher scales. To understand this, it is enough to consider two spatial scales of heterogeneity embodied in the flow velocity v,

$$v(y) = b(y) + \beta(y/a), \tag{7.4}$$

where "a" is a large scalar. Here fluctuations in b represent the effect of a local (or small) scale heterogeneity in the aquifer geometry and soil characteristics, while fluctuations in v which manifest only at a larger scale of distance (of the order a) are represented in $\beta(\cdot/a)$. Theorem 2.1 provides precise time scales ($t \ll a^{2/3}$, $t \ll a$ or $t \ll a^{4/3}$) over which the local scale b dominates and large scale fluctuations may be ignored. Here no specific assumptions are needed on $b(\cdot)$ or $\beta(\cdot)$, not even (7.2). The significance of this is that, irrespective of the nature of β, whenever a Gaussian approximation holds for the concentration corresponding to flow velocity $b(\cdot) + \beta(x_0)$ (assuming an initial point injection at ax_0) and diffusion matrix $D(x) \equiv ((D_{jj'}(x)))$, the same holds for the concentration with the actual flow velocity (7.4) and dispersion $D(x)$, provided $t \ll a^{2/3}$ (or $t \ll a$, $t \ll a^{4/3}$, as the case may be). Since Gaussian approximations for a single scale of fluctuations are known to be valid under assumptions of periodicity and almost periodicity of the coefficients, as well as under the assumption of their being an ergodic random field [see Bensoussan, Lions and Papanicolaou (1978); Bhattacharya (1985); Bhattacharya and Ramasubramanian (1988); Gelhar and Axness (1985); Kozlov (1979, 1980); Papanicolaou and Varadhan (1979); Winter, Newman and Neuman (1984)], a Gaussian approximation at the initial phase ($1 \ll t \ll a^{2/3}$) is expected to hold rather broadly in the present context (Theorem 2.2, Remark 2.1.3). Beyond this scale, as the effect of the large scale fluctuations gradually becomes manifest, this initial phase will break down. Under additional assumptions (on β), a different Gaussian approximation takes hold at a larger time scale. The latter approximation, along with its time scale, is provided in Theorems 5.2–5.4 for periodic flows satisfying assumptions (A1)–(A4), (A6) (Theorem 5.2), or (A1)–(A3), (A5), (A7) (Theorems 5.3, 5.4).

Under the hypotheses of Theorems 5.3, 5.4, the dispersivity grows from one constant D_{jj} to a larger constant, so that it is asymptotically a constant. Under the hypothesis of Theorem 5.2, the asymptotic growth in dispersivity is $O(a^2t/t) = O(a^2) = o(t)$ (since $t \gg a^2$ at the larger scale). Thus although dispersivity grows in the latter case, the growth is *sublinear* with time. In between the final and initial phases other *intermediate phases* appear. Examples 6.1, 6.2 in Section 6 illustrate this, along with a precise specification of the time scales for the initial, intermediate and final phases. A computation of dispersivity $d(t)$ in Example 6.1 through all these phases show a mostly sublinear growth,

$$\begin{gathered} d(t) = 1\,(t = O(1)), \qquad d(t) = 1 + \frac{c_1^2}{2\pi^2}(1 \ll t \ll a^{4/3}), \\ 1 \ll d(t) \ll t(a^{4/3} \ll t \ll a^2), \;\; d(t) \ll t(t \gg a^2). \end{gathered} \tag{7.5}$$

For the physical problem at hand, these are examples of multiscale versions of *stratified media* considered in Gupta and Bhattacharya (1986) and Guven and Molz (1986).

Because of the importance of the problem of solute transport in porous media in hydrology and environmental engineering, a number of field studies have been undertaken over the past two decades to monitor solute dispersion in aquifers [see, e.g., Adams and Gelhar (1992); Garabedian, LeBlanc, Gelhar and Celia (1991); LeBlanc Garbedian, Hess, Gelhar, Quadri, Stollenwerk and Wood (1991); Sauty (1980); Sudicky (1986)]. Such experiments are necessarily complex. They require the digging of many properly placed wells to monitor the solute concentration profile, often over a span of several years. The theoretical model most commonly fitted to the data is based on the important work of Gelhar and Axness (1983), where it is assumed that the coefficients of the Fokker–Planck equation governing solute concentration are ergodic random fields. An independent alternative mathematical approach under the same assumptions is given in Winter, Newman and Neuman (1984). Proofs of the validity of the

Gaussian approximation, along with a computation of its dispersion, may be found in Kozlov (1980) and Papanicolaou and Varadhan (1979) for the special case of the generator in divergence form. It seems that for the general case considered by Gelhar and Axness (1983) some mathematical details still need to be worked out, both for the CLT and for the analysis of the dispersion. As shown in Papanicolaou and Varadhan (1979), the periodic and almost periodic cases may be considered as special cases of the ergodic random field model.

The main thrust of the theoretical studies in the hydrology literature on solute dispersion in aquifers has been to explain the scale effect, that is, the increase in dispersivitiy with spatial scale. For example, the dispersivity at the field scales are observed to be larger by orders of magnitude from that at the laboratory scale. As pointed out in Bhattacharya and Gupta (1983), the validity of a hierarchy of Gaussian approximations at the laboratory and field scales, with increase in dispersivity with scale, can only be explained by the presence of multiple scales of heterogeneity in the medium. A single central limit theorem, such as mentioned in the preceding paragraph, cannot explain this phenomenon in a saturated aquifer whose dynamics are independent of time. The points of departure in the present article, following Bhattacharya and Götze (1995), are (1) the explicit introduction of multiple scales of heterogeneity in the velocity field and (2) determination of the time scales for changes from one Gaussian phase to the next. Although it is not claimed here that natural aquifers have periodic velocity fields, the detailed analysis of the periodic case with multiple scales provides a qualitative understanding of the scale effect in dispersion in general. Since under a random translation the periodic velocity field becomes an ergodic random field, the present study also provides an avenue for testing the validity of some of the informal theories and intuition on the nature of multiscale dispersion.

8. Final remarks. In the following series of remarks we mention some unresolved issues and research problems.

REMARK 8.1. The examples in Section 6 show that the time scale for the final Gaussian phase cannot in general be less than $t \gg a^2$ for divergence-free b and β. The additional logarithmic factors $(\log a)^2$ and $\log a$ in Theorems 5.2 and 5.4, respectively, are needed to offset the factor $a^{k/2}$ appearing in Theorem 4.5 in our estimate of the speed of convergence to equilibrium for diffusions on the big torus $\mathscr{T}_a$. We do not know if this factor $a^{k/2}$ can be removed in general. Among important recent methods for the estimation of the speed of convergence to equilibrium of Markov processes we would like to mention those of Chen and Wang (1994, 1997), and Diaconis and Saloff-Coste (1996).

The seemingly excessively large time scale $t \gg a^4(\log a)^2$ in Theorem 5.3 may be reduced to that given in Theorem 5.4, namely, $t \gg a^2 \log a$ if ag_j and a grad g_j can be shown to be bounded in sup norm rather than in the H^1-norm. We do not know if this is achievable in general.

REMARK 8.2. One may conjecture that the technical condition (A4)j in (3.68) is redundant for the validity of the conclusion of Theorem 5.2. We would also conjecture that, for Theorems 5.3 and 5.4, the assumption of continuity of the derivatives of p_j in (A5)j is redundant.

REMARK 8.3. It is easy to see that the condition that "$a \to \infty$ through integer values" may be relaxed to "$a \to \infty$ through a sequence of rational numbers with a bounded denominator." Can we relax this further in Theorem 5.2? Note that in Example 6.1 in Section 6 no restriction on "a" is needed (except that $a \to \infty$).

REMARK 8.4. As indicated by Theorems 5.5, 5.6 (also see Theorems 4.6, 4.7) for the one-dimensional case, multiscale multidimensional diffusions with periodic nondivergence-free velocity fields offer a rich diversity of behavior that needs to be explored further.

REMARK 8.5. An important problem, both from the point of view of mathematics and that of applications, is the analysis of multiscale diffusions whose coefficients constitute ergodic random fields. Methods employed in this article seem inapplicable for a general asymptotic analysis of such diffusions.

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MAJORIZING KERNELS AND STOCHASTIC CASCADES WITH APPLICATIONS TO INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

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ABSTRACT. A general method is developed to obtain conditions on initial data and forcing terms for the global existence of unique regular solutions to incompressible 3d Navier-Stokes equations. The basic idea generalizes a probabilistic approach introduced by LeJan and Sznitman (1997) to obtain weak solutions whose Fourier transform may be represented by an expected value of a stochastic cascade. A functional analytic framework is also developed which partially connects stochastic iterations and certain Picard iterates. Some local existence and uniqueness results are also obtained by contractive mapping conditions on the Picard iteration.

1. INTRODUCTION AND PRELIMINARIES

We develop two related approaches to obtain global and local existence, uniqueness and regularity, including spatial analyticity, of solutions to 3-dimensional incompressible Navier-Stokes (NS) equations governing fluid velocities

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = \nu \Delta u - \nabla p + g, \quad \nabla \cdot u = 0. \tag{1}$$

One approach is probabilistic and involves the construction of a multiplicative cascade solution to a related stochastic recursion in wave number Fourier space. The other approach is based on Picard iterations. Each of these approaches involves the notion of a *Fourier multiplier* which we formalize as follows.

Definition 1.1. Let $h : W_h \subseteq \mathbf{R}^n \backslash \{0\} \to (0, \infty)$ be a Lebesgue measurable function such that the closure of W_h is a semigroup and $h = 0$ on W_h^c with

$$0 < h * h(\xi) < \infty, \qquad \xi \in W_h. \tag{2}$$

The reciprocal function $1/h$ is referred to as a *Fourier multiplier*.

The probabilistic approach is based upon an interpretation of the integral equation governing Fourier transformed velocities scaled by a multiplier $1/h$. This is

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achieved in terms of expectation values of multiplicative cascade solutions to stochastic recursions generated by certain multi-type branching random walks in Fourier space. The transitions in wave-number are of the form $\xi \to (\xi_1, \xi_2), \xi_1 + \xi_2 = \xi$, with a transition probability kernel $h(\xi_1)h(\xi_2)/h * h(\xi)$. This generalizes branching random walks in the sense of LeJan and Sznitman [17] for $n = 3$ dimensions where $h(\xi) = |\xi|^{-2}, \xi \in W_h = \mathbf{R}^3\backslash\{0\}$. The essential requirement for this approach is that the above indicated expected values *exist*. Existence of these expected values is obtained in the present paper by constructions of a particular class of the Fourier multipliers, referred to as *majorizing kernels*, defined below.

The second approach is a purely analytic approach in which the Fourier multiplier $1/h$ is used to identify a Banach space norm for which iterations of the expected values may, under slightly more restrictive conditions, be interpreted as Picard iterates of successive approximations on a suitably identified function space defined via particular control of the Fourier transform by a majorizing Fourier multiplier, e.g. $u \in \mathcal{S}'$ such that $|\hat{u}(\xi, t)| \leq h(\xi)$. In particular, the Picard iteration may be expressed in terms of a contraction operator on such a space. It may be noted that a different function space for Picard iteration was identified by Kato [15] in efforts to obtain existence and uniqueness for Navier-Stokes equations.

As noted above, the probabilistic approach gives a representation of the Fourier transform $\hat{u}(\xi, t)$ of the solution of the evolution equation in the LeJan-Sznitman form of an expected value

$$\hat{u}(\xi, t) = h(\xi) E_{\xi_\theta = \xi} \chi(\theta, t). \tag{3}$$

Here χ is a random multiplicative functional of scalar values $m(\cdot)$ and Fourier transformed initial data and/or forcing (vector) values over the vertices of a multi-type branching random walk tree $\tau_\theta(t)$ initiated in time t from a single progenitor of type $\xi_\theta = \xi$. In general the scalar and vector value factors are evaluated at the wave-number (type) of the respective vertices appearing in the tree $\tau_\theta(t)$, with the initial and forcing terms appearing at the end-nodes. The holding times between branchings are determined from the principal part of the equation, while the branching probabilities depend on the lower order and forcing terms of the equation.

The framework developed here is also more generally applicable to diverse classes of evolution equations, including certain linear parabolic and fractional diffusion equations, semilinear reaction-diffusions, and some quasilinear equations such as incompressible Navier-Stokes equations in dimension $n \geq 2$, as well as one-dimensional Burgers' equations. The following extremely simple example is selected to illustrate some of the most basic graph theoretic and probabilistic ideas involved in this approach. It is so simple, however, that the notion of a Fourier multiplier is not required. Consider

$$u_t = a\Delta u + b \cdot \nabla u, \quad u(x, 0) = u_0(x), \tag{4}$$

in $n \geq 1$ dimensions, where $a > 0$, and $b \in \mathbf{R}^n$ are constants. To quickly get the flavor of the method, define the spatial Fourier transform of an integrable function f, or its distributional extension, by $\hat{f}(\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbf{R}}^n e^{-ix\cdot\xi} f(x)dx, \xi \in \mathbf{R}^n$. Then, from (4) one has

$$\hat{u}(\xi, t) = \hat{u}_0(\xi) e^{-a|\xi|^2 t} + \frac{ib \cdot \xi}{a|\xi|^2} \int_0^t a|\xi|^2 e^{-a|\xi|^2 s} \hat{u}(\xi, t-s) ds. \tag{5}$$

Now consider the random linear tree $\tau_\theta(t)$ rooted at a vertex θ of type $\xi_\theta = \xi$ which, after an exponential length of time, is replaced by a single vertex $\langle 1 \rangle$ of the same type $\xi_{\langle 1 \rangle} = \xi$. Proceeding in this manner one may calculate that the solution $\exp(-a|\xi|^2 + ib\cdot\xi)\hat{u}_0(\xi)$ is the expectation of the random product $\mathbb{X}(\theta, t)$ initialized by $\xi_\theta = \xi$ and consisting of factors $m(\xi) = ib\cdot\xi/a|\xi|^2$ at each vertex until termination, where one attaches the end factor $\hat{u}_0(\xi)$, i.e. $\mathbb{X}(\theta, t) = m(\xi)^{N(t)}\hat{u}_0(\xi)$, and

$$\hat{u}(\xi, t) = E_{\xi_\theta=\xi}\mathbb{X}(\theta, t) = E_{\xi_\theta=\xi}m(\xi)^{N(t)}\hat{u}_0(\xi), \tag{6}$$

where $N(t)$ is the Poisson process with parameter $\lambda(\xi) := a|\xi|^2$ which counts the number of times the exponential clocks ring before time t. In particular the Poisson process occupies a natural *dual* role to that played by the standard Brownian motion in the real space expectation formula. Similarly one may obtain a dual Feynman-Kac formula under the *complex measure condition* on coefficients given by Ito [14]; see Chen, Dobson, Guenther, Orum, Ossiander, Thomann, Waymire [7]. In particular this approach makes Ito's complex measure condition completely natural from a probabilistic point of view. One may also obtain a dual version of McKean's [18] branching Brownian motion formula for KPP, as well as other interesting equations which will be treated in a forthcoming monograph by the authors (in preparation). These also include, for example, the generalized fractional Burgers' equation of the type considered by Woyczynski, Biler, and Funaki [22], and the so-called "cheap Navier-Stokes equation" discussed by Montgomery-Smith [19] from the point of view of real-space iterative methods.

The primary focus of this paper is the 3d incompressible Navier-Stokes equation which may be expressed in the Fourier domain as follows:

$$\text{(FNS)} \qquad \begin{aligned} \hat{u}(\xi, t) = e^{-\nu|\xi|^2 t}\hat{u}_0(\xi) + \int_0^t e^{-\nu|\xi|^2 s}\big\{|\xi|(2\pi)^{-\frac{3}{2}} \\ \int_{\mathbf{R}^3} \hat{u}(\eta, t-s) \otimes_\xi \hat{u}(\xi - \eta, t-s)d\eta + \hat{g}(\xi, t-s)\big\}ds, \end{aligned}$$

where, for complex vectors w, z,

$$w \otimes_\xi z = -i(e_\xi \cdot z)\pi_{\xi^\perp}w, \ e_\xi = \frac{\xi}{|\xi|}, \text{ and } \pi_{\xi^\perp}w = w - (e_\xi \cdot w)e_\xi \tag{7}$$

is the projection of w onto the plane orthogonal to ξ, and $\nu > 0$ is the viscosity parameter. For $\xi \neq 0$, LeJan and Sznitman [17] rescale the equation (FNS) to normalize the integrating factor $e^{-\nu|\xi|^2 s}$ to the exponential probability density $\nu|\xi|^2 e^{-\nu|\xi|^2 s}$. Then they observe that the resulting equation is precisely the form for a branching random walk recursion for $\chi(\xi, t) := \nu|\xi|^2\hat{u}(\xi, t)$, for which the transition kernel $|\xi - \eta|^{-2}|\eta|^{-2}$ is naturally constrained by integrability to dimensions $d \geq 3$ for normalization to a probability.

Given a Fourier multiplier $1/h$ we consider the Fourier transformed equation (FNS) rescaled by factors $1/h(\xi)$, for $\xi \in W_h$. Namely, we consider the equation $(\text{FNS})_h$ defined by

$(\text{FNS})_h$

$$\begin{aligned} \chi(\xi, t) = e^{-\nu t|\xi|^2}\chi_0(\xi) + \int_0^t \nu|\xi|^2 e^{-\nu|\xi|^2 s}\big\{\frac{1}{2}m(\xi)\int_{W_h\times W_h} \chi(\eta_1, t-s) \\ \otimes_\xi \chi(\eta_2, t-s)H(\xi, d\eta_1 \times d\eta_2) + \frac{1}{2}\varphi(\xi, t-s)\big\}ds, \quad \xi \in W_h. \end{aligned}$$

Here

$$(8)\qquad m(\xi) = \frac{2h*h(\xi)}{\nu(2\pi)^{\frac{3}{2}}|\xi|h(\xi)}, \quad \chi_0(\xi) = \frac{\hat{u}_0(\xi)}{h(\xi)}, \quad \varphi(\xi,t) = \frac{2\hat{g}(\xi,t)}{\nu|\xi|^2h(\xi)},$$

and $H(\xi, d\eta_1 \times d\eta_2)$ is for $\xi \in W_h$ the transition probability kernel, with support contained in the set $\{(\eta_1,\eta_2) \in W_h \times W_h : \eta_1 + \eta_2 = \xi\}$, defined by

$$(9)\qquad \int_{W_h\times W_h} f(\eta_1,\eta_2)H(\xi,d\eta_1\times d\eta_2) = \int_{W_h} f(\xi-\eta,\eta)\frac{h(\xi-\eta)h(\eta)}{h*h(\xi)}d\eta$$

for bounded, Borel measurable $f : W_h \times W_h \to \mathbf{R}$. Finally we include the following additional *exterior condition* in defining $(\text{FNS})_h$:

$$(10)\qquad \chi(\xi,t) = 0, \qquad \xi \in W_h^c,\ t \geq 0.$$

Remark 1.1. One may easily check, using the semigroup requirement on W_h, that the exterior condition makes the equations (FNS) and $(\text{FNS})_h$ equivalent if and only if $\hat{u}_0(\xi) = 0$ and $\varphi(\xi,t) = 0$ for a.e. $\xi \in W_h^c, t \geq 0$. In many examples of interest to the present paper one has $W_h = R^n\backslash\{0\}$. It should also be noted that the re-scaled functions $\chi(\xi,t), \varphi(\xi,t)$ provide a convenient notational device for presenting the essential calculations. However, in the end the conditions and results are stated in terms of the respective functions $\hat{u}(\xi,t) = h(\xi)\chi(\xi,t)$, and $\hat{g}(\xi,t) = \frac{\nu}{2}|\xi|^2h(\xi)\varphi(\xi,t)$.

A first order approach to obtain finite expected values of the branching random walk cascade will be seen to result from the observation that the product $\otimes_\xi$ satisfies $|w\otimes_\xi z| \leq |w||z|, w, z \in C^n$, and the coefficients $m(\xi)$ may be controlled by selecting Fourier multipliers such that $m(\xi) \leq 1$. We refer to such a Fourier multiplier h as a majorizing kernel (with exponent one and constant $B = \frac{\nu(2\pi)^{\frac{3}{2}}}{2}$). The following slightly more general definition is suitable for extensions to generalized Navier-Stokes equations with *fractional Laplacian* and, as will be seen more fully in Section 4, for considerations of local solutions.

Definition 1.2. A positive locally integrable function h on $W_h \subset \mathbf{R}^n\backslash\{0\}$ whose closure $\overline{W}_h$ is a semigroup and such that (i) h is continuous on W_h, (ii) $h * h > 0$ a.e. on W_h, and (iii) $h * h(\xi) \leq B|\xi|^\theta h(\xi)$, for $\xi \in W_h$ and some real exponent θ and some $B > 0$, will be referred to as an *FNS-admissible majorizing kernel with constant B and exponent θ*. Majorizing kernels with a unit constant will be called *standard* kernels. We define $h = 0$ on W_h^c and refer to W_h as the *support* of h.

Since the focus of this paper is exclusively the Navier-Stokes equations, we will drop the prefix FNS-admissible in reference to majorizing kernels. Note that if h is a majorizing kernel with constant B, then $\frac{h}{B}$ is a standard majorizing kernel. Alternatively, if $\overline{h}$ is a standard majorizing kernel, then $h = B\overline{h}$ has constant B. If h is a majorizing kernel, then h/B, where $B = \sup\{h*h(\xi)/|\xi|^\theta h(\xi) : \xi \in W_h\}$, will be referred to as the *standardized* choice of h. Those majorizing kernels $h(\xi)$ which are defined and positive for all $\xi \neq 0$ are said to be *fully supported.* Some sense of the class of majorizing kernels may be derived by noting from Hölder's inequality that the set of fully supported majorizing kernels with a given exponent is a log-convex set. Also if $h(\xi)$ is a majorizing kernel, then so is $ce^{a\cdot\xi}h(\xi)$ for arbitrary fixed vector a and positive scalar c; note Theorems 2.1-2.4 in the next section in this general regard. Finally let us note that an exceptional role of $\xi = 0$ is linked to the use of the wave number ξ in defining the exponential waiting time distribution with mean $1/\nu|\xi|^2$.

Formulated in these terms, the results of LeJan and Sznitman [17] may be interpreted in terms of two exponent one, standardized majorizing kernels, $\pi^3/|\xi|^2$ and $\alpha e^{-\alpha|\xi|}/2\pi|\xi|$. These kernels are respectively non-integrable and integrable, with equality in (iii) of Definition 1.2. One may check that the only fully supported homogeneous majorizing kernels in $n \geq 3$ dimensions are those of degree $n-1$. Development of majorizing kernels is somewhat generally treated in Section 2. As will be demonstrated in subsequent Sections 3 and 4, apart from their role in existence, uniqueness and expected value representations, the majorizing kernels also play a role in constraining such structure of the solutions as regularity, support size, complexification, etc.

Now let us define a Banach space $\mathcal{F}_{h,\gamma,T}$ with a norm that depends on a Fourier multiplier $1/h$ as the completion of the set

$$(11) \qquad \{v \in \mathcal{S}' : \hat{v}(\xi,t) = 0, \xi \in W_h^c, \|v\|_{\mathcal{F}_{h,\gamma,T}} = \sup_{\substack{\xi \in W_h \\ 0 \leq t < T}} \frac{|\hat{v}(\xi,t)|}{e^{-\gamma\sqrt{t}|\xi|}h(\xi)} < \infty\}$$

under the indicated norm, where $\gamma \in \{0,1\}$ serves to conveniently index two different norms we wish to consider. Here $\mathcal{S}'$ is the space of tempered distributions on $\mathbf{R}^n$. Also, implicit to the definition of the Banach space $\mathcal{F}_{h,\gamma,T}$ is the requirement that tempered distributions belonging to this space have Fourier transforms which are functions. In the case $h(\xi) = |\xi|^{-2}$, $\mathcal{F}_{h,0,T}$ is the Besov type space introduced by Cannone and Planchon [4]. We will refer to such spaces $\mathcal{F}_{h,\gamma,T}$ as *majorizing spaces* in the case when h is a majorizing kernel. The spaces $\mathcal{F}_{h,1,T}$ generalize those introduced by Lemarié-Rieusset [16] to obtain conditions for spatial analyticity of solutions found by LeJan and Sznitman [17].

Note that if h is a majorizing kernel of exponent $\theta \leq 1$ and $u(x,t) \in \mathcal{F}_{h,\gamma,T} \cap C^1([0,T],\mathcal{S}')$ is such that $\hat{u}(\xi,t)$ is a solution of the (FNS), $u = \check{\hat{u}}$ is a mild solution of the Navier-Stokes. Indeed, the definition of majorizing kernel and of the function spaces $\mathcal{F}_{h,\gamma,T}$ imply that the product of distributions in $\mathcal{F}_{h,\gamma,T}$ is itself a distribution. To see this, note that if u and v are elements of $\mathcal{F}_{h,\gamma,T}$ for a standard majorizing kernel h of exponent θ, $|\hat{u} * \hat{v}(\xi)| \leq Mh * h(\xi) \leq M|\xi|^\theta h(\xi)$, where $M = \|u\|_{\mathcal{F}_{h,\gamma,T}}\|v\|_{\mathcal{F}_{h,\gamma,T}}$. Using the definition of a majorizing kernel, it follows that $\hat{u} * \hat{v}(\xi)$ is locally integrable. Thus, in particular one has $\widehat{B(u,u)}(\xi,t) = \hat{B}(\hat{u},\hat{u})(\xi,t)$ as needed, where $B(u,v) = \int_0^t e^{\nu\Delta s}P(u \cdot \nabla v)ds$ for the Leray projection P on divergence-free vector fields and

$$\hat{B}(\hat{u},\hat{v})(\xi,t) := \int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}} \int \{\hat{u}(\xi-\eta,t-s) \otimes_\xi \hat{v}(\eta,t-s)\} d\eta ds;$$

see Galdi [12], Temam [21]. Consequently, working in these function spaces, a direct relation between solutions obtained using the stochastic representation of Section 3 and the solutions obtained using Picard iteration methods can be seen. This is described in Section 4.

Remark 1.2. In order to restrict the solutions to correspond to (real) vector-valued incompressible flows, one may simply replace the Banach space $\mathcal{F}_{h,\gamma,T}$ by the closed subset

$$(12) \qquad \mathcal{G}_{h,\gamma,T} = \{v \in \mathcal{F}_{h,\gamma,T} : \xi \cdot \hat{v}(\xi,t) = 0, \hat{v}(-\xi,t) = \overline{\hat{v}(\xi,t)}, \xi \in W_h, 0 \leq t \leq T\}.$$

The main results of the paper use majorizing kernels of different exponents to establish existence, uniqueness and regularity properties of the solutions of the (FNS). Moreover these solutions have an expected value representation in terms of a suitably defined multiplicative stochastic functional $\chi(\theta, t)$ of a multitype branching random walk in Fourier wavenumber space. In the statements of these results, $(-\Delta)^\alpha$ denotes the fractional power of the Laplacian defined as the singular integral operator with symbol $|\xi|^{2\alpha}$. For example, using a majorizing kernel h of exponent 1, and working on the space $\mathcal{F}_{h,0,T}$, existence of solutions can be obtained for small enough initial data and forcing on a time interval that is solely constrained by the length of time for which the forcing remains small. Specifically one has the following theorem.

Theorem 1.1. *Let $h(\xi)$ be a standard majorizing kernel with exponent $\theta = 1$. Fix $0 < T \leq +\infty$. Suppose that $\|u_0\|_{\mathcal{F}_{h,0,T}} \leq (\sqrt{2\pi})^3\nu/2$ and $\|(-\Delta)^{-1}g\|_{\mathcal{F}_{h,0,T}} \leq (\sqrt{2\pi})^3\nu^2/4$. Then there is a unique solution u in the ball $\mathcal{B}_0(0, R)$ centered at 0 of radius $R = (\sqrt{2\pi})^3\nu/2$ in the space $\mathcal{F}_{h,0,T}$. Moreover the Fourier transform of the solution is given by $\hat{u}(\xi, t) = h(\xi)E_{\xi_\theta=\xi}\chi(\theta, t), \xi \in W_h$.*

It should be remarked that regularity properties of the solutions can be inferred from the particular majorizing kernel being used. For example, note that the majorizing kernel $h_0(\xi) = \pi^3/|\xi|^2$ gives existence and uniqueness, but no control over regularity of the solution. However, solutions obtained using the majorizing kernels $h_\beta^{(\alpha)} = |\xi|^{\beta-2}e^{-\alpha|\xi|^\beta}, 0 < \beta \leq 1, \alpha > 0$, maintain the same C^∞-regularity of the initial data, as can be seen from the bound on the Fourier transform of the solution. Moreover $\beta < 1$ permits smooth compactly supported initial data.

On the other hand, working in the function spaces $\mathcal{F}_{h,1,T}$ it is possible to use majorizing kernels to obtain spatial analyticity of the solution. However, it should be remarked that the size constraints imposed on the initial data and forcing are substantially more severe that those required in Theorem 1.1. Specifically one has

Theorem 1.2. *Let $h(\xi)$ be a standard majorizing kernel with exponent $\theta = 1$. Fix $0 < T \leq +\infty$. Assume that*

$$\|e^{\nu t\Delta}u_0(x)\|_{\mathcal{F}_{h,1,T}} \leq \frac{(\sqrt{2\pi})^3}{2}\rho\nu e^{-1/2\nu}$$

and that

$$\|(-\Delta)^{-1}g(x,t)\|_{\mathcal{F}_{h,1,T}} \leq \frac{(\sqrt{2\pi})^3}{4}\rho\nu^2 e^{-1/2\nu}$$

for some $0 \leq \rho < 1$. Then there is a unique solution u in the ball $\mathcal{B}_1(0, R)$ centered at 0 of radius $R = (\rho/2)(\sqrt{2\pi})^3\nu e^{-\frac{1}{2\nu}}$ in the space $\mathcal{F}_{h,1,T}$.

Under the conditions of Theorem 1.2 the asserted solution satisfies the following decay condition:

$$\sup_{0\leq t<T}\sup_{\xi\in\mathbf{R}^3}\frac{e^{\sqrt{t}|\xi|}|\hat{u}(\xi,t)|}{h(\xi)} < \infty. \tag{13}$$

Thus Theorem 1.2 provides another approach generalizing that of Lemarié-Rieusset [16] to obtain conditions for regularity in the stronger form of spatial analyticity. More specifically, for example, if $\exp(-d|\xi|)h(\xi) \in L^1$ for some $d \in \mathbf{R}$, then one may conclude that $u(x+iy,t)$ is complex analytic for $|y| < \sqrt{t} - d$. Thus the generalized Lemarié-Rieusset estimate (13) may be applied to obtain spatial analyticity for suitable majorizing kernels with exponent 1. In particular, Theorem 1.2 extends the results of Lemarié-Rieusset since there are majorizing kernels that are larger than $h_0(\xi) = \pi^3/|\xi|^2$ as (26) shows.

One may also obtain local existence and uniqueness from more relaxed conditions on the majorizing kernels as illustrated by the following.

Theorem 1.3. *Let $h(\xi)$ be a standard majorizing kernel with exponent $\theta < 1$. Fix $0 < T \leq +\infty, \gamma \in \{0,1\}$. Assume $e^{\nu t\Delta}u_0(x) \in \mathcal{F}_{h,\gamma,T}$ and for some $1 \leq \beta \leq 2$, $(-\Delta)^{-\frac{\beta}{2}}g(x,t) \in \mathcal{F}_{h,\gamma,T}$. Then there is a $0 < T_* \leq T$ for which one has a unique solution $u \in \mathcal{F}_{h,\gamma,T_*}$.*

Remark 1.3. Fujita and Kato [11] obtain global smooth solutions for initial velocities in L^2 with sufficiently small norm. In particular these results require finite energy conditions. Majorizing kernels can permit infinite energy and provide global smooth solutions if the initial data is sufficiently small in the norm $|\cdot|_h$. Kato [15] assumes initial velocity fields in L^3, and proves existence of smooth global solutions if the L^3 norm of the initial velocity is suitably small. While these results allow infinite energy, they do not cover the cases obtained under majorization by $h^{\alpha}_{\beta}, 0 \leq \beta \leq 1$.

Remark 1.4. Another variation on the general approach presented here leads to conditions for a local existence and uniqueness theory in all dimensions. Here one can use a particular perturbation to obtain results as follows: For a given $\nu > 0$ there is a time T_*, depending on ν, such that one has existence and uniqueness in a ball of $\mathcal{G}_{h,T_*}$ which does not otherwise depend on ν; see Orum [20].

The organization of this paper is as follows. In Section 2 we identify various majorizing kernels, including kernels applicable to Navier-Stokes in $n \geq 2$ dimensions. In Section 3 the stochastic recursion is defined and Theorem 1.1 is proved. In Section 4 the Picard iteration is defined and proofs of Theorems 1.2 and 1.3 are given. Conclusions and final remarks are presented in Section 5.

2. FNS-majorizing kernels

The FNS-admissible majorizing kernels play an important role in the development of our results. Recall that $h : W_h \to (0,\infty)$ is a standardized majorizing kernel with support $W_h \subset \mathbf{R}^n$ of exponent $\theta \geq 0$ if

$$h * h(\xi) \leq |\xi|^{\theta} h(\xi) \quad \text{for all} \quad \xi \in W_h.$$

The family of standard majorizing kernels of exponent θ on $\mathbf{R}^n$ is denoted by

$$\mathcal{H}_{n,\theta} = \{h : W_h \to (0,\infty) : h * h(\xi) \leq |\xi|^{\theta} h(\xi) \quad \text{for all} \quad \xi \in W_h \subset \mathbf{R}^n\}.$$

The first part of this section gives some building block structure of the sets $\mathcal{H}_{n,\theta}$ of majorizing kernels. The second part provides constructions of useful sub-families of $\mathcal{H}_{n,\theta}$. The main emphasis is on examples in $\mathcal{H}_{3,\theta}$ for $\theta = 0, 1$, although some examples are given in a more general setting. The section will close with some classes of examples of divergence-free vector fields which are majorized by specific kernels.

We begin by showing that the $\mathcal{H}_{n,\theta}$'s are logarithmically convex for fixed dimension n.

Theorem 2.1. *Suppose that* $\{q_j : 1 \le j \le m\}$ *satisfies* $q_j > 0$, *and* $\sum_1^m q_j = 1$. *Then for* $h_j \in \mathcal{H}_{n,\theta_j}$, $j = 1, ..., m$,

$$h(\xi) = \prod_{j=1}^{m} h_j^{q_j}(\xi) \in \mathcal{H}_{n,\sum_{j=1}^m q_j\theta_j}$$

with support $W_h = \bigcap_{j=1}^m W_{h_j}$.

Corollary 2.1. *Suppose that* $\{q_j : 1 \le j \le m\}$ *satisfies* $q_j > 0$, *and* $\sum_1^m q_j = 1$. *Then for* $h_j \in \mathcal{H}_{n,\theta}$, $j = 1, ..., m$,

$$h(\xi) = \prod_{j=1}^{m} h_j^{q_j}(\xi) \in \mathcal{H}_{n,\theta}$$

with support $W_h = \bigcap_{j=1}^m W_{h_j}$.

Proof. Take $q_1, q_2 > 0$ with $q_1 + q_2 = 1$. Take $h_1 \in \mathcal{H}_{n,\theta_1}$ and $h_2 \in \mathcal{H}_{n,\theta_2}$ and let $h(\xi) = h_1^{q_1}(\xi)h_2^{q_2}(\xi)$. Using Hölder's inequality,

$$\begin{aligned} h * h(\xi) &= \int_\eta (h_1(\eta)h_1(\xi-\eta))^{q_1}(h_2(\eta)h_2(\xi-\eta))^{q_2}\,d\eta \\ &\le (h_1 * h_1)^{q_1}(\xi)(h_2 * h_2)^{q_2}(\xi) \\ &\le |\xi|^{q_1\theta_1+q_2\theta_2} h_1^{q_1}(\xi)h_2^{q_2}(\xi) = |\xi|^{q_1\theta_1+q_2\theta_2} h(\xi). \end{aligned}$$

The complete result follows by induction. □

In addition, relationships between the $\mathcal{H}_{n,\theta}$'s as both n and θ vary are governed by a similar logarithmic convexity.

Theorem 2.2. *Fix* $n \ge 1$. *Suppose that* $k_1, \dots, k_m$ *is a partition of* n *and for each* $j = 1, \dots, m$, h_j *is in* $\mathcal{H}_{k_j,\theta_j}$. *Then*

$$h(\xi) = \prod_{j=1}^{m} h_j(\xi_j), \qquad \xi = (\xi_1, \dots, \xi_m) \text{ for } \xi_j \in \mathbf{R}^{k_j},$$

is in $\mathcal{H}_{n,\sum_{j=1}^m \theta_j}$ *with* $W_h = W_{h_1} \times ... \times W_{h_m}$.

Proof. For h as defined, taking $\eta = (\eta_1, ..., \eta_m)$ with $\eta_j \in \mathbf{R}^{k_j}$,

$$\begin{aligned} h * h(\xi) &= \int_{\eta \in \mathbf{R}^n} \prod_{j=1}^{m} h_j(\eta_j)h_j(\xi_j - \eta_j)\,d\eta \\ &= \prod_{j=1}^{m} \int_{\eta_j \in \mathbf{R}^{k_j}} h_j(\eta_j)h_j(\xi_j-\eta_j)\,d\eta_j \\ &\le \prod_{j=1}^{m} |\xi_j|^{\theta_j} h_j(\xi_j) \\ &= \prod_{j=1}^{m} |\xi_j|^{\theta_j} h(\xi) \\ &\le |\xi|^{\sum_{j=1}^m \theta_j} h(\xi). \end{aligned}$$

□

Theorem 2.3. *If A is an $n \times n$ invertible matrix and $h \in \mathcal{H}_{n,\theta}$, then defining $||A|| = \sup\{|A\mathbf{x}| : |\mathbf{x}| = 1\}$,*

$$h_A(\xi) := |detA| \cdot ||A||^{-\theta} h(A\xi) \in \mathcal{H}_{n,\theta}$$

with support $W_{h_A} = \{A^{-1}\xi : \xi \in W_h\}$.

Proof. Take A and h as given and define h_A as above. Then $W_{h_A} = \{\xi : 0 < h(A\xi) < \infty\} = \{A^{-1}\xi : 0 < h(\xi) < \infty\}$ and

$$\begin{aligned} h_A * h_A(\xi) &= |detA|^2 ||A||^{-2\theta} \int_{\mathbf{R}^n} h(A\eta) h(A(\xi - \eta)) d\eta \\ &= |detA| \cdot ||A||^{-2\theta} \int_{\mathbf{R}^n} h(\eta) h(A\xi - \eta) d\eta \\ &\le |detA| \cdot ||A||^{-2\theta} |A\xi|^\theta h(A\xi) \\ &\le |detA| \cdot ||A||^{-\theta} |\xi|^\theta h(A\xi) \\ &= |\xi|^\theta h_A(\xi). \end{aligned}$$

□

The $\mathcal{H}_{n,\theta}$'s are also closed under logarithmic translation both linearly and in norm.

Theorem 2.4. *If $h \in \mathcal{H}_{n,\theta}$ and $\psi : \mathbf{R}^n \to [0, \infty)$ satisfies $\psi(\xi) \le \psi(\eta) + \psi(\xi - \eta)$ for all $\eta, \xi \in W_h$, then*

$$h_\psi(\xi) = e^{-\psi(\xi)} h(\xi) \in \mathcal{H}_{n,\theta}.$$

Proof. $h_\psi * h_\psi(\xi) \le e^{-\psi(\xi)} h * h(\xi) \le |\xi|^\theta h_\psi(\xi)$. □

Corollary 2.2. *If $h \in \mathcal{H}_{n,\theta}$, then*

(i) *$e^{a\cdot\xi} h(\xi) \in \mathcal{H}_{n,\theta}$ for any fixed $a \in \mathbf{R}^n$,*

and, for any pseudo-metric ρ on a subset of $\mathbf{R}^3$ containing W_h,

(ii) *$e^{-a\rho(\xi_0,\xi)} h(\xi) \in \mathcal{H}_{n,\theta}$ for any $a > 0$ and ξ_0 fixed.*

Note. The example $e^{-a|\xi|^\beta} h(\xi) \in \mathcal{H}_{n,\theta}$ for any $a > 0$ and $0 < \beta \le 1$ is a noteworthy special case of part (ii) of Corollary 2.2.

The question of existence of majorizing kernels is non-trivial. For example, it can be shown that any piecewise continuous $h \in \mathcal{H}_{1,1}$ must have $W_h = (0, \infty)$ or $W_h = (-\infty, 0)$. This illustrates the tradeoff between n and θ; if exponent $\theta > 0$, the existence of majorizing kernels with support $\mathbf{R}^n \backslash \{0\}$ is problematic for smaller values of n. There are however fully supported majorizing kernels of exponent $\theta = 0$ for all $n \ge 1$.

Example 2.1. Let

$$h_1(\xi) = \frac{1}{2\pi(1 + \xi^2)} \text{ for } \xi \in \mathbf{R}.$$

Then

$$h_1 * h_1(\xi) = \frac{1}{2\pi(4 + \xi^2)} \le h_1(\xi)$$

for all $\xi \in \mathbf{R}$, so $h_1 \in \mathcal{H}_{1,0}$ with $W_{h_1} = \mathbf{R}$. Using Theorem 2.2, it is easy to see that for $n > 1$,

$$h_n(\xi) = (2\pi)^{-n} \prod_{j=1}^n (1 + \xi_j^2)^{-1} \in \mathcal{H}_{n,0}$$

with $W_h = \mathbf{R}^n$. The following rotationally invariant extension of h_1 is often more attractive:

$$\widetilde{h}_n(\xi) = \frac{\Gamma(\frac{n+1}{2})}{2\pi^{\frac{n+1}{2}}(1+|\xi|^2)^{\frac{n+1}{2}}}.$$

Then again

$$\widetilde{h}_n * \widetilde{h}_n(\xi) \leq \widetilde{h}_n(\xi) \qquad \text{for all} \qquad \xi \in \mathbf{R}^n, n \geq 1.$$

(See Folland [9], page 247, for an indication of the necessary computation.)

Propositions 2.1 and 2.2 below provide some examples of majorizing kernels in $\mathcal{H}_{3,1}$.

Proposition 2.1. *Suitably normalized, each of the following kernels $h_\beta^{(\alpha)}$ are in $\mathcal{H}_{3,1}$ with support $W = \mathbf{R}^3 \backslash \{0\}$:*

$$h_\beta^{(\alpha)}(\xi) = |\xi|^{\beta-2} e^{-\alpha|\xi|^\beta}, \ \xi \neq 0, \ 0 \leq \beta \leq 1, \ \alpha > 0.$$

Using Theorem 2.1 the following is immediate.

Corollary 2.3. *Suitably normalized, for each $\theta \in (0,1)$, $0 \leq \beta \leq 1$, and $\alpha > 0$,*

$$h_{\theta,\beta}^{(\alpha)}(\xi) = \frac{|\xi|^{\theta(\beta-2)} e^{-\alpha\theta|\xi|^\beta}}{(2\pi)^{3(1-\theta)} \prod_{j=1}^3 (1+\xi_j^2)^{(1-\theta)}}, \xi \neq 0,$$

and

$$\widetilde{h}_{\theta,\beta}^{(\alpha)}(\xi) = \frac{|\xi|^{\theta(\beta-2)} e^{-\alpha\theta|\xi|^\beta}}{(1+|\xi|^2)^{2(1-\theta)}}, \xi \neq 0,$$

are both in $\mathcal{H}_{3,\theta}$ with support $W = \mathbf{R}^3 \backslash \{0\}$.

The following lemma is sometimes useful for computing the convolution of two radially symmetric (rotationally invariant) functions, especially in dimension 3, due to the simplification of the integrand. It will be used in the proof of Proposition 2.1 below. Let $\sigma_n = 2\pi^{(n+1)/2}/\Gamma(\frac{n+1}{2})$ be the n-dimensional surface volume of a unit sphere S^n, and let

$$k(x,y,|\xi|) = \sqrt{(x+y+|\xi|)(-x+y+|\xi|)(x-y+|\xi|)(x+y-|\xi|)}$$

be 4 times the area of a triangle with side lengths x, y, and $|\xi|$.

Lemma 2.1. *Suppose $n \geq 2$, and that $h_1, h_2 : \mathbf{R}^n \to \mathbf{C}$ are each rotationally invariant, i.e. $h_1(\xi) = g_1(|\xi|)$ and $h_2(\xi) = g_2(|\xi|)$. Then the convolution $h_1 * h_2(\xi)$, if it exists, may be computed for $|\xi| \neq 0$ as*

$$h_1 * h_2(\xi) = \frac{\sigma_{n-2}}{2^{n-3}|\xi|^{n-2}} \iint_{T_{|\xi|}} g_1(x) g_2(y)\, xy\, [k(x,y,|\xi|)]^{n-3}\, dx dy, \tag{14}$$

where $T_{|\xi|} = \{(x,y) \in \mathbf{R}^2 : y \geq -x + |\xi|, x - |\xi| \leq y \leq x + |\xi|\}$.

Proof. The integrand in $h_1 * h_2(\xi) = \int h_1(\eta) h_2(\xi - \eta) d\eta$ is invariant under rotations around the axis defined by ξ (or reflection if $n = 2$). Such rotations leave invariant the unit sphere S^{n-2} centered at the origin in the hyperplane orthogonal to ξ. The following coordinates are therefore natural: $x = |\eta|$, $y = |\xi - \eta|$,

$\omega \in S^{n-2}$. We transform to this coordinate system by first passing to ordinary spherical coordinates:

$$
\begin{aligned}
\eta_1 &= r\cos\theta_1, & 0 \le \theta_1 \le \pi,\\
\eta_2 &= r\sin\theta_1\cos\theta_2, & 0 \le \theta_2 \le \pi,\\
\eta_3 &= r\sin\theta_1\sin\theta_2\cos\theta_3, & 0 \le \theta_3 \le \pi,\\
&\vdots & \vdots\\
\eta_{n-1} &= r\sin\theta_1 \cdots \sin\theta_{n-2}\sin\theta_{n-1}, & 0 \le \theta_{n-2} \le \pi,\\
\eta_n &= r\sin\theta_1 \cdots \sin\theta_{n-2}\cos\theta_{n-1}, & 0 \le \theta_{n-1} < 2\pi.
\end{aligned}
\tag{15}
$$

Here $r = |\eta|$, and θ_1 is the angle between η and ξ. The n-dimensional volume element is

$$
\begin{aligned}
d\eta_1 d\eta_2 \cdots d\eta_n &= r^{n-1}dr\sin^{n-2}\theta_1\sin^{n-3}\theta_2\cdots\sin\theta_{n-2}d\theta_1\cdots d\theta_{n-1}\\
&= r^{n-1}dr\sin^{n-2}\theta_1 d\theta_1 d\omega
\end{aligned}
$$

where $d\omega$ is the surface element for the sphere S^{n-2}. Using spherical coordinates and performing the integration over S^{n-2} gives, with $\theta = \theta_1$,

$$h_1 * h_2(\xi) = \sigma_{n-2}\int_0^\pi\int_0^\infty g_1(r)g_2\left(\sqrt{r^2+|\xi|^2-2r|\xi|\cos\theta}\right)r^{n-1}\sin^{n-2}\theta drd\theta.$$

Let $x = r = |\eta|$ and $y = \sqrt{r^2+|\xi|^2-2r|\xi|\cos\theta} = |\xi-\eta|$. The new region of integration becomes the set $T_{|\xi|}$ of all possible ordered pairs of triangle side lengths when the third side of the triangle has length $|\xi|$. The Jacobian is

$$\left|\frac{\partial(r,\theta)}{\partial(x,y)}\right| = \left|\frac{\partial(x,y)}{\partial(r,\theta)}\right|^{-1} = \left|\begin{matrix}\partial x/\partial r & 0\\ * & \partial y/\partial\theta\end{matrix}\right|^{-1} = \frac{y}{x|\xi|\sin\theta};$$

hence,

$$h_1 * h_2(\xi) = \frac{\sigma_{n-2}}{|\xi|}\iint_{T_{|\xi|}} g_1(x)g_2(y)xy\,[x\sin\theta]^{n-3}\,dxdy. \tag{16}$$

Expressed in terms of x and y, $x\sin\theta = |2\xi|^{-1}k(x,y,|\xi|)$, giving (14). □

Proof of Proposition 2.1. The cases $\beta = 0$ and $\beta = 1$ are treated by LeJan and Sznitman [17]. They are included for completeness here. The case $\beta = 0$ is treated first. Clearly $h_0^{(\alpha)} * h_0^{(\alpha)}(\xi)$ is finite for all $|\xi| \neq 0$. From Lemma 2.1,

$$
\begin{aligned}
h_0^{(\alpha)} * h_0^{(\alpha)}(\xi) &= 2\pi e^{-2\alpha}|\xi|^{-1}\iint_{T_{|\xi|}}\frac{1}{xy}\,dx\,dy\\
&= 2\pi e^{-2\alpha}|\xi|^{-1}\iint_{T_1}\frac{1}{xy}\,dx\,dy\\
&= 2\pi e^{-\alpha}\iint_{T_1}\frac{1}{xy}\,dx\,dy\,|\xi|\,h_0^{(\alpha)}(\xi).
\end{aligned}
$$

For $\alpha > 0$ and $\beta \in (0,1]$ fixed we have $h_\beta^{(\alpha)}(\xi) = g(|\xi|)$ where $g(r) = r^{\beta-2}e^{-\alpha r^\beta}$. Note that for $r, x > 0$, $(x+r)^{\beta-1} - x^{\beta-1} \le 0$ and for $0 \le x \le r$, $x^\beta + (r-x)^\beta \ge r^\beta$.

For $|\xi| = r$ then

$$\begin{aligned}
h * h(\xi) &= 2\pi r^{-1} \iint_{T_r} x g(x) y g(y)\, dx\, dy \\
&= \frac{2\pi r^{-1}}{\alpha\beta} \int_{x=0}^{\infty} x^{\beta-1} e^{-\alpha x^\beta} \int_{y=|r-x|}^{r+x} \alpha\beta y^{\beta-1} e^{-\alpha y^\beta}\, dy\, dx \\
&= \frac{2\pi r^{-1}}{\alpha\beta} \int_{x=0}^{\infty} x^{\beta-1} e^{-\alpha x^\beta} (e^{-\alpha|r-x|^\beta} - e^{-\alpha(r+x)^\beta})\, dx \\
&\leq \frac{2\pi r^{-1}}{\alpha\beta} (\int_{x=0}^{r} x^{\beta-1} e^{-\alpha x^\beta - \alpha(r-x)^\beta}\, dx \\
&+ \int_{x=0}^{\infty} (x+r)^{\beta-1} e^{-\alpha(x+r)^\beta - \alpha x^\beta}\, dx - \int_{x=0}^{\infty} x^{\beta-1} e^{-\alpha x^\beta - \alpha(x+r)^\beta}\, dx) \\
&\leq \frac{2\pi r^{-1}}{\alpha\beta} e^{-\alpha r^\beta} \int_{x=0}^{r} x^{\beta-1}\, dx \\
&= \frac{2\pi r^{\beta-1}}{\alpha\beta^2} e^{-\alpha r^\beta}.
\end{aligned}$$

□

One may also show that certain Bessel kernels and similar transforms provide further interesting examples of majorizing kernels in $\mathcal{H}_{n,1}$ for $n \geq 3$, as in the following proposition. These kernels are closely related to the Bessel kernels of Aronszajn and Smith [2]. They can also be combined with the kernels of Example 2.1 to construct kernels in $\mathcal{H}_{n,\theta}$ for $0 < \theta < 1$.

Proposition 2.2. *For $n \geq 3$ and (β, γ) with $0 \leq \beta \leq 1$ and $1 \leq \gamma \leq 1 + \beta$, suitably normalized, each of the following radially symmetric functions is in $\mathcal{H}_{n,1}$ with support $\mathbf{R}^n \backslash \{0\}$:*

$$h_{n,\beta,\gamma}(\xi) = \int_{t>0} t^{\frac{\gamma-n}{2}-1} e^{-t^\beta - |\xi|^2/t}\, dt, \ \xi \in \mathbf{R}^n.$$

Remark 2.1. One may apply the Laplace method for estimating integrals to show that the Bessel type kernels $h = h_{n,\beta,\gamma}$ are also regularizing kernels in the sense that the distributions in the corresponding function space $\mathcal{F}_{h,0,T}$ are C^∞-functions.

The following lemma provides a comparison between the kernels of Propositions 2.1 and 2.2.

Lemma 2.2. (i) *For each $\alpha \in (0, 1)$, there exists a constant $c^{(\alpha)}$ with*

$$h_{3,1,2}(\frac{\xi}{2}) \leq c^{(\alpha)} h_1^{(\alpha)}(\xi).$$

(ii) *For each $\alpha > 0$ and $\beta \in [0, 1]$, there exists a constant $c_\beta^{(\alpha)}$ with*

$$h_{3,1,1+\beta}(\frac{\xi}{2}) \leq c_\beta^{(\alpha)} h_\beta^{(\alpha)}(\xi).$$

Proof. Fix $\beta \in (0,1]$ and choose $\delta \in (0,1)$. Then

$$\begin{aligned} h_{3,1,1+\beta}(\frac{\xi}{2}) &= \int_{t>0} t^{\frac{\beta}{2}-2} e^{-\frac{|\xi|^2}{4t}-t}\,dt \\ &= e^{-\delta|\xi|}\int_{t>0} t^{\frac{\beta}{2}-2} e^{-\frac{(1-\delta^2)|\xi|^2}{4t}-(\sqrt{t}-\frac{\delta|\xi|}{2\sqrt{t}})^2}\,dt \\ &\le e^{-\delta|\xi|}\int_{t>0} t^{\frac{\beta}{2}-2} e^{-\frac{(1-\delta^2)|\xi|^2}{4t}}\,dt \\ &= (\frac{(1-\delta^2)|\xi|^2}{4})^{\frac{\beta}{2}-1} e^{-\delta|\xi|}\int_{s>0} s^{-\beta/2}e^{-s}\,ds \\ &= (\frac{(1-\delta^2)}{4})^{\frac{\beta}{2}-1}\Gamma(1-\beta/2)|\xi|^{\beta-2}e^{-\delta|\xi|}. \end{aligned}$$

For $|\xi| \ge 1$, trivially $e^{-\delta|\xi|} \le e^{-\delta|\xi|^\beta}$. For $|\xi| < 1$, $|\xi|^\beta - |\xi| \le (1-\beta)\beta^{\frac{\beta}{1-\beta}}$. Taking $\delta = \alpha$, this gives, for $0 < \beta \le 1$ and $0 < \alpha < 1$,

$$h_{3,1,1+\beta}(\frac{\xi}{2}) \le C_\beta^{(\alpha)} h_\beta^{(\alpha)}(\xi)$$

for $C_\beta^{(\alpha)} = 2^{2-\beta}\Gamma(1-\frac{\beta}{2})(1-\alpha^2)^{\frac{\beta}{2}-1}e^{\alpha(1-\beta)\beta^{\frac{\beta}{1-\beta}}}$.

For $0<\beta<1,\ 0<\delta<1$ and $\alpha \ge 1$,

$$e^{-\delta|\xi|} \le e^{-\alpha|\xi|^\beta} \quad \text{for } |\xi| \ge (\frac{\alpha}{\delta})^{\frac{1}{1-\beta}}.$$

For $|\xi| < (\frac{\alpha}{\delta})^{\frac{1}{1-\delta}}$, $-\delta|\xi| + \alpha|\xi|^\beta$ is maximized at $|\xi| = (\frac{\alpha\beta}{\delta})^{\frac{1}{1-\beta}}$ with a maximum of $(1-\beta)\alpha^{\frac{1}{1-\beta}}(\frac{\beta}{\delta})^{\frac{\beta}{1-\beta}}$. This gives

$$h_{3,1,1+\beta}(\frac{\xi}{2}) \le C_\beta^{(\alpha)} h_\beta^{(\alpha)}(\xi)$$

for $C_\beta^{(\alpha)} = 2^{2-\beta}\Gamma(1-\frac{\beta}{2})\inf_{0<\delta<1}(1-\delta^2)^{\frac{\beta}{2}-1}e^{(1-\beta)\alpha^{\frac{1}{1-\beta}}}(\frac{\beta}{\delta})^{\frac{\beta}{1-\beta}}$. □

The majorizing kernels of Proposition 2.2 arise as weighted integrals of the function $t^{-\frac{n}{2}}e^{-\frac{|\xi|^2}{t}}$. The method of deriving these kernels can also be used to derive families of non-radial kernels as follows. Fix $\alpha \in (0,2]$ and define

$$f_\alpha(x) = \frac{1}{2\pi}\int_{\lambda\in\mathbf{R}} e^{-|\lambda|^\alpha + i\lambda x}\,d\lambda \qquad \text{for } x \in \mathbf{R}.$$

These f_α's correspond to the symmetric stable densities; for example, $f_1(x) = (\pi(1+x^2))^{-1}$ and $f_2(x) = \frac{1}{2\sqrt{\pi}}e^{-x^2/4}$. The convolution and scaling properties of the f_α's give

(17)

$$(s+t)^{-\frac{1}{\alpha}}f_\alpha((s+t)^{-1/\alpha}x) = \int_{y\in\mathbf{R}}(st)^{-1/\alpha}f_\alpha(s^{-1/\alpha}(x-y))f_\alpha(t^{-1/\alpha}y)\,dy$$

for $s,t>0,\ x\in\mathbf{R}$.

For $n \ge 1,\ 0<\alpha\le 2$, and $g:\mathbf{R}^+ \to \mathbf{R}$ define

$$T_{n,\alpha}g(x) = \int_{s>0} g(s)s^{-n/\alpha}\prod_{i=1}^n f_\alpha(s^{-1/\alpha}x_i)\,ds$$

for all $x \in \mathbf{R}^n$ such that this integral converges.

Lemma 2.3. *Suppose $g_1, g_2 : \mathbf{R}^+ \to \mathbf{R}$ such that $T_{n,\alpha} g_1$, $T_{n,\alpha} g_2$, $g_1 * g_2$ and $T_{n,\alpha} g_1 * T_{n,\alpha} g_2$ each exist a.e. with respect to Lebesgue measure. Then*

$$T_{n,\alpha} g_1 * T_{n,\alpha} g_2(x) = T_{n,\alpha}(g_1 * g_2)(x) \text{ a.e.}$$

Proof. Use Fubini's Theorem and (17) above to check the result. □

Proof of Proposition 2.2. For $\xi \in \mathbf{R}^n$, $h_{n,\beta,\gamma}(\xi) = 2^n \pi^{n/2} T_{n,2} h_{\beta,\gamma}(\xi)$ where

$$h_{\beta,\gamma}(t) = t^{\frac{\gamma}{2}-1} e^{-t^\beta} \cdot \mathbf{1}_{(0,\infty)}(t).$$

Note that since $u^\beta + (1-u)^\beta \geq 1$ for $0 \leq u \leq 1$ and $0 \leq \beta \leq 1$,

$$\begin{aligned} h_{\beta,\gamma} * h_{\beta,\gamma}(t) &= \int_{s=0}^{t} s^{\frac{\gamma}{2}-1}(t-s)^{\frac{\gamma}{2}-1} e^{-s^\beta-(t-s)^\beta}\, ds \\ &= t^{\gamma-1} \int_{u=0}^{1} u^{\frac{\gamma}{2}-1}(1-u)^{\frac{\gamma}{2}-1} e^{-t^\beta(u^\beta+(1-u)^\beta)}\, du \\ &\leq t^{\gamma-1} e^{-t^\beta} \int_{u=0}^{1} u^{\frac{\gamma}{2}-1}(1-u)^{\frac{\gamma}{2}-1}\, du \\ &= B(\frac{\gamma}{2}, \frac{\gamma}{2}) h_{\beta,2\gamma}(t). \end{aligned}$$

This gives, for $\beta \in [0,1]$ and $\gamma > 0$,

$$h_{n,\beta,\gamma} * h_{n,\beta,\gamma}(\xi) \leq B(\frac{\gamma}{2}, \frac{\gamma}{2}) h_{n,\beta,2\gamma}(\xi)$$

for all ξ such that $h_{n,\beta,\gamma}(\xi)$ exists.

We proceed by showing that, for (β,γ) in the range given, the $h_{n,\beta,\gamma}$'s exist and the ratio

$$\frac{h_{n,\beta,2\gamma}(\xi)}{|\xi| h_{n,\beta,\gamma}(\xi)} \tag{18}$$

is bounded uniformly in $\xi \in \mathbf{R}^n$. For $z > 0$ and $\beta \in [0,1]$ define

$$g_{\beta,\alpha}(z) = \int_0^\infty t^{\alpha-1} e^{-\frac{z^2}{t} - t^\beta}\, dt.$$

For $|\xi| = z$ we have

$$h_{n,\beta,\gamma}(\xi) = g_{\beta,\frac{\gamma-n}{2}}(z)$$

and

$$h_{n,\beta,2\gamma}(\xi) = g_{\beta,\gamma-\frac{n}{2}}(z).$$

The following lemma is useful.

Lemma 2.4. *For $\beta \in (0,1]$ and $z > 0$,*

(i) *For $\alpha > 0$, $g_{\beta,\alpha}(z) \leq \frac{1}{\beta}\Gamma(\frac{\alpha}{\beta})$.*
(ii) *For $\alpha = 0$, $g_{\beta,0}(z) \leq \frac{1}{\beta} e^{-1} + \int_{s=z^2}^\infty s^{-1} e^{-s}\, ds$.*
(iii) *For $\alpha < 0$, $z^{-2\alpha} g_{\beta,\alpha}(z) \leq \Gamma(-\alpha)$ with $\lim_{z\downarrow 0} z^{-2\alpha} g_{\beta,\alpha}(z) = \Gamma(-\alpha)$.*

Proof of Lemma 2.4. Both $g_{\beta,\frac{\gamma-n}{2}}$ and $g_{\beta,\gamma-\frac{n}{2}}$ are continuous functions on $(0,\infty)$ for all (β,γ) with $0 \leq \beta \leq 1$ and $1 \leq \gamma \leq 1+\beta$. For any $\alpha \in \mathbf{R}$ and $0 < \beta \leq 1$, the charge of variables $x = \frac{z^2}{t}$ gives

$$g_{\beta,\alpha}(z) = z^{2\alpha} \int_0^\infty s^{-\alpha-1} e^{-s-s^{-\beta} z^{2\beta}}\, ds. \tag{19}$$

In particular $z^{-2\alpha}g_{\beta,\alpha}(z)$ is continuous and strictly decreasing in $z>0$. For $\alpha<0$, $\lim_{z\searrow 0} z^{-2\alpha}g_{\beta,\alpha}(z)=\Gamma(-\alpha)$. Thus we see immediately that $g_{\beta,\frac{\gamma-n}{2}}$ is a continuous and decreasing function of z specified by β and γ, and $g_{\beta,\gamma-\frac{n}{2}}$ is a continuous and decreasing function of z for $\gamma<\frac{n}{2}$. Next consider the case $n=3$, $\beta\in[\frac{1}{2},1]$ and $\gamma=\frac{3}{2}$:

$$\begin{aligned} g_{\beta,0}(z) &\leq \int_1^\infty t^{\beta-1}e^{-t^\beta}\,dt+\int_0^1 t^{-1}e^{-\frac{z^2}{t}}\,dt \\ &= \frac{1}{\beta}e^{-1}+\int_{z^2}^\infty s^{-1}e^{-s}\,ds. \end{aligned}$$

The case $n=3$, $\gamma\in(\frac{3}{2},1+\beta)$ for $\beta\in(\frac{1}{2},1]$ is handled as follows. For $\alpha>0$, the change of variables $s=t^\beta$ gives

$$\begin{aligned} g_{\beta,\alpha}(z) &= \frac{1}{\beta}\int_0^\infty s^{\frac{\alpha}{\beta}-1}e^{-s-z^2s^{-\frac{1}{\beta}}}\,ds \\ &\leq \frac{1}{\beta}\Gamma(\frac{\alpha}{\beta}). \end{aligned}$$

□

Returning to the proof of Proposition 2.2 we see that the key to bounding (18) uniformly in $\xi\in\mathbf{R}^n$ is showing that

$$\limsup_{z\searrow 0}\frac{g_{\beta,\gamma-\frac{n}{2}}(z)}{zg_{\beta,\frac{\gamma-n}{2}}(z)}$$

and

$$\limsup_{z\nearrow\infty}\frac{g_{\beta,\gamma-\frac{n}{2}}(z)}{zg_{\beta,\frac{\gamma-n}{2}}(z)}$$

are both finite.

First consider the case $(\beta,\gamma)=(0,1)$. From (19), for all $n\geq 3$,

$$\frac{g_{0,1-\frac{n}{2}}(z)}{zg_{0,\frac{1-n}{2}}(z)}=\frac{\Gamma(\frac{n}{2}-1)}{\Gamma(\frac{n-1}{2})}<\infty.$$

Next consider $\beta\in(1,2]$ and $\gamma\in[1,1+\beta]\cap[1,\frac{n}{2})$. From (iii) of Lemma 2.4

$$\begin{aligned} \limsup_{z\searrow 0}\frac{g_{\beta,\gamma-\frac{n}{2}}(z)}{zg_{\beta,\frac{\gamma-n}{2}}(z)} &= \limsup_{z\searrow 0} z^{\gamma-1}\frac{z^{n-2\gamma}g_{\beta,\gamma-\frac{n}{2}}(z)}{z^{n-\gamma}g_{\beta,\frac{\gamma-n}{2}}(z)} \\ &= \begin{cases}\frac{\Gamma(\frac{n}{2}-1)}{\Gamma(\frac{n-1}{2})}, & \gamma=1,\\ 0, & \gamma\in(1,1+\beta]\cap(1,\frac{n}{2}).\end{cases} \end{aligned}$$

For $n=3$, $\gamma=\frac{3}{2}$, and $\beta\in[\frac{1}{2},1]$, using (ii) and (iii) of Lemma 2.4,

$$\begin{aligned} \limsup_{z\searrow 0}\frac{g_{\beta,0}(z)}{zg_{\beta,-\frac{3}{4}}(z)} &= \frac{1}{\Gamma(\frac{3}{4})}\lim_{z\searrow 0} z^{\frac{1}{2}}g_{\beta,0}(z) \\ &\leq \frac{1}{\Gamma(\frac{3}{4})}\limsup_{z\searrow 0}(z^{\frac{1}{2}}\int_{z^2}^1 s^{-1}\,ds+z^{\frac{1}{2}}\int_1^\infty e^{-s}\,ds) \\ &\leq \frac{2}{\Gamma(\frac{3}{4})}\lim_{z\searrow 0} z^{\frac{1}{2}}\ln z=0. \end{aligned}$$

For $n = 4$, $\gamma = 2$ and $\beta = 1$, again using (ii) and (iii) of Lemma 2.4

$$\limsup_{z\searrow 0} \frac{g_{1,0}(z)}{zg_{1,-1}(z)} \le \lim_{z\searrow 0} zg_{1,0}(z) = 0.$$

For $n = 3$, $\beta \in (\frac{1}{2}, 1]$ and $\gamma \in (\frac{3}{2}, 1+\beta]$,

$$\begin{aligned}\limsup_{z\searrow 0} \frac{g_{\beta,\gamma-\frac{3}{2}}(z)}{zg_{\beta,\frac{\gamma-3}{2}}(z)} &\le \frac{\Gamma(\frac{\gamma-\frac{3}{2}}{\beta})}{\beta\Gamma(\frac{3-\gamma}{2})} \lim_{z\searrow 0} z^{2-\gamma}, \\ &= \begin{cases} 1 & \text{for } \beta = 1,\ \gamma = 2, \\ 0 & \text{for } \beta \in (\frac{1}{2}, 1],\ \gamma \in (\frac{3}{2}, 1+\beta] \cap (\frac{3}{2}, 2). \end{cases}\end{aligned}$$

Now consider the limit of the ratio as $z \nearrow \infty$. Fix $\beta \in (0, 1]$ and $\gamma \in [1, 1+\beta]$. For the minute fix $z \ge 1$ and consider $f(t) = \frac{z^2}{t} + t^\beta$. Then f is minimized at $t_0 = (\frac{z^2}{\beta})^{\frac{1}{\beta-1}}$, decreases on $(0, t_0)$ and increases to ∞ on (t_0, ∞). Fix $r \ge 2^{\frac{2}{n-\gamma}}\beta^{-\frac{1}{\beta-1}}$ sufficiently large to satisfy

$$\frac{1}{r} + r^\beta \le \frac{1}{2}(\frac{1}{r^2} + r^{2\beta}).$$

In particular this gives

$$f(rz^{\frac{2}{\beta+1}}) \le \frac{1}{2} f(r^2 z^{\frac{2}{\beta+1}}) \tag{20}$$

and $rz^{\frac{2}{\beta+1}} \ge t_0$. Then

$$\begin{aligned} g_{\beta,\frac{\gamma-n}{2}}(z) &\ge \int_{t_0}^{rz^{\frac{2}{\beta+1}}} t^{\frac{\gamma-n}{2}-1} e^{-f(t)}\, dt \\ &\ge e^{-f(rz^{\frac{2}{\beta+1}})} \cdot \frac{2}{n-\gamma}(t_0^{\frac{\gamma-n}{2}} - (rz^{\frac{2}{\beta+1}})^{\frac{\gamma-n}{2}}) \\ &= \frac{2z^{\frac{\gamma-n}{\beta+1}}}{n-\gamma} e^{-f(rz^{\frac{2}{\beta-1}})} (\beta^{\frac{n-\gamma}{2(\beta+1)}} - r^{\frac{\gamma-n}{2}}) \\ &\ge \frac{\beta^{\frac{n-\gamma}{2(\beta+1)}}}{n-\gamma} z^{\frac{\gamma-n}{\beta+1}} e^{-f(rz^{\frac{2}{\beta-1}})} \end{aligned} \tag{21}$$

and

$$\begin{aligned} \int_{r^2 z^{\frac{2}{\beta+1}}}^{\infty} t^{\gamma-\frac{n}{2}-1} e^{-f(t)}\, dt &\le e^{-\frac{1}{2}f(r^2 z^{\frac{2}{\beta+1}})} \int_{r^2 z^{\frac{2}{\beta+1}}}^{\infty} t^{\gamma-\frac{n}{2}-1} e^{-\frac{1}{2}t^\beta}\, dt \\ &= e^{-\frac{1}{2}f(r^2 z^{\frac{2}{\beta+1}})} z^{\frac{2\gamma-n}{\beta+1}} \int_{r^2}^{\infty} s^{\gamma-\frac{n}{2}-1} e^{-\frac{z^{\frac{2\beta}{\beta+1}}}{2}s^\beta}\, ds. \end{aligned} \tag{22}$$

Combining (20), (21) and (22),

(23)

$$\frac{\int_{r^2 z^{\frac{2}{\beta+1}}}^{\infty} t^{\gamma-\frac{n}{2}-1} e^{-f(t)}\, dt}{zg_{\beta,\frac{\gamma-n}{2}}(z)} \le (n-\gamma)\beta^{\frac{\gamma-n}{2(\beta+1)}} z^{\frac{\gamma}{\beta+1}-1} \int_{r^2}^{\infty} s^{\gamma-\frac{n}{2}-1} e^{\frac{-z^{\frac{2\beta}{\beta-1}}}{2}s^\beta}\, ds.$$

For $\gamma \le 1+\beta$, this goes to 0 as $z \to \infty$.

For $z \ge 1$, $t \le r^2 z^{\frac{2}{\beta+1}}$ gives

$$t^{\frac{\gamma}{2}} \le r^\gamma z^{\frac{\gamma}{\beta+1}} \le r^\gamma z,$$

so that

(24)

$$z^{-1}\int_0^{r^2 z^{\frac{2}{\beta+1}}} t^{\gamma-\frac{n}{2}-1}e^{-f(t)}\,dt \le r^\gamma \int_0^{r^2 z^{\frac{2}{\beta+1}}} t^{\frac{\gamma-n}{2}-1}e^{-f(t)}\,dt \le r^\gamma g_{\beta,\frac{\gamma-n}{2}}(z).$$

Using (23) and (24), for $\beta \in (0,1]$ and $\gamma \in [1, 1+\beta]$,

$$\limsup_{z\nearrow\infty} \frac{g_{\beta,\gamma-\frac{n}{2}}(z)}{z g_{\beta,\frac{\gamma-n}{2}}(z)} \le r^\gamma < \infty.$$

□

The same general technique that gave the kernels of Proposition 2.2 gives families of non-radial kernels that are not fully supported. These are the *larger* kernels that permit broader existence and uniqueness results for given initial data u_0^λ of (FNS); see Remark 2.2 below.

Proposition 2.3. *For each $\alpha \in (0,1]$ and $n \ge 3$,*

$$H_{n,\alpha}(\xi) = \int_{t>0} t^{-\frac{n-1+\alpha}{\alpha}} \prod_{i=1}^n f_\alpha(t^{-\frac{1}{\alpha}}\xi_i)\,dt$$

is suitably normalized in $\mathcal{H}_{n,1}$ with support $W_{n,\alpha} = \{\xi \in \mathbf{R}^n : \sum_1^n \mathbf{1}_{[\xi_i=0]} < \frac{n\alpha+1}{\alpha+1}\}$.

Proof. Fix $\alpha \in (0,1]$ and $n \ge 3$. Let $g_\gamma(t) = t^{\gamma-1}$ for $\gamma, t > 0$ and set

$$H_{n,\alpha}(\xi) = T_{n,\alpha} g_{\frac{1}{\alpha}}(\xi)$$

for all $\xi \in \mathbf{R}^n$ for which $T_{n,\alpha}g_{\frac{1}{\alpha}}(\xi)$ converges. The convolution $g_\gamma * g_\gamma(t) = B(\gamma,\gamma)g_{2\gamma}(t)$, so from Lemma 2.3,

$$H_{n,\alpha} * H_{n,\alpha}(\xi) = B(\frac{1}{\gamma},\frac{1}{\gamma})T_{n,\alpha}g_{\frac{2}{\alpha}}(\xi).$$

In order to check convergence of $T_{n,\alpha}g_\gamma(\xi)$ for $\gamma = \frac{1}{\alpha}, \frac{2}{\alpha}, \alpha \in (0,1]$, we rely on a series expansion of $f_\alpha(x)$ for $\alpha \in (0,1]$ and $|x|$ large given by Feller [8], p. 583:

$$f_\alpha(x) = \frac{1}{\pi|x|}\sum_{k\ge1} \frac{\Gamma(k\alpha+1)}{k!}(-1)^{k+1}|x|^{-\alpha k}\sin(\frac{k\alpha\pi}{2}).$$

In particular, using this expansion it is straightforward to show that for $\alpha \in (0,1]$ and $|x| > 2^{\frac{1}{\alpha}}$, $f_\alpha(x) < c_\alpha|x|^{-1-\alpha}$ where c_α is a constant depending on α. In addition, it is easy to see that $f_\alpha(x)$ is maximized at $x = 0$.

Fix $n \ge 3$ and $x \in \mathbf{R}^n$ with $|x| > 0$. The change of variables $s = t|x|^{-\alpha}$ gives

$$T_{n,\alpha}g_\gamma(x) = |x|^{\gamma\alpha-n}T_{n,\alpha}g_\gamma(\frac{x}{|x|}). \tag{25}$$

Let $J(x) = \{i : x_i \neq 0\}$, $j = j(x) = \sum_1^n \mathbf{1}_{[x_i=0]}$ and $r(x) = \min\{\frac{1}{2}(\frac{|x_j|}{|x|})^\alpha : j \in J(x)\}$. Then

$$\begin{aligned}\int_{s=0}^{r(x)} s^{\gamma-\frac{n}{\alpha}-1}\prod_1^n f_\alpha(\frac{x_i}{|x|}s^{-\frac{1}{\alpha}})\,ds &\leq f_\alpha^j(0)\int_{s=0}^{r(x)} s^{\gamma-\frac{n}{\alpha}-1}\prod_{i\in J(x)} c_\alpha(\frac{|x_i|}{|x|}s^{-\frac{1}{\alpha}})^{-1-\alpha}\,ds \\ &= f_\alpha^j(0)c_\alpha^{n-j}\prod_{i\in J(x)}(\frac{|x_i|}{|x|})^{-1-\alpha} \\ &\quad\cdot\int_{s=0}^{r(x)} s^{\gamma-\frac{n-(n-j)(1+\alpha)}{\alpha}-1}\,ds.\end{aligned}$$

For $\gamma = \frac{1}{\alpha}, \frac{2}{\alpha}$ this integral converges for $j < \frac{n\alpha+1}{\alpha+1}$. Also for $\gamma < \frac{n}{\alpha}$,

$$\int_{r(x)}^{\infty} s^{\gamma-\frac{n}{\alpha}-1}\prod_1^n f_\alpha(\frac{x_i}{|x|}s^{-\frac{1}{\alpha}})\,ds < f_\alpha^n(0)\int_{r(x)}^{\infty} s^{\gamma-\frac{n}{\alpha}-1}\,ds < \infty.$$

Together these give

$$T_{n,\alpha}g_\gamma(\frac{x}{|x|}) < \infty$$

for $\gamma = \frac{1}{\alpha}, \frac{2}{\alpha}$ and $\sum_1^n \mathbf{1}_{[x_i=0]} < \frac{n\alpha+1}{\alpha+1}$. From (25) we see that to verify that $H_{n,\alpha}$ is a majorizing kernel, we need to show that for a constant $c_{n,\alpha} \in (0,\infty)$,

$$T_{n,\alpha}g_{\frac{2}{\alpha}}(\frac{x}{|x|}) \leq c_{n,\alpha}T_{n,\alpha}g_{\frac{1}{\alpha}}(\frac{x}{|x|})$$

for all x with $\sum_1^n \mathbf{1}_{[x_i=0]} < \frac{n\alpha+1}{\alpha+1}$. Fix $n \geq 3, \alpha \in (0,1]$, and $y \in \mathbf{R}^n$ with $|y| = 1$ and $\sum_1^n \mathbf{1}_{[y_i=0]} < \frac{n\alpha+1}{\alpha+1}$. For $\gamma = \frac{1}{\alpha}, \frac{2}{\alpha}$ let

$$I_\gamma^{(1)}(y) = \int_{s=0}^{1} s^{\gamma-\frac{n}{\alpha}-1}\prod_1^n f_\alpha(y_i s^{-\frac{1}{\alpha}})\,ds$$

and

$$I_\gamma^{(2)}(y) = \int_{s=1}^{\infty} s^{\gamma-\frac{n}{\alpha}-1}\prod_1^n f_\alpha(y_i s^{-\frac{1}{\alpha}})\,ds.$$

Immediately

$$I_{\frac{2}{\alpha}}^{(1)}(y) \leq I_{\frac{1}{\alpha}}^{(1)}(y).$$

Using Yamazato [23] we see that $f_\alpha(x)$ is uni-modal and strictly decreasing on $(0,\infty)$. This gives

$$I_{\frac{1}{\alpha}}^{(2)}(y) \geq \int_{s>1} s^{\frac{1-n}{\alpha}-1}\prod_1^n f_\alpha(1)\,ds = \frac{\alpha}{n-1}f_\alpha^n(1)$$

and

$$T_{n,\alpha}g_{\frac{2}{\alpha}}(x) \leq c_{n,\alpha}|x|T_{n,\alpha}g_{\frac{1}{\alpha}}(x) \quad \text{for} \quad c_{n,\alpha} = \frac{n-1}{n-2}(\frac{f_\alpha(0)}{f_\alpha(1)})^n B(\frac{1}{\gamma},\frac{1}{\gamma}).$$

□

Remark 2.2. In the case $n = 3, \alpha = 1$ the kernel $H_{3,1}$ can be written as

$$H_{3,1}(\xi) = \frac{1}{|\xi|^2}G(\frac{\xi}{|\xi|}), \tag{26}$$

where G is defined a.e. on the unit sphere with $G(\theta) \to \infty$ as θ approaches the points $(0,0,\pm 1), (0,\pm 1, 0)$, and $(\pm 1, 0, 0)$, respectively. In particular the growth of $H_{3,1}$ along particular directions is much larger than $h_0(\xi) = 1/|\xi|^2$. Transforming $H_{3,1}$ via a rotation as suggested in Theorem 2.3 permits such growth in any direction.

In view of the role of majorizing kernels in providing bounds on the Fourier transformed forcing and/or initial data, the theory contains a dual problem which is to identify classes of divergence-free vector fields in physical space which are so dominated.

The first example is a class of divergence-free vector fields on $\mathbf{R}^3$ whose Fourier transforms are dominated by $h_{3,\beta,\gamma}(\xi)$.

Example 2.2. Fix $0 \le \beta \le 1$ and $1 \le \gamma \le 1+\beta$. For $1 \le j \le 3$ let $m_j(t)$ be measurable functions on $[0,\infty)$ such that $|m_j(t)| \le t^{\frac{3}{2}-1} e^{-t^{\beta}}$ and $\int_{t>0} t^{-3/2}|m_j(t)|dt < \infty$. Let $v(x)$ be the vector field whose components $v_j(x)$ are the Laplace transforms of $m_j(t)$ evaluated at $|x|^2/4$; that is,

$$v_j(x) = \int_0^\infty e^{-t|x|^2/4} m_j(t)dt.$$

Let $u(x)$ be the divergence-free projection of $v(x)$. Then the following calculation shows that

$$|\hat{u}(\xi)| \le c h_{3,\beta,\gamma}(\xi).$$

After using Tonelli's Theorem to check integrability, Fubini's Theorem gives

$$\begin{aligned} |\hat{v}_j(\xi)| &= c \,\Big| \int_{t>0} \int_{\mathbf{R}^3} e^{-i\xi\cdot x} e^{\frac{-t|x|^2}{4}} m_j(t) dx\, dt \Big| \\ &\le c \int_{t>0} t^{-3/2} |m_j(t)| e^{-|\xi|^2/t} dt \\ &\le c\, h_{3,\beta,\gamma}(\xi). \end{aligned}$$

The projection of the vector field $v(x)$ onto the divergence-free component $u(x)$ becomes, on the Fourier side, $\hat{u}(\xi) = \hat{v}(\xi) - \frac{\xi}{|\xi|}(\hat{v}(\xi)\cdot\frac{\xi}{|\xi|}) = \pi_{\xi^\perp}\hat{v}(\xi)$. This contraction gives

$$|\hat{u}(\xi)| \le |\hat{v}(\xi)| \le c h_{3,\beta,\gamma}(\xi) \qquad \text{for all} \qquad \xi \in \mathbf{R}^3\backslash\{0\}.$$

For the next example we consider majorization by the kernels $h_\beta^{(\alpha)}$.

Example 2.3. Let $\mathcal{M}$ denote the space of finite signed measures on $\mathbf{R}^3$ with total variation norm $\|\ \|$. Let $0 < \beta \le 1$ and denote the "Fourier transformed Bessel kernel" of order β by $G_\beta(x) = (1+|x|^2)^{-\frac{1-\beta}{2}}$. Then for each $g = G_\beta * \mu, \mu \in \mathcal{M}$, one has for $\beta = 1,\ \alpha \in (0,1)$ and for $\beta \in (0,1),\ \alpha > 0$,

$$|\hat{g}(\xi)| \le C_\beta^{(\alpha)} h_\beta^{(\alpha)}(\xi)\|\mu\|, \quad \xi \ne 0,$$

for a constant $C_\beta^{(\alpha)} > 0$. In particular, if $v \in L^1$ is a divergence-free vector field, then $g = G_\beta * v$ is also a divergence-free vector field whose Fourier transform is dominated by $h_\beta^{(\alpha)}$. To verify this class of examples it suffices to check that

$$|\hat{G}_\beta(\xi)| \le C_\beta^{(\alpha)} h_\beta^{(\alpha)}(\xi), \tag{27}$$

for some constant $C_\beta^{(\alpha)}$. For this we take the Fourier transform of $(1+|x|^2)^{-\frac{1+\beta}{2}}$ and then use Lemma 2.2. First notice that for any $a > 0$,

$$\Gamma(\frac{\beta+1}{2}) = a^{\frac{\beta+1}{2}} \int_0^\infty t^{\frac{\beta-1}{2}} e^{-at}\,dt.$$

Solving for $a^{-\frac{\beta+1}{2}}$ and then taking $a = 1+|x|^2$, we obtain

$$G_\beta(x) = \frac{1}{\Gamma(\frac{\beta+1}{2})} \int_0^\infty t^{\frac{\beta-1}{2}} e^{-(1+|x|^2)t}\,dt$$

and

$$\begin{aligned}
\hat{G}_\beta(\xi) &= \frac{(2\pi)^{-\frac{3}{2}}}{\Gamma(\frac{\beta+1}{2})} \int_0^\infty t^{\frac{\beta-1}{2}} e^{-t} \int_{x\in\mathbf{R}^3} e^{-ix\cdot\xi-|x|^2 t}\,dx\,dt \\
&= \frac{2^{-\frac{3}{2}}}{\Gamma(\frac{\beta+1}{2})} \int_0^\infty t^{\frac{\beta-2}{2}-1} e^{-t-\frac{|\xi|^2}{4t}}\,dt \\
&= \frac{2^{-\frac{3}{2}}}{\Gamma(\frac{\beta+1}{2})} h_{3,1,\beta+1}(\frac{\xi}{2}).
\end{aligned}$$

Then (27) follows from Lemma 2.2 with $C_\beta^{(\alpha)} = \frac{2^{-\frac{3}{2}}}{\Gamma(\frac{\beta+1}{2})} c_\beta^{(\alpha)}$.

The following example uses the $h_\beta^{(\alpha)}$ majorizing kernels to give smooth divergence-free vector fields, including some with compact support.

Example 2.4. Let $m_j(t), t > 0, j = 1,2,3$, be measurable functions such that $\int_0^\infty e^{-|x|^2 t}|m_j(t)|dt < \infty, x \in \mathbf{R}^3, j = 1,2,3$. Define a vector field with components $v_j, j = 1,2,3$, by

$$v_j(x) = \int_0^\infty e^{-|x|^2 t} m_j(t)dt, x \in \mathbf{R}^3.$$

Let u be the divergence-free projection of v. Then,

(i) If $|m_j(t)| \le ct^{-\frac{1}{2}}$, then $|\hat{u}_j(\xi)| \le c' h_0^{(\alpha)}(\xi)$ for some $c' > 0, j = 1,2,3$.
(ii) If $|m_j(t)| \le ce^{-2\alpha^2 t}$, then $|\hat{u}_j(\xi)| \le c' h_1^{(\alpha)}(\xi)$ for some $c' > 0, j = 1,2,3$.
(iii) For arbitrary $\epsilon > 0$ there is a smooth probability density function k_ϵ supported on $[-\epsilon,\epsilon]^3$ such that

$$|\hat{k}_\epsilon(\xi)| \le c(\beta,\epsilon)\exp\{-|\epsilon\xi|^\beta\}, \xi \in \mathbf{R}^3, c(\beta,\epsilon) > 0.$$

Let v be any divergence-free integrable vector field such that $|\hat{v}(\xi)| \le c|\xi|^{-2},\ \xi \ne 0$. Then the componentwise perturbation $u = k_\epsilon * v$ is a divergence-free infinitely differentiable vector field such that $|\hat{u}_j(\xi)| \le c' h_\beta^{(\alpha)}(\xi)$, for $\alpha = \epsilon^\beta$ and some $c' > 0, j = 1,2,3$.

To verify (i) and (ii) first recall that

$$(2\pi)^{-\frac{3}{2}} \int_{\mathbf{R}^3} e^{-ix\cdot\xi-|x|^2 t}\,dx = (2t)^{-\frac{3}{2}} e^{-\frac{|\xi|^2}{4t}},$$

and therefore

$$|\hat{u}_j(\xi)| \le 2^{-\frac{3}{2}} \int_{t>0} t^{-\frac{3}{2}} |m_j(t)| e^{-\frac{|\xi|^2}{4t}}\,dt.$$

For $|m_j(t)| \le ct^{-\frac{1}{2}}$,

$$\begin{aligned} |\hat{u}_j(\xi)| &\le c2^{-\frac{3}{2}} \int_{t>0} t^{-2} e^{-\frac{|\xi|^2}{4t}}\, dt \\ &= c2^{\frac{1}{2}} |\xi|^{-2} \\ &= c2^{\frac{1}{2}} e^{\alpha} h_0^{(\alpha)}(\xi) \end{aligned}$$

for $j = 1, 2, 3$. For $|m_j(t)| \le ce^{-2\alpha^2 t}$, using the change of variables $s = \frac{|\xi|^2}{8t}$,

$$\begin{aligned} |\hat{u}_j(\xi)| &\le c2^{-\frac{3}{2}} \int_{t>0} t^{-\frac{3}{2}} e^{-2\alpha^2 t - \frac{|\xi|^2}{4t}}\, dt \\ &= c|\xi|^{-1} \int_{s>0} s^{-\frac{1}{2}} e^{-2s - \frac{\alpha^2|\xi|^2}{4s}}\, ds \\ &= c|\xi|^{-1} e^{-\alpha|\xi|} \int_{s>0} s^{-\frac{1}{2}} e^{-s-(\sqrt{s} - \frac{\alpha|\xi|}{2\sqrt{s}})^2}\, ds \\ &\le c\Gamma(\frac{1}{2}) h_1^{(\alpha)}(\xi). \end{aligned}$$

To check (iii) one may apply Theorem 10.2 of Bhattacharya and Rao [3] to see that for any fixed $\beta \in (0,1)$ there exists a probability measure on $(\mathbf{R}, \mathcal{B})$ with density k whose support is contained in $[-1, 1]$ and

$$|\hat{k}(\xi)| \le c(\beta) \exp\{-3^{\frac{\beta}{2}-1} |\xi|^{\beta}\} \quad \text{for } \xi \in \mathbf{R}.$$

Without loss of generality we can assume that k is symmetric and infinitely differentiable. Fix $\epsilon > 0$ and take k_ϵ to be the density of the probability measure on $\mathbf{R}^3$ given by

$$K_\epsilon(A) = \iiint_{A_\epsilon} k(x_1)k(x_2)k(x_3)\, dx_1\, dx_2\, dx_3$$

where $A_\epsilon = \{\frac{x}{\epsilon} : x \in A\}$. Then k_ϵ has support contained in $[-\epsilon, \epsilon]^3$ and

$$\begin{aligned} |\hat{k}_\epsilon(\xi)| &\le c^3(\beta) e^{-3^{\frac{\beta}{2}-1} \epsilon^{\beta} \sum_{i=1}^{3} |\xi_i|^{\beta}} \\ &\le c^3(\beta) e^{-\epsilon^{\beta}|\xi|^{\beta}} \end{aligned}$$

using Jensen's inequality in the exponent. If v is an integrable divergence-free vector field on $\mathbf{R}^3$ with $|\hat{v}(\xi)| \le c|\xi|^{-2}$, then $u = k_\epsilon * v$ is both divergence-free and infinitely differentiable with

$$\begin{aligned} |\hat{u}_j(\xi)| &= |\hat{k}_\epsilon|\, |\hat{v}_j(\xi)| \\ &\le c^3(\beta) e^{-\epsilon^{\beta}|\xi|^{\beta}} \min\{c|\xi|^{-2},\ |\hat{v}_j(\xi)|\}. \end{aligned}$$

For $|\xi| \ge 1$ then

$$|\hat{u}_j(\xi)| \le c'(\beta) h_{\beta}^{(\epsilon^{\beta})}(\xi)$$

with $c'(\beta) = c \cdot c^3(\beta)$. For $|\xi| \le 1$,

$$|\hat{u}_j(\xi)| \le c''(\beta) h_{\beta}^{(\epsilon^{\beta})}(\xi)$$

for $c''(\beta) = c^3(\beta)||v_j||$, where $||v_j||$ denotes the L^1-norm of v_j.

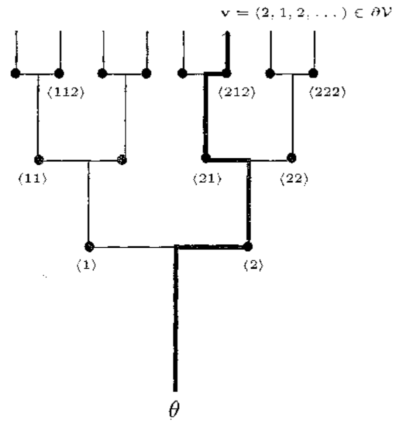

FIGURE 1. Full binary tree with index set $\mathcal{V}$ and boundary $\partial\mathcal{V}$. The path $\mathbf{v} = (2, 1, 2, \dots) \in \partial\mathcal{V}$ is indicated in bold, with $\mathbf{v}|0 = \theta$, $\mathbf{v}|1 = \langle 2\rangle$, $\mathbf{v}|2 = \langle 21\rangle$, and $\mathbf{v}|3 = \langle 212\rangle$.

3. STOCHASTIC RECURSION

The vertex set $\mathcal{V}$ of a complete binary tree rooted at θ may be coded as (see Figure 1)

$$\mathcal{V} = \bigcup_{j=0}^{\infty}\{1,2\}^j = \{\theta, \langle 1\rangle, \langle 2\rangle, \langle 11\rangle, \dots\}, \tag{28}$$

where $\{1,2\}^0 = \{\theta\}$. Also let $\partial\mathcal{V} = \prod_{j=0}^{\infty}\{1,2\} = \{1,2\}^{\mathbb{N}}$.

A stochastic model consistent with $(\mathrm{FNS})_h$ is obtained by consideration of a multitype branching random walk of non-zero Fourier wavenumbers ξ, thought of as particle *types*, as follows: A particle of type $\xi \neq 0$ initially at the root θ holds for an exponentially distributed length of time S_θ with holding time parameter $\lambda(\xi) = \nu|\xi|^2$; i.e. $ES_\theta = \frac{1}{\nu|\xi|^2}$. When this exponential clock rings, a coin κ_θ is tossed and either with probability $\frac{1}{2}$ the event $[\kappa_\theta = 0]$ occurs and the particle is terminated, or with probability $\frac{1}{2}$ one has $[\kappa_\theta = 1]$ and the particle is replaced by two offspring particles of types η_1, η_2 selected from the set $\eta_1+\eta_2 = \xi$ according to the probability kernel $H(\xi, d\eta_1 \times d\eta_2)$ defined by (9). This process is repeated independently for the particle types η_1, η_2 rooted at the vertices $\langle 1\rangle, \langle 2\rangle$, respectively.

A more precise mathematical description of the stochastic model requires a bit more notation. For $\mathbf{v} = (v_1, v_2, \dots, v_k) \in \mathcal{V}$, let $\mathbf{v}|j = (v_1, \dots, v_j), j \leq k$. Also let $|\mathbf{v}| = k$, $|\theta| = 0$, denote the geneological length of the vertex $\mathbf{v} \in \mathcal{V}$. For $\mathbf{v} = (v_1, v_2, \dots) \in \partial\mathcal{V}$, and $j = 0, 1, 2, \dots$ let $\mathbf{v}|j = (v_1, \dots v_j)$, $\mathbf{v}|0 = \theta$. That is, for $\mathbf{v} \in \partial\mathcal{V}$, $\mathbf{v}|0, \mathbf{v}|1, \mathbf{v}|2, \dots$ may be viewed as a non-terminating *path* through vertices of the tree starting from the root $\mathbf{v}|0 = \theta$. For $\mathbf{u}, \mathbf{v} \in \partial\mathcal{V}$, or in $\mathcal{V}$, let $|\mathbf{u} \wedge \mathbf{v}| = \inf\{m \geq 1 : \mathbf{u}|m \neq \mathbf{v}|m\}$.

The following requirements provide the defining properties of the underlying stochastic model. The model depends on the initial frequency (wave number) ξ and the choice of majorizing kernel h. Fix h and let $W_h \subseteq \mathbf{R}^3\backslash\{0\}$ denote the support of h. Let $\mathcal{B}_h$ denote the Borel subsets of W_h. For fixed $\xi \in W_h$, let $\{(\xi_{\mathbf{v}}, \kappa_{\mathbf{v}}) : \mathbf{v} \in \mathcal{V}\}$ be the tree-indexed stochastic process starting at $(\xi_\theta, \kappa_\theta)$ with $\xi_\theta = \xi \in W_h$, $\kappa_\theta \in \{0,1\}$, taking values in the state space $W_h \times \{0,1\}$, and defined on a probability space $(\Omega, \mathcal{F}, P_\xi)$ by the following properties:

(1) $P_\xi(\xi_\theta \in B,\ \kappa_\theta = \kappa) = \frac{1}{2}\delta_\xi(B),\ B \in \mathcal{B}_h,\ \kappa \in \{0,1\}$.

(2) For any fixed $\mathbf{v} \in \partial\mathcal{V}$, the sequence $(\xi_{\mathbf{v}|0}, \kappa_{\mathbf{v}|0}), (\xi_{\mathbf{v}|1}, \kappa_{\mathbf{v}|1}), (\xi_{\mathbf{v}|2}, \kappa_{\mathbf{v}|2}), \ldots$ is a Markov chain with transition probabilities

$$P_\xi(\xi_{\mathbf{v}|n+1} \in B,\ \kappa_{\mathbf{v}|n+1} = \kappa | \sigma(\{(\xi_{\mathbf{u}}, \kappa_{\mathbf{u}}) : |\mathbf{u}| \le n\})) = \frac{1}{2}\int_B \frac{h(\xi_{\mathbf{v}|n} - \eta)h(\eta)}{h * h(\xi_{\mathbf{v}|n})}d\eta \tag{29}$$

for $B \in \mathcal{B}_h, \kappa \in \{0,1\}$. In particular, for $\mathbf{v} \in \mathcal{V}$, $\xi_{\mathbf{v}1} + \xi_{\mathbf{v}2} = \xi_{\mathbf{v}}$ P_ξ-*a.s.*, where $\mathbf{v}j = (v_1 \ldots v_n)j := (v_1 \cdots v_n, j)$, $j = 1, 2, \ldots$ is the concatenation operation.

(3) For any $\mathbf{u}, \mathbf{v}, \in \partial\mathcal{V}$, $\{(\xi_{\mathbf{u}|m}, \kappa_{\mathbf{u}|m})\}_{m=0}^\infty$ and $\{(\xi_{\mathbf{v}|m}, \kappa_{\mathbf{v}|m})\}_{m=0}^\infty$ are conditionally independent given $\sigma(\{(\xi_{\mathbf{w}}, \kappa_{\mathbf{w}}) : |\mathbf{w}| \le |\mathbf{u} \wedge \mathbf{v}|\})$.

(4) Let $\{\overline{S}_{\mathbf{v}} : \mathbf{v} \in \mathcal{V}\}$ be a sequence of *iid* mean one exponentially distributed random variables defined on $(\Omega, \mathcal{F}, P_\xi)$ and independent of $\{(\xi_{\mathbf{v}}, \kappa_{\mathbf{v}}) : \mathbf{v} \in \mathcal{V}\}$. Define $\lambda(\eta) = \nu|\eta|^2$ for $\eta \in W_h$ and

$$S_{\mathbf{v}} = \lambda(\xi_{\mathbf{v}})^{-1} \cdot \overline{S}_{\mathbf{v}},\ \mathbf{v} \in \mathcal{V}.$$

Conditionally given $\{\xi_{\mathbf{v}} : \mathbf{v} \in \mathcal{V}\}$, the collection $\{S_{\mathbf{v}} : \mathbf{v} \in \mathcal{V}\}$ consists of independent exponentially distributed random variables having respective conditional means $\{\lambda(\xi_{\mathbf{v}})^{-1} : \mathbf{v} \in \mathcal{V}\}$.

Remark 3.1. The above properties, although not an explicit construction, define the stochastic model; see Harris [13] for an approach to construction of the underlying probability space.

Our objective now is to use the stochastic branching model represented by the collection of random variables $\{\xi_{\mathbf{v}}, \kappa_{\mathbf{v}}, S_{\mathbf{v}} : \mathbf{v} \in \mathcal{V}\}$ to recursively define a random functional related to (FNS) through its expected value. Namely, for measurable functions $\chi_0 : W_h \to \mathbf{C}^3$ and $\varphi : W_h \times [0,\infty) \to \mathbf{C}^3$, and for $\xi_\theta = \xi \in W_h, t \ge 0$, the stochastic functional $\mathbb{X}(\theta, t)$ is recursively defined by

$$\mathbb{X}(\theta,t) = \begin{cases} \chi_0(\xi_\theta), & \text{if } S_\theta > t, \\ \varphi(\xi_\theta, t - S_\theta), & \text{if } S_\theta \le t, \kappa_\theta = 0, \\ m(\xi_\theta)\mathbb{X}(\langle 1\rangle,\ t - S_\theta) \otimes_{\xi_\theta} \mathbb{X}(\langle 2\rangle, t - S_\theta), & \text{otherwise,} \end{cases} \tag{30}$$

where the product $\otimes_\xi$ and factors $m(\xi)$ are defined in (7) and (8), respectively, and where $\langle 1\rangle$ and $\langle 2\rangle$ are root vertices of the shifted full binary trees

$$\mathcal{V}_{\langle i\rangle} := \{\langle i\rangle, \langle i,1\rangle, \langle i,2\rangle, \langle i,1,1\rangle, \langle i,1,2\rangle, \langle i,2,1\rangle, \ldots\}, \tag{31}$$

types $\xi_{\langle i\rangle}, i = 1, 2$, respectively.

For evaluation of the stochastic functional $\mathbb{X}(\theta, t)$, for a given $\xi_\theta = \xi$, it is useful to identify a particular tree structure intrinsic to the stochastic branching model

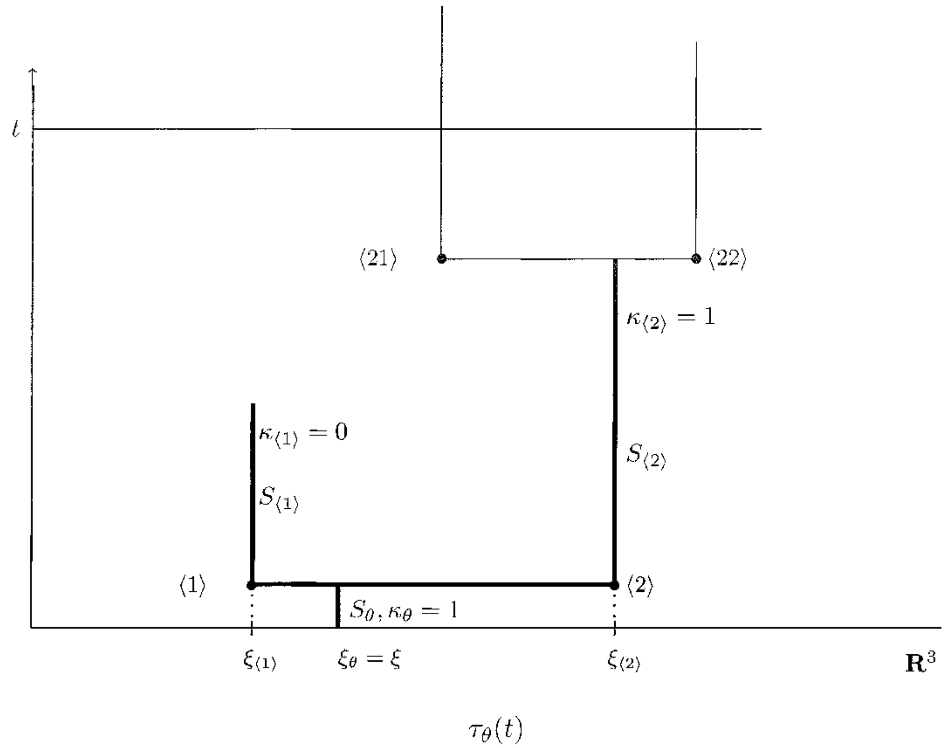

FIGURE 2. Schematic of a tree indexed branching random walk with $\tau_\theta(< t)$ denoted in bold lines

by (see Figure 2)

$$\tau_\theta(t) = \{\mathbf{v} \in \mathcal{V} : \prod_{j=0}^{|\mathbf{v}|-1} k_{\mathbf{v}|j} = 1,\ B_\mathbf{v} \le t\} \tag{32}$$

where

$$B_\theta = 0, \qquad B_\mathbf{v} = \sum_{j=0}^{|\mathbf{v}|-1} S_{\mathbf{v}|j}, \quad \theta \neq \mathbf{v} \in \mathcal{V}. \tag{33}$$

It is helpful to have a bit more notation and further decompose $\tau_\theta(t)$ into sets of vertices of two types. We say that $\mathbf{v} \in \mathcal{V}$, *born* at time $B_\mathbf{v}$, *survives* for a time $S_\mathbf{v}$ until the *clock ring* at time $R_\mathbf{v} := B_\mathbf{v} + S_\mathbf{v} = \sum_{j=0}^{|\mathbf{v}|} S_{\mathbf{v}|j}$. In this way we can partition $\tau_\theta(t)$ into the vertices born before time t with clock rings before and after time t; see Figure 2. Namely,

$$\tau_\theta(t) = \tau_\theta(< t) \cup \tau_\theta(> t)$$

where

$$\begin{aligned} \tau_\theta(< t) &= \{\mathbf{v} \in \tau_\theta(t) : R_\mathbf{v} \le t\}, \\ \tau_\theta(> t) &= \{\mathbf{v} \in \tau_\theta(t) : B_\mathbf{v} \le t < R_\mathbf{v}\}. \end{aligned}$$

Since the discrete branching process defined by $\{\mathbf{v} \in \mathcal{V} : \prod_{j=0}^{|\mathbf{v}|} \kappa_{\mathbf{v}|j} = 1\}$ is a critical binary Galton-Watson process, the recursion will terminate in a finite number of iterations with probability one. In particular, $\mathbb{X}(\theta, t)$ is simply a *finite* product of values of χ_0 and/or φ. For example, the functional evaluation of the sample tree in Figure 2 is given by

$$\mathbb{X}(\theta, t) = m(\xi_\theta)m(\xi_{\langle 2\rangle})\varphi(\xi_{\langle 1\rangle}, t - R_{\langle 1\rangle}) \otimes_{\xi_\theta} [\chi_0(\xi_{\langle 21\rangle}) \otimes_{\xi_{\langle 2\rangle}} \chi_0(\xi_{\langle 22\rangle})].$$

In particular, the product is over vertices $\mathbf{v} \in \tau_\theta(t)$ with evaluations of factors at the *leaves* $\mathbf{v}$ of $\tau_\theta(< t)$ as $\varphi(\xi_\mathbf{v},\ t - R_\mathbf{v})$ and at the *leaves* $\mathbf{v}$ of $\tau_\theta(> t)$ as $\chi_0(\xi_\mathbf{v})$; here a *leaf* refers to a terminal vertex, while a non-terminating vertex is referred to as a *branch point*. No essential use of graph theoretic notions is made beyond their descriptive role in this development.

Remark 3.2. The branching random walk constructed here differs from that introduced by LeJan and Sznitman [17] in that by constructing the process forward in time we eliminate the dependence of the model $(\Omega, \mathcal{F}, P_\xi)$ on t. Secondly, a larger class of transition probabilities is furnished by the respective class of majorizing kernels. In order to relate the stochastic framework to (FNS) and/or $(\mathrm{FNS})_h$, we require a notion of *solution*. The first is a variant on one formulated by LeJan and Sznitman [17] for solutions to $(\mathrm{FNS})_h$ in the special case $h = h_0^{(\alpha)}$. Since we do not wish to exclude the analysis of complex valued solutions, we do not include their condition $\overline{h(\xi)\chi(\xi,t)} = h(-\xi)\chi(-\xi,t)$ in the definition of solution, but choose to consider it as a possible subsequent property of solutions.

Definition 3.1. A function $\chi : W_h \times [0,T] \to C^3$ which is

(1) continuous in $t \in [0,T]$ for each fixed $\xi \in W_h$,
(2) measurable in $\xi \in W_h$ for each fixed $t \in [0,T]$,
and satisfies
(3) $\int_0^T \int_{W_h \times W_h} |\chi(\xi_1, s) \cdot e_\xi| \cdot |\pi_{\xi^\perp}\chi(\xi_2, s)| H(\xi, d\xi_1 \times d\xi_2) < \infty$ for a.e. $\xi \in W_h$,
and
(4) $\chi(\xi, t) \cdot \xi = 0,\ 0 \le t \le T$,

will be called a *solution* to $(\mathrm{FNS})_h$ for initial data $\chi_0 : W_h \to \mathbf{C}^3,\ \chi_0(\xi) \cdot \xi = 0$, and forcing $\varphi : W_h \times [0,T] \to \mathbf{C}^3,\ \int_0^T |\varphi(\xi,t)|dt < \infty,\ \varphi(\xi,t)\cdot\xi = 0$, provided $(\mathrm{FNS})_h$ holds for *a.e.* $\xi \in W_h$.

Remark 3.3. Global solutions are defined by requiring the conditions of the definition for all $T > 0$. In the case that a solution to $(\mathrm{FNS})_h$ also satisfies

$$\overline{h(\xi)\chi(\xi,t)} = h(-\xi)\chi(-\xi,t),$$

we will say that $\chi(\xi,t)$ is a *solution in the sense of LeJan-Sznitman.*

Although our focus is on *majorizing kernels*, the stochastic model may be constructed for any measurable $h : W_h \to (0,\infty)$ such that $h * h(\xi) < \infty$. With this in mind we make the following definition.

Definition 3.2. Let $1/h$ be a Fourier multiplier on W_h. We say that the pair (u_0, g) is $(\mathrm{FNS})_h$-admissible if

(1) $\hat{u}_0(\xi) = \hat{g}(\xi,t) = 0$ for a.e. $\xi \in W_h^c, t \ge 0$.
(2) $\mathbf{E}_{\xi_\theta=\xi}|\mathbb{X}(\theta,t)| < \infty$ for a.e. $\xi \in W_h,\ t \ge 0$,

where $\chi_0(\xi) = \hat{u}_0(\xi)/h(\xi)$, and $\varphi(\xi,t) = 2\hat{g}(\xi,t)/(\nu|\xi|^2 h(\xi)), t \ge 0$, as in (8).

Theorem 3.1 (Existence). *If (u_0, g) is (FNS)$_h$-admissible for a given Fourier multiplier $1/h$, then*

$$\hat{u}(\xi, t) \quad = \quad \begin{cases} h(\xi)\mathbf{E}_{\xi_\theta=\xi}\mathbb{X}(\theta, t), & \text{if } \xi \in W_h, \ t \geq 0, \\ 0, & \text{if } \xi \in W_h^c, t \geq 0, \end{cases}$$

is a solution to (FNS).

Proof. As noted in Remark 1.1, it suffices to consider (FNS)$_h$. To verify that (FNS)$_h$ is satisfied, decompose $\mathbb{X}(\theta, t)$ as

$$\begin{aligned} \mathbb{X}(\theta, t) \quad = \quad & \mathbb{X}(\theta, t)\mathbf{1}[S_\theta > t] + \mathbb{X}(\theta, t)\mathbf{1}[S_\theta \leq t, \kappa_\theta = 0] \\ & + \mathbb{X}(\theta, t)\mathbf{1}[S_\theta \leq t, \kappa_\theta = 1], \end{aligned}$$

take expectation starting at ξ, and use the strong Markov property and conditional independence in the recursive definition of $\mathbb{X}(\theta, t)$ on $[S_\theta \leq t, \kappa_\theta = 1]$. Specifically,

$$\begin{aligned} & \mathbf{E}_{\xi_\theta=\xi}\{m(\xi_\theta)\mathbb{X}(\langle 1\rangle, t - S_\theta) \otimes_{\xi_\theta} \mathbb{X}(\langle 2\rangle, t - S_\theta)\mathbf{1}[S_\theta \leq t, \kappa = 1]\} \\ = \quad & m(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[S_\theta \leq t, \kappa_\theta = 1]\mathbf{E}\{\mathbb{X}(\langle 1\rangle, t - S_\theta) \\ & \otimes_{\xi_\theta}\mathbb{X}(\langle 2\rangle, t - S_\theta)|\xi_{\langle 1\rangle}, \xi_{\langle 2\rangle}, S_\theta, \kappa_\theta\}\} \\ = \quad & m(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[S_\theta \leq t, \kappa_\theta = 1]\chi(\xi_{\langle 1\rangle}, t - S_\theta) \otimes_{\xi_\theta} \chi(\xi_{\langle 2\rangle}, t - S_\theta)\} \\ = \quad & \frac{1}{2}m(\xi)\int_0^t \lambda(\xi)e^{-\lambda(\xi)s}\int_{W_h \times W_h} \chi(\eta_1, t - s) \otimes_\xi \chi(\eta_2, t - s)H(\xi, d\eta_1 \times d\eta_2)ds. \end{aligned}$$

The continuity requirement in (1) of Definition 3.1 is evident in the representation of $\chi(\xi, t)$ by (FNS)$_h$. The measurability (2) may be obtained from the measure theoretic construction of the stochastic branching model. The condition (3) is contained in the (FNS)$_h$-admissibility definition. To check the incompressibility condition (4) simply observe that samplepointwise one has

$$\mathbb{X}(\theta, t) \cdot \xi_\theta = 0$$

by the definition of $\mathbb{X}(\theta, t)$, orthogonality of $\pi_{\xi\perp}$, and corresponding hypothesis on $\chi_0(\xi)$ and $\varphi(\xi, t)$. □

The proof of the existence part of Theorem 1.1 stated in the Introduction now follows as a corollary to Theorem 3.1 as follows:

Proof of existence in Theorem 1.1. Defining $c_\nu = \nu(2\pi)^{\frac{3}{2}}/2$, the conditions of Theorem 1.1 state that

$$\text{(i) } h * h(\xi) \leq |\xi|h(\xi), \quad \text{(ii) } |\hat{u}_0(\xi)| \leq c_\nu h(\xi), \quad \text{(iii) } |\hat{g}(\xi, t)| \leq \nu c_\nu|\xi|^2 h(\xi)/2.$$

Thus one may define a majorizing kernel h_ν with constant c_ν by

$$h_\nu(\xi) = c_\nu h(\xi), \xi \in W_{h_\nu} = W_h.$$

The conditions (i)-(iii) may then be expressed with respect to the majorizing kernel h_ν as

$$\text{(i) } m(\xi) = h_\nu * h_\nu(\xi)/(c_\nu|\xi|h_\nu(\xi)) \leq 1, \quad \text{(ii) } |\chi_0(\xi)| \leq 1, \quad \text{(iii) } |\varphi(\xi, t)| \leq 1,$$

where $\chi_0(\xi) = \hat{u}_0(\xi)/h_\nu(\xi)$, and $\varphi(\xi, t) = 2\hat{g}(\xi, t)/\nu|\xi|^2 h_\nu(\xi)$. In particular it follows that $|\mathbb{X}(\theta, t)| \leq 1$ for this choice of majorizing kernel, and hence Theorem 3.1 applies. Now one may check that cancellations make the formula defining the solution $\hat{u}(\xi, t)$

invariant under rescalings of h by constants. Specifically, it follows from the defining stochastic recursion (30) that for any positive constant $c > 0$ one has

$$c\chi_{ch}(\theta, t) = \chi_h(\theta, t) \quad \text{a.s.,} \tag{34}$$

where χ_h denotes the functional corresponding to the Fourier multiplier h. Note that the stochastic functional is always a.s. finite since the stochastic recursion terminates in a finite number of steps a.s. □

Remark 3.4. Note that for a Fourier multiplier $1/h$ induced by a majorizing kernel h with constant $B > 0$, the corresponding factor $m(\xi)$ is bounded by one provided that this constant is sufficiently small, i.e. $B \le c_\nu = \nu(2\pi)^{\frac{3}{2}}/2$. In this case one sees that (u_0, g) is (FNS)$_h$-admissible under the condition that $|\hat{u}_0(\xi)| \le Bh(\xi)$, and $|\hat{g}(\xi, t)| \le B\nu|\xi|^2 h(\xi)/2$ by virtue of the implied a.s. unit bound on the functional χ. In particular there is an implied competition over the size of the majorizing constant B in this approach. Recently Chris Orum [20] has shown that one may further exploit incompressibility as reflected in the geometry of the product $\otimes_\xi$ to obtain (FNS)$_h$-admissible majorizing kernels with constants which are twice as large as these.

Under the additional hypothesis that $h(\xi) = h(-\xi)$ one may check that

$$\overline{\chi(\theta, t)}|_{\xi_\theta = \xi} \stackrel{dist}{=} \chi(\theta, t)|_{\xi_\theta = -\xi}.$$

As a result it will follow that $\chi(\xi, t) = \mathbf{E}_{\xi_\theta = \xi}\chi(\theta, t)$ is also a solution in the sense of LeJan-Sznitman under this additional condition. However, we shall also see in a later section that this assumption is not necessary for the expected value.

The above proof of the existence part of Theorem 1.1 provides a global solution in the ball $\mathcal{B}_0(0, R)$ in the space $\mathcal{F}_{h,0,T}, T > 0$, of radius $R = c_\nu = \nu(2\pi)^{\frac{3}{2}}/2$. For uniqueness of solutions within this ball an argument along the lines of that used by LeJan and Sznitman [17] may be applied to obtain the following.

Theorem 3.2 (Uniqueness). *Let $h(\xi)$ be a standard majorizing kernel with exponent $\theta = 1$. Fix $0 < T \le +\infty$. Suppose that $\|u_0\|_{\mathcal{F}_{h,0,T}} \le \nu(\sqrt{2\pi})^3/2$ and $\|\Delta^{-1}g\|_{\mathcal{F}_{h,0,T}} \le \nu^2(\sqrt{2\pi})^3/4$. Then the solution*

$$\hat{u}(\xi, t) = \begin{cases} h(\xi)\mathbf{E}_{\xi_\theta = \xi}\chi(\theta, t), & \text{if } \xi \in W_h,\ t \ge 0, \\ 0, & \text{if } \xi \in W_h^c, t \ge 0, \end{cases}$$

is unique in the ball $\mathcal{B}_0(0, R)$ centered at 0 of radius $R = \nu(\sqrt{2\pi})^3/2$ in the space $\mathcal{F}_{h,0,T}$.

Proof. Suppose that $\hat{w}(\xi, t)$ is another solution to (FNS) with $|\hat{w}(\xi, t)| \le Rh(\xi)$. As in the proof of Theorem 1.1, without loss of generality one may replace h by $h_\nu = c_\nu h$, where $c_\nu \equiv R = \nu(2\pi)^{\frac{3}{2}}/2$ and define

$$\gamma(\xi, t) = \hat{w}(\xi, t)/h_\nu(\xi).$$

Then

$$\sup_{\substack{\xi \in W_h \\ 0 \le t \le T}} |\gamma(\xi, t)| \le 1.$$

Define a truncation of $\tau_\theta(t)$ by

$$\tau_\theta^{(n)}(t) = \{\mathbf{v} \in \tau_\theta(t) : |\mathbf{v}| \le n\}, \quad n = 0, 1, 2, \ldots.$$

Let $Y(\tau_\theta^{(n)}(t))$ be the recursively defined random functional given by

$$Y(\tau_\theta^{(n)}(t)) = \begin{cases} \chi_0(\xi_\theta) & \text{if } S_\theta > t, \\ \varphi(\xi_\theta, t - S_\theta) & \text{if } S_\theta \le t, \kappa_\theta = 0, \\ m(\xi_\theta) Y(\tau_{\langle 1\rangle}^{(n-1)}(t - S_\theta)) \otimes_{\xi_\theta} Y(\tau_{\langle 2\rangle}^{(n-1)}(t - S_\theta)), & \text{otherwise,} \end{cases}$$

for $n = 1, 2, \ldots$, where $\chi_0(\xi) = \hat{u}_0(\xi)/h_\nu(\xi)$, $\varphi(\xi, t) = 2\hat{g}(\xi, t)/(\nu|\xi|^2 h_\nu(\xi))$, $m(\xi) = 2h_\nu * h_\nu(\xi)/(\nu(2\pi)^{3/2}|\xi| h_\nu(\xi)) \le 1$, and

$$Y(\tau_\theta^{(0)}(t)) = \begin{cases} \chi_0(\xi_\theta) & \text{if } S_\theta > t, \\ \varphi(\xi_\theta, t - S_\theta) & \text{if } S_\theta \le t, \kappa_\theta = 0, \\ m(\xi_\theta)\gamma(\xi_{\langle 1\rangle}, t - S_\theta) \otimes_{\xi_\theta} \gamma(\xi_{\langle 2\rangle}, t - S_\theta), & \text{otherwise.} \end{cases}$$

Observe that since $\hat{w}(\xi, t)$ is an assumed solution to (FNS) it follows directly from $(\text{FNS})_{h_\nu}$ that

$$\mathbf{E}_{\xi_\theta = \xi} Y(\tau_\theta^{(0)}(t)) = \gamma(\xi, t).$$

Moreover, using $(\text{FNS})_{h_\nu}$ and conditioning on

$$\mathcal{F}_n = \sigma(\{S_{\mathbf{v}}, \xi_{\mathbf{v}}, \kappa_{\mathbf{v}} : |\mathbf{v}| \le n\}),$$

this extends by induction to yield

$$\gamma(\xi, t) = \mathbf{E}_{\xi_\theta = \xi} Y(\tau_\theta^{(n)}(t)) \quad \text{for } n = 0, 1, 2, \ldots.$$

Specifically, one has

$$\begin{aligned} & \mathbf{E}_{\xi_\theta = \xi} Y(\tau_\theta^{(n+1)}(t)) \\ = \; & \chi_0(\xi) e^{-\lambda(\xi)t} + \frac{1}{2}\int_0^t \lambda(\xi) e^{-\lambda(\xi)s} \varphi(\xi, t - s) ds \\ & + m(\xi) \mathbf{E}_{\xi_\theta = \xi}\{Y(\tau_{\langle 1\rangle}^{(n)}(t - S_\theta)) \otimes_\xi Y(\tau_{\langle 2\rangle}^{(n)}(t - S_\theta)) \mathbf{1}[S_\theta \le t, \kappa_\theta = 1]\} \\ = \; & \chi_0(\xi) e^{-\lambda(\xi)t} + \frac{1}{2}\int_0^t \varphi(\xi, t - s)\lambda(\xi) e^{-\lambda(\xi)s} ds + m(\xi)\frac{1}{2}\int_0^t \lambda(\xi) e^{-\lambda(\xi)s} \\ & \cdot \int \mathbf{E}_{\xi_{\langle 1\rangle}} Y(\tau_{\langle 1\rangle}^{(n)}(t - s)) \otimes_\xi \mathbf{E}_{\xi_{\langle 2\rangle}} Y(\tau_{\langle 2\rangle}^{(n)}(t - s)) H(\xi, d\xi_{\langle 1\rangle} \times d\xi_{\langle 2\rangle})\, ds. \end{aligned}$$

Now observe that

$$Y(\tau_\theta^{(0)}(t)) = \chi(\theta, t) \quad \text{on } [\tau_\theta^{(0)}(t) = \tau_\theta(t)],$$

and more generally, since the terms $\gamma(\xi_{\mathbf{v}}, t - R_{\mathbf{v}})$ appear in Y only at truncated vertices,

$$Y(\tau_\theta^{(n)}(t)) = \chi(\theta, t) \quad \text{on } [\tau_\theta^{(n)}(t) = \tau_\theta(t)].$$

Thus, since

$$\mathbf{E}|Y(\tau_\theta^{(n)}(t))| \le 1 \quad \text{for all } n$$

and

$$\mathbf{E}|\chi(\theta, t)| \le 1 \quad \text{for all } n$$

we have

$$\begin{aligned} |\gamma(\xi, t) - \mathbf{E}\chi(\theta, t)| &= |\mathbf{E}\{Y(\tau_\theta^{(n)}(t)) - \chi(\theta, t)\mathbf{1}[\tau_0^{(n)}(t) \ne \tau_\theta(t)]\}| \\ &\le 2P(\tau_\theta^{(n)}(t) \ne \tau_\theta(t)) \to 0 \quad \text{as } n \to \infty. \end{aligned}$$

□

Corollary 3.1. *Under the conditions of the theorem one has*

$$Y(\tau_\theta^{(n)}(t)) = \mathbf{E}_{\xi_\theta=\xi}\{\chi(\theta,t)|\mathcal{F}_n\}, \quad n = 0,1,2,\ldots,$$

where

(1) $\mathcal{F}_n = \sigma(\{S_{\mathbf{v}}, \xi_{\mathbf{v}1}, \xi_{\mathbf{v}2}, \kappa_{\mathbf{v}} : |\mathbf{v}| \le n\})$,
(2)

$$Y(\tau_\theta^{(0)}(t)) = \begin{cases} \chi_0(\xi_\theta) & \text{if } S_\theta > t, \\ \varphi(\xi_\theta, t - S_\theta) & \text{if } S_\theta \le t, \kappa_\theta = 0, \\ m(\xi_\theta)\mathbf{E}_{\xi_{\langle 1\rangle}}\chi(\langle 1\rangle, t - S_\theta) & \\ \quad \otimes_{\xi_\theta}\mathbf{E}_{\xi_{\langle 2\rangle}}\chi(\langle 2\rangle, t - S_\theta), & \text{otherwise.} \end{cases}$$

In particular, $\{Y(\tau_\theta^{(n)}(t)) : n = 0,1,2,\ldots\}$ *is a martingale with respect to the filtration* $\{\mathcal{F}_n : n \ge 0\}$.

Proof. First note from the recursive definition of the functional $Y(\tau_\theta^{(n)}(t))$ that for any $N \ge n$,

$$\mathbf{E}(Y(\tau_\theta^{(N)}(t))|\mathcal{F}_n) = Y(\tau_\theta^{(n)}(t)), \; N \ge n.$$

Let $G = G(S_{\mathbf{v}}, \xi_{\mathbf{v}1}, \xi_{\mathbf{v}2}, \kappa_{\mathbf{v}} : |\mathbf{v}| \le n)$ be a bounded $\mathcal{F}_n$-measurable function. Then, for $N \ge n$,

$$\begin{aligned} \mathbf{E}\{G \cdot Y(\tau_\theta^{(n)}(t))\} &= \mathbf{E}\{G \cdot \mathbf{E}\{Y(\tau_\theta^{(N)}(t))|\mathcal{F}_n\}\} \\ &= \mathbf{E}\{\mathbf{E}\{G \cdot Y(\tau_\theta^{(N)}(t))|\mathcal{F}_n\}\} \\ &= \mathbf{E}\{G \cdot Y(\tau_\theta^{(N)}(t))\} \\ &= \lim_{N\to\infty} \mathbf{E}\{GY(\tau_\theta^{(N)}(t))\} \\ &= \mathbf{E}\{\lim_{N\to\infty} GY(\tau_\theta^{(N)}(t))\mathbf{1}[\tau_\theta^{(N)}(t) = \tau_\theta(t)]\} \\ &= \mathbf{E}\{G\chi(\theta,t)\}. \end{aligned}$$

□

4. Picard iterations of a contraction map

In this section we show how majorizing kernels can be used to obtain local or global solutions of the Navier-Stokes equations following a contraction mapping argument. At the same time, relations of the stochastic cascade theory with a Picard iteration scheme are established.

Recall that the (FNS) equations are

$$\begin{aligned} \hat{u}(\xi,t) &= e^{-\nu|\xi|^2 t}\hat{u}_0(\xi) + \hat{B}(\hat{u},\hat{u})(\xi,t) \\ &+ \int_0^t e^{-\nu|\xi|^2 s}\hat{g}(\xi,t-s)ds := \hat{Q}[\hat{u};\hat{u}_0,\hat{g}](\xi,t) \end{aligned} \tag{35}$$

where

$$\hat{B}(\hat{u},\hat{v})(\xi,t) := \int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}} \int \left\{\hat{u}(\xi-\eta,t-s) \otimes_\xi \hat{v}(\eta,t-s)\right\}d\eta ds.$$

Consider the Picard iteration scheme naturally associated with the (projected) Navier-Stokes equation

$$u_{n+1}(x,t) = F(x,t) + B(u_n, u_n)(x,t) \tag{36}$$

where $F(x,t) = e^{t\nu\Delta}u_0(x) + \int_0^t e^{s\nu\Delta}g(x,t-s)ds$, $u^{(0)}(x,t) = e^{t\nu\Delta}u_0(x)$ and $u_1(x,t) = F(x,t) + B(u^{(0)}, u^{(0)})(x,t)$. The convergence of the iterates follows from showing that Q is a contraction in an appropriate ball in $\mathcal{F}_{h,\gamma,T}$.

Remark 4.1. In the case $\gamma = 1$ the smaller ball for existence and uniqueness is related to the increased regularity, namely spatial analyticity, implied by the decay on the Fourier transform in this case. Existence and uniqueness results in the larger balls obtained with $\gamma = 0$ are aimed at C^∞-smoothness.

The following lemmas summarize some of the technical details.

Lemma 4.1. *Let $0 \le \beta \le 2$, $\mu > 0$ and $M(\beta) = \sup_{\lambda>0} \frac{1-e^{-\lambda}}{\lambda^{(2-\beta)/2}}$. Then*

$$\int_0^t |\xi|^\beta e^{-\mu|\xi|^2 s} ds \le t^{(2-\beta)/2}\mu^{-\beta/2}M(\beta).$$

Proof. A direct calculation gives for $0 \le \beta \le 2$,

$$\int_0^t |\xi|^\beta e^{-\mu|\xi|^2 s} ds = \frac{1-e^{-\mu|\xi|^2 t}}{\mu|\xi|^{2-\beta}} = \frac{t^{(2-\beta)/2}}{\mu^{\beta/2}}\frac{1-e^{-\lambda}}{\lambda^{(2-\beta)/2}}$$

where $\lambda = \mu|\xi|^2 t$ and the result follows immediately. □

In the spirit of Foias and Temam [10] and Lemarié-Rieusset [16], one has the following estimate.

Lemma 4.2. *Let $\xi, \eta \in R^n$, $0 \le s \le t$. Then*

$$e^{-\nu s|\xi|^2 - \sqrt{t-s}|\xi-\eta| - \sqrt{t-s}|\eta|} \le e^{1/(2\nu)}e^{-\sqrt{t}|\xi|}e^{-\nu s|\xi|^2/2}.$$

Proof. Using the triangle inequality, it suffices to show that

$$f(|\xi|) := \frac{1}{2\nu} + \frac{1}{2}\nu|\xi|^2 s + \sqrt{t-s}|\xi| - \sqrt{t}|\xi| \ge 0.$$

A simple calculation shows that $f(r)$ achieves its minimum value at

$$r = (\sqrt{t} - \sqrt{t-s})/(\nu s) = 1/[\nu(\sqrt{t} + \sqrt{t-s})]$$

of

$$\frac{1}{\nu}\frac{\sqrt{t-s}}{\sqrt{t}+\sqrt{t-s}}$$

which is non-negative for $0 \le s \le t$. □

Using the above lemmas, it is possible to estimate the bilinear form $B(u,v)$. When considering the majorizing kernel of exponent 1, it is the size of the data that is used to show that Q is a contraction on a small ball centered at the origin. For this pointwise estimates of $\hat{B}$ will be needed.

Proposition 4.1. *Let h be a standard majorizing kernel of exponent $\theta = 1$. For $\gamma = 0$ or 1, let $C(1,\gamma) = (2\pi)^{-3/2}2^\gamma$. Then for $u(x,t), v(x,t) \in \mathcal{F}_{h,\gamma,T}$, and $0 \le t \le T$,*

$$|\hat{B}(\hat{u},\hat{v})(\xi,t)| \le |u|_{\mathcal{F}_{h,\gamma,T}}|v|_{\mathcal{F}_{h,\gamma,T}}h(\xi)e^{-\gamma\sqrt{t}|\xi|}C(1,\gamma)\frac{1-e^{-\nu|\xi|^2 t/2^\gamma}}{\nu}e^{\gamma/(2\nu)}.$$

Proof. Considering the case $\gamma = 0$ first one has

$$\begin{aligned}
|\hat{B}(\hat{u},\hat{v})(\xi,t)| &\leq \|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} \int_0^t [e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}} \int h(\xi-\eta)h(\eta)d\eta]ds \\
&\leq \|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} h(\xi)(2\pi)^{-\frac{3}{2}} \int_0^t e^{-\nu|\xi|^2 s}|\xi|^2 ds \\
&\leq \|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} h(\xi)(2\pi)^{-\frac{3}{2}} \frac{1}{\nu}(1-e^{-\nu|\xi|^2 t}).
\end{aligned}$$

Similarly, for $\gamma = 1$ and using Lemma 4.2,

$$\begin{aligned}
|\hat{B}(\hat{u},\hat{v})(\xi,t)| &\leq \|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} \int_0^t \Big[e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}} \\
&\qquad \int h(\xi-\eta)h(\eta)e^{-\sqrt{t-s}|\xi-\eta|}e^{-\sqrt{t-s}|\eta|}d\eta\Big] ds \\
&\leq \|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} h(\xi)e^{-\sqrt{t}|\xi|}e^{1/(2\nu)}(2\pi)^{-\frac{3}{2}} \int_0^t e^{-\nu|\xi|^2 s/2}|\xi|^2 ds \\
&\leq \|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} h(\xi)e^{-\sqrt{t}|\xi|}e^{1/(2\nu)}(2\pi)^{-\frac{3}{2}} \frac{2}{\nu}(1-e^{-\nu|\xi|^2 t/2}).
\end{aligned}$$

□

When using majorizing kernels of exponent $\theta < 1$, estimates on the norm of the bilinear form $B(u,v)$ are obtained using the time integral as follows.

Proposition 4.2. *Let h be a standard majorizing kernel of exponent $\theta < 1$ and let $C(\theta,\gamma) = M(\theta+1)(2\pi)^{-3/2}2^{\gamma(\theta+1)/2}$ where $M(\theta+1)$ is defined in Lemma 4.1. Then for $u, v \in \mathcal{F}_{h,\gamma,T}$,*

$$\|B(u,v)\|_{\mathcal{F}_{h,\gamma,T}} \leq \|u\|_{\mathcal{F}_{h,\gamma,T}}\|v\|_{\mathcal{F}_{h,\gamma,T}} C(\theta,\gamma)T^{(1-\theta)/2}\left(\frac{1}{\nu}\right)^{(\theta+1)/2} e^{\gamma/(2\nu)}.$$

Proof. Considering $\gamma = 0$ one has

$$\begin{aligned}
|\hat{B}(\hat{u},\hat{v})|(\xi,t) &\leq (2\pi)^{-3/2}\|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} \int_0^t |\xi| \left[e^{-\nu|\xi|^2 s}\int h(\xi-\eta)h(\eta)d\eta\right] ds \\
&\leq (2\pi)^{-3/2}\|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} h(\xi)\int_0^T |\xi|^{1+\theta}e^{-\nu|\xi|^2 s}ds \\
&\leq (2\pi)^{-3/2}\|u\|_{\mathcal{F}_{h,0,T}}\|v\|_{\mathcal{F}_{h,0,T}} h(\xi)M(1+\theta)\left(\frac{1}{\nu}\right)^{(\theta+1)/2} T^{(1-\theta)/2}.
\end{aligned}$$

Similarly, for $\gamma = 1$ use Lemma 4.1 and Lemma 4.2 to get

$$\begin{aligned}
|\hat{B}(\hat{u},\hat{v})|(\xi,t) &\leq (2\pi)^{-3/2}\|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} \int_0^t |\xi|e^{-\nu|\xi|^2 s}\int e^{-\sqrt{t-s}|\xi-\eta|}e^{-\sqrt{t-s}|\eta|} \\
&\qquad h(\xi-\eta)h(\eta)d\eta ds \\
&\leq (2\pi)^{-3/2}e^{1/(2\nu)}\|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} h(\xi)e^{-\sqrt{t}|\xi|}\int_0^t |\xi|^{1+\theta}e^{-\nu|\xi|^2 s/2}ds \\
&\leq (2\pi)^{-3/2}e^{1/(2\nu)}\|u\|_{\mathcal{F}_{h,1,T}}\|v\|_{\mathcal{F}_{h,1,T}} h(\xi)e^{-\sqrt{t}|\xi|} \\
&\qquad \cdot M(1+\theta)\left(\frac{2}{\nu}\right)^{(\theta+1)/2} T^{(1-\theta)/2}. \quad \square
\end{aligned}$$

The first result on global existence is an immediate consequence of these propositions assuming that the initial data and forcing are small. As noted in the Introduction, the solution determined by this theorem exists for the same time interval on which the forcing remains small.

Theorem 4.1. *Let h be a standard majorizing kernel of exponent $\theta = 1$. For $\gamma = 0$ or 1, let $\rho_\gamma = \rho_\gamma(\nu) < \min\{1, (\nu/2)(1/C(1,\gamma))\}$ where $C(1,\gamma)$ is defined in Proposition 4.1. Then, if $\|e^{\nu t\Delta}u_0(x)\|_{\mathcal{F}_{h,\gamma,T}} \le \rho_\gamma e^{-\gamma/(2\nu)}$ and $\|(\Delta)^{-1}g(x,t)\|_{\mathcal{F}_{h,\gamma,T}} \le \rho_\gamma(\nu/2)e^{-\gamma/(2\nu)}2^{-\gamma}$, the Navier-Stokes equations have a unique solution $u(x,t) \in \mathcal{F}_{h,\gamma,T}$ satisfying $\|u\|_{\mathcal{F}_{h,\gamma,T}} \le \rho_\gamma$.*

Proof. Let $\hat{F}(\xi,t) = e^{-\nu|\xi|^2 t}\hat{u}_0(\xi) + \int_0^t e^{-\nu|\xi|^2 s}\hat{g}(\xi, t-s)ds$.

Consider the case $\gamma = 0$ first. Then

$$|\hat{F}(\xi,t)| \le \rho_0 h(\xi)\left(e^{-\nu|\xi|^2 t} + \frac{1}{2}(1 - e^{-\nu|\xi|^2 t})\right). \tag{37}$$

Also, if $\|u\|_{\mathcal{F}_{h,0,T}} \le \rho_0$, it follows from the choice of ρ_0 and Proposition 4.1 that

$$|\hat{B}(\hat{u},\hat{u})(\xi,t)| \le \rho_0 h(\xi)\frac{1}{2}(1 - e^{-\nu|\xi|^2 t}). \tag{38}$$

Thus, using (37) and (38), one has

$$|\hat{Q}[\hat{u};\hat{u}_0,\hat{g}](\xi,t)| \le |\hat{F}(\xi,t)| + |\hat{B}(\hat{u},\hat{u})(\xi,t)| \le \rho_0 h(\xi).$$

Also if $\|v\|_{\mathcal{F}_{h,0,T}} \le \rho_0$, using Proposition 4.1 one has

$$\begin{aligned} \|B(u,u) - B(v,v)\|_{\mathcal{F}_{h,0,T}} &= \|B(u,u-v) + B(u-v,v)\|_{\mathcal{F}_{h,0,T}} \\ &\le \rho_0 C(1,0)(2/\nu)(\|u-v\|_{\mathcal{F}_{h,0,T}}). \end{aligned}$$

The result follows by the contraction mapping theorem since $\rho_0 C(1,0)(2/\nu) < 1$.

Considering $\gamma = 1$, note that $|\hat{u}_0(\xi)|/h(\xi) \le \rho_1 e^{-1/(2\nu)}$ so

$$e^{-\nu|\xi|^2 t}|\hat{u}_0(\xi)| \le \rho_1 h(\xi)e^{-1/(2\nu)}e^{-\nu|\xi|^2 t} \le \rho_1 h(\xi)e^{-\sqrt{t}|\xi|}e^{-\nu|\xi|^2 t/2} \tag{39}$$

where in the last step, Lemma 4.2 with $s = t$ was used. Similarly,

$$\begin{aligned} \left|\int_0^t e^{-\nu|\xi|^2 s}\hat{g}(\xi,t-s)ds\right| &\le \rho_1 h(\xi)\frac{1}{2}\frac{\nu}{2}e^{-1/(2\nu)}\int_0^t e^{-\nu|\xi|^2 s}|\xi|^2 e^{-\sqrt{t-s}|\xi|}ds \\ &\le \rho_1 h(\xi)e^{-\sqrt{t}|\xi|}\frac{1}{2}\frac{\nu}{2}\int_0^t e^{-\nu|\xi|^2 s/2}|\xi|^2 ds \\ &\le \rho_1 h(\xi)e^{-\sqrt{t}|\xi|}\frac{1}{2}(1 - e^{-\nu|\xi|^2 t/2}) \end{aligned} \tag{40}$$

where in the last step, Lemma 4.2 with $\eta = 0$ was used. Thus, from (39) and (40) it follows that

$$|\hat{F}(\xi,t)| \le \rho_1 h(\xi)e^{-\sqrt{t}|\xi|}\left[e^{-\nu|\xi|^2 t/2} + \frac{1}{2}(1 - e^{-\nu|\xi|^2 t/2})\right]. \tag{41}$$

As before, if $\|u\|_{\mathcal{F}_{h,1,T}} \le \rho_1$, it follows from the choice of ρ_1 and Proposition 4.1 that

$$|\hat{B}(\hat{u},\hat{u})(\xi,t)| \le \rho_1 h(\xi)e^{-\sqrt{t}|\xi|}\frac{1}{2}(1 - e^{-\nu|\xi|^2 t/2}). \tag{42}$$

Thus, using (41) and (42), one has for $\|u\|_{\mathcal{F}_{h,1,T}} \le \rho_1$,

$$|\hat{Q}[\hat{u}; \hat{u}_0, \hat{g}](\xi, t)| \le \rho_1 h(\xi) e^{-\sqrt{t}|\xi|}.$$

Also if $\|v\|_{\mathcal{F}_{h,1,T}} \le \rho_1$,

$$\begin{aligned} \|\hat{Q}[\hat{u}; \hat{u}_0, \hat{g}](\xi, t) - \hat{Q}[\hat{v}; \hat{u}_0, \hat{g}](\xi, t)\|_{\mathcal{F}_{h,1,T}} &= \|B(u,u) - B(v,v)\|_{\mathcal{F}_{h,1,T}} \\ &= \|B(u, u-v) + B(u-v, v)\|_{\mathcal{F}_{h,1,T}} \\ &\le \rho_1 C(1,1)\frac{2}{\nu}(\|u - v\|_{\mathcal{F}_{h,0,T}}), \end{aligned}$$

and as before the proposition follows by the contraction mapping theorem. □

It is possible to show that solutions exist locally in time when the forcing satisfies a bound involving fractional powers of the Laplace operator. A result along this line is given by the following theorem.

Theorem 4.2. *Let h be a standard majorizing kernel of exponent $\theta = 1$ and let ρ_γ be as in Theorem 4.1. Then if $\|e^{\nu t\Delta} u_0(x)\|_{\mathcal{F}_{h,\gamma,T}} \le \rho_\gamma$ and for some $0 \le \beta < 2$, $(-\Delta)^{-\beta/2} g(x,t) \in \mathcal{F}_{h,\gamma,T}$, then there exists T_* and $u(x,t) \in \mathcal{F}_{h,\gamma,T_*}$ satisfying the Navier-Stokes equation and $\|u\|_{\mathcal{F}_{h,\gamma,T_*}} \le \rho_\gamma$.*

Proof. New estimates are required for the forcing term. Considering $\gamma = 0$ first, note that $0 \le t \le T$:

$$\begin{aligned} \left|\int_0^t e^{-\nu|\xi|^2 s} \hat{g}(\xi, t-s) ds\right| &\le \|g\|_{\mathcal{F}_{h,0,T}} h(\xi) \int_0^t e^{-\nu|\xi|^2 s} |\xi|^\beta ds \\ &\le \|g\|_{\mathcal{F}_{h,0,T}} h(\xi) M(\beta) t^{(2-\beta)/2} \nu^{-\beta/2} \end{aligned}$$

where in the last step, Lemma 4.1 was used.

As in the proof of Theorem 4.1 one has for $0 \le t \le T$

$$\begin{aligned} |\hat{Q}[\hat{u}; \hat{u}_0, \hat{g}](\xi, t)| \le\ & h(\xi) \Big[\|e^{\nu t\Delta} u_0\|_{\mathcal{F}_{h,0,T}} e^{-\nu|\xi|^2 t} \\ & + \|g\|_{\mathcal{F}_{h,0,T}} M(\beta) t^{(2-\beta)/2} \nu^{-\beta/2} + \|u\|^2_{\mathcal{F}_{h,0,T}} (2\pi)^{-3/2} \frac{1}{\nu}(1 - e^{-\nu|\xi|^2 t}) \Big]. \end{aligned}$$

The result follows by choosing T_* small enough so that $\hat{Q}$ is a contraction of the ball of radius ρ_γ centered at the origin into itself.

Similarly, for $\gamma = 1$, one has

$$\begin{aligned} \left|\int_0^t e^{-\nu|\xi|^2 s} \hat{g}(\xi, t-s) ds\right| &\le \|g\|_{\mathcal{F}_{h,1,T}} h(\xi) \int_0^t e^{-\nu|\xi|^2 s} |\xi|^\beta e^{-\sqrt{t-s}|\xi|} ds \\ &\le \|g\|_{\mathcal{F}_{h,1,T}} h(\xi) e^{-\sqrt{t}|\xi|} e^{1/(2\nu)} \int_0^t e^{-\nu|\xi|^2 s/2} |\xi|^\beta ds \\ &\le \|g\|_{\mathcal{F}_{h,1,T}} h(\xi) e^{-\sqrt{t}|\xi|} M(\beta) t^{(2-\beta)/2} (\nu/2)^{-\beta/2}. \end{aligned}$$

Thus,

$$\begin{aligned} |\hat{Q}[\hat{u}; \hat{u}_0, \hat{g}](\xi, t)| \le\ & h(\xi) e^{-\sqrt{t}|\xi|} \Big[\|e^{\nu t\Delta} u_0\|_{\mathcal{F}_{h,1,T}} e^{-\nu|\xi|^2 t} \\ & + \|g\|_{\mathcal{F}_{h,1,T}} M(\beta) t^{(2-\beta)/2} \nu^{-\beta/2} + \|u\|^2_{\mathcal{F}_{h,1,T}} (2\pi)^{-3/2} \frac{1}{\nu}(1 - e^{-\nu|\xi|^2 t}) \Big]. \end{aligned}$$

As before, the result follows by choosing T_* small enough so that the contraction mapping theorem can be applied to $\hat{Q}$ as a mapping on the ball or radius ρ_γ centered at the origin. □

Finally, a further local existence result can be obtained if majorizing kernels of exponent $\theta < 1$ are considered.

Theorem 4.3. *Let h be a standard majorizing kernel of exponent $\theta < 1$. Assume that for some $1 \leq \beta \leq 2$,*

$$(\Delta)^{-\beta/2} g(x,t) \in \mathcal{F}_{h,\gamma,T}. \tag{43}$$

Then, for any initial data such that $e^{\nu t\Delta} u_0(x) \in \mathcal{F}_{h,\gamma,T}$ and forcing satisfying (43) there exists $T_* \leq T$ and a unique $u(x,t) \in \mathcal{F}_{h,\gamma,T_*}$ satisfying the Navier-Stokes equation.

Proof. A straightforward calculation shows that

$$\hat{F}(\xi,t) = e^{-\nu|\xi|^2 t}\hat{u}_0(\xi) + \int_0^t e^{-\nu|\xi|^2 s}\hat{g}(\xi, t-s)ds$$

satisfies

$$\|F\|_{\mathcal{F}_{h,\gamma,T}} \leq M$$

for an appropriate M.

Using Proposition 4.2, it follows for suitable constants C, independent of T,

$$\begin{aligned} \|Q[\hat{u};\hat{u}_0,\hat{g}] - F\|_{\mathcal{F}_{h,\gamma,T}} &\leq \|B(u,u)\|_{\mathcal{F}_{h,\gamma,T}} \\ &\leq \left[\|u-F\|_{\mathcal{F}_{h,\gamma,T}} + \|F\|_{\mathcal{F}_{h,\gamma,T}}\right]^2 CT^{(1-\theta)/2}. \end{aligned} \tag{44}$$

Similarly,

$$\begin{aligned} \|Q[\hat{u};\hat{u}_0,\hat{g}] - Q[\hat{v};\hat{u}_0,\hat{g}]\|_{\mathcal{F}_{h,\gamma,T}} &\leq \|B(u,u) - B(v,v)\|_{\mathcal{F}_{h,\gamma,T}} \\ &\leq \|B(u,(u-v)) + B(u-v,v)\|_{\mathcal{F}_{h,\gamma,T}} \\ &\leq C(\|u\|_{\mathcal{F}_{h,\gamma,T}} + \|v\|_{\mathcal{F}_{h,\gamma,T}}) \\ &\quad \cdot \|u-v\|_{\mathcal{F}_{h,\gamma,T}} T^{(1-\theta)/2}. \end{aligned} \tag{45}$$

Now, use (44) and (45) to choose $T_* \leq T$ such that if for some $\rho > 0$,

$$\|u - F\|_{\mathcal{F}_{h,\gamma,T_*}} < \rho,$$

Q is a contraction in the ball centered at F of radius ρ. □

Remark 4.2. Theorem 4.3 establishes uniqueness and regularity for solutions to (FNS) on a finite time interval $[0, T_*)$ for all initial $u_0 \in \mathcal{F}_{h,\gamma,T_*}$ without further restricting $\|u_0\|_{\mathcal{F}_{h,\gamma,T_*}}$. Here $T_* \to 0$ as $\nu \to 0$. This is consistent with other known local existence and uniqueness theorems; e.g. see Temam [21] and Kato [15].

Remark 4.3. Recall that a Banach space X is called a *limit space* for the Navier-Stokes equations iff $\|u\|_X = \|u_\lambda\|_X$ where $u_\lambda = \lambda u(\lambda x, \lambda^2 t)$. If h is a majorizing kernel with exponent $\theta = 1$, then $h_\lambda(\xi) = \lambda^{-2}h(\xi/\lambda)$ is also a majorizing kernel of the same exponent. Moreover, if $u \in \mathcal{F}_{h,\gamma,T}$, $u_\lambda \in \mathcal{F}_{h_\lambda,\gamma,T}$ and $\|u\|_{\mathcal{F}_{h,\gamma,T}} = \|u_\lambda\|_{\mathcal{F}_{h_\lambda,\gamma,T}}$. Thus an exponent one majorizing kernel h such that $h = h_\lambda$ defines a limit space $X = \mathcal{F}_{h,\gamma,T}$ in the usual sense, whereas the relation $\|u\|_{\mathcal{F}_{h,\gamma,T}} = \|u_\lambda\|_{\mathcal{F}_{h_\lambda,\gamma,T}}$ defines a slightly more general version of this notion. Nonetheless the global existence result of Theorem 4.1 is in agreement with the similar results known for the usual limit spaces; cf. Cannone and Meyer [5], Cannone and Planchon [4], and Chen and Xin [6].

Finally, the relation between the iteration scheme and the expected value representation of the solution obtained in Section 3 is established in the following proposition. For reference, recall that the replacement time of a vertex $\mathbf{v}$ is defined as

$$R_{\mathbf{v}} = \sum_{k=0}^{|\mathbf{v}|} S_{\mathbf{v}|k}.$$

Introduce

$$A_n(\theta, t) = [|\mathbf{v}| \le n \ \forall \mathbf{v} \in \tau_\theta(t)] \cap [R_{\mathbf{v}} > t \ \forall \mathbf{v} \in \{\mathbf{u} \in \tau_\theta(t) : |\mathbf{u}| = n\}],$$

and let $\mathbf{1}[n; \theta, t]$ be the indicator of the event $A_n(\theta, t)$. Observe that the definition of the event $A_n(\theta, t)$ and its indicator extends to $A_n(\langle i \rangle, t - S_\theta), i = 1, 2$, and inductively to $A_n(\mathbf{v}, t - B_{\mathbf{v}})$, using the shifted binary tree defined by (31) and the time shift $t - S_\theta$.

Proposition 4.3. *Let*

$$\begin{aligned} v_k(\xi, t) &= h(\xi)\chi_k(\xi, t) \\ &= h(\xi)\mathbf{E}_\xi\{\mathbf{1}[k; \xi, t]\chi(\theta, t)\} \end{aligned}$$

and denote by $\hat{u}_k(\xi, t)$ the Fourier transform of the k^{th} iterate of the iteration scheme defined in (36). *Then $v_k(\xi, t) = \hat{u}_k(\xi, t)$.*

Proof. The proof is by induction on k. Note that

$$\begin{aligned} v_0(\xi, t) &= h(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[0; \theta, t]\chi(\theta, t)\} \\ &= h(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\chi(\theta, t)|S_\theta > t\}\mathbf{P}[S_\theta > t] \\ &= h(\xi)\chi_0(\xi)e^{-\nu|\xi|^2 t} \\ &= \hat{u}^{(0)}(\xi). \end{aligned}$$

The proof for the general case rests on the following identity:

(46)
$$\begin{aligned} &h(\xi)\mathbf{E}_{\xi_\theta=\xi}\left\{\mathbf{E}_{\xi_\theta=\xi}\left\{\mathbf{1}[k+1; \theta, t]\mathbf{1}[\kappa_\theta = 1]\mathbf{1}[S_\theta < t]m(\xi_\theta)\right.\right. \\ &\quad \left.\left. \cdot \chi(\langle 1 \rangle, t - S_\theta) \otimes_{\xi_\theta} \chi(\langle 2 \rangle, t - S_\theta)|\xi_{\langle 1 \rangle}, \xi_{\langle 2 \rangle}, S_\theta\right\}\right\} \\ = &\int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}} \int_{\mathbf{R}^3} \chi_k(\eta, t-s) \otimes_\xi \chi_k(\xi - \eta, t - s)h(\eta)h(\xi - \eta)d\eta. \end{aligned}$$

To see this, recall that $\mathbf{P}[\kappa_\theta = 1] = 1/2$ as well as both the recursive definition of the χ functional together with the following factorization on the event $[\kappa_\theta = 1, S_\theta < t]$:

$$\mathbf{1}[k+1; \theta, t] = \mathbf{1}[k; \langle 1 \rangle, t - S_\theta]\mathbf{1}[k; \langle 2 \rangle, t - S_\theta]. \tag{47}$$

Also recall the exterior condition (10) and the definitions of m given in (8) and of the transition probability kernel given in (9). With these in mind, the left-hand side of (46) can be computed as

$$h(\xi)\frac{1}{2}\int_0^t e^{-\nu|\xi|^2 s}\nu|\xi|^2\frac{2h*h(\xi)}{\nu(2\pi)^{\frac{3}{2}}|\xi|h(\xi)}\int_{\mathbf{R}^3}\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[k;\langle 1\rangle,t-s]\mathsf{X}(\langle 1\rangle,t-s)$$
$$\otimes_\xi \mathbf{1}[k;\langle 2\rangle,t-s]\mathsf{X}(\langle 2\rangle,t-s)|\xi_{\langle 1\rangle}=\eta,\xi_{\langle 2\rangle}=\xi-\eta\}\frac{h(\xi-\eta)h(\eta)}{h*h(\xi)}d\eta ds$$
$$=\int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}}\mathbf{E}_{\xi_\theta=\xi}\{\int_{\mathbf{R}^3}\mathbf{1}[k;\langle 1\rangle,t-s]\mathsf{X}(\langle 1\rangle,t-s)$$
$$\otimes_\xi \mathbf{1}[k;\langle 2\rangle,t-s]\mathsf{X}(\langle 2\rangle,t-s)|\xi_{\langle 1\rangle}=\eta,\xi_{\langle 2\rangle}=\xi-\eta\}h(\eta)h(\xi-\eta)d\eta ds.$$

Thus, using the conditional independence of the recursive functional it follows that the last equation can be written as

$$\int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}}\int_{\mathbf{R}^3}\left[h(\eta)\mathbf{E}_{\xi_{\langle 1\rangle}=\eta}\{\mathsf{X}(\langle 1\rangle,t-s)\mathbf{1}[k;\langle 1\rangle,t-s]\}\right]$$
$$\otimes_\xi\left[h(\xi-\eta)\mathbf{E}_{\xi_{\langle 2\rangle}=\xi-\eta}\{\mathsf{X}(\langle 2\rangle,t-s)\mathbf{1}[k;\langle 2\rangle,t-s]\}\right]d\eta ds$$

as needed to establish (46).

To complete the proof, with condition on the value of the first clock ring S_θ, recall the definitions of m and φ given in (8) and use (46) to get

$$\begin{aligned}
v_{k+1}(\xi,t) &= h(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[k+1;\theta,t]\mathsf{X}(\theta,t)|\xi_{\langle 1\rangle},\xi_{\langle 2\rangle},S_\theta\}\} \\
&= h(\xi)\left[\chi_0(\xi)e^{-\nu|\xi|^2 t}+\frac{1}{2}\int_0^t e^{-\nu|\xi|^2 s}\nu|\xi|^2\varphi(\xi,t-s)ds\right] \\
&\quad + h(\xi)\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{E}_{\xi_\theta=\xi}\{\mathbf{1}[k+1;\theta,t]\mathbf{1}[\kappa_\theta=1]\mathbf{1}[S_\theta<t]m(\xi)\mathsf{X}(\langle 1\rangle,t-S_\theta) \\
&\qquad \otimes_{\xi_\theta}\mathsf{X}(\langle 2\rangle,t-S_\theta)|\xi_{\langle 1\rangle},\xi_{\langle 2\rangle},S_\theta\}\} \\
&= \hat{u}^{(0)}(\xi)+\int_0^t e^{-\nu|\xi|^2 s}\hat{g}(\xi,t-s)ds \\
&\quad + \int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}}\int_{\mathbf{R}^3}v_k(\eta,t-s)\otimes_\xi v_k(\xi-\eta,t-s)d\eta ds \\
&= \hat{F}(\xi,t)+\int_0^t e^{-\nu|\xi|^2 s}|\xi|(2\pi)^{-\frac{3}{2}}\int_{\mathbf{R}^3}\hat{u}_k(\eta,t-s)\otimes_\xi \hat{u}_k(\xi-\eta,t-s)d\eta ds
\end{aligned}$$

by the induction hypothesis and the definition of $\hat{F}$. This last equation is $\hat{u}_{k+1}(\xi,t)$ as claimed. □

A consequence of the proposition is that the convergence of the iteration scheme (36) and the existence of the expected value in Theorem 3.1 are essentially equivalent.

5. Conclusions and remarks

The Introduction and identification of majorizing kernels provides a way to obtain existence and uniqueness of mild solutions of Navier-Stokes equations and track regularity of initial data to solutions. The same methods may be applied to the Fourier coefficients in the case of periodic initial data and forcing. In fact the identification of majorizing kernels is somewhat simpler here due to the fact that on the integer lattice the origin need not be a singularity of the majorizing kernel. One may use a lattice version of the theory for constructions of majorizing kernels (e.g. Theorems 2.1-2.2) to construct fully supported majorizing kernels on the integer lattice in all dimensions $d \geq 2$. In the case $d = 1$ one also obtains cascade representations of solutions to Burgers' equation by these techniques. For example majorizing kernels supported on the positive half-line, $h(\xi) = \mathbf{1}[\xi > 0]$, also appear naturally and yield an existence/uniqueness theory for complex-valued solutions in Hardy spaces H^p.

As emphasized in the Introduction, in principle the theory may be approached from the perspective of identifying Fourier multipliers for which $E_{\xi_\theta=\xi}|X(\theta,t)| < \infty$. While majorizing kernels are sufficient for this purpose, this neither exploits the geometric structure of the product $\otimes_\xi$ nor the "size"(number of vertices) of the underlying stochastic tree structure beyond simple first order considerations.

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Part VI
Stochastic Foundations in Applied Sciences III: Statistics

Chapter 17
Nonparametric Statistical Methods on Manifolds

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Abstract One of the many fundamental contributions that Rabi Bhattacharya, together with his coauthors, has made is the development of a general nonparametric theory of statistical inference on manifolds, in particular related to both intrinsic and extrinsic Fréchet means of probability distributions thereon (cf. Bhattacharya and Bhattacharya 2012, Bhattacharya, Patrangenaru 2013 and 2005). With the increasing importance of statistical analysis for non-Euclidean data in many applications, there is much scope for further advances related to this particular broad area of research. In the following, we concentrate on two particular important themes in data analysis on manifolds: nonparametric bootstrap methods and nonparametric curve fitting.

17.1 Bootstrap Methods

A major application of the central limit results in [4] and [5] for intrinsic and extrinsic means on general manifolds is to statistical inference, e.g., the construction of confidence regions and multi-sample tests via bootstrap methods.

The bootstrap, see [8], provides a way of estimating, on the basis of an observed sample, the sampling distribution of a statistic $T(S; F)$, where $S = \{X_1, \ldots, X_n\}$ is an independent random sample from a probability distribution F. Here we will assume that F is a distribution on a Riemannian manifold $\mathcal{M}$ and that the target for inference is a population location parameter $\mu = \mu(F) \in \mathcal{M}$. Let $\hat{F}$ denote the empirical distribution function (EDF) based on the sample S; so for $A \subset \mathcal{M}$,

$$\hat{F}(A) = n^{-1} \sum_{i=1}^{n} \delta_{X_i}(A),$$

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where $\delta_{X_i}(A) = 1$ if $X_i \in A$ and zero otherwise. Let $S^* = \{X_1^*, \ldots, X_n^*\}$ denote a sample of size n drawn randomly with replacement from the original sample S, with corresponding EDF $\hat{F}^*$. Then Efron's bootstrap principle is that the distribution of $\hat{\mu} = \mu(\hat{F})$ based on an i.i.d. sample $\{X_1, \ldots, X_n\}$ from F is approximately the same as the distribution of $\hat{\mu}^* = \mu(\hat{F}^*)$ based on an i.i.d. sample $\{X_1^*, \ldots, X_n^*\}$ from $\hat{F}$. The usefulness of this result is that the distribution of $\hat{\mu}^*$ can be approximated with arbitrary accuracy by simulation and hence used as a basis for inference about μ.

Two very basic but commonly arising inference problems concerning μ are as follows: (i) given a sample $S = \{X_1, \ldots, X_n\}$, construct a confidence region for $\mu \in \mathcal{M}$; and (ii) given $k \geq 2$ independent samples $S_1, \ldots, S_k$, test the hypothesis that $\mu_1 = \cdots = \mu_k$, where $\mu_i = \mu(F_i)$ and F_i is the population distribution from which the sample $S_i = \{X_{i,1}, \ldots, X_{i,n_i}\}$ is drawn.

There are many possible ways to construct bootstrap procedures to address (i) and (ii), but doing so using *pivotal* statistics has well-known advantages; see, for example, [10] and [12]. A pivotal statistic is one whose asymptotic distribution does not depend on unknown parameters. Pivotal statistics for bootstrapping in the setting where μ is an extrinsic mean and $\mathcal{M}$ is the unit sphere were devised in [10], and the approach was generalized in [4] and [5] to general $\mathcal{M}$.

Consider the following strategy for constructing a pivotal statistic for an extrinsic mean. Suppose that $\{X_1, \ldots, X_n\}$ is an i.i.d. sample from a subset of a finite-dimensional linear space, represented as $\mathbb{R}^q$ or $\mathbb{C}^q$, in which $\mathcal{M}$ is embedded. Assume that a location parameter of interest can be written as

$$\mu = \phi(\Xi) \quad \text{where} \quad \Xi = E[X_1],$$

where $\phi(\Xi)$ is a smooth map with codomain of dimension t, say. Typically, extrinsic means can be written in this form.

Suppose that the sample mean $\hat{\Xi} = n^{-1} \sum_{i=1}^{n} X_i$ satisfies a central limit theorem, so that as $n \to \infty$,

$$n^{1/2}(\hat{\Xi} - \Xi) \to N_q(0, V)$$

in distribution. Since $\phi(\cdot)$ is smooth, then, by the delta method,

$$n^{1/2}\{\phi(\hat{\Xi}) - \phi(\Xi)\} \approx L(\hat{\Xi} - \Xi),$$

where L is a matrix of derivatives, and

$$n^{1/2}\{\phi(\hat{\Xi}) - \phi(\Xi)\} \to N_t(0, LVL^\top)$$

in distribution. Then, provided $LVL^\top$ has full rank,

$$n\{\phi(\hat{\Xi}) - \phi(\Xi)\}^\top (LVL^\top)^{-1}\{\phi(\hat{\Xi}) - \phi(\Xi)\}$$

converges in distribution to χ_t^2 when $\Xi = E[X_1]$. In practice it is convenient to replace $LVL^\top$ with its asymptotically equivalent sample analogue $\hat{L}\hat{V}\hat{L}^\top$, leading to the pivotal statistic

$$T(\mu) = n\{\phi(\hat{\Xi}) - \mu\}^\top (\hat{L}\hat{V}\hat{L}^\top)^{-1}\{\phi(\hat{\Xi}) - \mu\}. \quad (17.1)$$

A bootstrap version of this statistic is

$$T^*(\mu) = n\{\phi(\hat{\Xi}^*) - \mu\}^\top (\hat{L}^* \hat{V}^* \hat{L}^{*\top})^{-1} \{\phi(\hat{\Xi}^*) - \mu\}, \tag{17.2}$$

which can be used to construct bootstrap algorithms to address problems (i) and (ii) as follows.

Algorithm 1: Bootstrap confidence region for $\mu \in \mathcal{M}$.

Step 1. Starting with the original sample $S = \{X_1, \ldots, X_n\}$, calculate $\hat{\mu} = \mu(\hat{F})$.

Step 2. Generate B bootstrap resamples $S_1^*, \ldots, S_B^*$ randomly with replacement from the original sample S. For $b = 1, \ldots, B$, calculate $c_b = T_b^*(\hat{\mu})$, the value of the bootstrap version of the pivotal statistic based on resample S_b^* evaluated at $\hat{\mu}$.

Step 3. Order the c-values to obtain $c_{(1)} \leq \ldots \leq c_{(B)}$.

Step 4. Return the approximate $100(1-\alpha)\%$ confidence region

$$\{\mu \in \mathcal{M} : T(\mu) \leq c_{([B(1-\alpha)]+1)}\},$$

where $T(\mu)$ is the pivotal statistic based on the original sample S.

Algorithm 2: Bootstrap test for equality of means $\mu_1 = \cdots = \mu_k$.

Step 1. Given samples $S_1, \ldots, S_k$, calculate the quantities needed to evaluate the pivotal statistics $T_1(\mu), \ldots, T_k(\mu)$.

Step 2. Find $\hat{\mu}_{\text{pooled}}$ to minimize $\sum_{j=1}^{k} T_j(\mu)$ over μ, and write

$$\hat{\tau} = \sum_{j=1}^{k} T_j(\hat{\mu}_{\text{pooled}}).$$

Step 3. Set up the bootstrap null hypothesis H_{Boot} by adjusting the empirical distribution functions $\hat{F}_1, \ldots, \hat{F}_k$ to $\hat{F}_1^{\text{adj}}, \ldots, \hat{F}_k^{\text{adj}}$, in such a way that

$$\mu(\hat{F}_1^{\text{adj}}) = \cdots = \mu(\hat{F}_k^{\text{adj}}) = \hat{\mu}_{\text{pooled}}.$$

One can adjust the $\hat{F}_j$ either by transforming the samples in some way, or by resampling with nonuniform resampling probabilities, or maybe a combination of the two.

Step 4. Generate B independent resamples under the bootstrap null hypothesis H_{Boot} to obtain resamples $\{S_{11}^*, \ldots, S_{k1}^*\}, \ldots, \{S_{1B}^*, \ldots, S_{kB}^*\}$. For $b = 1, \ldots, B$, perform Step 2 to obtain $\hat{\mu}_{\text{pooled},b}$, and calculate

$$\tau_1^* = \sum_{j=1}^{k} T_{j1}^*(\hat{\mu}_{\text{pooled},1}^*), \ldots, \tau_B^* = \sum_{j=1}^{k} T_{jB}^*(\hat{\mu}_{\text{pooled},B}^*),$$

where T_{jb}^* is the pivotal statistic based on $S_{1b}^*, \ldots, S_{kb}^*$.

Step 5. Calculate the bootstrap p-value

$$\frac{1}{B}\#\{b : \hat{\tau} > \hat{\tau}_b\}.$$

Types of manifold-valued data for which bootstrap algorithms of this kind have been developed include directions and axes and 2D and 3D shape (cf. [1, 2, 10, 23] and [24]). In 2D shape analysis, for example, preshapes (configurations of landmarks with location and scale information removed) can be written as complex unit vectors $Z_1, \ldots, Z_n$. Taking $X_i = Z_i Z_i^*$, where * denotes conjugate transpose, further removes rotation information, then the space of all possible X_i can be identified with 2D similarity shape space (cf. [5]). The population and sample extrinsic mean shapes are the unit eigenvectors corresponding to the largest eigenvalues of $\Xi = E(X_1)$ and $\hat{\Xi} = n^{-1} \sum X_i$, respectively. Defining $\phi(\hat{\Xi})$ as the maximum eigenvalue of $\hat{\Xi}$ leads to straightforward calculations for $\hat{L}$ and $\hat{V}$ in (17.1) (cf. [2]). In 3D shape analysis with p landmarks, preshapes can be written as 3-by-$(p-1)$ matrices, Z_i, satisfying trace $(Z_i^\top Z_i) = 1$. Taking $X_i = Z_i^\top Z_i$ removes rotation (as well as reflection) information. A map $\phi(\hat{\Xi})$ defined to project $\hat{\Xi}$ onto the space of positive-definite matrices of rank ≤ 3 can be interpreted as an extrinsic mean reflection shape (cf. [7]). Calculations for $\hat{L}$ and $\hat{V}$ are lengthier but tractable. An important issue, however, is that the limiting χ^2 distribution of (17.1) has $3p - 7$ degrees of freedom, and unless sample sizes are very large then $\hat{L}^* \hat{V}^* \hat{L}^{*\top}$ can be singular or ill-conditioned under bootstrap resampling. This leads to poor coverage accuracy even with reasonably large sample sizes. Using regularized test statistics, such as (17.1) and (17.2) with adjustments made to the smaller eigenvalues of $LVL^\top$, appears necessary, and numerical evidence suggests such an approach is very effective (cf. [23] and [24]).

In summary, the pivotal statistic for Algorithms 1 and 2 requires: a central limit theorem for the extrinsic mean (as provided by [5] in a general manifold setting), and a smooth map $\phi(\cdot)$ that defines a meaningful location parameter, for which the calculations of L and V are tractable. If any ingredient is missing, one may still develop bootstrap approaches which are nonpivotal; see examples for analysis of projective shape in [21], and planar curves in [9].

A broadly applicable nonpivotal bootstrap approach addressing problem (i) above is the following, in which d is a metric on $\mathcal{M}$.

Algorithm 3: Nonpivotal bootstrap confidence region for $\mu \in \mathcal{M}$.

Step 1: Starting with the original sample $S = \{X_1, \ldots, X_n\}$, calculate $\hat{\mu} = \mu(\hat{F})$.

Step 2: Generate B independent resamples

$$S_1^* = \{X_{11}^*, \ldots, X_{1n}^*\}, \ldots, S_B^* = \{X_{B1}^*, \ldots, X_{Bn}^*\},$$

sampled randomly with replacement from the original sample S, and calculate $\hat{\mu}_b^* = \mu(\hat{F}_b^*)$, where $\hat{F}_b$ is the empirical distribution function based on resample S_b^*.

Step 3: order the values $d(\hat{\mu}, \hat{\mu}_1^*), \ldots, d(\hat{\mu}, \hat{\mu}_B^*)$ to obtain $c_{(1)} \leq c_{(2)} \leq \cdots \leq c_{(B)}$.

Step 4: return the (approximate) $100(1-\alpha)\%$ confidence region

$$\mathcal{R}_\alpha = \{\mu \in \mathcal{M} : d(\mu, \hat{\mu}) \leq c_{([B(1-\alpha)]+1)}\},$$

where [.] denotes integer part.

It remains an open question how best to develop effective bootstrap algorithms on more general spaces, such as stratified manifolds and, more generally, various types of metric space of potential interest in applications. For the example of "open books" (disjoint copies of half-spaces glued along their boundary hyperplanes), the central limit theorem has a limit distribution which is a mixture of components (cf. [16]), which is a nonstandard setting from a bootstrap perspective.

17.2 Curve Fitting

Other classical statistical methodology, such as the widely used method of principal component analysis, can be adapted and developed to analyze the variability of manifold-valued data further. The most straightforward way to apply principal component analysis to manifold-valued data is to perform the standard principal component analysis on the tangent space at the Fréchet mean of the data, i.e., obtain the eigendecomposition of the sample covariance of tangent coordinates, with eigenvectors giving the principal components ordered by the corresponding eigenvalues. In other words, the data are first transferred, using the inverse exponential map or other similar maps, to the tangent space at their Fréchet mean, and then principal component analysis is applied to the transferred data to find the lower dimensional subspace in that tangent space that maximizes the variance of the projection of the transferred data. This method, combined with generalized Procrustean analysis, is widely used in statistical shape analysis (cf. [6]). If the first principal component obtained in this way has a sufficiently high eigenvalue, a unit vector in the resulting 1-dimensional sub-tangent space determines a geodesic which often gives a good approximation to indicate the variability of the data.

This idea of using geodesics to model the variability of the data can be refined by replacing the use of the tangent space by working directly on the manifold, leading to the concept of *principal geodesic component analysis*, as introduced in [14]. Applications of principal geodesic component analysis so defined to Kendall's shape spaces can be found in [13] & [15], and to medially defined anatomical shapes can be found in [11]. For a set of data $\{X_1, \ldots, X_n\}$ in a given Riemannian manifold $\mathcal{M}$ with induced metric d, the first principal geodesic γ_0 to this set of data is defined to be

$$\gamma_0 = \arg\min_{\gamma \in G(\mathcal{M})} \sum_{i=1}^{n} d(X_i, \gamma)^2,$$

where $G(\mathcal{M})$ denotes the set of all possible maximal geodesics in $\mathcal{M}$ and the distance between a given point and a geodesic is defined as the minimum of the distances between that given point and points on the geodesic. To find such an optimal γ_0, we note that, up to re-parametrization and translation along its curve, any geodesic γ can be expressed, using the exponential map, in terms of a point x on γ and a unit tangent vector v at x as $\gamma(t) = \exp_x(tv)$. Then, the above minimization problem can be expressed in a more tractable way as

$$\begin{aligned} &\min_{x \in \mathcal{M}, v \in T_x(\mathcal{M}), \|v\|=1} \sum_{i=1}^{n} d(X_i, \gamma)^2 \\ &= \min_{x \in \mathcal{M}, v \in T_x(\mathcal{M}), \|v\|=1} \sum_{i=1}^{n} \min_{t_i \in \mathbb{R}} d(\exp_x(t_i v), X_i)^2 \\ &= \min_{x \in \mathcal{M}, v \in T_x(\mathcal{M}), \|v\|=1, t_i \in \mathbb{R}} \sum_{i=1}^{n} d(\exp_x(t_i v), X_i)^2. \end{aligned}$$

This will allow us to use iterative computer algorithms to approximate the first principal geodesic. However, on account of the ambiguity in the choice of reference point x, mentioned above, the solution to such a minimization problem is no longer unique.

We can also consider searching for an optimal curve among other prescribed sets of curves to capture the main features of the data, for example the use of the set of small circles for data lying on a sphere. The method of *principal nested spheres* (PNS), proposed in [17], introduces a general framework for a novel non-geodesic decomposition of variability of data lying on high-dimensional spheres. Instead of searching for an optimal small circle directly, it decomposes a high-dimensional sphere into a sequence of sub-manifolds with decreasing intrinsic dimensions, which can be interpreted as an analogue of principal component analysis. The procedure for finding the PNS involves iterative reduction of the data dimension. To describe it more explicitly, we assume that $\{X_1, \ldots, X_n\}$ is a sample in the unit m-sphere $\mathcal{S}^m$, where $m > 1$. Then the best fitting sub-sphere for this set of data is defined as the sub-sphere of dimension $m - 1$ in $\mathcal{S}^m$ minimizing, among all possible such sub-spheres, the sum of the squares of the distances of the data points to it. Since any sub-sphere A_{m-1} of dimension $m-1$ can be characterized by an $r \in (0, \pi/2]$ and a direction $x \in \mathcal{S}^m$ as

$$A_{m-1}(x, r) = \{x' \in \mathcal{S}^m \mid d(x, x') = r\},$$

where d denotes the intrinsic distance on $\mathcal{S}^m$, the problem of finding the best fitting sub-sphere becomes searching for $(\hat{x}, \hat{r})$ which solves

$$\arg\min_{x \in \mathcal{S}^m, r \in (0, \pi/2]} \sum_{i=1}^{n} (d(X_i, x) - r)^2.$$

Then, each step of the iterative procedure for fitting principal nested spheres repeats this, after rescaling to standardize the radius of the spheres, for the (orthogonally) projected data onto the best fitting sub-sphere obtained in the previous step. If $\hat{r} = \pi/2$, then the best fitting sub-sphere is a great sub-sphere, so that this method generalizes the method of finding principal geodesics, similar to those from previous approaches to manifold principal component analysis.

The procedure for implementing PNS makes it clear that the method can also be used for dimension reduction of spherical data. Moreover, although the PNS method is primarily proposed for data lying on spheres as suggested by its name, the idea could possibly be generalized to fit more general manifold-valued data using principal nested sub-manifolds defined by a sequence of constraints. For example, [17] did include principal nested 2D shape spaces, which is a simple generalization. This would expand the range of techniques for the analysis of variability of such data. Nevertheless, this would require the understanding of the geometry of the underlying manifold. One of the challenging issues here is the careful choice of the class of sub-manifolds so that it is possible to implement the method and the interpretation is meaningful.

The methods mentioned above all use some form of orthogonal projection from the observed data to an estimated curve. However, this is not always adequate for the interpolation of time-indexed observed data on manifolds, so that it is necessary to adapt other classical techniques, such as generalizing Euclidean cubic spline fitting. Recall first that, for a given data set $\{X_1, \ldots, X_n\}$ in $\mathbb{R}^m$, where X_j is observed at time $t_j \in T$, $j = 0, \ldots, n$, the cubic spline in $\mathbb{R}^m$ fitted to this dataset with smoothing parameter λ is the function $f(\cdot, \lambda) : T \to \mathbb{R}^m$ that minimizes

$$\sum_{i=0}^{n} \|f(t_j, \lambda) - X_j\|^2 + \lambda \int_T \|f''(t, \lambda)\|^2 dt, \tag{17.3}$$

among all C^2-functions, where T is a time interval containing all the time points.

One way to generalize the Euclidean cubic spline to manifolds is to use *parallel transport* to transfer data to tangent spaces, preserving the inter-relationships among the data as much as possible, and then to use the known procedure in Euclidean space to find the cubic spline for the transported data. More precisely, for a given dataset $S = \{X_1, \cdots, X_n\}$ in a manifold $\mathcal{M}$, where X_j is observed at time t_j, and smoothing parameter λ, the $\mathcal{M}$-valued smoothing spline fitted to S with parameter λ is defined to be the C^2-function

$$\gamma(\cdot, \lambda) : [t_0, t_n] \to \mathcal{M}$$

such that its unrolling $\gamma^\dagger$ onto the tangent space of $\mathcal{M}$ at $\gamma(t_0, \lambda)$ is the cubic smoothing spline fitted to the data $S^\dagger$ obtained by unwrapping S at times t_j, with respect to γ, into the tangent space of $\mathcal{M}$ at $\gamma(t_0, \lambda)$. For a more formal definition, see [18]. The terms *unrolling* and *unwrapping* are both intuitive descriptions of moving the curve and general points on the manifold using the concept of parallel transport. The $\mathcal{M}$-valued smoothing spline defined in this way is, except at the data times, the solution to the 4th order differential equation

$$\nabla^4 f = 0,$$

where ∇ denotes the covariant derivative (cf. [18]). For a given data set, the search for the $\mathcal{M}$-valued smoothing spline involves a straightforward iterative algorithm: given an estimate $\gamma^{(i)}$ at the ith stage, fit a Euclidean smoothing spline $(\gamma^{(i+1)})^\dagger$ with parameter λ, in the tangent space at $\gamma^{(i)}(t_0)$, to the unwrapped data $S^\dagger$ with respect to $\gamma^{(i)}$; and then wrap $(\gamma^{(i+1)})^\dagger$ at the corresponding times back onto the manifold with respect to $\gamma^{(i)}$ to define $\gamma^{(i+1)}$. This method was introduced in [18] for solving a nonparametric smoothing problem on the sphere. Subsequent developments have included applications to regression problems and extensions to more complicated manifolds (cf. [19] and [20]). However, for the construction of $\mathcal{M}$-valued splines of this type to be feasible, it is crucial to have knowledge of parallel transport in the manifold $\mathcal{M}$.

A more direct generalization of the Euclidean spline to manifold-valued data $\{X_1, \ldots, X_n\}$ in $\mathcal{M}$, where X_i is observed at time t_i, is to find the solution to the analogue for manifolds of the minimization problem (17.3), i.e., to find the solution to the problem of minimizing

$$E(\gamma) = \sum_{i=0}^{n} d(\gamma(t_j, \lambda), X_j)^2 + \lambda \int_T \left\| \frac{\nabla^2 \gamma(t, \lambda)}{dt^2} \right\|^2 dt$$

within a certain set of C^2-curves on $\mathcal{M}$. Then, the minimizing function is four-times differentiable and satisfies the differential equation

$$\nabla^4 f + \|\nabla f\|^2 \nabla^2 f - \langle \nabla^2 f, \nabla f \rangle \nabla f = 0,$$

except at the data times. Clearly, this differential equation is heavily entangled with the geometry of the manifold, and so to find the minimizing curve requires full knowledge of that geometry. Rather than directly solving such a, usually complicated, differential equation, it is possible to search for the minimizer using the steepest-descent direction iteratively (cf. [25]): at each step γ is replaced by γ^τ, where

$$\gamma^\tau(t) = \exp_{\gamma(t)}(-\tau \operatorname{grad}(E(\gamma))(t))$$

and τ is a predetermined positive constant. To be able successfully to implement this procedure, the crucial feature is the use of the second order Palais metric defined by

$$\langle\langle v, w\rangle\rangle_\gamma = \langle v(0), w(0)\rangle_{\gamma(0)} + \left\langle \frac{\nabla v}{dt}(0), \frac{\nabla w}{dt}(0)\right\rangle_{\gamma(0)} + \int_0^T \left\langle \frac{\nabla^2 v}{dt^2}, \frac{\nabla^2 w}{dt^2}\right\rangle_{\gamma(t)} dt,$$

for any tangent vector fields v and w along γ. With this metric, the gradient of E has a relatively simple closed expression in terms of the curvature tensor, together with the parallel transport. Compared with the previous method, this requires more detailed knowledge of the geometry of manifolds. However, it has proved possible to carry it out (cf. [26]). In general, the model choice appropriate to the problem needs to take into account the balance between the need to respect to geometry of the manifold in order to preserve the inter-relation among the data and the requirement to know that geometry in detail.

If the data points are not indexed in some natural order, it is also possible to fit a curve to capture patterns of nonlocal variation by using the differential equations, as implied by the method of *principal flows* in [22]. The idea behind the method is that, at each point on the curve, the derivative of the fitted curve is the first principal component generated by a *local* tangent principal component, so that the curve always follows the direction of maximal variability. For a given set of data $\{X_1, \ldots, X_n\}$ in $\mathcal{M}$, the method relies on the introduction of the localized version of the tangent covariance matrix which is a tensor on a suitably restricted open set of $\mathcal{M}$ defined by

$$\Sigma_\lambda(x) = \frac{1}{\sum_{i=1}^n \kappa_\lambda(X_i, x)} \sum_{i=1}^n \left\{\exp_x^{-1}(X_i) \otimes \exp_x^{-1}(X_i)\right\} \kappa_\lambda(X_i, x).$$

The positive constant λ is used to control the size of the neighborhood and $\kappa_\lambda(X_i, x) = K(\lambda^{-1} d(X_i, x))$ for a smooth nonincreasing univariate kernel K on $[0, \infty)$. Then, the local tangent principal component is the vector field $W(x)$ defined to be the first principal unit eigenvector of $\Sigma_\lambda(x)$. Assuming that Σ_λ is defined and has distinct first and second eigenvalues on an open set containing the Fréchet mean $\hat{x}$ of the data set, then the principal flow is the curve γ that solves

$$\dot{\gamma}(t) = W(\gamma(t)), \qquad \gamma(0) = \hat{x}.$$

The principal flow γ can be extended in both directions at $\hat{x}$ by choosing the opposite sign for $W(\hat{x})$: otherwise the sign of W is determined by requiring $\dot{\gamma}$ to be smooth. Note that $W(x)$ so defined is always tangent to the manifold and so the solution γ lies in $\mathcal{M}$. The rigidity or flexibility of the principal flows can be controlled by varying λ.

Over the last decade there have been many models proposed for curve fitting techniques on manifolds: the preceding selection is by no means complete. On the other hand, although some statistical analysis, such as inference, has been carried out for the estimated curves (cf. [19]), their asymptotic properties have so far been relatively less explored. Whereas similar behavior to their Euclidean counterparts is expected, the extent of the role played by the geometry of the underlying manifolds and its effect on that behavior is certainly unclear. Methodology based on extensions of the work of Rabi Bhattacharya, e.g., the bootstrap in [4] and [5], is one plausible avenue to explore.

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Chapter 18
Nonparametric Statistics on Manifolds and Beyond

Stephan Huckemann and Thomas Hotz

Abstract We review some aspects of the Bhattacharya-Patrangenaru asymptotic theory for intrinsic and extrinsic means on manifolds, some of the problems involved, many of which are still open, and survey some of its impacts on the community.

18.1 Before "Large Sample Theory of Intrinsic and Extrinsic Sample Means on Manifolds"

Let us start with a famous quote by [16]:

> *The theory of errors was developed by Gauss primarily in relation to the needs of astronomers and surveyors, making rather accurate angular measurements. Because of this accuracy it was appropriate to develop the theory in relation to an infinite linear continuum, or, as multivariate errors came into view, to a Euclidean space of the required dimensionality. The actual topological framework of such measurements, the surface of a sphere, is ignored in the theory as developed, with a certain gain in simplicity.*

Indeed, this "certain gain in simplicity" is huge. In Euclidean spaces, measurements can be averaged, error (co)variances are well defined, and in consequence, over time, a rich toolbox of parametric and nonparametric descriptive and inferential statistics has been developed and applied with grand success. In contrast, already on the sphere, which is one of the very simplest non-Euclidean spaces, where there is no concept of adding and subtracting points, the notions of averages, typical points, means, and covariances are neither trivial nor canonically uniquely defined.

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In the second half of the last century, a new challenge arose, when statistics of *shape* became of interest. Although the problem of relating shape to tractable covariates dates back to antiquity, e.g., when Aristotle's student Theophrast of Eresos in Lesbos (ca. 371–287 BC) in his *περί φυτών α'ίτιών (On the Causes of Plants)* discusses some views of Democritos (ca. 460–370 BC) on the relationship of a tree's shape and its speed of growth (see [55, I.8.2 and II.11.7]), a scientific treatment of the topic had only comparatively recently been undertaken in the context of biological *allometry*, the phrase having been coined by [33], cf. [18].

Statistical analysis of shape then followed several approaches. One is to consider only certain parameters describing either shape or size and the discovery that in principle only one size variable can be statistically independent of a specific shape variable (see [49]) may be quite surprising. A more holistic approach takes into account that the underlying data space is essentially a Euclidean space modulo a group action. For landmark based similarity shape, this is a matrix space of landmark configurations modulo the similarity group. The naïve quotient, however, gives a non-Hausdorff space – all configurations can be rescaled to arbitrary size, in any neighborhood of the shape $\varDelta$ of configurations with all landmarks coinciding – a dead end to statistical ambition. In consequence, some configurations may have to be removed, and the canonical quotient structure would have to be suitably altered. In *Generalized Procrustes analysis*, $\varDelta$ is removed and shape representatives are picked via a constrained minimization procedure, cf. [19]. This provides the concept of a *Procrustes mean* and a corresponding (co)variance. Asymptotics for such Procrustes coordinates, however, remained in the dark for some time. In fact, it took a while to realize that centers of a perturbation model in the configuration space cannot always be consistently estimated by Procustes means (e.g., [46, 41, 45, 30]).

In the approach initiated by [11], for similarity shape of d-dimensional configurations ($d \in \mathbb{N}$), say, only those configurations were considered, the first $d-1$ landmarks of which provide for a $(d-1)$-dimensional frame. The resulting data space of *Bookstein coordinates* is Euclidean, allowing in particular, for asymptotic inferential statistics. As there is no rose without thornes, the usually undesirable price to be paid is that statistically obtained results may hinge on the order of landmarks.

The need for statistical inference under the lack of a satisfying nonparametric theory led to the blossoming of parametric models, among others, for spheres and shape spaces (overviews in [12, 47]). Also, it was realized that Procrustes coordinates can be viewed as coordinates in some tangent space. In fact, [37] showed that the spaces of planar similarity shapes without $\varDelta$ can be given the manifold structure of complex projective spaces. In this context, without exploiting a possible manifold structure though, a first nonparametric two-sample test for equality of two shape distributions was proposed by [58].

It was near the turn of the millennium when [25] considered nonparametric asymptotics of the mean direction on spheres. Since every manifold has a second order spherical approximation, [23, 24] showed that on a manifold embedded in a Euclidean space the asymptotic distribution of the corresponding mean location – the usual average in the ambient space orthogonally projected to the embedded manifold, the projection not being defined on a negligible set only [21, 22] – follows a $1/\sqrt{n}$ Gaussian Central Limit Theorem (CLT) supported in the tangent space with higher order terms confined to the normal space.

At this point, Rabi Bhattacharya enters the stage with Vic Patrangenaru, who was his PhD student at that time, originally trained as a geometer.

18.2 "Large Sample Theory of Intrinsic and Extrinsic Sample Means on Manifolds"

Underlying their seminal twin papers [6, 7] is the notion of a *Fréchet mean* of a random variable X on a manifold M with respect to a metric $d : M \times M \to [0, \infty))$, given by minimizers μ of the Fréchet functional

$$M \to [0, \infty),\ p \mapsto F(p) = \mathbb{E}[d(p, X)^2]\,,$$

cf. [17]. Of special interest are the *intrinsic* geodesic distance $d = d_I$ due to a Riemannian structure on M, and the chordal or *extrinsic* distance $d_E(p, q) = \|p - q\|$ $(p, q \in M)$ due to some embedding of M in a Euclidean space $\mathbb{R}^D$ of dimension $D \in \mathbb{N}$ with norm $\|\cdot\|$. (The extrinsic distance had been the subject of the work of Hendriks and collaborators above). Although [6, 7] only consider these distances, their asymptotic theory easily extends to other distances, e.g., to Ziezold or Procrustes distances (cf. [30, 31]). The concept of extrinsics is pushed further by [15] when they embed infinite dimensional planar shape spaces in a Hilbert space.

The first stop on the road towards a CLT for these Fréchet means is consistency. To this end consider a sample $X_1, \ldots, X_n \sim X$ on M and define the sets of sample and population Fréchet means

$$E_n^{(d)} = \operatorname*{arg\,min}_{p \in M} \frac{1}{n} \sum_{j=1}^{n} d(p, X_j)^2, \quad E^{(d)} = \operatorname*{arg\,min}_{p \in M} \mathbb{E}[d(p, X_j)^2]\,.$$

For the more general case of random variables on separable metric spaces, [57] derived a version of strong consistency (actually, he required a quasi-metric on a separable space only):

$$\text{if } F(p) < \infty \text{ for at least one } p \in M \text{ then } \bigcap_{n=1}^{\infty} \overline{\bigcup_{k=n}^{\infty} E_k^{(d)}} \subset E^{(d)} \text{ a.s.}$$

Notably, Ziezold's version of the Strong-Law does not prevent a.s. that cluster points of sample means may diffuse to "infinity." To ensure this, [6] showed under additional conditions that

$$\text{for every } \epsilon > 0 \text{ there is a random number } n \in \mathbb{N} \text{ such that}$$
$$\textstyle\bigcup_{k=n}^{\infty} E_k^{(\rho)} \subset \{p \in P : d(E^{(d)}, p) \le \epsilon\} \text{ a.s.}\,,$$

the *Bhattacharya-Patrangenaru Strong-Law*.

For a $1/\sqrt{n}$-Central-Limit-Theorem (CLT) to hold we require several conditions. First a conditions in equation:

(A) uniqueness: $E^{(d)} = \{\mu\}$.

For the intrinsic geodesic distance $d = d_I$, with a local chart (U, ϕ) near $\mu \in U \subset M$, $\phi : U \to \mathbb{R}^D$, $\phi(\mu) = 0$, [7] show that under additional conditions one has

$$\sqrt{n}\phi(\mu_n) \to \mathcal{N}(0, \Sigma_\phi) \text{ as } n \to \infty \text{ for every measurable choice } \mu_n \in E_n^{(d)} \tag{18.1}$$

with a covariance matrix that depends on the choice of the chart. With the function

$$f_X : U \to [0, \infty), x \mapsto d(X, \phi^{-1}(x))^2$$

and $x_n = \phi^{-1}(\mu_n)$ the reasoning behind (18.1) is the Taylor expansion

$$\begin{aligned} 0 &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \operatorname{grad} f_{X_j}(x_n) \\ &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \operatorname{grad} f_{X_j}(0) + \left(\frac{1}{n} \sum_{j=1}^{n} \operatorname{Hess} f_{X_j}(0) \right) \sqrt{n} x_n \qquad (18.2) \\ &\quad + \left(\frac{1}{n} \sum_{j=1}^{n} (\operatorname{Hess} f_{X_j}(y_n) - \operatorname{Hess} f_{X_j}(0)) \right) \sqrt{n} x_n \qquad (18.3) \end{aligned}$$

with some random $y_n \in \mathbb{R}^D$ on the line segment between 0 and x_n. This Taylor expansion is valid a.s. under the additional condition

(B) a.s. local twice continuous differentiability: f_X is a.s. twice continuously differentiable at $x = 0$.

From the "Euclidean" CLT we have that the first term in (18.2) tends to $\mathcal{N}(0, \operatorname{Cov}[\operatorname{grad} f_X(x)])$ in distribution, and from the Strong-Law that the first factor of the second to $\mathbb{E}[\operatorname{Hess} f_X(0)]$ a.s. while the first factor of the first term in (18.3) tends to zero a.s. under the following additional conditions

(C) finite second moments: $\operatorname{Cov}[\operatorname{grad} f_X(x)], \mathbb{E}[\operatorname{Hess} f_X(x)]$ exist at $x = 0$.

(D) continuous expectation of the Hessian: $\mathbb{E}[\operatorname{Hess} f_X(x)]$ exists near $x = 0$ and is continuous there.

Finally, to obtain the limiting covariance for $\sqrt{n}x_n$ it is required to invert the expected Hessian, i.e., we require

(E) positive definite expectation of the Hessian: $\mathbb{E}[\operatorname{Hess} f_X(0)] > 0$.

Let us now discuss the above conditions. To this end we need the notion of the *cut locus* $C(p)$ of $p \in M$ comprising all points q such that the extension of a length minimizing geodesic joining p to q is no longer minimizing beyond q. Note that cut loci are void on manifolds with non-positive sectional curvatures.

Uniqueness (A).
If M has non-positive sectional curvatures then there is a unique Fréchet mean, cf. [35]. This is the case for the space of positive definite matrices with one of the canonical structures (e.g., [42]) which in applications is the similarity shape space of simplices (e.g., [44]) or that of diffusion matrices (e.g., [14]). If M also features positive sectional curvatures, there are examples of nonuniqueness. For example, $E^{(d)} = M$ if M is a sphere on which X is uniformly distributed. Uniqueness could be shown only if the support of X is sufficiently concentrated. In fact, in a series of publications [35, 39, 43, 20], the condition on concentration could be, among others, relaxed to that of a geodesic half sphere due to [1]. Realistically in many applications, as is also the case for most parametric models (von Mises, Fisher, Bingham, etc.) one would have to assume a support on the entire sphere, however. Only for the circle (which features no sectional curvatures) exhaustive results with respect to uniqueness of intrinsic means are known. One of such is that for X with a density g with respect to arc measure, intrinsic means are unique if the circle decomposes into two subintervals sharing only the endpoints, in the interior of one of which $g > 0$ and $g < 0$ in the other, cf. [26].

A.s. local twice continuous differentiability (B) and continuous expectation of the Hessian (D).
This is the case if there is a neighborhood V of the cut locus $C(\mu)$ of the unique intrinsic mean μ such that $X \notin V$ a.s. It seems, however, that this is in general not necessary for a $1/\sqrt{n}$-CLT to hold, as examples on the circle teach, cf. [26].

Finite second moments (C).
This is a natural condition for a CLT that cannot be relaxed.

Positive definite expectation of the Hessian (E).
This is again a conditions in equation, for otherwise in directions of eigenvectors of vanishing eigenvalues, higher order Taylor expansions are necessary, yielding slower rates of convergence than those of (18.1). In violation of this condition, as exemplified in [26], arbitrarily slow rates of convergence may result.

18.3 Beyond "Large Sample Theory of Intrinsic and Extrinsic Sample Means on Manifolds"

Although the *Bhattacharya-Patrangenaru asymptotic CLT* (BP-CLT) covers many important cases as a suite of subsequent publications show (e.g., [51, 14, 56, 28, 9, 40]), cases with non-manifold data-spaces, however, are not covered. As such the spaces of phylogenetic trees (cf. [10]) have recently gained attention (e.g., [2, 50, 53]), also Kendall's shape spaces Σ_m^k [36] for higher dimensional ($m \geq 3$) objects with k landmarks are no longer manifolds. In fact for the latter at singularities, some sectional curvatures are unbounded (cf. [38] and [29]). While for $m = 2$ the popular Procrustes means turn out to be extrinsic means (or equivalently, mean locations) of the Veronese-Whitney embedding, cf. [6, 7], for $m \geq 3$ the asymptotics of Procrustes means – notably being neither intrinsic nor extrinsic – remained open until [30].

All these non-manifold spaces mentioned above are manifold stratified spaces. In fact, the *general shape space* $Q = M/G$ is such, as it is the canonical quotient of a compact Riemannian manifold M modulo a smooth, proper (hence all orbits are closed), and isometric action of a Lie group G, cf. [52, Theorems 1.3.16 and 4.3.7]. For Σ_m^k, the rotational group acts on unit size centered configurations. Recall from [48, pp. 3,4] that a space

$$Q = \bigcup_{1 \leq j \leq J} Q_j \subset \mathbb{R}^D$$

for some $D, J \in \mathbb{N}$ is a *stratified space* if all *strata* Q_j are disjoint manifolds satisfying the *axiom of the frontier*

if $\mathrm{cl}(Q_i) \cap Q_j \neq \emptyset$ then $Q_j \subset \mathrm{cl}(Q_i)$.

It is a Whitney stratified space if additionally the Whitney condition "b" is fulfilled:

if $x_k \in Q_i, y_k \in Q_j$, with $x_k, y_k \to y \in Q_j$ as $k \to \infty$, $1 \leq i \neq j \leq J$ and $L_k = x_k - y_k \to L$ then $L \in \lim_{k\to\infty} T_{x_k} Q_i$.

Let us call a stratified space Q as above a *Riemannian stratified space* if all strata are Riemannian manifolds with metrics induced by $\mathbb{R}^D$. The stratum with the highest dimension is the *top stratum* Q^*, also called the *manifold part* of Q.

In order to directly apply the BP-CLT one would have to make sure that the following additional condition holds.

(F) Manifold stability: $E^{(d)} \subset Q^*$ for all random variables with support not disjoint from Q^*.

Manifold stability (F)
holds for general shape spaces with the intrinsic geodesic distance, but in case of Kendall's shape spaces Σ_m^k, $m \geq 3$, there are counterexamples for the full Procrustes distance (cf. [32]). On phylogenetic tree spaces, although being stratified non-positive curvature spaces thus featuring unique means (cf. [54]), "worse" things can happen for the canonical intrinsic distance. We have not only $\mu = 0 \in Q \setminus Q^*$ for distributions that are symmetric about the origin 0 (which stands for the "star tree" having no interior edge), minor arbitrary perturbations of this distributions do not move the mean away from the origin: The mean *sticks* to the origin giving rise to degenerate limiting sample mean distributions that cannot be assessed via the BP-CLT and that reach the population mean in finite random time, cf. [27, 4].

For suitable embeddings $Q \subset \mathbb{R}^D$ manifold stability may also be given with respect to the extrinsic distance. Since extrinsic means are orthogonal projections of averages in the ambient space, one would have to make sure that singular strata are not protruding into the ambient space. For Kendall's *reflection shape space* (which is obtained from unit size centered configurations modulo the full orthogonal group), among others, Rabi Bhattacharya's student [5] showed manifold stability of the extrinsic mean, cf. also [13, 3].

(Semi-)intrinsic statistical analysis.

In all of the previous considerations, data descriptors namely Fréchet means have been taken from the data space. In view of dimension reduction, data descriptors have become of interest that live in separate spaces, such as geodesics on Σ_m^k (cf. [29, 31]) in the space of geodesics or principal nested small-spheres on spheres by [34] in the corresponding spaces of small spheres. It turns out that Ziezold's Strong Law as well as the BP Strong Law and BP-CLT can be suitably adapted to this more general scenario of a Fréchet ρ-mean

$$\operatorname*{arg\,min}_{p\in P} \mathbb{E}[\rho(X,p)^2]$$

on a descriptor space P due to random data $X \in Q$ where the spaces are linked via a continuous function $\rho : Q \times P \to [0,\infty)$ conveying the notion of a distance between a datum and a descriptor (the orthogonal distance of a data point to a geodesic, say). This analysis is intrinsic because intrinsic data descriptors are sought for, it may be semi-intrinsic if for asymptotic considerations extrinsic embeddings are considered that facilitate computations considerably, cf. [8].

18.4 Conclusion

This short survey covers a detail of Rabi Bhattacharya's recent work and its impact on statistics on non-Euclidean spaces which is an active field of research now. In fact, the general viewpoint taken by [6, 7], considering the strong laws of large numbers for Fréchet means on manifolds with intrinsic and extrinsic means as special cases, utilizing these for statistical inference of shapes by deriving confidence regions via the bootstrap, consolidated this research area and provided it with a new impetus. Indeed, the several hundreds of citations of these articles bear witness to the amount of research to which they led. By exposing extrinsic and intrinsic methods side-by-side, they further highlighted the analyst's freedom to choose the metric on the manifold, immediately raising questions such as which metric one "ought" to choose which go beyond mere mathematical statistics but have to be answered for each application anew, based on the mathematical properties that have been shown.

When the two authors of the present manuscript returned to academia about a decade ago, rather free to choose future fields, we were struck by these two seminal papers which not only proposed a new approach filling a long-standing gap but also paved the way for further research in ample exciting directions, along some of which we gladly traveled ourselves. We are truly grateful for this inspiring work.

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Chapter 19
Reprints: Part VI

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LARGE SAMPLE THEORY OF INTRINSIC AND EXTRINSIC SAMPLE MEANS ON MANIFOLDS. I

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Sufficient conditions are given for the uniqueness of intrinsic and extrinsic means as measures of location of probability measures Q on Riemannian manifolds. It is shown that, when uniquely defined, these are estimated consistently by the corresponding indices of the empirical $\hat{Q}_n$. Asymptotic distributions of extrinsic sample means are derived. Explicit computations of these indices of $\hat{Q}_n$ and their asymptotic dispersions are carried out for distributions on the sphere S^d (directional spaces), real projective space $\mathbb{R}P^{N-1}$ (axial spaces) and $\mathbb{C}P^{k-2}$ (planar shape spaces).

1. Introduction. The aim of this article is to develop nonparametric statistical inference procedures for measures of location of distributions on general manifolds, which are complete as metric spaces. Although the main applications are to distributions on (i) spheres S^d (spaces of directions), (ii) real projective spaces $\mathbb{R}P^{N-1}$ (axial spaces) and (iii) complex projective spaces $\mathbb{C}P^{k-2}$ (planar shape spaces), a general theory for both compact and noncompact manifolds is sought. In this introduction a summary of the main results is presented, along with a brief review of the literature on the subject.

A natural index of location for a probability measure Q on a metric space M with the distance ρ is the so-called *Fréchet mean* which minimizes $F(p) = \int \rho^2(p,x)Q(dx)$, if there is a unique minimizer. In general, the set of all minimizers is called the *Fréchet mean set*. In the case M is a d-dimensional connected C^∞ Riemannian manifold with a metric tensor g and geodesic distance d_g, we will assume that (M, d_g) is complete and we will refer to the Fréchet mean (set) as the *intrinsic mean* (*set*). We say that the *intrinsic mean exists* if there is a unique minimizer, and denote it by $\mu_I(Q)$. It is shown in Theorem 2.1 that (i) the intrinsic mean set is compact, (ii) for each point m in the intrinsic mean set, the Euclidean mean of the distribution on the tangent space at m of the inverse of the exponential map is zero and (iii) in the case of simply connected M of nonpositive curvature, the intrinsic mean exists if F is finite; a particular case of this result, when M is a Bookstein's shape space of labeled triangles, with a Riemannian metric of constant negative curvature is due to Le and Kume (2000). From a result of Karcher (1977) it follows that if the distribution is

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sufficiently concentrated then the intrinsic mean exists. For planar shape spaces $\mathbb{C}P^{k-2}$, a useful necessary and sufficient condition for the existence of an intrinsic mean is proved by Le (1998) for distributions Q which are absolutely continuous (w.r.t. the volume measure) with a density that is a function only of the distance from a given point.

An important question on the estimation of location is that of *consistency*. Theorem 2.3 says that if M is a metric space such that all closed bounded subsets of M are compact then, with probability 1, given any $\varepsilon > 0$, the Fréchet sample mean set based on a random sample from Q will be within a distance less than ε from the Fréchet mean set of Q for all sufficiently large sample sizes. Thus if M is a complete Riemannian manifold and if the intrinsic mean exists then, almost surely, all measurable choices from the intrinsic sample mean set converge uniformly to the intrinsic mean of Q. In particular, this generalizes and strengthens the strong consistency result for compact M that follows from an earlier result of Ziezold (1977). [Also see Kent and Mardia (1997) and Le (1998).]

Much of the literature in the field deals with special cases of what we call the *extrinsic mean*, perhaps because of the technical difficulties involved in proving the existence of an intrinsic mean and in computing the intrinsic sample mean, even when it exists. To define an extrinsic mean of Q with respect to an embedding j of M in a Euclidean space $(\mathbb{R}^k, d_0)$, consider first the set of all points p of $\mathbb{R}^k$ such that there is a *unique* point x in $j(M)$ having the smallest distance from p, that is, satisfying $d_0(p, j(M)) = d_0(p, x)$. Such points p are called *nonfocal*, and points which are not nonfocal are called *focal*. For example, the only focal point of S^d in $\mathbb{R}^{d+1}$ is the origin. For an embedding j of M in $\mathbb{R}^k$ a probability measure Q on M *is* said to be *nonfocal* if, when viewed as a measure on $\mathbb{R}^k$ via j, its mean μ is a nonfocal point. The *extrinsic mean* $\mu_{\mathrm{E}}(Q)$ of a nonfocal Q is the j-preimage of the projection $P_{j(M)}(\mu)$ of μ on $j(M)$, that is, $j(\mu_{\mathrm{E}}(Q))$ is the point of $j(M)$ closest to μ. One may show that the set of all focal points is closed and has Lebesgue measure zero in $\mathbb{R}^k$ (Theorem 3.2). Being thus guaranteed that most probability measures on M are nonfocal, one proceeds to show that the *extrinsic sample mean* $\overline{X}_{\mathrm{E}} = \mu_{\mathrm{E}}(\hat{Q}_n)$ based on a random sample is a *strongly consistent* estimate of the (population) extrinsic mean $\mu_{\mathrm{E}}(Q)$ of a nonfocal Q (Theorem 3.4). Here $\hat{Q}_n$ is the empirical distribution of the random sample. As far as the estimation of the intrinsic mean $\mu_{\mathrm{I}}(Q)$ is concerned, Theorem 3.3(b) in the present article proves that under an equivariant embedding one has $\mu_{\mathrm{I}}(Q) = \mu_{\mathrm{E}}(Q)$ provided M is a compact two point homogeneous space other than a round sphere, and Q is nonfocal and invariant under the subgroup of isometries leaving a given point fixed. In particular, under the assumed symmetries, the extrinsic sample mean is a strongly consistent estimator of the intrinsic mean $\mu_{\mathrm{I}}(Q)$ if the latter exists.

As indicated above, for an embedding of M in an Euclidean space $\mathbb{R}^k$, the extrinsic mean $\mu_{\mathrm{E}}(Q)$ exists under broad verifiable conditions. The next important task, beyond consistency, is to derive the asymptotic distribution of the extrinsic sample mean and use this to construct confidence regions for $\mu_E(Q)$ and, therefore, of $\mu_I(Q)$ when the intrinsic and extrinsic means coincide. A general method is presented for this. Let $\overline{X}$ be the sample mean, when the observations X_i are viewed as points in the ambient space $\mathbb{R}^k$. In Theorem 3.6, the projection $H(\overline{X})$ of $\overline{X}$ on the tangent space to M at $\mu_E(Q)$ is shown to be asymptotically normal centered at $\mu_E(Q)$, and a computation of the asymptotic dispersion is given. One derives bootstrap-based confidence regions for $\mu_E(Q)$ (Corollary 3.7) by Efron's percentile method [Efron (1982)] with a coverage error $O_p(n^{-1/2})$ for general Q, which is particularly useful in those cases where the asymptotic dispersion matrix is difficult to compute. Note once again that, under the hypothesis of symmetry in Theorem 3.3(b), if the intrinsic mean exists then the above confidence regions apply to it.

Finally, Section 4 applies the preceding theory to (i) real projective spaces $\mathbb{R}P^{N-1}$, or the *axial spaces*, and to (ii) complex projective spaces $\mathbb{C}P^{k-2}$, or the *planar shape spaces*. Under the so-called *Veronese–Whitney embedding*, the explicit formulas for the extrinsic mean of a nonfocal distribution on an axial space are given in Theorem 4.2. For planar shape spaces the corresponding results are presented in Theorem 4.4. It is also pointed out in Example 4.3 that inconsistent Procrustes estimators in some parametric models arise when Q is focal, thus clarifying an issue raised in Dryden and Mardia (1998), page 280. As an application both intrinsic the extrinsic (*Procrustean*) sample means are computed using some data from Bookstein (1991) on children with the so-called Apert syndrome. This is presented in graphical form. Also, the extrinsic sample mean of 13 complete observations of Apert data is used to estimate a missing landmark in one incomplete observation. The data here are quite concentrated, which makes the extrinsic sample mean almost indistinguishable from the intrinsic sample mean.

We now briefly mention some of the earlier literature on statistical inference on Riemannian manifolds. In parametric statistical inference, the *information matrix* has been used as a Riemannian metric on the parameter space ever since Rao (1945). For more recent treatments and advances in this direction, we refer to Amari (1985), Barndorff-Nielson and Cox (1994), Burbea and Rao (1982), Efron (1975) and Oller and Corcuera (1995). Pioneering work on directional analysis was carried out by G. S. Watson beginning in the 1950s [see Watson (1983) and Mardia and Jupp (1999) and the references in both]. Some classes of semiparametric models were analyzed by Beran (1979), Watson (1983) and others. Statistical analysis for axial and shape spaces similar in spirit to the inference for extrinsic means presented here may be found in Kent (1992), Kent and Mardia (1997), Le (1998) and Prentice and Mardia (1995). Nonparametric bootstrap methods for inference on extrinsic means of axes have been employed in Beran and Fisher (1998) and in Fisher, Hall, Jing and Wood (1996). The recent books by Dryden and Mardia (1998) and Kendall, Barden, Carne and Le (1999) are good sources for readable accounts of various methodologies in the field, emphasizing their applications.

2. Intrinsic means and moments of a probability measure on a Riemannian manifold. Let (M, g) be a d-dimensional connected and complete Riemannian manifold, that is, M is a d-dimensional C^∞ connected manifold with a complete Riemannian metric g. Denote by d_g the (geodesic) distance under g. We consider M-valued random variables X, that is, measurable maps on a probability space $(\Omega, \mathcal{A}, P)$ into $(M, \mathcal{B})$, where $\mathcal{B}$ denotes the Borel sigma-algebra of M. All probability measures on M below are defined on $\mathcal{B}$. Note that every closed bounded subset of M is compact [do Carmo (1992), pages 146–149].

For the following definition we consider, more generally, a metric space (M, d) and a probability measure Q on the Borel sigma-algebra $\mathcal{B}$ of M.

DEFINITION 2.1. Let Q be a probability measure on the metric space (M, d). The *Fréchet mean set* of Q is the set of all minimizers of the map F on M defined by

$$F(p) = \int d^2(p, x) Q(dx), \qquad p \in M. \tag{2.1}$$

If there is a unique minimizer, this is called the *Fréchet mean* of Q. If M is a Riemannian manifold, the Fréchet mean (set) w.r.t. the geodesic distance $d = d_g$ is defined to be the *intrinsic mean* (*set*) of Q; if the minimizer is unique, the intrinsic mean will be labeled $\mu_I(Q)$. If X is an M-valued random variable having distribution Q, then the above are also referred to as the *Fréchet*, or *intrinsic mean* (*set*) *of* X, as the case may be.

Riemannian manifolds are "curved," so that geodesics starting at a point p may meet for a second time in the cut locus of p. Technical details on cut locus and normal coordinates are as follows. If the manifold is complete, the *exponential map* at q is defined on the tangent space T_qM by $\exp_q v = \gamma(1)$, where $\gamma : t \to \gamma(t)$ is the geodesic with $\gamma(0) = q$, $\dot\gamma(0) = v$. An open set $U \subset M$ is said to be a *normal neighborhood* of q $(\in U)$, if $\exp_q$ is a diffeomorphism on a neighborhood V of the origin of T_qM onto U, with V such that $tv \in V$ for $0 \le t \le 1$, if $v \in V$. Suppose $U = \exp_q V$ is a normal neighborhood of q. Then $(x^1, x^2, \dots, x^d)$ are said to be the *normal coordinates* of a point $p \in U$ w.r.t. a fixed orthobasis $(v_1, v_2, \dots, v_d)$ of T_qM if $p = \exp_q (x^1 v_1 + x^2 v_2 + \cdots + x^d v_d)$.

Let $v \in T_qM$ be such that $g(v, v) = 1$. The set of numbers $s > 0$, such that the geodesic segment $\{\exp_q tv : 0 \le t \le s\}$ is minimizing is either $(0, \infty)$ or $(0, r(v)]$, where $r(v) > 0$. We will write $r(v) = \infty$ in the former case. If $r(v)$ is finite, then $\exp_q r(v)v$ is the *cut point of* q *in the direction* v [Kobayashi and Nomizu (1996), page 98]. Let $S_qM = \{v \in T_qM : g(v, v) = 1\}$; then the largest open subset of M in which a normal coordinate system around q is defined is $\exp_q(V(q))$, where $V(q) = \{tv : 0 \le t < r(v),\ v \in S_qM\}$. The *cut locus* of q is $C(q) = \exp_q\{r(v)v : v \in S_qM,\ r(v) \text{ finite}\}$ [Kobayashi and Nomizu (1996), page 100]. Note that $C(q)$ has volume measure 0, and M is the disjoint union of $\exp_q(V(q))$ and $C(q)$. The *injectivity radius at the point* q is $r_q = \inf\{r(v): v \in S_q M\}$.

EXAMPLE 2.1. For the d-dimensional unit sphere, $M = \mathbb{S}^d = \{p \in \mathbb{R}^{d+1}: \|p\| = 1\}$, with the Riemannian metric induced by the Euclidean metric on $\mathbb{R}^{d+1}$, the exponential map is given by

$$\exp_p(v) = \cos(\|v\|)p + \sin(\|v\|)\|v\|^{-1}v, \qquad v \in T_p S^d,\ v \neq 0. \tag{2.2}$$

Also, $V(p) = \{v \in T_p S^d : \|v\| < \pi\}$ and $C(p) = -p$. We may now determine the exponential map when M is a real (complex) projective space $\mathbb{R}P^d$ ($\mathbb{C}P^{d/2}$ for d even) of constant (constant holomorphic) curvature. In this case M is a quotient of a round sphere S, and the projection map $\pi : S \to M$ is a Riemannian submersion. If we denote by *exp* the exponential map for both the sphere and projective space, we have $\exp_{\pi(p)} d\pi(v) = \pi(\exp_p(v))$. If $p \in \mathbb{S}^d$, then since $\mathbb{R}P^d$ is homogeneous, for $[p] \in \mathbb{R}P^d$, we may assume without loss of generality that $p = (1, 0, \dots, 0)$. Then $C([p]) = \{[q] : q = (0, q^1, \dots, q^d) \in \mathbb{S}^d\} = \mathbb{R}P^{d-1}$ is the *projective hyperplane from infinity* of the point $[p]$. Similarily, we may assume that the point $[p] \in \mathbb{C}P^{d/2}$ is represented by $p = (1, 0, \dots, 0)$ and in this case $C([p])$ is $\mathbb{C}P^{d/2-1}$, the *complex projective hyperplane at infinity* of the point $[p]$.

If $Q(C(q)) = 0$, we will denote by $\lambda_Q = \lambda_{Q,q}$ the *image measure of* Q *under* $\exp_q^{-1}$ on $M \backslash C(q)$. We will suppress q in $\lambda_{Q,q}$.

THEOREM 2.1. *Assume* (M, g) *is a complete connected Riemannian manifold. Let* $I(Q)$ *be the intrinsic mean set of* Q *and set* $C(Q) = \bigcup_{q \in I(Q)} C(q)$. (a) *If there is a point* p *on* M *such that* $F(p)$ *is finite, then the intrinsic mean set is a nonempty compact set.* (b) *If* $q \in I(Q)$ *and* $Q(C(Q)) = 0$, *then*

$$\int_{V(q)} v\lambda_Q(dv) = 0. \tag{2.3}$$

(c) *Suppose* (M, g) *has nonpositive curvature, and* M *is simply connected. Then every probability measure* Q *on* M *has an intrinsic mean, provided* $F(p)$ *is finite for some* p.

PROOF. (a) It follows from the triangle inequality (for d_g) that if $F(p)$ is finite for some p, then F is finite and continuous on M. To show that a minimizer exists, let l denote the infimum of F and let $p_n \in M$ be such that $F(p_n) \to l$ as $n \to \infty$. By the triangle and the Schwarz inequalities, and by integration w.r.t. Q, one has

$$\begin{aligned} &d_g^2(p_n, p_1) \le 2d_g^2(p_n, x) + 2d_g^2(x, p_1) \qquad \forall x \in M, \\ &d_g^2(p_n, p_1) \le 2(F(p_n) + F(p_1)). \end{aligned} \tag{2.4}$$

Hence since $F(p_n)$ $(n \ge 1)$ is a bounded sequence, so is p_n $(n \ge 1)$. By completeness of M, p_n has a subsequence converging to some point p^*. Then

$F(p^*) = l$, so that p^* is a minimizer. Also the inequalities (2.4) applied this time to p^* and an arbitrary minimizer m show that $d_g^2(m, p^*) \leq 4l$. In other words, the set of minimizers is bounded. It is also a closed set, since its complement is clearly open, proving compactness of the intrinsic mean set. To prove (b), note that $\exp_q(V(q))$ has Q-probability 1. Consider an arbitrary point x in $\exp_q(V(q))$; then with probability 1 there is a unique geodesic, say $\gamma_{x,\mu}$ joining x and μ with $\gamma_{x,\mu}(0) = x$, $\gamma_{x,\mu}(1) = \mu$. Also let $\mu_v(t)$ be the geodesic starting at μ $[\mu_v(0) = \mu]$ with tangent vector v $[(d\mu_v(t)/dt)(0) = v]$. Let $\alpha_{v,x}$ be the angle made by the vectors tangent to these geodesics at μ. Then [see Helgason (1978), page 77, and Oller and Corcuera (1995), Proposition 2.10]

$$d_\mu F(v) = 2 \int d_g(x, \mu) \|v\| \cos(\alpha_{v,x}) Q(dx). \tag{2.5}$$

Select a point $q \in I(Q)$ and write the integral in (2.5) in normal coordinates on $T_q M$. If $\mu \in I(Q)$, then μ is a critical point of F. Then we select $\mu = q$, and evaluate the right-hand side of (2.5) at $v = v_i = \frac{\partial}{\partial x^i}$. Note that given that $\exp_q$ is a radial isometry, the right-hand side of (2.5) in this case is $2 \int x^i \lambda_Q(dx)$, where x^i are the normal coordinates of an arbitrary point of $\exp_q(V(q))$. Then in such coordinates, (2.5) becomes (2.3).

For part (c) of the theorem, we adapt the proof of Kobayashi and Nomizu (1996), Theorem 9.1, to our situation as follows. By part (a) there is a point q in the intrinsic mean set. By a classical result due to J. Hadamard [see Helgason (1978), page 74], since M is simply connected and complete, $C(q) = \varnothing$, and we define a map G on M by

$$G(p) = \int_M \| \exp_q^{-1}(p) - v\|^2 \lambda_Q(dv). \tag{2.6}$$

Since on a simply connected manifold of nonpositive curvature $\exp_q$ is expanding, we have $G(p) \leq F(p)$. On the other hand by part (b), $G(p) = G(q) + \|\exp_q^{-1}(p)\|^2$ and, since $\exp_q$ is a radial isometry, $F(q) = G(q)$. Therefore, q is in fact the unique minimizer of F. □

REMARK 2.1. If M has nonpositive curvature and is not simply connected, the intrinsic mean does not exist in general. If M is flat a sufficient condition for the existence of the intrinsic mean is that the support of Q is contained in a geodesically convex open normal neighborhood of M and $F(p)$ is finite for some p. In general, if the infimum of the injectivity radii is a positive number $r(M)$ and the *scalar curvature* of (M, g) is bounded from above by $(\pi/r(M))^2$ and if the support of Q is contained in a closed geodesic ball $\overline{B}_\rho$ of radius $\rho = r(M)/4$, then the intrinsic mean exists. To see this note that, when restricted to the closed geodesic ball $\overline{B}_{2\rho}$, F has a unique minimum at some point in $\overline{B}_\rho$ [see Karcher (1977), Theorem 1.2]. Clearly, this minimum value is no more than ρ^2. On the other hand, if $p \in (\overline{B}_{2\rho})^c$, then $F(p) \geq d_g^2(p, \overline{B}_\rho) > \rho^2$. This proves the uniqueness of the minimum of F in M, when the support of Q is contained in $\overline{B}_\rho$. Necessary and sufficient conditions for the existence of the intrinsic mean of absolutely continuous radially distributed probability measures on $\mathbb{C}P^{d/2}$ are given in Le (1998) and Kendall, Barden, Carne and Le (1999).

REMARK 2.2. Mean values of a random variable on a manifold were defined in Oller and Corcuera (1995) and previously in Emery and Mokobodzki (1991), as exponential barycenters. The mean values in the sense of Oller and Corcuera (1995) turn out to be critical points of F, while the intrinsic means defined here are minimizers of F. This explains, for example, why in Oller and Corcuera (1995) the von Mises distribution on S^d is found to have two mean values, while in fact there is only one intrinsic mean. Note that the density at $x \in S^d$ of the *von Mises distribution* w.r.t. the volume form is a constant multiple of $\exp(mx)$.

In the case of a Riemannian manifold, the points in the intrinsic mean set are points of local minima of F and are therefore *Karcher means* [Kendall (1990) and Le (1998)].

REMARK 2.3. If $C(q)$ has Q-measure zero, for some $q \in M$, an *intrinsic moment w.r.t. a given set of normal coordinates* of an arbitrary *order* $s = (s^1, \dots, s^d) \in Z_+^d$ can be defined by $\int x^s \lambda_Q(dx)$ where $x^s = (x^1)^{s^1} \cdots (x^d)^{s^d}$, if the latter is finite.

REMARK 2.4. As the proof shows, part (a) of Theorem 2.1 holds for the Fréchet mean set of a probability measure Q on any metric space M with the property that all closed bounded subsets of M are compact.

For the structure of probability measures which are invariant under a group of isometries one has the following simple result.

PROPOSITION 2.2. *Suppose K is a group of isometries of (M, g) which leaves the measure Q invariant. Then the intrinsic mean set is left invariant by K. In this case Q induces a quotient measure on the space of orbits M/K and the mean set of Q is a union of orbits.*

PROOF. An isometry τ of (M, g) is a diffeomorphism of M such that $g(d\tau(v), d\tau(v)) = g(v, v)$ for all $v \in T_q M$. Since $d_g(p, q) = d_g(\tau(p), \tau(q))$ for all $p, q \in M$, if Q is invariant under τ then one has $F(\tau(p)) = F(p)$ [see (2.1)]. In particular, this is true when p is a minimizer of F and $\tau \in K$. The claim follows from these observations. □

EXAMPLE 2.2. If Q is rotationally symmetric on S^d (such as the von Mises measure), then the intrinsic mean set of Q is a union of parallel $(d-1)$-dimensional spheres or poles of the axis of rotation, since the space of orbits is one-dimensional. Let $SO(d)$ be the *special orthogonal group* (or group of rotations).

The $SO(d)$ invariant measures on S^d depend on one function of one real variable, as shown in Watson [(1983), Section 4.2]. The uniform distribution on a compact Riemannian manifold whose density is $1/\operatorname{vol}(M)$ w.r.t. the volume measure is an example of an invariant distribution. Recall that the volume measure of a Riemannian manifold in a local chart is given by

$$\operatorname{vol}(A) = \int_A \det\left(g_x\left(\frac{\partial}{\partial x^i}, \frac{\partial}{\partial x^j}\right)\right)^{1/2} \lambda(dx), \tag{2.7}$$

where λ is the Lebesgue measure. The intrinsic mean set of the uniform distribution is M.

DEFINITION 2.2. Let $X_1, \dots, X_n$ be independent random variables with a common distribution Q on a metric space (M, d), and consider their *empirical distribution* $\hat{Q}_n = \frac{1}{n}\sum_{k=1}^n \delta_{X_k}$. The *Fréchet sample mean* (*set*) is the Fréchet mean (set) of $\hat{Q}_n$, that is, the (set of) minimizer(s) m of $p \to \frac{1}{n}\sum_{j=1}^n d^2(X_j, p)$. If M is a Riemannian manifold, then the Fréchet sample mean (set) of $\hat{Q}_n$ for the distance $d = d_g$ is called the *intrinsic sample mean* (*set*).

The following result establishes the strong consistency of the Fréchet sample mean as an estimator of the Fréchet mean of the underlying distribution.

THEOREM 2.3. *Let Q be a probability measure on a metric space (M, d) such that every closed bounded subset of M is compact. Assume F is finite on M.* (a) *Then, given any $\varepsilon > 0$, there exist a P-null set N and $n(\omega) < \infty$ $\forall \omega \in N^c$, such that the Fréchet* (*sample*) *mean set of $\hat{Q}_n = \hat{Q}_{n,\omega}$ is contained in the ε-neighborhood of the Fréchet mean set of Q for all $n \geq n(\omega)$.* (b) *If the Fréchet mean of Q exists then every measurable choice from the Fréchet* (*sample*) *mean set of $\hat{Q}_n$ is a strongly consistent estimator of the Fréchet mean of Q.*

PROOF. (a) We will first prove that for every compact subset K of M one has

$$\begin{aligned} &\sup_{p \in K} |F_{n,\omega}(p) - F(p)| \to 0 \qquad \text{a.s. as } n \to \infty, \\ &F_{n,\omega}(p) := \int d^2(x, p)\hat{Q}_{n,\omega}(dx) \equiv \frac{1}{n}\sum_{j=1}^n d^2(X_j, p). \end{aligned} \tag{2.8}$$

To prove (2.8) first observe that for a given $p_0 \in K$ one has, in view of the strong law of large numbers (SLLN) applied to $\frac{1}{n}\sum_{j=1}^n d(X_j, p_0)$,

$$\begin{aligned} \sup_{p \in K} \frac{1}{n}\sum_{j=1}^n d(X_j, p) &\leq \frac{1}{n}\sum_{j=1}^n d(X_j, p_0) + \sup_{p \in K} d(p, p_0) \\ &\leq \int d(x, p_0)Q(dx) + 1 + \operatorname{diam}(K) = A, \text{ say,} \end{aligned} \tag{2.9}$$

which holds for all $n \geq n_1(\omega)$, where $n_1(\omega) < \infty$ outside a P-null set N_1. Fix $\varepsilon' > 0$. From (2.9) one obtains, using the inequality $|d^2(X_j, p) - d^2(X_j, p')| \leq \{d(X_j, p) + d(X_j, p')\}d(p, p')$, the bound

$$\sup_{\{p,p' \in K : d(p,p') < \delta_1\}} |F_{n,\omega}(p) - F_{n,\omega}(p')| \leq 2A\delta_1 = \varepsilon'/3 \qquad \forall n \geq n_1(\omega)\ (\omega \notin N_1), \tag{2.10}$$

where $\delta_1 := A/6\varepsilon'$. For the next step in the proof of (2.8), let $\delta_2 > 0$ be such that $|F(p) - F(p')| < \varepsilon'/3$ if $p, p' \in K$ and $d(p, p') < \delta_2$. Let $\delta = \min\{\delta_1, \delta_2\}$, and $\{q_1, q_2, \ldots, q_r\}$ be a δ-net in K, that is, $\forall\, p \in K$, there exists $q(p) \in \{q_1, \ldots, q_r\}$ such that $d(p, q(p)) < \delta$. By the SLLN, there exist a P-null set N_2 and $n_2(\omega) < \infty$ $\forall\, \omega \notin N_2$ such that

$$\max_{i=1,2,\ldots,r} |F_{n,\omega}(q_i) - F(q_i)| < \varepsilon'/3 \qquad \forall n \geq n_2(\omega)\ (\omega \notin N_2). \tag{2.11}$$

Note that by (2.10), (2.11) and the fact that $|F(q(p)) - F(p)| < \varepsilon'/3\ \forall\, p \in K$, one has

$$\begin{aligned}
&\sup_{p\in K} |F_{n,\omega}(p) - F(p)| \\
&\quad \leq \sup_{p\in K} |F_{n,\omega}(p) - F_{n,\omega}(q(p))| + \sup_{p\in K} |F_{n,\omega}(q(p)) - F(q(p))| \\
&\qquad + \sup_{p\in K} |F(q(p)) - F(p)| \\
&\quad < \varepsilon'/3 + \varepsilon'/3 + \varepsilon'/3 = \varepsilon' \qquad \forall n \geq n(\omega) := \max\{n_1(\omega), n_2(\omega)\},
\end{aligned}$$

outside the P-null set $N_3 = N_1 \cup N_2$. This proves (2.8).

To complete the proof of (a), fix $\varepsilon > 0$. Let C be the (compact) Fréchet mean set of Q, $\ell := \min\{F(p) : p \in C\}$. Write $C^\varepsilon := \{p : d(p, C) < \varepsilon\}$. It is enough to show that there exist $\theta(\varepsilon) > 0$ and $n(\omega) < \infty$ $\forall \omega$, outside a P-null set N such that

$$\begin{aligned}
F_{n,\omega}(p) &\leq \ell + \theta(\varepsilon)/2 && \forall\, p \in C, \\
F_{n,\omega}(p) &\geq \ell + \theta(\varepsilon) && \forall\, p \in M\backslash C^\varepsilon,\ \forall n \geq n(\omega)\ (\omega \notin N).
\end{aligned} \tag{2.12}$$

For (2.12) implies that $\min\{F_{n,\omega}(p) : p \in M\}$ is not attained in $M\backslash C^\varepsilon$ and, therefore, the Fréchet mean set of $\hat{Q}_{n,\omega}$ is contained in C^ε, provided $n \geq n(\omega)$ $(\omega \notin N)$. To prove (2.12) we will first show that *there exist a compact set D containing C and $n_3(\omega) < \infty$ outside a P-null set N_3 such that both $F(p)$ and $F_{n,\omega}(p)$ are greater than $\ell + 1$ $\forall\, p \in M\backslash D$, for all $n \geq n_3(\omega)$* $(\omega \notin N_3)$. If M is compact then this is trivially true, by taking $M = D$. So assume M is noncompact. Fix $p_0 \in C$ and use the inequality $d(x, q) \geq |d(q, p_0) - d(x, p_0)|$ to get

$$\int d^2(x, q)Q(dx) \geq \int \{d^2(q, p_0) + d^2(x, p_0) - 2d(q, p_0)d(x, p_0)\}Q(dx)$$

or

$$F(q) \geq d^2(q, p_0) + F(p_0) - 2d(q, p_0)F^{1/2}(p_0). \tag{2.13}$$

Similarly, using $\hat{Q}_{n,\omega}$ in place of Q,

$$F_{n,\omega}(q) \geq d^2(q, p_0) + F_{n,\omega}(p_0) - 2d(q, p_0)F_{n,\omega}^{1/2}(p_0). \tag{2.14}$$

Since M is unbounded, one may take q at a sufficiently large distance Δ from C such that, by (2.13), $F(q) > \ell + 1$ on $M\backslash D$, where $D := \{q : d(q, C) \leq \Delta\}$. Since $F_{n,\omega}(p_0) \to F(p_0)$ a.s., by (2.14) one may find a P-null set N_3 and $n_3(\omega) < \infty$ such that $F_{n,\omega}(q) > \ell + 1$ on $M\backslash D$ $\forall n \geq n_3(\omega)$ $(\omega \notin N_3)$. This proves the italicized statement above.

Finally, let $D_\varepsilon := \{p \in D : d(p, C) \geq \varepsilon\}$. Then D_ε is compact and $\ell_\varepsilon := \min\{F(p) : p \in D_\varepsilon\} > \ell$, so that there exists $\theta = \theta(\varepsilon)$, $0 < \theta(\varepsilon) < 1$, such that $\ell_\varepsilon > \ell + 2\theta$. Now apply (2.8) with $K = D$ to find $n_4(\omega) < \infty$ outside a P-null set N_4 such that $\forall n \geq n_4(\omega)$, one has (i) $F_{n,\omega}(p) \leq \ell + \theta/2$ $\forall p \in C$ and (ii) $F_{n,\omega}(p) > \ell + \theta$ $\forall p \in D_\varepsilon$. Since $F_{n,\omega}(p) > \ell + 1$ on $M\backslash D$ $\forall n \geq n_3(\omega)$ $(\forall \omega \notin N_3)$, one has $F_{n,\omega}(p) > \ell + \theta$ $\forall p \in D_\varepsilon \cup (M\backslash D) = M\backslash C^\varepsilon$ if $n \geq n(\omega) := \max\{n_3(\omega), n_4(\omega)\}$ for $\omega \notin N$, where $N = N_3 \cup N_4$. This proves (2.12), and the proof of part (a) is complete.

Part (b) is an immediate consequence of part (a). □

REMARK 2.5. A theorem of Ziezold (1977) for general separable (pseudo) metric spaces implies the conclusion of part (b) of Theorem 2.3 for *compact metric spaces M*, but not for noncompact M. In metric spaces such that all closed bounded subsets are compact, the present theorem provides (i) strong consistency for Fréchet sample means and (ii) *uniform convergence* to the Fréchet mean of Q of arbitrary measurable selections from the sample mean set. This applies to both intrinsic and extrinsic means of Q and $\hat{Q}_n$ on manifolds.

REMARK 2.6. Under the hypothesis of Theorem 2.3(a), the Hausdorff distance between the intrinsic sample mean set and the intrinsic mean set does not in general go to 0, as the following example shows. Consider n independent random variables $X_1, \ldots, X_n$ with the same distribution on the unit circle, that is, absolutely continuous w.r.t. the uniform distribution. Then with probability 1, we may assume that for $i \neq j$, $X_i \neq X_j$. Assume $X_j = e^{i\theta_j}$ and let $X_j^* = e^{i\theta_j^*} = -X_j$, where the arguments θ_j^* are in the increasing order of their indices. $F(e^{i\theta})$ is periodic with period 2π and is a piecewise quadratic function; on each interval $[\theta_j^*, \theta_{j+1}^*]$, $F(e^{i\theta}) = \sum_{k=1}^n (2\pi\varepsilon_{k,j} + (-1)^{\varepsilon_{k,j}}(\theta - \theta_k))^2$ where $\varepsilon_{k,j} \in \{0, 1\}$. Therefore, the points of local minima have the form $\frac{1}{n}\sum_{k=1}^n(\theta_k + 2\pi\varepsilon_{j,k}(-1)^{\varepsilon_{j,k}})$ and each local minimum value $m_j = m_j(\theta_1, \theta_2, \ldots, \theta_n)$ is a quadratic form in $\theta_1, \ldots, \theta_n$. Since $\varepsilon_{k,j} \in \{0, 1\}$, there are at most 2^n such possible distinct quadratic polynomials. Given that the each of the variables θ_j^* is continuous, the probability that there is a fixed pair of indices $i \neq j$, such that $m_i(\theta_1, \dots, \theta_n) = m_j(\theta_1, \dots, \theta_n)$ is 0. This shows that, with probability 1, all the local minima are distinct and the intrinsic sample mean exists. On the other hand, the intrinsic mean set of the uniform measure on the circle is the whole circle, proving that in this case the Hausdorff distance between the intrinsic sample mean set and the intrinsic mean set is π with probability 1.

REMARK 2.7. The computation of the intrinsic mean set of a probability measure on a nonflat manifold M often involves nonstandard numerical algorithms, even if M has a Riemannian metric of maximum degree of mobility. For this reason, in the next section we will focus on a different approach to indices of location of probability measures on manifolds.

3. Extrinsic means of distributions on submanifolds. Since most of the literature on directional and shape analysis is concerned with parametric inference (e.g., MLEs, likelihood ratios, etc.), there has not been much emphasis on intrinsic analysis. For purposes of nonparametric or semiparametric inference, however, statistical analysis of intrinsic indices such as the intrinsic mean is very important. But it is generally not easy to prove the existence (i.e., uniqueness) of the intrinsic mean. Also intrinsic means, when they exist, are often very difficult to compute. On the other hand, a manifold can be also looked at as a submanifold of some Euclidean space, and a probability measure on it can be regarded as a probability measure in that ambient linear space. Such an approach has been employed in directional analysis in Mardia and Jupp (1999), Watson (1983) and Fisher, Hall, Jing and Wood (1996), and in shape analysis in Kent (1992), Dryden and Mardia (1993) and Le (1998).

In this section we give a general treatment of the notion of an extrinsic mean, and of statistical inference for it. We will also show that under special structures of invariance and symmetry the intrinsic and extrinsic means coincide, and therefore the extrinsic sample mean, which is easier to compute, can be used as a consistent estimator of the intrinsic sample mean.

Assume M is a closed submanifold of the Euclidean space $\mathbb{E}^k = (\Re^k, d_0)$ where d_0 denotes the Euclidean distance, $d_0(x, y) = \|y - x\|$. Let Q be a probability measure on M. Let G^c be the set of nonfocal points of M in E^k. The *projection map* $P_M : G^c \to M$ is defined as $P_M(p) = x$ if $d_0(p, M) = d_0(p, x)$.

In this case, the Fréchet function is defined on M by

$$F_0(p) = \int_M \|p - x\|^2 Q(dx). \tag{3.1}$$

DEFINITION 3.1. The *extrinsic mean set* of Q is the set of all minimizers of F_0 on M. If there is a unique minimizer, this is called the *extrinsic mean* of Q and will be labeled $\mu_E(Q)$.

PROPOSITION 3.1. *Assume* μ *is the mean of* Q *as a probability measure on* $\mathbb{R}^k$. *Then* (a) *the extrinsic mean set is the set of all points* $m \in M$, *with* $d_0(\mu, m) = d_0(\mu, M)$, *and* (b) *if* $\mu_{\mathrm{E}}(Q)$ *exists then* μ *exists and is nonfocal and* $\mu_{\mathrm{E}}(Q) = P_M(\mu)$.

PROOF. (a) If $p, x \in M$, then $\|p - x\|^2 = \|p - \mu\|^2 + 2\langle p - \mu, \mu - x\rangle + \|\mu - x\|^2$ and if we integrate this identity over M w.r.t. Q, given that $\int_M x Q(dx) = \int_{\mathbb{R}^k} x Q(dx) = \mu$, we get

$$F_0(p) = \|p - \mu\|^2 + \int_M \|\mu - x\|^2 Q(dx). \tag{3.2}$$

In particular, for any points $p, m \in M$, $F_0(p) - F_0(m) = d_0^2(\mu, p) - d_0^2(\mu, m)$ and (a) follows by selecting m to be a minimizer of F_0. (b) If $\mu_{\mathrm{E}}(Q)$ exists then μ exists and from part (a) it follows that the distance from an arbitrary point on M to μ has the unique minimizer $\mu_{\mathrm{E}}(Q)$, that is, μ is nonfocal and since $d_0(\mu_{\mathrm{E}}(Q), \mu) = d_0(\mu, M)$, $\mu_{\mathrm{E}}(Q) = P_M(\mu)$. □

THEOREM 3.2. *The set of focal points of a submanifold* M *of* E^k *is a closed subset of* $\mathbb{E}^k$ *of Lebesgue measure* 0.

PROOF. A point p is nonfocal, with $d_0(p, M) = r$, if and only if the (hyper)sphere $S(p, r)$ of radius r centered at p has a unique point x in common with M. In this case the interior of the ball $B(p, r)$ is included in $\mathbb{E}^k \backslash M$ and $T_x M \subseteq T_x S(p, r)$; x is the point of absolute minimum of the function L_p defined on M by $L_p(y) = d_0^2(p, y)$. Let $u = (u^1, \dots, u^d)$ be coordinates of points $y = y(u)$ on M, with $y(0) = x$. In Milnor [(1963), page 36] it is shown that x is a degenerate critical point of L_p if and only if p is a focus. Moreover, from the computations in Milnor [(1963), page 35] it follows that if $K_1, K_2, \dots, K_s$ are the nonzero principal curvatures of M at the point x and $|t| < \min\{|K_1|^{-1}, |K_2|^{-1}, \dots, |K_s|^{-1}\}$ for any unit vector ν in $\nu_x M$, the normal space at the point x, the matrix

$$((\partial y/\partial u^i(0))(\partial y/\partial u^j(0)) - t\nu(\partial^2 y/\partial u^i \partial u^j(0)))$$

is positive definite. In particular, since $r < \min\{|K_1|^{-1}, |K_2|^{-1}, \dots, |K_s|^{-1}\}$, the matrix

$$((\partial y/\partial u^i(0))(\partial y/\partial u^j(0)) - (p - y(0))(\partial^2 y/\partial u^i \partial u^j(0)))$$

is positive definite. There are a neighborhood N of p and an open neighborhood U of 0 such that, for any $u \in U$ and $q \in N$, the matrix of the second partial derivatives of $L_q(y(u))$, namely,

$$((\partial y/\partial u^i(u))(\partial y/\partial u^j(u)) - (q - y(u))(\partial^2 y/\partial u^i \partial u^j(u)))$$

is positive definite. Since the manifold topology of M coincides with the induced topology, one may assume that there is a ball $B(x,\varepsilon)$, such that $y(U) = M \cap B(x,\varepsilon)$. Let ε be as small as necessary. Since x is the only common point of M and $S(p,r)$, and the set $M \setminus \operatorname{Int} B(x,\varepsilon)$ is closed, there is a number δ, $r > \delta > 0$, such that $d_0(p, M \setminus \operatorname{Int} B(x,\varepsilon)) = r + \delta$. Let $q \in \operatorname{Int} B(p, \delta/2)$ and $z \in M \setminus \operatorname{Int} B(x,\varepsilon)$. Then $d_0(q,z) > |d_0(q,p) - d_0(p,z)| > r + \delta - \delta/2 > d_0(q,x)$. It follows that $d_0(q,M) = d_0(q, M \cap \operatorname{Int} B(x,\varepsilon))$. If $y \in \operatorname{Int} B(x,\varepsilon) \setminus \{x\}$ is such that $d_0^2(q,y) = d_0^2(q,M)$, it follows by the positive definiteness of the displayed matrix above that y is an isolated point of minimum of L_q, proving that the set of nonfocal points is open.

Let $G(\infty)$ be the set of foci of M, and let G be the set of focal points. It is known [Milnor (1963), page 33] that $G(\infty)$ has Lebesgue measure zero. If x is a point on M, we define $G(x)$ to be the set of all points f in E^k such that there is at least another point x' $(\neq x)$ on M with $d_0(x,f) = d_0(x',f) = d_0(f,M)$. Another description of $G(x)$ is as the set of all centers f of spheres of E^k that are tangent to M at least at two points, one of which is x, and whose interiors are disjoint from M. The tangent space $T_x M$ is included in the tangent space at x to such a sphere. Therefore the normal line at x to such a sphere is included in the normal space $\nu_x M$, which means that a point in $G(x)$ is in $\nu_x M$. We show that on each ray starting at x in $\nu_x M$ (x is the zero element, if $\nu_x M$ is regarded as a vector space) there is at most one point in $G(x)$. Indeed if f_1, f_2 are two distinct points on such a ray starting at x, assume f_1 is closer to x than f_2. Let x', x'' be such that $d_0(x', f_1) = d_0(x, f_1) = d_0(f_1, M)$, $d_0(x'', f_2) = d_0(x, f_2) = d_0(f_2, M)$. Then x' is a point of M in the interior of $S(f_2, d_0(f_2, M))$, a contradiction. Given that $G(x)$ intersects the radii coming out of x in $\nu_x M$ at most at one point, the Lebesgue measure of $G(x)$ in $\nu_x M$ is zero.

Let NM be the disjoint union of $\nu_x M$, $x \in M$. NM is the normal bundle of M and it is a manifold of dimension k. We define the map $N : NM \to \mathbb{R}^k$ by $N(x, v_x) = x + v_x$. One may show [Milnor (1963)] that the critical values of N are the foci of M. Therefore if $f = N(x, v_x)$ is a focal point that is not a focus, f is a regular value of N. Thus, if λ represents the Lebesgue volume form in $\mathbb{R}^k$, then $N^*\lambda$ is a volume form on $N^{-1}(\mathbb{R}^k \setminus G(\infty))$, and the Lebesgue measure of $G \setminus G(\infty)$ is

$$\lambda(G \setminus G(\infty)) \le \int_{NM \setminus G(\infty)} N^*\lambda.$$

If we apply Fubini's theorem integrating over the base M the integral in each fiber (normal space $\nu_x M$), we see that the integrand in $\nu_x M$ is a volume form that is a multiple $C(x)$ of the Lebesgue measure in $\nu_x M$. Therefore

$$\int_{NM \setminus G(\infty)} N^*\lambda = \int_M C(x) \left(\int_{G(x)} \lambda_x(dv) \right) \operatorname{vol}_M(dx),$$

which is zero since

$$\int_{G(x)} \lambda_x(dv) = \lambda_x(G(x)) = 0. \qquad \square$$

Now we extend the notion of extrinsic means to embeddings of manifolds.

DEFINITION 3.2. Assume Q is a probability measure on M and $j : M \to \mathbb{R}^k$ is an embedding, such that $j(M)$ is closed . We say that Q is *nonfocal w.r.t.* j if Q regarded as a measure $j(Q)$ on $\mathbb{R}^k$ has a mean $\mu(j(Q)) = \int_{\mathbb{R}^k} x(j(Q))(dx)$ which is a nonfocal point of $j(M)$. The extrinsic mean of a probability measure Q which is nonfocal w.r.t. j is $\mu_{\mathrm{E}}^j(Q) := j^{-1}(P_{j(M)}(\mu(j(Q))))$.

Since the embedding j is assumed to be given, we will normally drop the superscript j and write $\mu_{\mathrm{E}}(Q)$ for $\mu_{\mathrm{E}}^j(Q)$.

DEFINITION 3.3. A *Riemannian embedding* is an embedding $j : M \to \mathbb{R}^k$ which pulls back the induced Riemannian structure on $j(M)$ to the Riemannian structure of M. A Riemannian embedding is said to be *equivariant* at a point p of M, if every isometry of $j(M)$ that keeps $j(p)$ fixed is the restriction of an Euclidean isometry. A *two point homogeneous space* is a Riemannian manifold such that for each two pairs of its points (p, q), (p', q') with $d_g(p, q) = d_g(p', q')$, there is an isometry τ with $\tau(p) = p'$ and $\tau(q) = q'$.

To simplify notation, we will often write p for $j(p)$ and M for $j(M)$, in case of a Riemannian embedding j. It is known that M is a two-point homogeneous space if and only if, for each $p \in M$, the *isotropy group* H_p of all isometries of M which keep p fixed is *transitive* on every *geodesic sphere* $S(p, r) := \{x \in M : d_g(x, p) = r\}$, $r > 0$ [Chavel (1993), page 147]. That is, given q, $q' \in S(p, r)$, there exists $h \in H_p$ such that $h(q) = h(q')$.

The following theorem links the intrinsic mean of Q on a Riemannian manifold with its extrinsic mean under an embedding which is equivariant at a point p. Note that for every $h \in H_p$ the *differential* dh maps T_pM into itself.

THEOREM 3.3. *Let $j : M \to \mathbb{R}^k$ be a Riemannian embedding which is equivariant at p. Assume that $0 \equiv (p, 0)$ is the only fixed point of T_pM under the family of maps $\{dh : h \in H_p\}$. Assume also that Q is a probability measure on M which is invariant under H_p, and $\mu(j(Q))$ is finite and nonfocal.* (a) *Then either $\mu_{\mathrm{E}}(Q) = p$ or $\mu_{\mathrm{E}}(Q) \in C(p)$, the cut locus of p. The same holds for the intrinsic mean $\mu_{\mathrm{I}}(Q)$ if it exists.* (b) *If, in addition to the hypothesis above, M is a compact two point homogeneous space other than the round sphere and $\mu_{\mathrm{I}}(Q)$ exists, then $\mu_{\mathrm{I}}(Q) = \mu_{\mathrm{E}}(Q) = p$.*

PROOF. (a) The mean $\mu(j(Q))$ of $j(Q)$, regarded as a measure on the ambient Euclidean space, is invariant under each Euclidean isometry $\hat{h}$, say, which extends $h \in H_p$. For Q, as a measure on the Euclidean space, is invariant under $\hat{h}$ $\forall h \in H_p$, due to the equivariant embedding at p and the invariance of Q on M under H_p. It now follows that $\mu_{\mathrm{E}}(Q)$ is invariant under H_p. Suppose now that $\mu_{\mathrm{E}}(Q) \neq p$. We will show that in that case $\mu_{\mathrm{E}}(Q) \in C(p)$. If this is not so then $\mu_{\mathrm{E}}(Q) \in \exp_p(V(p))$. Then there exists a unique minimizing geodesic joining p and $\mu_{\mathrm{E}}(Q)$. Because of uniqueness this geodesic, say, γ, is left invariant by the isometries $h \in H_p$. Then $\dot{\gamma}(0)$ is invariant under dh $\forall h \in H_p$, contradicting the hypothesis that 0 is the only invariant vector in T_pM under $\{dh : h \in H_p\}$.

Suppose next that $\mu_{\mathrm{I}}(Q)$ exists. Then $\mu_{\mathrm{I}}(Q)$ is invariant under H_p, since $F(y) = F(hy)$, $\forall h \in H_p$, due to the invariance of Q under H_p. The same argument as above now shows that either $\mu_{\mathrm{I}}(Q) = p$ or $\mu_{\mathrm{I}}(Q) \in C(p)$.

(b) It follows from a classification theorem due to Wang (1952) that besides the round spheres, there are only four types of two-point homogeneous spaces, namely, the real projective spaces, complex projective spaces, quaternionic projective spaces and the Cayley projective planes [see also Helgason (1978), page 535]. It is known from Warner (1965) that for any point $p \in M$, $C(p)$ is a strong deformation retract of $M \backslash \{p\}$, and, in particular, $C(p)$ has the homotopy type of $M \backslash \{p\}$. On the other hand, if M is one of the two-point homogeneous spaces other than a sphere given by Wang's classification, then the cohomology of $M \backslash \{p\}$ is not trivial. This shows that in this case $M \backslash \{p\}$ is not homotopically trivial and therefore $C(p)$ is also not homotopically trivial. This implies that if M is not a sphere, $C(p)$ has at least two points q, q'. Moreover, since the isotropy group H_p is transitive on the geodesic sphere $S(p, d_g(p,q))$, we may assume that $d_g(p,q) = d_g(p,q') = r$. Hence if $\mu_{\mathrm{E}}(Q) \in C(p)$ there exists $q' \in C(p) \backslash \{\mu_{\mathrm{E}}(Q)\}$ such that $d_g(p, \mu_{\mathrm{E}}(Q)) = d_g(p, q')$. By the transitivity of H_p on $S(p,r)$, there exists $h \in H_p$ such that $h(\mu_{\mathrm{E}}(Q)) = q'$, contradicting the invariance of $\mu_{\mathrm{E}}(Q)$. By (a), $\mu_{\mathrm{E}}(Q) = p$.

The same argument applies to $\mu_{\mathrm{I}}(Q)$ if it exists. □

EXAMPLE 3.1. Let Q be a probability measure on a sphere, with $\mu(j(Q)) \neq 0$, such that the group leaving Q invariant is the stabilizer of a given point p. Then $\mu_{\mathrm{E}}(Q)$ is either p or the antipodal point of p on the sphere. The same is true of $\mu_{\mathrm{I}}(Q)$ if it exists. Such examples of probability distributions are given in Watson [(1983), page 136] and Fisher (1993), including the von Mises distributions. Another example of an invariant distribution is given by the *Dimroth–Watson distribution* on the real projective plane $\mathbb{R}P^2$, whose Radon–Nykodim derivative at the point $[x]$ w.r.t. the volume measure of a constant curvature Riemannian structure on $\mathbb{R}P^2$ is proportional to $\exp[k(p \cdot x)^2]$, $x \in S^2$, and is $O(2)$ invariant. A general $O(2)$ invariant measure with a density on $\mathbb{R}P^2$ has the Radon–Nykodim derivative w.r.t. the volume form at the point $[x]$ proportional to $f((p \cdot x)^2)$, $x \in S^2$, where f is a density of an absolutely continuous positive measure on a finite interval. An example of equivariant embedding of $\mathbb{R}P^2$ furnished with a Riemannian structure with constant curvature into the space of symmetric matrices $S(3, \mathbb{R})$ is provided by the Veronese-like map $j[u] = uu^t$. The Euclidean distance d_0 on $S(3, \mathbb{R})$ is given by $d_0^2(A, B) := \mathrm{Tr}((A - B)(A - B))$. As such if u, v are in $\mathbb{S}^2$, $d_0^2(j[u], j[v]) = \mathrm{Tr}(uu^t - vv^t)(uu^t - vv^t) = \mathrm{Tr}(uu^t uu^t - 2uu^t vv^t + vv^t vv^t) = 2(1 - (u \cdot v)^2)$. The fact that the embedding is equivariant follows from the action of isometries of $O(3)$ on $S(3, \mathbb{R})$, by simultaneous left and right multiplication. By Theorem 3.3(b), if the intrinsic mean direction of a rotationally invariant measure on $\mathbb{R}P^2$ (the space of directions in the three-dimensional Euclidean space) exists, it is the same as the extrinsic mean. Note that proportional distances yield the same Fréchet mean set, and therefore the intrinsic mean sets of a probability measure on $\mathbb{R}P^2$ obtained after scaling $\mathbb{S}^2$ to different radii are all the same. Finally, note that Kobayashi (1968) gave a general construction of an isometric embedding of a compact symmetric space, which can be used to provide an equivariant embedding of any two-point homogeneous space (including the Cayley plane) into a Euclidean space.

DEFINITION 3.4. Assume $X = (X_1, \dots, X_n)$ are i.i.d. M-valued random variables whose common distribution is a nonfocal measure Q on (M, j) and the function $p \to \sum_{r=1}^n \|j(p) - j(X_r)\|^2$ has a unique minimizer on M; this minimizer is the *extrinsic least squares sample mean.* If the mean $\overline{j(X)}$ of the sample $j(X) = (j(X_1), \dots, j(X_n))$ is a nonfocal point, the *extrinsic sample mean* is

$$\overline{X}_{\mathrm{E}} := j^{-1}\big(P_{j(M)}(\overline{j(X)})\big) \equiv \mu_{\mathrm{E}}^{j}(\hat{Q}_n), \tag{3.3}$$

where $\hat{Q}_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ is the empirical distribution.

From now on, we will occasionally omit the embedding, that is we assume M is a submanifold of the Euclidean space and j is the inclusion map. To ease notational complexity in this case, we will often write X_i for $j(X_i)$ and $\overline{X}$ for $\overline{j(X)} = \frac{1}{n}\sum_{i=1}^n j(X_i)$.

THEOREM 3.4. *Assume Q is a nonfocal probability measure on the manifold M and $X = \{X_1, \dots, X_n\}$ is a random sample from Q.* (a) *If the sample mean $\overline{X}$ is a nonfocal point then the least squares sample mean equals the extrinsic sample mean $\overline{X}_{\mathrm{E}}$.* (b) *$\overline{X}_{\mathrm{E}}$ is a strongly consistent estimator of $\mu_{\mathrm{E}}(Q)$.*

PROOF. (a) If $\overline{X}$ is a nonfocal point then by Proposition 3.1, applied to the empirical $\hat{Q}_n$, the extrinsic least squares sample mean is the extrinsic sample mean. (b) By the SLLN, $\overline{X}$ converges to $\mu[j(Q)]$ almost surely. Since F^c is open, by Proposition 3.2, and the projection P_M from F^c to M is continuous, $j^{-1}(P_M(\overline{X}))$ converges to $\mu_{\mathrm{E}}(Q)$ almost surely. □

In particular, from Theorem 3.4 we get the following consequence.

REMARK 3.1. If Q is focal, the extrinsic mean set has at least two points. Therefore by Theorem 2.3(a) the extrinsic sample mean set may have more than one point, and a selection from the extrinsic sample mean set sequence may not have a limit.

COROLLARY 3.5. *Assume M, Q and the equivariant embedding j are as in Theorem* 3.3(b). *Then the extrinsic least squares sample mean is a strongly consistent estimator of the intrinsic mean of Q.*

We now consider a method for constructing confidence regions for extrinsic means $\mu_{\mathrm{E}}(Q)$ on regular submanifolds. For the formulas below we omit summation symbols for any repeated index in the same monomial.

Let H be the projection on the affine subspace $\mu_{\mathrm{E}}(Q) + T_{\mu_{\mathrm{E}}}M$. We would like to determine the asymptotic distribution of $H(\overline{X})$. While $H(\overline{X})$ is not the same as $P_M(\overline{X})$, its asymptotic distribution is easier to compute. For large samples the extrinsic sample mean is close to the extrinsic mean and, therefore, $H(\overline{X})$ and $P_M(\mu)$ will be close to each other. When M is a linear variety, the two maps coincide. Thus for concentrated data the delta method for H gives a good estimate of the distribution of the extrinsic sample mean. Assume that around $P_M(\mu)$ the implicit equations of M are $F^1(x) = \cdots = F^c(x) = 0$, where $F^1, \dots, F^c$ are functionally independent. Then $\overline{X} - H(\overline{X})$ is in $\nu_{P_M(\mu)}M$, the orthocomplement of $T_{P_M(\mu)}M$; thus it is a linear combination of the gradients $\operatorname{grad}_{P_M(\mu)} F^1, \dots, \operatorname{grad}_{P_M(\mu)} F^c$. We need to evaluate the differential of the map H at μ, in terms of $F^1, \dots, F^c$. Set $\nu_\alpha = \|\operatorname{grad}_{P_M(\mu)} F^\alpha\|^{-1} \operatorname{grad}_{P_M(\mu)} F^\alpha$ ($\alpha = 1, \dots, c$) and

$$h_{\alpha\beta}(\mu) = \nu_\alpha \nu_\beta,$$
$$(h^{\alpha\beta}(\mu))_{\alpha,\beta=1,\dots,c} = \left((h_{\alpha\beta}(\mu))_{\alpha,\beta=1,\dots,c}\right)^{-1}.$$

Then $x - H(x) = t^\beta(x,\mu)\nu_\beta$ where $t^\beta(x,\mu) = h^{\alpha\beta}(\mu)(x - P_M(\mu))\nu_\alpha$. Therefore, $H(x) = x + h^{\alpha\beta}(\mu)((P_M(\mu) - x)\nu_\alpha)\nu_\beta$, $d_\mu H(v) = v - h^{\alpha\beta}(\mu)(v\nu_\alpha)\nu_\beta$, that is,

$$G_i^j = \frac{\partial H^j}{\partial x^i}(\mu) = \delta_{ij} - h^{\alpha\beta}(\mu)\nu_\alpha^i \nu_\beta^j, \tag{3.4}$$

where $\delta_{ij} = 1$ or 0 according as $i = j$ or $i \neq j$. By the delta method we arrive at the following theorem.

THEOREM 3.6. *Let $\{X_k\}_{k=1,\dots,n}$ be a random sample from a nonfocal distribution Q on the submanifold M, given in a neighborhood of $\mu_{\mathrm{E}}(Q)$ by the equations $F^1(x) = \cdots = F^c(x) = 0$. Assume Q has mean μ and covariance matrix Σ as a distribution in the ambient numerical space. If G is the matrix given by* (3.4), *then $n^{1/2}(H(\overline{X}) - P_M(\mu))$ converges weakly to $N(0, G\Sigma G^t)$ in the tangent space of M at the extrinsic mean $\mu_{\mathrm{E}}(Q) = P_M(\mu)$ of Q.*

Sometimes the matrix $\Gamma = G\Sigma G^t$ may be difficult to compute and one may use nonpivotal bootstrap, that is, Efron's percentile bootstrap to obtain a confidence region for $\mu_{\mathrm{E}}(Q)$. We state this as follows [see Efron (1982)]:

COROLLARY 3.7. *Under the hypothesis of Theorem* 3.6, *one may construct an asymptotic* $(1-\alpha)$*-confidence region for* $\mu_{\mathrm{E}}(Q) = P_M(\mu)$, *using the bootstrapped statistic* $n^{1/2}(\overline{H}(\overline{X}^*) - \overline{H}(\overline{X}))$. *Here* $\overline{H}$ *is the projection on the affine subspace* $\overline{X}_{\mathrm{E}} + T_{\overline{X}_{\mathrm{E}}}M$ *and* $\overline{X}^*$ *is the mean of a random sample with repetition of size n from the empirical* $\hat{Q}_n$ *considered as a probability measure on the Euclidean space in which M is embedded.*

REMARK 3.2. Suppose F is finite and Q is nonfocal. By Theorem 3.2, there exists $\delta > 0$ such that $\overline{X}$ is nonfocal if $\|\overline{X} - \mu\| < \delta$. Since $P(\|\overline{X} - \mu\| \geq \delta) = O(n^{-1})$, one may define $\overline{X}_E$ to be any measurable selection from the sample extrinsic mean set if $\overline{X}$ is focal. Theorem 3.6 and a corresponding version of Corollary 3.7 hold for this $\overline{X}_{\mathrm{E}}$.

EXAMPLE 3.2. Let $M = S^d$, j the usual embedding (inclusion) in $\mathbb{R}^{d+1}$ and Q a nonfocal probability measure on S^d, that is, $\mu = \int_{\mathbb{R}^{d+1}} xQ(dx) \neq 0$. Let $m = P_M\mu$. Then $H(\overline{X}) - m = \overline{X} - m - \{(\overline{X} - m)\cdot m\}m = \overline{X} - (\overline{X}\cdot m)m = \overline{X} - \mu - \{(\overline{X} - \mu)\cdot m\}m$. Hence $\sqrt{n}(H(\overline{X}) - m)$ converges in distribution to a d-dimensional normal distribution supported by the tangent space $T_m S^d$ identified with $\{x \in \mathbb{R}^{d+1} : xm = 0\}$. As a measure on $\mathbb{R}^{d+1}$ this normal distribution has mean 0 and covariance matrix $\Gamma := \Sigma + (m^t\Sigma m)mm^t - 2\Sigma(mm^t)$, where Σ is the covariance matrix of Q viewed as a measure on $\mathbb{R}^{d+1}$. An asymptotic $(1-\alpha)$-confidence region for m may now be constructed using the estimate of Γ obtained by replacing in its expression (i) Σ by the sample covariance matrix S and (ii) m by $\overline{X}/|\overline{X}|$. Alternatively, one may use the bootstrap procedure of Corollary 3.7.

4. Means of distributions on axial spaces, planar shape spaces and their Veronese–Whitney embeddings. The space of all directions in $\mathbb{R}^N$, or axial space, is an $(N-1)$-dimensional real projective space. It is the space $\mathbb{R}P^{N-1}$ of equivalence classes on a round sphere in $\mathbb{R}^N$ with antipodal points identified. As such this space carries a Riemannian structure of constant positive curvature, since the antipodal map is an isometry of the round sphere. This is the space of elliptic geometry, and the total group of isometries $SO(N)$ has maximum mobility. Given that this elliptic space is locally isometric with a round sphere, if the support of a distribution w.r.t. the stabilizer of a point [which is a subgroup of $SO(N)$ isomorphic to $SO(N-1)$] has small diameter, then the intrinsic mean exists (see Remark 2.1).

In this section we would like to consider the general situation when the distribution is not concentrated. Note that for N odd, $\mathbb{R}P^{N-1}$ cannot be embedded in $\mathbb{R}^N$.

Usually, in directional statistics, one regards an axial distribution as one corresponding to an $\mathbb{S}^{N-1}$-valued random variable X such that X and $-X$ have the same distribution [Watson (1983), Chapter 5; Fisher, Hall, Jing and Wood (1996); and Beran and Fisher (1998)]. One may show that the Veronese–Whitney map defined in Section 3 for $N = 3$, and given for arbitrary N by the same formula $j([u]) = u\ u^t$ ($\|u\| = 1$), is an equivariant embedding of $\mathbb{R}P^{N-1}$ into a $\frac{1}{2}N(N+1)$-dimensional Euclidean space. To see this, let $S(N, \mathbb{R})$ denote the set of all real $N \times N$ symmetric matrices. Since the Euclidean distance d_0 between two symmetric matrices is

$$d_0(A, B) = \operatorname{Tr}\big((A - B)(A - B)^t\big) = \operatorname{Tr}\big((A - B)^2\big), \tag{4.1}$$

the group $O(N)$ acts as a group of isometries of $(S(N, \mathbb{R}), d_0)$ via

$$T(A) = TAT^t \tag{4.2}$$

and leaves $M = j(\mathbb{R}P^{N-1})$ invariant. It is known that $O(N)$ acts transitively on $\mathbb{S}^{N-1}$, that is, if $u, v \in \mathbb{R}^N$, $\|u\| = \|v\| = 1$, there is a $T \in O(N)$ such that $Tu = v$. Then $T(j[u]) = Tuu^tT^t = vv^t = j([v])$, showing that $O(N)$ acts transitively on M. The stabilizer of this action is $O(N-1)$. Therefore $\mathbb{R}P^{N-1}$ with the Riemannian metric induced by j is a homogeneous space, with a group of isometry of largest dimension. From Theorem 3.1 in Kobayashi (1972), it turns out that with this metric $\mathbb{R}P^{N-1}$ has constant positive curvature, and j is an equivariant embedding of $\mathbb{R}P^{N-1}$ into $S(N, \mathbb{R})$. Also $M = j(\mathbb{R}P^{N-1})$ is included in the set $S_+(N, \mathbb{R})$ of symmetric nonnegative definite N by N real matrices. $S_+(N, \mathbb{R})$ is convex, so the mean under Q of matrices in $S_+(N, \mathbb{R})$ is a matrix in $S_+(N, \mathbb{R})$. Therefore, we are interested in determining only the projection of a semipositive matrix on M. If A is in $S(N, \mathbb{R})$ and T is an orthogonal matrix, then $d_0(A, M) = d_0(T(A), M)$. Given A in $S_+(N, \mathbb{R})$, there is T in $O(N)$ such that $T(A) = \operatorname{diag}(\eta_a)_{a=1,\dots,N} = D$, and the entries of D are all nonnegative, in increasing order. Let $x = (x^a)$ be a unit vector in $\mathbb{R}^N$. After elementary computations we get

$$d_0^2(D, j([x])) = 1 + \sum \eta_a^2 - 2\sum \eta_a (x^a)^2 \geq d_0^2(D, j([e_N])), \tag{4.3}$$

where e_N is the eigenvector of D of unit length corresponding to the highest eigenvalue. Note that if η_N has multiplicity two or more, then for any $t \in [0, 2\pi]$ and for any unit vector $x = (x^a) \in \mathbb{R}^N$, we have

$$d_0^2(D, j[x]) \geq d_0^2(D, j[\cos t e_{N-1} + \sin t e_N]) = d_0^2(D, j[e_N])$$

and D is focal. If η_N is simple, that is, has multiplicity one, then $d_0^2(D, j[x]) \geq d_0^2(D, j[e_N])$ and the equality holds only if $[x] = [e_N]$. In this last case, D is a nonfocal and $P_M(D) = j([e_N])$. We will call such an eigenvector of length 1 a *highest eigenvector* of D. One then obtains the following:

PROPOSITION 4.1. *The set F of the focal points of $M = j(\mathbb{R}P^{N-1})$ in $S_+(N,\mathbb{R})$ is contained in the set of matrices in $S_+(N,\mathbb{R})$ whose largest eigenvalues are of multiplicity at least 2. The projection $P_M : S_+(N,\mathbb{R})\backslash F \to M$ associates to each nonnegative definite symmetric matrix A with a highest eigenvalue of multiplicity one, the matrix $j([m])$ where m is a highest unit eigenvector of A.*

If Q is a probability measure on $\mathbb{R}P^{N-1}$, assume $[X]$, $\|X\| = 1$ is a $\mathbb{R}P^{N-1}$-valued random variable with distribution Q. As a consequence of Corollary 3.5 and Proposition 4.1 we obtain the theorem:

THEOREM 4.2. *Assume $[X_r]$, $\|X_r\| = 1$, $r = 1,\dots,n$, is a random sample from a probability measure Q on $\mathbb{R}P^{N-1}$. Then* (a) *Q is nonfocal if the highest eigenvalue of $E[X_1X_1^t]$ is simple and in this case $\mu_E(Q) = [m]$, where m is a unit eigenvector of $E[X_1X_1^t]$ corresponding to this eigenvalue.* (b) *Under the hypothesis of* (a) *the extrinsic sample mean $\overline{[X]}_{\mathrm{E}}$ is a strongly consistent estimator of $\mu_{\mathrm{E}}(Q)$.*

Note that when it exists, $\overline{[X]}_{\mathrm{E}}$ is given by $\overline{[X]}_{\mathrm{E}} = [m]$, where m is a unit eigenvector of $S_n = \frac{1}{n}\sum_{n=1}^{n} X_rX_r^t$. It may be noted that in this case $\overline{[X]}_{\mathrm{E}}$ is also the MLE for the mean of a Bingham distribution [Prentice (1984) and Kent (1992)] and for the mean of the Dimroth–Watson distribution, whose density function at $[x]$ is proportional to $\exp(k(\mu\cdot x)^2)$, where k is a constant. For these or more general parametric families, MLE asymptotics or bootstrap methods [Fisher and Hall (1992)] are commonly used. Nonparametric techniques of estimation of extrinsic means will be presented in a forthcoming second part of this article.

We turn now to planar shape spaces [see Kendall (1984)].

DEFINITION 4.1. *A planar k-ad* is an ordered set $(z_1, z_2,\dots,z_k)$ of k points in the Euclidean plane at least two of which are distinct. Two k-ads $(z_1, z_2,\dots,z_k)$ and $(z_1', z_2',\dots,z_k')$ are said to have the *same shape* if there is a direct similarity T in the plane, that is, a composition of a rotation, a translation and a homothety such that $T(z_j) = z_j'$ for $j = 1,\dots,k$. Having the same shape is an equivalence relationship in the space of planar k-ads, and the set of all equivalence classes of k-ads is called the *planar shape space of k-ads,* or the space $\sum_2^k$. Without loss of generality one may assume that two k-ads that have the same shape also have the same center of mass, that is, $\sum z_j = \sum z_j' = 0$, and they have the same shape if there is a composition of a transformation T which keeps the origin fixed, and is a rotation followed by a homothety such that $T(z_j) = z_j'$ for $j = 1,\dots,k-1$. Such a transformation T is determined by a nonzero complex number, that is to say, the two k-ads with center of mass 0 have the same shape if there is a $z \in \mathbb{C}\backslash\{0\}$ such that $zz_j = z_j'$ for $j = 1,\dots,k-1$. Thus the shape equivalence class of a planar

k-ad is uniquely determined by a point in $\mathbb{C}P^{k-2}$, that is to say, $\sum_2^k$ is identified with $\mathbb{C}P^{k-2}$. Kendall (1984) pointed out that there is no unique way to identify $\sum_2^k$ with $\mathbb{C}P^{k-2}$ and indeed our method of identification differs from Kendall's method.

Tests appropriate for mismatch of shapes of k-ads were introduced in Sibson (1978) based on the so-called *Procrustes statistic*. The *Procrustean distance*, in our terminology, is the distance induced by the Euclidean distance on $\mathbb{C}P^{k-2}$ via a quadratic Veronese–Whitney embedding into a unit sphere of the linear space $S(k-1, \mathbb{C})$ of *selfadjoint complex matrices of order* $k-1$. In order to define $j: \mathbb{C}P^{k-2} \to S(k-1, \mathbb{C})$ it is useful to note that $\mathbb{C}P^{k-2} = \mathbb{S}^{2k-3}/\mathbb{S}^1$, where $\mathbb{S}^{2k-3}$ is the space of complex vectors $\mathbb{C}^{k-1}$ of norm 1, and the equivalence relation on $\mathbb{S}^{2k-3}$ is by multiplication with scalars in $\mathbb{S}^1$ (complex numbers of modulus 1). If $z = (z^1, z^2, \dots, z^{k-1})$ is in $\mathbb{S}^{2k-3}$, we will denote by $[z]$ the equivalence class of z in $\mathbb{C}P^{k-2}$. The *Veronese–Whitney* (or simply *Veronese*) *map* is in this case $j([z]) = zz^*$ where, if z is considered as a column vector, z^* is the adjoint of z, that is, the conjugate of the transpose of z. The Euclidean distance in the space of Hermitian matrices $S(k-1, \mathbb{C})$ is $d_0^2(A, B) = \mathrm{Tr}((A-B) \times (A-B)^*) = \mathrm{Tr}((A-B)^2)$.

Kendall (1984) (see his Theorem 1) has shown that the Euclidian distance in $S(k-1, \mathbb{C})$ induces via j a Riemannian structure on $\mathbb{C}P^{k-2}$, which is known in literature as the *Fubini–Study metric* and has a highest dimensional group of isometries on $\mathbb{C}P^{k-2}$ among all the Riemannian metrics on this manifold. The isometry group is the special unitary group $SU(k-1)$ of all $(k-1) \times (k-1)$ complex matrices A, with $A^*A = I$, $\det(A) = 1$. By analogy with the action of the orthogonal group in the real projective space, one may show that the group $SU(k-1)$ acts transitively as a group of isometries and up to a scaling factor, j is an equivariant embedding of $\mathbb{C}P^{k-2}$ into the space of self adjoint matrices $S(k-1, \mathbb{C})$.

Since $M = j(\mathbb{C}P^{k-2})$ is $SU(k-1)$ invariant, the techniques used for $j(\mathbb{R}P^{N-1})$ can be adapted to determine the focal points of M in $S_{-}(k-1, \mathbb{C})$, the space of nonnegative definite self-adjoint $(k-1) \times (k-1)$ complex matrices. We are then led to the following:

PROPOSITION 4.3. *The focal points of* $M = j(\mathbb{C}P^{N-1})$ *in* $S_+(k-1, \mathbb{C})$ *are the nonnegative definite symmetric matrices with the highest eigenvalue of multiplicity at least* 2. *The projection* $P_M: S_+(k-1, \mathbb{C}) \setminus F \to M$ *associates to each matrix* $A \in S_+(k-1, \mathbb{C})$ *with a highest eigenvalue of multiplicity* 1, *the matrix* $j([m])$, *where* m *is a highest unit eigenvector of* A.

The following result, which follows from Theorem 3.4 and Proposition 4.3, addresses the question of consistency of Procrustes estimators [see Dryden and Mardia (1998), page 280].

THEOREM 4.4. *Let Q be a probability distribution on $\mathbb{C}P^{k-2}$ and let $\{[Z_r], \|Z_r\| = 1\}_{r=1,\dots,n}$ be a random sample from Q.* (a) *Q is nonfocal iff λ, the largest eigenvalue of $E[Z_1 Z_1^*]$, is simple and in this case $\mu_{\mathrm{E}}(Q) = [m]$, where m is an eigenvector of $E[Z_1 Z_1^*]$ corresponding to λ, with $\|m\| = 1$.* (b) *The extrinsic sample mean $\overline{[Z]}_{\mathrm{E}}$ is a consistent estimator of $\mu_{\mathrm{E}}(Q)$ iff λ is simple.*

EXAMPLE 4.1. The *Dryden–Mardia distribution* on $\mathbb{C}P^{k-2}$ is induced by a $\mathbb{C}^{k-1}$-valued random variable Z which has a multivariate normal distribution with mean ν and covariance matrix $\sigma^2 I_{2k-2}$. The variable X on $\mathbb{C}P^{k-2}$ corresponding to Z is $X = [Z] = \{\lambda Z, \lambda \in \mathbb{C}^*\}$. Kent and Mardia (1997) showed that $E(j(X)) = \alpha I_{k-1} + \beta \nu\nu^*$, where $\alpha > 0$, $\alpha + \beta > 0$. If we write this quadratic form w.r.t. orthogonal coordinates with the first axis along ν, we notice that as a matrix, $E(j(X))$ is conjugate with a diagonal matrix whose diagonal entries are all α except for the entry $\alpha + \beta$ in the upper left corner, showing that $E(j(X))$ is nonfocal for j. By Theorem 4.4 the extrinsic mean of the Dryden–Mardia distribution exists and the extrinsic sample mean is a consistent estimator of the extrinsic mean.

EXAMPLE 4.2. The complex unit sphere is $\mathbb{C}S^{k-2} = \{z \in \mathbb{C}^{k-1} \mid \|z\| = 1\}$. Kent (1994) defines on $\mathbb{C}S^{k-2}$ the complex Bingham distribution associated with a Hermitian matrix as a parameter by the probability density function

$$f_A(z) = C(A)^{-1} \exp(z^* A z), \qquad z \in \mathbb{C}S^{k-2}. \tag{4.4}$$

This density is constant along the orbit of z via the action of $\mathbb{C}S^0$ given by $(e^{i\theta}, z) \mapsto e^{i\theta} z$. The space of orbits is $\mathbb{C}P^{k-2}$ and the image of the volume measure of $\mathbb{C}S^{k-2}$ on $\mathbb{C}P^{k-2}$ in this projection is the volume measure associated with the Fubini–Study metric. Therefore $f_A(z)$ induces a probability density function on $\mathbb{C}P^{k-2}$, which we call the density of the *complex Bingham distribution for planar shapes,* given by

$$g_A([z]) = f_A(z), \qquad [z] \in \mathbb{C}S^{k-2}. \tag{4.5}$$

Assume λ_A is the largest eigenvalue of A and let V_A be the eigenspace corresponding to λ_A. Then the extrinsic mean set of the complex Bingham distribution for planar shapes is the set $\{[\mu] \mid \mu \in V_A \backslash 0\}$. The extrinsic mean exists only if V_A has dimension one over $\mathbb{C}$. Therefore if $\dim_{\mathbb{C}} V_A \geq 2$, even if the Procrustes estimate (extrinsic sample mean) exists, it is inconsistent.

In general, if $[z_r] = [(z_r^1, \dots, z_r^{k-1})]$, $\|z_r\| = 1$, $r = 1, \dots, n$, are independent observations from a random variable on $\mathbb{C}P^{k-2}$, the extrinsic sample mean $\overline{[z]}_{\mathrm{E}}$ is $[m]$, where m is a highest unit eigenvector of

$$K := \frac{1}{n} \sum_{r=1}^{n} z_r z_r^*. \tag{4.6}$$

Note that $\overline{[z]}_{\mathrm{E}}$ is the full Procrustes estimate for parametric families such as Dryden–Mardia distributions or complex Bingham distribution for planar shapes [Kent (1992)]. Unlike other authors [Kent (1994) and Kendall (1984)], in our computations we do not make any use of the so-called Helmert transform. We simply center the raw landmark data $u_r = (u_r^1, \dots, u_r^k)$, $r = 1, \dots, n$, get $w_r = (w_r^1, \dots, w_r^k)$ with $w_r^j = u_r^j - \overline{u}_r$ and rescale the first $k-1$ transformed coordinates by taking $z_r = \|\tilde{w}_r\|^{-1}\tilde{w}_r$, where $w_r = (\tilde{w}_r^t, w_r^k)$. Then we evaluate K in (4.6) and take the highest eigenvector of K as a representative of $\overline{[z]}_{\mathrm{E}}$. As noted before, given that our identification of Σ_2^k to $\mathbb{C}P^{k-2}$ differs from Kendall's identification, the values of $\overline{[z]}_{\mathrm{E}}$ using the two identification methods may differ. This difference will be small in the case of a highly concentrated distribution, as in the example below.

REMARK 4.1. The extrinsic sample mean can be used to determine missing coordinates when most of the landmarks in a new observation are known. We consider the case of one missing landmark although for more missing landmarks the same principle works. Assume $\overline{[z]}_E = [\zeta]$, $\zeta \in \mathbb{C}S^{k-2}$, is the sample mean of a number of complete observations and $o = (z^1, \dots, z^{k-1}, z)$ are the raw coordinates of a new observation, with z unknown (we may assume w.l.o.g. that the missing landmark is the last one). After centering and rescaling we get

$$(4.7)\qquad w^j = \left(z^j - \frac{1}{k}\left(z + \sum_{s=1}^{k-1} z^s\right)\right) \Big/ \left(\sum_{j=1}^{k}\left|z^j - \frac{1}{k}\left(z + \sum_{s=1}^{k-1} z^s\right)\right|^2\right)^{1/2}.$$

Minimizing $d_0([o], [\zeta])$ amounts to maximizing

$$(4.8)\qquad h(z) = \frac{(\sum_{j=1}^{k-1} |w^j \overline{\zeta^j}|^2)}{\sum_{j=1}^{k-1} |w^j|^2},$$

where w^j are given in (4.7), and the solution gives the missing landmark z conditionally on the sample data and the other landmarks in o. We will call this the *XM method* of retrieval for a single missing landmark.

If $z, w \in \mathbb{C}S^{k-2}$, the Fubini–Study distance $d_g([z], [w])$ is proportional to $\arccos|z^t\overline{w}|$. Therefore the intrinsic mean $\overline{[z]}_{\mathrm{I}}$ of the sample $[z_r]$, $\|z_r\| = 1$, $r = 1, \dots, n$, is a minimizer of

$$(4.9)\qquad g([\zeta]) = \sum_{r=1}^{n} \arccos^2(|z_r^t\overline{\zeta}|), \qquad \|\zeta\| = 1.$$

The minimizer can be determined by selecting $\zeta = (\zeta^1, \dots, \zeta^{k-1})$ with $\zeta^{k-1} > 0$. If for $r = 1, \dots, n$ and $j = 1, \dots, k-1$, we have $\zeta^j = \xi^j + i\eta^j$ and $z_r^j = x_r^j + iy_r^j$, such a minimizer is obtained by using numerical methods for the objective function of $2(k-2)$ real variables

$$\begin{aligned} & g(\xi^1, \xi^2, \ldots, \xi^{k-2}, \eta^1, \eta^2, \ldots, \eta^{k-2}) \\ & = \sum_{r=1}^{n} \arccos^2 \left| z_r^{k-1} \sqrt{1 - \sum_{j=1}^{k-2} ((\xi^j)^2 + (\eta^j)^2)} + \sum_{j=1}^{k-2} z_r^j \overline{\zeta^j} \right|. \end{aligned} \tag{4.10}$$

Because the intrinsic distance is larger than the extrinsic distance (chord $<$ arc) outliers have more influence on the intrinsic sample mean, which makes the use of the extrinsic mean preferable in practice if strong outliers are present. For concentrated data the two means are very close to each other.

We close with an example to compute the mean *Apert syndrome upper midface*, and to use it to estimate a missing landmark. In our example, based on data from Bookstein (1991), we determine the extrinsic mean of a group of 8 landmarks on the Apert syndrome upper midface. The data set represents coordinates of the following landmarks: the Anterior nasal spine, Sella, Spheno-ethmoid registration, Nasion, Orbitale, Inferior zygoma, Pterygomaxillary fissure and Posterior nasal spine taken from lateral X-rays of a group of 14 children suffering from the Apert syndrome. The data are displayed in Figure 1. Note that the coordinates of landmark 7 from "child 9" are missing. The shape variable (in our case, shape of the 8 landmarks on the upper face) is valued in a planar shape space $\mathbb{C}P^6$ (real dimension $= 12$). The usual statistical methods fail when applied to $\mathbb{C}P^{k-2}$ because, as a Riemannian manifold, $\mathbb{C}P^{k-2}$ is not locally Euclidean, whatever the metric we consider on it. As a special case of Theorem 3.3(b), one may show that if the i.i.d. $\mathbb{C}P^{k-2}$-valued observations have a Dryden–Mardia distribution, then the intrinsic and extrinsic means are the same. Thus the extrinsic sample mean is a consistent estimator of the intrinsic mean of Q, by Theorem 2.3 or by Ziezold (1977). This result is due to Kent and Mardia (1997) and Le (1998).

Using MINITAB, from the 13 complete observations, after rescaling, we found the following representative for the extrinsic sample mean shape corresponding to $\overline{[z]}_E = [z^1 : z^2 : z^3 : z^4 : z^5 : z^6 : z^7] \in \mathbb{C}P^6$:

$$\begin{aligned} z^1 &= -0.174205 + 0.351359i, & z^2 &= 0.258564 - 0.431477i, \\ z^3 &= -0.112506 - 0.233028i, & z^4 &= -0.527492 - 0.069521i, \\ z^5 &= -0.117264 + 0.109873i, & z^6 &= 0.113351 + 0.209546i, \\ z^7 &= 0.279319 + 0.000000i, & z^8 &= 0.280233 + 0.063249i. \end{aligned}$$

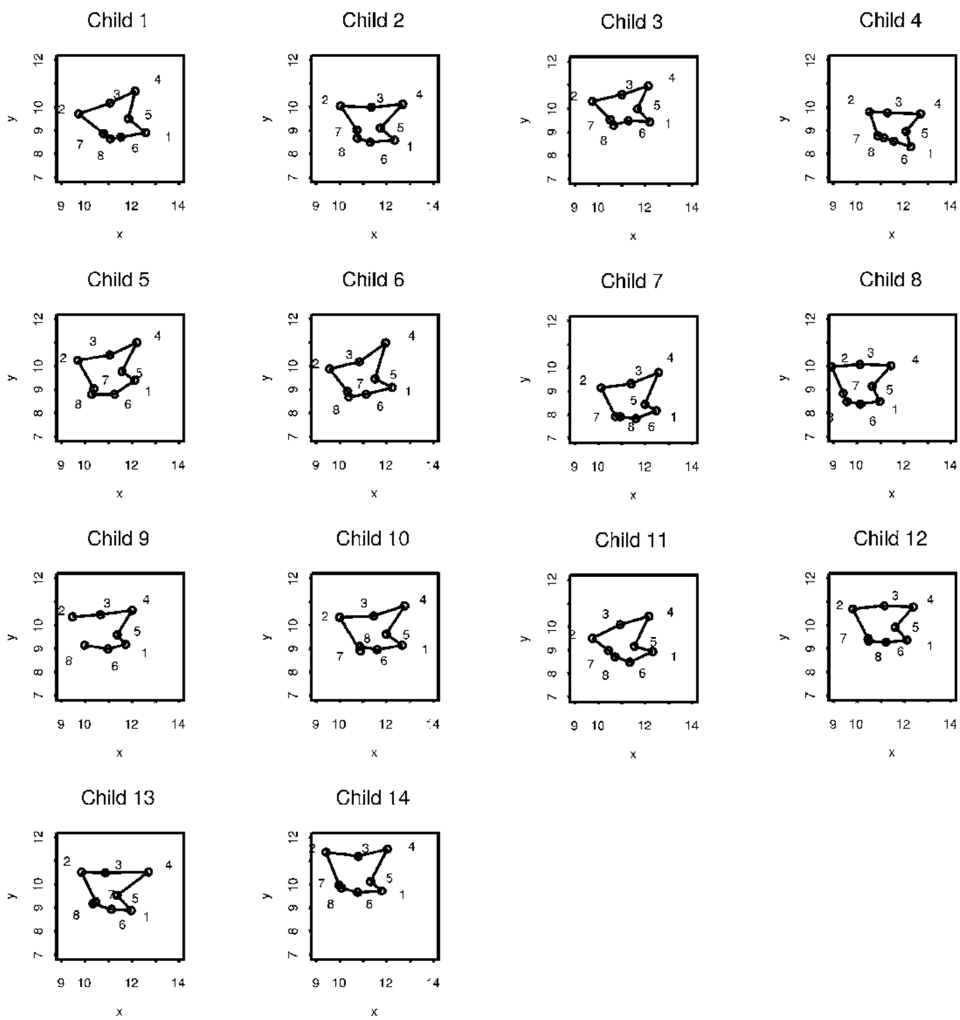

FIG. 1. *Apert data.*

Using MATHEMATICA for the function g in (4.10), we obtained a representative for the intrinsic sample mean shape corresponding to $\overline{[z]}_I = [z^1 : z^2 : z^3 : z^4 : z^5 : z^6 : z^7] \in \mathbb{C}P^6$, which after rescaling, is given by

$$z^1 = -0.174180 + 0.351085i, \qquad z^2 = 0.258289 - 0.431400i,$$
$$z^3 = -0.112757 - 0.232802i, \qquad z^4 = -0.527627 - 0.069441i,$$
$$z^5 = -0.117257 + 0.109764i, \qquad z^6 = 0.113449 + 0.209658i,$$
$$z^7 = 0.279347 + 0.000000i, \qquad z^8 = 0.280736 + 0.063136i.$$

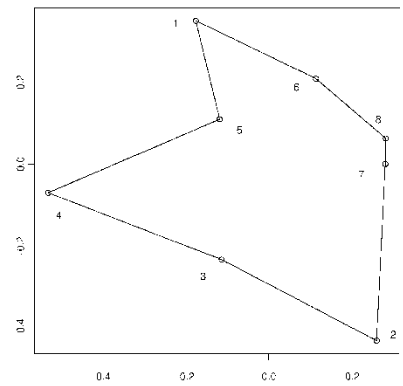

FIG. 2. *Extrinsic sample mean of the* 13 *complete Apert observations.*

The representative of the intrinsic sample mean, including the resulting coordinate $z^8 = -\sum_{j=1}^{7} z^j$, is displayed in Figure 3; it cannot be distinguished from the extrinsic sample mean (cf. Figure 2) since the coordinates of corresponding landmarks are identical to the third decimal.

As explained above, we used a different method of identification of a shape with a point in $\mathbb{C}P^6$. For this reason our result slightly difers from the extrinsic mean obtained using Kendall's method of identification. We also include a representative of the extrinsic sample mean, using Kendall's method of identification [for details on Kendall's method see Kendall (1984)], provided by one of the referees:

$$z^1 = -0.1764454 + 0.3503738i, \qquad z^2 = 0.2619642 - 0.4296601i,$$
$$z^3 = -0.1109860 - 0.2335313i, \qquad z^4 = -0.5270207 - 0.0731476i,$$
$$z^5 = -0.1178114 + 0.1094137i, \qquad z^6 = 0.1123381 + 0.2108623i,$$
$$z^7 = 0.2771263 + 0.0000000i, \qquad z^8 = 0.2808349 + 0.0656893i.$$

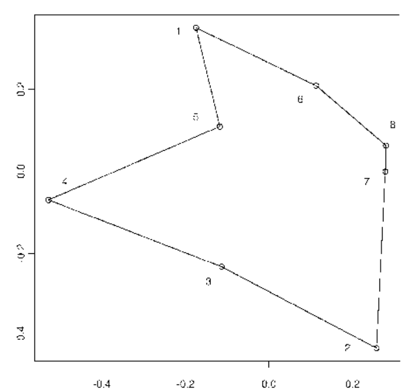

FIG. 3. *Intrinsic sample mean of the* 13 *complete Apert observations.*

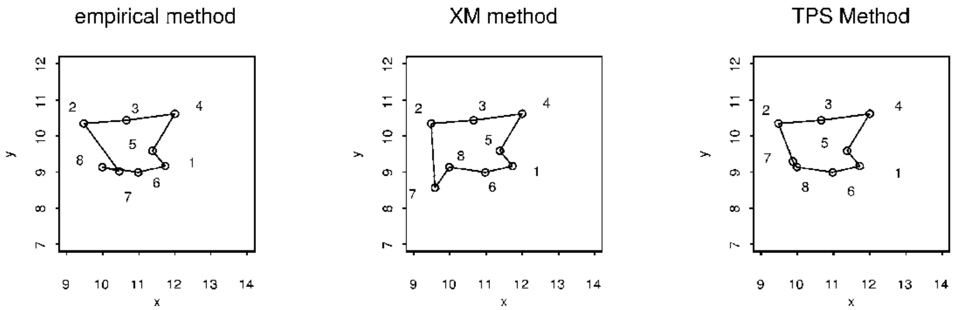

FIG. 4. *Retrival of landmark 7 in observation 9.*

Finally, in Figure 4 we display observation 9 completed by various methods. Our XM method, from formulas (4.7)–(4.8), yields for the missing landmark the coordinate $z_7 = 9.59 + 8.57i$. Unlike the empirical method which yields $z_7 = 10.46 + 9.02i$, the XM method places landmark 7 to the left of landmark 8, in agreement with 9 out of the complete 13 observations.

However, when applied to the Apert data, both the empirical method and the XM method perform worse than the TPS (thin-plate spline) method [see Dryden and Mardia (1998), page 206]. We owe to one of the referees of this paper the value of $z_7 = 9.88 + 9.307i$ based on the TPS method, thus putting landmark 7 above landmark 8, which is the case for 12 out of 13 observations.

For work on missing landmark data see Bookstein and Mardia (2000).

REMARK 4.2. While the computations for Apert data are only illustrative, we believe that similar computations for random samples of clinically normal children from various groups of populations, may be useful in reconstructive plastic surgery.

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LARGE SAMPLE THEORY OF INTRINSIC AND EXTRINSIC SAMPLE MEANS ON MANIFOLDS—II

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This article develops nonparametric inference procedures for estimation and testing problems for means on manifolds. A central limit theorem for Fréchet sample means is derived leading to an asymptotic distribution theory of intrinsic sample means on Riemannian manifolds. Central limit theorems are also obtained for extrinsic sample means w.r.t. an arbitrary embedding of a differentiable manifold in a Euclidean space. Bootstrap methods particularly suitable for these problems are presented. Applications are given to distributions on the sphere S^d (directional spaces), real projective space $\mathbb{R}P^{N-1}$ (axial spaces), complex projective space $\mathbb{C}P^{k-2}$ (planar shape spaces) w.r.t. Veronese–Whitney embeddings and a three-dimensional shape space Σ_3^4.

1. Introduction. Statistical inference for distributions on manifolds is now a broad discipline with wide-ranging applications. Its study has gained momentum in recent years, especially due to applications in biosciences and medicine, and in image analysis. Including in the substantial body of literature in this field are the books by Bookstein [10], Dryden and Mardia [15], Kendall, Barden, Carne and Le [33], Mardia and Jupp [41], Small [49] and Watson [52]. While much of this literature focuses on parametric or semiparametric models, the present article aims at providing a general framework for nonparametric inference for location. This is a continuation of our earlier work [7, 8] where some general properties of extrinsic and intrinsic mean sets on general manifolds were derived, and the problem of consistency of the corresponding sample indices was explored. The main focus of the present article is the derivation of asymptotic distributions of intrinsic and extrinsic

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sample means and confidence regions based on them. We provide classical CLT-based confidence regions and tests based on them, as well as those based on Efron's bootstrap [17].

Measures of location and dispersion for distributions on a manifold M were studied in [7, 8] as Fréchet parameters associated with two types of distances on M. If $j:M \to \mathbb{R}^k$ is an embedding, the Euclidean distance restricted to $j(M)$ yields the *extrinsic mean set* and the *extrinsic total variance*. On the other hand, a *Riemannian distance* on M yields the *intrinsic mean set* and *intrinsic total variance.*

Recall that the *Fréchet mean* of a probability measure Q on a complete metric space (M,ρ) is the minimizer of the function $F(x) = \int \rho^2(x,y)Q(dy)$, when such a minimizer exists and is unique [21]. In general the set of minimizers of F is called the *Fréchet mean set.* The intrinsic mean $\mu_I(Q)$ is the Fréchet mean of a probability measure Q on a *complete* d-dimensional Riemannian manifold M endowed with the geodesic distance d_g determined by the Riemannian structure g on M. It is known that if Q is sufficiently concentrated, then $\mu_I(Q)$ exists [see Theorem 2.2(a)]. The *extrinsic mean* $\mu_E(Q) = \mu_{j,E}(Q)$ of a probability measure Q on a manifold M w.r.t. an embedding $j:M \to \mathbb{R}^k$ is the Fréchet mean associated with the restriction to $j(M)$ of the Euclidean distance in $\mathbb{R}^k$. In [8] it was shown that the extrinsic mean of Q exists if the ordinary mean of $j(Q)$ is a *nonfocal point* of $j(M)$, that is, if there is a *unique* point x_0 on $j(M)$ having the smallest distance from the mean of $j(Q)$. In this case $\mu_{j,E}(Q) = j^{-1}(x_0)$.

It is easier to compute the intrinsic mean if the Riemannian manifold has zero curvature in a neighborhood containing $\operatorname{supp} Q$ [45]. In particular this is the case for distributions on linear projective shape spaces [42]. If the manifold has nonzero curvature around $\operatorname{supp} Q$, it is easier to compute the extrinsic sample mean. It may be pointed out that if Q is highly concentrated as in our medical examples in [8] and in Section 5, the intrinsic and extrinsic means are virtually indistinguishable.

We now provide a summary of the main results in this article. Section 2 is devoted to nonparametric inference for the Fréchet mean of a probability measure Q on a manifold M for which there is a domain U of a chart $\phi: U \to \mathbb{R}^d$ such that $Q(U) = 1$. In Theorem 2.1 it is shown that in this case, under some rather general assumptions, the image of the Fréchet sample mean under ϕ is asymptotically normally distributed around the image of the Fréchet mean of Q. This leads to the asymptotic distribution theory of the intrinsic sample mean on a Riemannian manifold M (Theorems 2.2, 2.3). In Corollaries 2.3 and 2.4 bootstrap confidence regions are derived for the Fréchet mean, with or without a pivot.

Section 3 is devoted to asymptotics of extrinsic sample means. The ideas behind the main result here are essentially due to Hendriks and Landsman [27] and Patrangenaru [44]. The two approaches are somewhat different.

We present in this article an extension of the latter approach. Extrinsic means are commonly used in directional, axial and shape statistics. In the particular case of directional data analysis, that is, when $M = S^{d-1}$ is the unit sphere in $\mathbb{R}^d$, Fisher, Hall, Jing and Wood [19] provided an approach for inference using computationally efficient bootstrapping which gets around the problem of increased dimensionality associated with the embedding of the manifold M in a higher-dimensional Euclidean space. In Corollary 3.2 confidence regions are derived for the extrinsic mean $\mu_{j,E}(Q)$. Nonparametric bootstrap methods on abstract manifolds are also derived in this section (Theorem 3.2, Proposition 3.2).

If one assumes that Q has a nonzero absolutely continuous component with respect to the volume measure on M, then from some results of Bhattacharya and Ghosh [6], Babu and Singh [1], Beran [2] and Hall [24, 25], one derives bootstrap-based confidence regions for $\mu_E(Q)$ with coverage error $O_p(n^{-2})$ (Theorem 3.4) (also see [5, 9]). One may also use the nonpivotal bootstrap to construct confidence regions based on the percentile method of Hall [25] for general Q with a coverage error no more than $O_p(n^{-d/(d+1)})$, where d is the dimension of the manifold (see Remark 2.4 and Proposition 3.2). This is particularly useful in those cases where the asymptotic dispersion matrix is difficult to compute.

Section 4 applies the preceding theory to (i) real projective spaces $\mathbb{R}^{N-1}$—the *axial spaces*, and (ii) complex projective spaces $\mathbb{C}P^{k-2}$—the *shape spaces*. Another application to products of real projective spaces $(\mathbb{R}P^m)^{k-m-1}$, or the so-called *projective shape spaces*, will appear in [42].

As an application of Corollary 3.3, large sample confidence regions for mean axes are described in Corollary 4.2. A similar application to projective shape spaces, combining bootstrap methods for directional data from [3], appears in [42]. Other applications to axial spaces are given in Theorem 4.3 and Corollary 4.4, and to planar shape spaces in Theorem 4.5.

Finally in Section 5 we apply the results of Sections 2 and 4 to construct (1) a 95% large sample confidence region for the intrinsic mean location of the magnetic South Pole from a directional data set given in [20], (2) simultaneous confidence intervals for the affine coordinates of the extrinsic sample mean shape in a medical application and (3) a test for the difference between three-dimensional mean shapes in a glaucoma detection problem.

2. A central limit theorem for Fréchet sample means and bootstrapping. A d-dimensional *differentiable manifold* is a locally compact separable Hausdorff space M, together with an *atlas* $\mathcal{A}_M$ comprising a family of *charts* (U_α, ϕ_α) of open sets U_α covering M, and for each α a homeomorphism ϕ_α of U_α onto an open subset of $\mathbb{R}^d$ for which the transition maps $\phi_\alpha \cdot \phi_\beta^{-1} : \phi_\beta(U_\alpha \cap U_\beta) \to \phi_\alpha(U_\alpha \cap U_\beta)$ are of class $\mathcal{C}^\infty$. The sets U_α

are often called *coordinate neighborhoods*. One may show that a differentiable manifold is metrizable. We briefly recall some basic notion associated with Riemannian manifolds. For details the reader may refer to any standard text on differential geometry (e.g., [13, 26], or [38]). A *Riemannian metric* g on a differentiable manifold M is a $\mathcal{C}^\infty$ symmetric positive definite tensor field of type $(2,0)$, that is, a family of inner products $g_p = \langle\cdot,\cdot\rangle_p$ on the tangent spaces $T_pM, p \in M$, which is differentiable w.r.t. p. A *Riemannian manifold* M is a connected differentiable manifold endowed with a Riemannian metric g. The distance ρ_g induced by g is called the *geodesic distance*. For $p, q \in M, \rho_g(p,q)$ is the infimum of lengths $\int_a^b \langle \dot{x}(t), \dot{x}(t)\rangle_{x(t)}^{1/2}\,dt$ of all $\mathcal{C}^1$-curves $x(t), a \le t \le b$, with $x(a) = p, x(b) = q$. The minimizer satisfies a variational equation whose solution is a *geodesic curve*. There is a unique such geodesic curve $t \to \gamma(t)$ for any initial point $\gamma(0) = p$ and initial tangent vector $\dot{\gamma}(0) = v$. A classical result of Hopf and Rinow states that (M, ρ_g) is complete as a metric space if and only if (M, g) is *geodesically complete* [i.e., every geodesic curve $\gamma(t)$ is defined for all $t \in \mathbb{R}$]. These two equivalent properties of completeness are in turn equivalent to a third property: *all closed bounded subsets of* (M, ρ_g) *are compact* ([13], pages 146 and 147).

Given $q \in M$, the *exponential map* $\mathrm{Exp}_q : U \to M$ is defined on an open neighborhood U of $0 \in T_qM$ by the correspondence $v \to \gamma_v(1)$, where $\gamma_v(t)$ is the unique geodesic satisfying $\gamma(0) = q, \dot{\gamma}(0) = v$, provided $\gamma(t)$ extends at least to $t = 1$. Thus if (M, g) is geodesically complete or, equivalently, (M, ρ_g) is complete as a metric space, then Exp_q is defined on all of T_qM. In this article, unless otherwise specified, all *Riemannian manifolds are assumed to be complete*.

Note that if $\gamma(0) = p$ and $\gamma(t)$ is a geodesic, it is generally not true that the geodesic distance between p and $q = \gamma(t_1)$, say, is minimized by $\gamma(t), 0 \le t \le t_1$ (consider, e.g., the great circles on the sphere S^2 as geodesics). Let $t_0 = t_0(p)$ be the supremum of all $t_1 > 0$ for which this minimization holds. If $t_0 < \infty$, then $\gamma(t_0)$ is the *cut point of* p *along* γ. The *cut locus* $C(p)$ of p is the union of all cut points of p along all geodesics γ starting at p [e.g., $C(p) = \{-p\}$ on S^2].

In this article we deal with both intrinsic and extrinsic means. Hence we will often consider a general distance ρ on a differentiable manifold M, but assume that (M, ρ) is complete as a metric space. We consider only those probability measures Q on M for which the Fréchet mean $\mu_{\mathcal{F}} = \mu_{\mathcal{F}}(Q)$ exists. Moreover *we assume that there is a chart* (U, ϕ) *such that* $Q(U) = 1$, *and* $\mu_{\mathcal{F}} \in U$.

REMARK 2.1. The assumption above on the existence of a chart (U, ϕ) such that $Q(U) = 1$ is less restrictive than it may seem. If g is a Riemannian structure on M and Q is absolutely continuous w.r.t. the volume measure, then, for any given p, the complement U of the cut locus $C(p)$ is the domain of definition of such a local coordinate system (the coordinate map being the inverse of Exp_p, the exponential map at p) (see [38], page 100, for details).

EXAMPLE 2.1. For the d-dimensional unit sphere, $M = S^d = \{p \in \mathbb{R}^{d+1} : \|p\| = 1\}$, with the Riemannian metric induced by the Euclidean metric on $\mathbb{R}^{d+1}$, the exponential map at a given point $p \in S^d$ is defined on the tangent space T_pM and is given by

$$\mathrm{Exp}_p(v) = \cos(\|v\|)p + \sin(\|v\|)\|v\|^{-1}v \qquad (v \in T_pS^d, v \neq 0). \tag{2.1}$$

If $x \in S^d, x \neq -p$, then there is a unique vector $u \in T_pM$ such that $x = \mathrm{Exp}_p u$, and we will label this vector by $u = \mathrm{Log}_p x$. Since $T_pS^d = \{v \in \mathbb{R}^{d+1}, v \cdot p = 0\}$, it follows that

$$\mathrm{Log}_p x = (1 - (p \cdot x)^2)^{-1/2} \arccos(p \cdot x)(x - (p \cdot x)p). \tag{2.2}$$

In particular, for $d = 2$ we consider the orthobasis $e_1(p), e_2(p) \in T_pS^2$, where $p = (p_1, p_2, p_3)^t \in S^2 \backslash \{N, S\}$ $[N = (0, 0, 1), S = (0, 0, -1)]$:

$$\begin{aligned} e_1(p) &= ((p_1)^2 + (p_2)^2)^{-1/2}(-p_2, p_1, 0)^t, \\ e_2(p) &= (-((p_1)^2 + (p_2)^2)^{-1/2} p_1 p_3, \\ &\qquad -(x^2 + y^2)^{-1/2} p_2 p_3, ((p_1)^2 + (p_2)^2)^{1/2})^t. \end{aligned} \tag{2.3}$$

The *logarithmic coordinates* of the point $x = (x_1, x_2, x_3)^T$ are given in this case by

$$\begin{aligned} u^1(p) &= e_1(p) \cdot \mathrm{Log}_p x, \\ u^2(p) &= e_2(p) \cdot \mathrm{Log}_p x. \end{aligned} \tag{2.4}$$

For computations one may use $a \cdot b = a^t b$.

Now the image measure Q^ϕ of Q under ϕ has the Fréchet mean $\mu = \phi(\mu_{\mathcal{F}})$ w.r.t. the distance $\rho^\phi(u, v) := \rho(\phi^{-1}(u), \phi^{-1}(v)), u, v \in \phi(U)$. Similarly, if X_i $(i = 1, \dots, n)$ are i.i.d. with common distribution Q and defined on a probability space $(\Omega, \mathcal{A}, P)$, let $\mu_{n,\mathcal{F}}$ be a measurable selection from the Fréchet mean set (w.r.t. ρ) of the empirical $\hat{Q}_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$. Then $\mu_n = \phi(\mu_{n,\mathcal{F}})$ is a measurable selection from the Fréchet mean set (w.r.t. ρ^ϕ) of $\hat{Q}_n^\phi = \frac{1}{n}\sum_{i=1}^n \delta_{\tilde{X}_i}$, where $\tilde{X}_i = \phi(X_i)$. Assuming twice continuous differentiability of $\theta \to (\rho^\phi)^2(u, \theta)$, write the Euclidean gradient as

$$\Psi(u; \theta) = \mathrm{grad}_\theta (\rho^\phi)^2(u, \theta) = \left(\frac{\partial}{\partial \theta^r}(\rho^\phi)^2(u, \theta)\right)_{r=1}^d = (\Psi^r(u; \theta))_{r=1}^d. \tag{2.5}$$

Now μ is the point of minimum of

$$F^\phi(\theta) := \int (\rho^\phi)^2(u, \theta) Q^\phi(du) \tag{2.6}$$

and μ_n is a local minimum of

$$F_n^{\phi}(\theta) := \int (\rho^{\phi})^2(u,\theta)\hat{Q}_n^{\phi}(du).$$

Therefore, one has the Taylor expansion

$$\begin{aligned} 0 &= \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\Psi^r(\tilde{X}_i;\mu_n) \\ &= \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\Psi^r(\tilde{X}_i;\mu) \\ &\quad + \frac{1}{n}\sum_{i=1}^{n}\sum_{r'=1}^{d} D_{r'}\Psi^r(\tilde{X}_i;\mu)\sqrt{n}(\mu_n^{r'}-\mu^{r'}) + R_n^r \qquad (1 \le r \le d), \end{aligned} \tag{2.7}$$

where

$$R_n^r = \sum_{r'=1}^{d}\sqrt{n}(\mu_n^{r'}-\mu^{r'})\frac{1}{n}\sum_{i=1}^{n}\{D_{r'}\Psi^r(\tilde{X}_i;\theta_n) - D_{r'}\Psi^r(\tilde{X}_i;\mu)\} \tag{2.8}$$

and θ_n lies on the line segment joining μ and μ_n (for sufficiently large n). We will assume

$$\begin{aligned} E|\Psi(\tilde{X}_i;\mu)|^2 &< \infty, \\ E|D_{r'}\Psi^r(\tilde{X}_i;\mu)|^2 &< \infty \qquad (\forall\, r, r'). \end{aligned} \tag{2.9}$$

To show that R_n^r is negligible, write

$$u^{r,r'}(x,\varepsilon) := \sup_{\{\theta:\, \|\theta-\mu\|\le\varepsilon\}} |D_{r'}\Psi^r(x;\theta) - D_{r'}\Psi^r(x;\mu)|$$

and assume

$$\delta^{r,r'}(c) := Eu^{r,r'}(\tilde{X}_i, c) \to 0 \qquad \text{as } c \downarrow 0 \ (1 \le r, r' \le d). \tag{2.10}$$

One may then rewrite (2.7) in vectorial form as

$$0 = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\Psi(\tilde{X}_i;\mu) + (\Lambda + \delta_n)\sqrt{n}(\mu_n - \mu), \tag{2.11}$$

where

$$\Lambda = E((D_{r'}\Psi^r(\tilde{X}_i;\mu)))_{r,r'=1}^{d} \tag{2.12}$$

and $\delta_n \to 0$ in probability as $n \to \infty$, if $\mu_n \to \mu$ in probability. If, finally, we assume Λ is nonsingular, then (2.11) leads to the equation

$$\sqrt{n}(\mu_n - \mu) = \Lambda^{-1}\left(\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\Psi(\tilde{X}_i;\mu)\right) + \delta_n', \tag{2.13}$$

where δ_n' goes to zero in probability as $n \to \infty$. We have then arrived at the following theorem.

THEOREM 2.1 (CLT for Fréchet sample means). *Let Q be a probability measure on a differentiable manifold M endowed with a metric ρ such that every closed and bounded set of (M,ρ) is compact. Assume* (i) *the Fréchet mean $\mu_{\mathcal{F}}$ exists,* (ii) *there exists a coordinate neighborhood (U,ϕ) such that $Q(U)=1$,* (iii) *the map $\theta \to (\rho^\phi)^2(\theta,u)$ is twice continuously differentiable on $\phi(U)$,* (iv) *the integrability conditions* (2.9) *hold as well as the relation* (2.10) *and* (v) *Λ, defined by* (2.12), *is nonsingular. Then* (a) *every measurable selection μ_n from the (sample) Fréchet mean set of $\hat{Q}_n^\phi = \frac{1}{n}\sum_{i=1}^n \delta_{\tilde{X}_i}$ is a consistent estimator of μ, and* (b) $\sqrt{n}(\mu_n - \mu) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Lambda^{-1}C(\Lambda^t)^{-1})$, *where C is the covariance matrix of $\Psi(\tilde{X}_i;\mu)$.*

PROOF. Part (a) follows from Theorem 2.3 in [8]. The proof of part (b) is as outlined above, and it may also be derived from standard proofs of the CLT for M-estimators (see, e.g., [29], pages 132–134). □

As an immediate corollary one obtains:

COROLLARY 2.1. *Let (M,g) be a Riemannian manifold and let $\rho=\rho_g$ be the geodesic distance. Let Q be a probability measure on M whose support is compact and is contained in a coordinate neighborhood (U,ϕ). Assume that* (i) *the intrinsic mean $\mu_I=\mu_{\mathcal{F}}$ exists,* (ii) *the map $\theta \to (\rho^\phi)^2(\theta,u)$ is twice continuously differentiable on $\phi(U)$ for each $u\in\phi(U)$ and Λ, defined by* (2.12), *is nonsingular. Then the conclusions of Theorem* 2.1 *hold for the intrinsic sample mean $\mu_{n,I}=\mu_{n,\mathcal{F}}$ of $\hat{Q}_n=\frac{1}{n}\sum_{i=1}^n \delta_{X_i}$, with $\mu=\phi(\mu_I)$.*

We now prove one of the main results of this section.

THEOREM 2.2 (CLT for intrinsic sample means). *Let (M,g) be a Riemannian manifold and let $\rho=\rho_g$ be the geodesic distance. Let Q be a probability measure on M whose support is contained in a closed geodesic ball $\overline{B}_r \equiv \overline{B}_r(x_0)$ with center x_0 and radius r which is disjoint from the cut locus $C(x_0)$. Assume $r<\frac{\pi}{4K}$, where K^2 is the supremum of sectional curvatures in $\overline{B}_r$ if this supremum is positive, or zero if this supremum is nonpositive. Then* (a) *the intrinsic mean μ_I (of Q) exists, and* (b) *the conclusion of Theorem* 2.1 *holds for the image $\mu_n=\phi(\mu_{n,I})$ of the intrinsic sample mean $\mu_{n,I}$ of $\hat{Q}_n=\frac{1}{n}\sum_{i=1}^n \delta_{X_i}$, under the inverse ϕ of the exponential map, $\phi=(\mathrm{Exp}_{x_0})^{-1}$.*

PROOF. (a) It is known that under the given assumptions, there is a *local minimum* μ_I, say, of the Fréchet function F which belongs to B_r and that this minimum is also the *unique* minimum in $\overline{B}_{2r}$ [30, 34, 40]. We now show that μ_I is actually the unique *global minimum* of F. Let $p \in (\overline{B}_{2r})^c$. Then $\rho(p,x) > r, \forall\, x \in \overline{B}_r$. Hence

$$F(p) = \int_{\overline{B}_r} \rho^2(p,x)Q(dx) > \int_{\overline{B}_r} r^2 Q(dx) = r^2. \tag{2.14}$$

On the other hand,

$$F(\mu_I) \le F(x_0) = \int_{\overline{B}_r} \rho^2(x_0,x)Q(dx) \le r^2, \tag{2.15}$$

proving $F(p) > F(\mu_I)$.

(b) In view of Corollary 2.1, we only need to show that the Hessian matrix $\Lambda \equiv \Lambda(\mu)$ of $F \circ \phi^{-1}$ at $\mu := \phi(\mu_I)$ is nonsingular, where $\phi = \mathrm{Exp}_{x_0}^{-1}$. Now according to [30], Theorem 1.2, for every geodesic curve $\gamma(t)$ in $B_r, t \in (c,d)$ for some $c < 0, d > 0$,

$$\frac{d^2}{dt^2} F(\gamma(t)) > 0 \qquad (c < t < d). \tag{2.16}$$

Let $\psi = \mathrm{Exp}_{\mu_I}$ denote the exponential map at μ_I, and let $\gamma(t)$ be the unique geodesic with $\gamma(0) = \mu_I$ and $\dot\gamma(0) = v$, so that $\gamma(t) = \psi(tv)$. Here we identify the tangent space $T_{\mu_I}M$ with $\mathbb{R}^d$. Applying (2.16) to this geodesic (at $t = 0$), and writing $G = F \circ \psi$, one has

$$\left.\frac{d^2}{dt^2} F(\psi(tv))\right|_{t=0} = \sum v^i v^j (D_i D_j G)(0) > 0 \qquad (\forall\, v \neq 0), \tag{2.17}$$

that is, the Hessian of G is positive definite at $0 \in \mathbb{R}^d$. If $x_0 = \mu_I$, this completes the proof of (b).

Next let $x_0 \neq \mu_I$. Now $F \circ \phi^{-1} = G \circ (\psi^{-1} \circ \phi^{-1})$ on a domain that includes $\mu = \phi(\mu_I) \equiv (\mathrm{Exp}_{x_0})^{-1}(\mu_I)$. Write $\psi^{-1} \circ \phi^{-1} = f$. Then in a neighborhood of μ,

$$\begin{aligned} \frac{\partial^2 (G \circ f)}{\partial u^r\, \partial u^{r'}}(u) &= \sum_{j,j'} (D_j D_{j'} G)(f(u)) \frac{\partial f^j}{\partial u^r}(u) \frac{\partial f^{j'}}{\partial u^{r'}}(u) \\ &\quad + \sum_j (D_j G)(f(u)) \frac{\partial^2 f^j}{\partial u^r\, \partial u^{r'}}(u). \end{aligned} \tag{2.18}$$

The second sum in (2.18) vanishes at $u = \mu$, since $(D_jG)(f(\mu)) = (D_jG)(0) = 0$ as $f(\mu) = \psi^{-1}\phi^{-1}(\mu) = \psi^{-1}(\mu_I) = 0$ is a local minimum of G. Also f is a diffeomorphism in a neighborhood of μ. Hence, writing $\Lambda_{r,r'}(\mu)$ as the (r,r') element of $\Lambda(\mu)$,

$$\Lambda_{r,r'}(\mu) = \frac{\partial^2 (F \circ \phi^{-1})}{\partial u^r\, \partial u^{r'}}(\mu) = \sum_{j,j'} (D_j D_{j'} G)(0) \frac{\partial f^j}{\partial u^r}(\mu) \frac{\partial f^{j'}}{\partial u^{r'}}(\mu).$$

This shows, along with (2.17), that $\Lambda = \Lambda(\mu)$ is positive definite. $\square$

REMARK 2.2. If the supremum of the sectional curvatures (of a complete manifold M) is nonpositive, and the support of Q is contained in $\overline{B}_r$, then the hypotheses of Theorem 2.2 are satisfied, and the conclusions (a), (b) hold. One may apply this even with $r = \infty$.

REMARK 2.3. The assumptions in Theorem 2.2 on the support of Q for the existence of μ_I are too restrictive for general applications. But without additional structures they cannot be entirely dispensed with, as is easily shown by letting Q be the uniform distribution on the equator of S^2. For the complex projective space $\mathbb{C}P^{d/2}$, d even, necessary and sufficient conditions for the existence of the intrinsic mean μ_I of an absolutely continuous (w.r.t. the volume measure) Q with radially symmetric density are given in [33, 39].

It may be pointed out that it is the assumption of some symmetry, that is, the invariance of Q under a group of isometries, that often causes the intrinsic mean set to contain more than one element (see, e.g., [8], Proposition 2.2). The next result is, therefore, expected to be more generally applicable than Theorem 2.2.

THEOREM 2.3 (CLT for intrinsic sample means). *Let Q be absolutely continuous w.r.t. the volume measure on a Riemannian manifold (M, g). Assume that* (i) *μ_I exists,* (ii) *the integrability conditions* (2.9) *hold,* (iii) *the Hessian matrix Λ of $F \circ \phi^{-1}$ at $\mu = \phi(\mu_I)$ is nonsingular and* (iv) *the covariance matrix C of $\Psi(\tilde{X}_i; \mu)$ is nonsingular. Then $\sqrt{n}(\mu_n - \mu) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Gamma)$, where $\Gamma = \Lambda^{-1}C(\Lambda^t)^{-1}$.*

This theorem follows from Theorem 2.1 and Remark 2.1.

In order to obtain a confidence region for $\mu_{\mathcal{F}}$ using the CLT in Theorem 2.1 in the traditional manner, one needs to estimate the covariance matrix $\Gamma = \Lambda^{-1}C(\Lambda^t)^{-1}$. For this one may use proper estimates of Λ and C, namely,

$$\begin{aligned} \hat{\Lambda}(\theta) &:= \frac{1}{n}\sum_{i=1}^{n}(\operatorname{Grad}\Psi)(\tilde{X}_i, \mu_n), &\qquad \hat{C} &= \operatorname{Cov}\hat{Q}_n^{\phi}, \\ \hat{\Gamma} &:= \hat{\Lambda}^{-1}\hat{C}(\hat{\Lambda}^t)^{-1}, &\qquad \hat{\Gamma}^{-1} &= \hat{\Lambda}^t\hat{C}^{-1}\hat{\Lambda}. \end{aligned} \tag{2.19}$$

The following corollary is now immediate. Let $\chi^2_{d,1-\alpha}$ denote the $(1-\alpha)$th quantile of the chi-square distribution with d degrees of freedom.

COROLLARY 2.2. *Under the hypothesis of Theorem 2.1, if C is nonsingular, a confidence region for $\mu_{\mathcal{F}}$ of asymptotic level $1-\alpha$ is given by $U_{n,\alpha} := \phi^{-1}(D_{n,\alpha})$, where $D_{n,\alpha} = \{v \in \phi(U) : n(\mu_n - v)^t\hat{\Gamma}^{-1}(\mu_n - v) \le \chi^2_{d,1-\alpha}\}$.*

EXAMPLE 2.2. In the case of the sphere S^2 from Example 2.1, it follows that if we consider an arbitrary data point $u = (u^1, u^2)$, and a second point $\theta = \mathrm{Log}_p \lambda = (\theta^1, \theta^2)$, and evaluate the matrix of second-order partial derivatives w.r.t. θ^1, θ^2 of

$$G(u,\theta) = \arccos^2\left(\cos\|u\| + \frac{\sin\|u\|}{\|u\|}(u^1\theta^1 + u^2\theta^2) - \frac{1}{2}\|\theta\|^2\cos\|u\|\right), \tag{2.20}$$

then

$$\frac{\partial^2 G}{\partial\theta^r\,\partial\theta^s}(u;0) = \frac{2u^r u^s}{\|u\|^2}\left(1 - \frac{\|u\|}{\tan\|u\|}\right) + \frac{2\delta_{rs}\|u\|}{\tan\|u\|}, \tag{2.21}$$

where δ_{rs} is the Kronecker symbol and $\|u\|^2 = (u^1)^2 + (u^2)^2$. The matrix $\hat\Lambda = (\lambda_{rr'})_{r,r'=1,2}$ has the entries

$$\lambda_{rr'} = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial^2 G}{\partial\theta^r\,\partial\theta^{r'}}(u_i;0). \tag{2.22}$$

Assume $\hat C$ is the sample covariance matrix of $u_j, j = 1,\dots,n$; a large sample confidence region for the intrinsic mean is given by Corollary 2.2 with $\mu_n = 0$.

We now turn to the problem of bootstrapping a confidence region for $\mu_{\mathcal F}$. Let $X^*_{i,n}$ be i.i.d. with common distribution $\hat Q_n$ (conditionally, given $\{X_i : 1 \le i \le n\}$). Write $\tilde X^*_{i,n} = \phi(X^*_{i,n}), 1 \le i \le n$, and let μ^*_n be a measurable selection from the Fréchet mean set of $\hat Q^{*,\phi}_n := \frac{1}{n}\sum_{i=1}^n \delta_{\tilde X^*_{i,n}}$. Let $E^*_{n,\alpha}$ be a subset of $\phi(U)$, such that $P^*(\mu^*_n - \mu_n \in E^*_{n,\alpha}) \to 1-\alpha$ in probability, where P^* denotes the probability under $\hat Q_n$.

COROLLARY 2.3. *In addition to the hypothesis of Theorem 2.1, assume C is nonsingular. Then $\phi^{-1}(\{(\mu_n - E^*_{n,\alpha}) \cap \phi(U)\})$ is a confidence region for $\mu_{\mathcal F}$ of asymptotic level $(1-\alpha)$.*

PROOF. One may write (2.7) and (2.8) with μ and μ_n replaced by μ_n and μ^*_n, respectively, also replacing $\tilde X_i$ by $\tilde X^*_i$ in (2.8). To show that a new version of (2.11) holds with similar replacements (also replacing Λ by $\hat\Lambda$), with a δ^*_n (in place of δ_n) going to zero in probability, one may apply Chebyshev's inequality with a first-order absolute moment under $\hat Q_n$, proving that $\hat\Lambda^* - \hat\Lambda$ goes to zero in probability. Here $\hat\Lambda^* = \frac{1}{n}\sum_{i=1}^n (\mathrm{Grad}\,\Psi)(\tilde X^*_i; \mu^*_n)$. One then arrives at the desired version of (2.7), replacing $\mu_n, \mu, \Lambda, \tilde X_i$ by $\mu^*_n, \mu_n, \hat\Lambda, \tilde X^*_i$, respectively, and with the remainder (corresponding to δ'_n) going to zero in probability. □

REMARK 2.4. In Corollary 2.3, we have considered the so-called *percentile bootstrap* of Hall [25] (also see [17]), which does not require the computation of the standard error $\hat{\Lambda}$. For this as well as for the CLT-based confidence region given by Corollary 2.2, one can show that the coverage error is no more than $O_p(n^{-d/(d+1)})$ or $O(n^{-d/(d+1)})$, as the case may be [4]. One may also use the bootstrap distribution of the *pivotal statistic* $n(\mu_n-\mu)^T\hat{\Gamma}^{-1}(\mu_n-\mu)$ to find $c^*_{n,\alpha}$ such that

$$P^*(n(\mu^*_n-\mu_n)^T\hat{\Gamma}^{*-1}(\mu^*_n-\mu_n)\le c^*_{n,\alpha})\simeq 1-\alpha, \tag{2.23}$$

to find the confidence region

$$D^*_{n,\alpha}=\{v\in\phi(U):n(\mu_n-v)^T\hat{\Gamma}^{-1}(\mu_n-v)\le c^*_{n,\alpha}\}. \tag{2.24}$$

In particular, if Q has a nonzero absolutely continuous component w.r.t. the volume measure on M, then so does Q^ϕ w.r.t. the Lebesgue measure on $\phi(U)$ (see [13], page 44). Then assuming (a) $c^*_{n,\alpha}$ is such that the P^*-probability in (2.23) equals $1-\alpha+O_p(n^{-2})$ and (b) some additional smoothness and integrability conditions of the third derivatives of Ψ, one can show that the coverage error [i.e., the difference between $1-\alpha$ and $P(\mu\in D^*_{n,\alpha})$] is $O_p(n^{-2})$ (see [5, 6, 12, 24, 25]). It follows that the coverage error of the confidence region $\phi^{-1}(D^*_{n,\alpha}\cap\phi(U))$ for $\mu_{\mathcal{F}}$ is also $O(n^{-2})$. We state one such result precisely.

COROLLARY 2.4 (Bootstrapping the intrinsic sample mean). *Suppose the hypothesis of Theorem 2.3 holds. Then*

$$\sup_{r>0}|P^*(n(\mu^*_n-\mu_n)^T\hat{\Gamma}^{*-1}(\mu^*_n-\mu_n)\le r)$$
$$-P(n(\mu_n-\mu)^T\hat{\Gamma}^{-1}(\mu_n-\mu)\le r)|=O_p(n^{-2}),$$

and the coverage error of the pivotal bootstrap confidence region is $=O_p(n^{-2})$.

REMARK 2.5. The assumption of absolute continuity of Q in Theorem 2.3 is reasonable for most applications. Indeed this is assumed in most parametric models in directional and shape analysis (see, e.g., [15, 52]).

REMARK 2.6. The results of this section may be extended to the two-sample problem, or to paired samples, in a fairly straightforward manner. For example, in the case of paired observations $(X_i,Y_i), i=1,\dots,n$, let X_i have (marginal) distribution Q, and intrinsic mean μ_I, and let Q_2 and ν_I be the corresponding quantities for Y_i. Let $\phi=\mathrm{Exp}^{-1}_{x_0}$ for some x_0, and let μ,ν and μ_n,ν_n be the images under ϕ of the intrinsic population and sample means. Then one arrives at the following [see (2.13)]:

$$\sqrt{n}(\mu_n-\mu)-\sqrt{n}(\nu_n-\nu)\xrightarrow{\mathcal{L}}\mathcal{N}(0,\Gamma), \tag{2.25}$$

where Γ is the covariance matrix of $\Lambda_1^{-1}\Psi(\tilde{X}_i;\mu) - \Lambda_2^{-1}\Psi(\tilde{Y}_i;\nu)$. Here Λ_i is the Hessian matrix of $F \circ \phi^{-1}$ for Q_i $(i = 1, 2)$. Assume Γ is nonsingular. Then a CLT-based confidence region for $\gamma := \mu - \nu$ is given in terms of $\gamma_n := \mu_n - \nu_n$ by $\{v \in \mathbb{R}^d : n(\gamma_n - v)\hat{\Gamma}^{-1}(\gamma_n - v) \le \chi^2_{d,1-\alpha}\}$. Alternatively, one may use a bootstrap estimate of the distribution of $\sqrt{n}(\gamma_n - \gamma)$ to derive a confidence region.

In Section 5 we consider two applications of results in this section (and one application of the results in Sections 3 and 4). Application 1 deals with the data from a paleomagnetic study of the possible migration of the Earth's magnetic poles over geological time scales. Here $M = S^2$ and the geodesic distance between two points is the arclength between them measured on the great circle passing through them.

Application 3 analyzes some recent three-dimensional image data on the effect of a (temporary) glaucoma-inducing treatment in 12 Rhesus monkeys. On each animal $k = 4$ carefully chosen landmarks are measured on each eye—the normal eye and the treated eye. For each observation (a set of four points in $\mathbb{R}^3$) the effects of translation, rotation and size are removed to obtain a sample of 12 points on the five-dimensional shape orbifold Σ_3^4. We use the so-called three-dimensional Bookstein coordinates to label these points (see [15], pages 78–80). In order to apply Theorem 2.3 (i.e., its analog indicated above), a somewhat flat Riemannian structure is chosen so that the necessary assumptions can be verified.

3. The CLT for extrinsic sample means and confidence regions for the extrinsic mean. From Theorem 2.1 one may derive a CLT for extrinsic sample means similar to Corollary 2.1. In this section, however, we use another approach which, for extrinsic means, is simpler to apply and generally less restrictive.

Recall that the extrinsic mean $\mu_{j,E}(Q)$ of a nonfocal probability measure Q on a manifold M w.r.t. an embedding $j : M \to \mathbb{R}^k$, when it exists, is given by $\mu_{j,E}(Q) = j^{-1}(P_j(\mu))$, where μ is the mean of $j(Q)$ and P_j is the projection on $j(M)$ (see [8], Proposition 3.1, e.g.). Often the extrinsic mean will be denoted by $\mu_E(Q)$, or simply μ_E, when j and Q are fixed in a particular context. To ensure the existence of the extrinsic mean set, in this section we will assume that $j(M)$ is closed in $\mathbb{R}^k$.

Assume $(X_1, \dots, X_n)$ are i.i.d. M-valued random objects whose common probability distribution is Q, and let $\overline{X}_E := \mu_E(\hat{Q}_n)$ be the *extrinsic sample mean*. Here $\hat{Q}_n = \frac{1}{n}\sum_{j=1}^n \delta_{X_j}$ is the empirical distribution.

A CLT for the extrinsic sample mean on a *submanifold* M of $\mathbb{R}^k$ (with j the inclusion map) was derived by Hendriks and Landsman [27] and, independently, by Patrangenaru [44] by different methods. Differentiable manifolds that are not a priori submanifolds of $\mathbb{R}^k$ arise in new areas of data analysis such as in shape analysis, in high-level image analysis, or in signal and image processing (see, e.g., [15, 16, 22, 31, 32, 33, 42, 51]). These manifolds, known under the names of shape spaces and projective shape spaces, are quotient spaces of submanifolds of $\mathbb{R}^k$ (spaces of orbits of actions of Lie groups), rather than submanifolds of $\mathbb{R}^k$. Our approach is a generalization of the adapted frame method of Patrangenaru [44] to closed embeddings in $\mathbb{R}^k$. This method leads to an appropriate dimension reduction in the CLT and, thereby, reduces computational intensity. This method extends the results of Fisher et al. [19] who considered the case $M = S^d$. We expect that with some effort the results of Hendriks and Landsman [27] may be modified to yield the same result.

Assume j is an embedding of a d-dimensional manifold M such that $j(M)$ is closed in $\mathbb{R}^k$, and Q is a j-nonfocal probability measure on M such that $j(Q)$ has finite moments of order 2 (or of sufficiently high order as needed). Let μ and Σ be, respectively, the mean and covariance matrix of $j(Q)$ regarded as a probability measure on $\mathbb{R}^k$. Let $\mathcal{F}$ be the set of focal points of $j(M)$, and let $P_j : \mathcal{F}^c \to j(M)$ be the projection on $j(M)$. P_j is differentiable at μ and has the differentiability class of $j(M)$ around any nonfocal point. In order to evaluate the differential $d_\mu P_j$ we consider a special orthonormal frame field that will ease the computations. Assume $p \to (f_1(x), \ldots, f_d(x))$ is a local frame field on an open subset of M such that, for each $x \in M$, $(dj(f_1(x)), \ldots, dj(f_d(x)))$ are orthonormal vectors in $\mathbb{R}^k$. A local frame field $(e_1(p), e_2(p), \ldots, e_k(p))$ defined on an open neighborhood $U \subseteq \mathbb{R}^k$ is *adapted to the embedding* j if it is an orthonormal frame field and $\forall x \in j^{-1}(U)$, $(e_r(j(x)) = d_p j(f_r(x))$, $r = 1, \ldots, d$. Let $e_1, e_2, \ldots, e_k$ be the canonical basis of $\mathbb{R}^k$ and assume $(e_1(p), e_2(p), \ldots, e_k(p))$ is an adapted frame field around $P_j(\mu) = j(\mu_E)$. Then $d_\mu P_j(e_b) \in T_{P_j(\mu)} j(M)$ is a linear combination of $e_1(P_j(\mu)), e_2(P_j(\mu)), \ldots, e_d(P_j(\mu))$:

$$d_\mu P_j(e_b) = \sum (d_\mu P_j(e_b)) \cdot e_a(P_j(\mu)) e_a(P_j(\mu)). \tag{3.1}$$

By the delta method, $n^{1/2}(P_j(\overline{j(X)}) - P_j(\mu))$ converges weakly to $N(0, \Sigma_\mu)$, where $\overline{j(X)} = \frac{1}{n}\sum_{i=1}^n j(X_i)$ and

$$\begin{aligned} \Sigma_\mu = {} & \left[\sum_{a=1}^d d_\mu P_j(e_b) \cdot e_a(P_j(\mu)) e_a(P_j(\mu))\right]_{b=1,\ldots,k} \Sigma \\ & \times \left[\sum d_\mu P_j(e_b) \cdot e_a(P_j(\mu)) e_a(P_j(\mu))\right]^t_{b=1,\ldots,k}. \end{aligned} \tag{3.2}$$

Here Σ is the covariance matrix of $j(X_1)$ w.r.t. the canonical basis $e_1, e_2, \ldots, e_k$. The asymptotic distribution $N(0, \Sigma_\mu)$ is degenerate and can be regarded as a distribution on $T_{P_j(\mu)} j(M)$, since the range of $d_\mu P_j$ is $T_{P_j(\mu)} j(M)$. Note that

$$d_\mu P_j(e_b) \cdot e_a(P_j(\mu)) = 0 \qquad \text{for } a = d+1, \ldots, k.$$

REMARK 3.1. An asymptotic distribution of the extrinsic sample mean can be obtained as a particular case of Theorem 2.1. The covariance matrix in that theorem depends both on the way the manifold is embedded and on the chart used. We provide below an alternative CLT, which applies to arbitrary embeddings, leads to pivots and is independent of the chart used.

The tangential component $\tan(v)$ of $v \in \mathbb{R}^k$ w.r.t. the basis $e_a(P_j(\mu)) \in T_{P_j(\mu)}j(M), a = 1, \dots, d$, is given by

$$\tan(v) = (e_1(P_j(\mu))^t v, \dots, e_d(P_j(\mu))^T v)^t. \tag{3.3}$$

Then the random vector $(d_{\mu_E} j)^{-1}(\tan(P_j(j(\overline{X})) - P_j(\mu))) = \sum_{a=1}^d \overline{X}_j^a f_a$ has the following covariance matrix w.r.t. the basis $f_1(\mu_E), \dots, f_d(\mu_E)$:

$$\begin{aligned} \Sigma_{j,E} &= e_a(P_j(\mu))^t \Sigma_\mu e_b(P_j(\mu))_{1 \le a,b \le d} \\ &= \left[\sum d_\mu P_j(e_b) \cdot e_a(P_j(\mu))\right]_{a=1,\dots,d} \Sigma \\ &\quad \times \left[\sum d_\mu P_j(e_b) \cdot e_a(P_j(\mu))\right]^t_{a=1,\dots,d}. \end{aligned} \tag{3.4}$$

DEFINITION 3.1. The matrix $\Sigma_{j,E}$ given by (3.4) is the *extrinsic covariance matrix* of the j-nonfocal distribution Q (of X_1) w.r.t. the basis $f_1(\mu_E), \dots, f_d(\mu_E)$.

When j is fixed in a specific context, the subscript j in $\Sigma_{j,E}$ will be omitted. If, in addition, rank $\Sigma_\mu = d$, $\Sigma_{j,E}$ is invertible and we define the *j-standardized mean vector*

$$\overline{Z}_{j,n} =: n^{1/2} {\Sigma_{j,E}}^{-1/2} (\overline{X}_j^1, \dots, \overline{X}_j^d)^T. \tag{3.5}$$

PROPOSITION 3.1. *Assume $\{X_r\}_{r=1,\dots,n}$ is a random sample from the j-nonfocal distribution $j(Q)$, and let $\mu = E(j(X_1))$ and assume the extrinsic covariance matrix $\Sigma_{j,E}$ of Q is finite. Let $(e_1(p), e_2(p), \dots, e_k(p))$ be an orthonormal frame field adapted to j. Then* (a) *the extrinsic sample mean $\overline{X}_E$ has asymptotically a normal distribution in the tangent space to M at $\mu_E(Q)$ with mean* 0 *and covariance matrix $n^{-1}\Sigma_{j,E}$, and* (b) *if $\Sigma_{j,E}$ is nonsingular, the j-standardized mean vector $\overline{Z}_{j,n}$ given in* (3.5) *converges weakly to $N(0, I_d)$.*

As a particular case of Proposition 3.1, when j is the inclusion map of a submanifold of $\mathbb{R}^k$, we get the following result for nonfocal distributions on an arbitrary closed submanifold M of $\mathbb{R}^k$:

COROLLARY 3.1. *Assume $M \subseteq \mathbb{R}^k$ is a closed submanifold of $\mathbb{R}^k$. Let $\{X_r\}_{r=1,\dots,n}$ be a random sample from the nonfocal distribution Q on M,* *and let* $\mu = E(X_1)$ *and assume the covariance matrix* Σ *of* $j(Q)$ *is finite. Let* $(e_1(p), e_2(p), \ldots, e_k(p))$ *be an orthonormal frame field adapted to* M. *Let* $\Sigma_E := \Sigma_{j,E}$, *where* $j : M \to \mathbb{R}^k$ *is the inclusion map. Then* (a) $n^{1/2}\tan(j(\overline{X}_E) - j(\mu_E))$ *converges weakly to* $N(0, \Sigma_E)$, *and* (b) *if* Σ *induces a nonsingular bilinear form on* $T_{j(\mu_E)}j(M)$, *then* $\|\overline{Z}_{j,n}\|^2$ *converges weakly to the chi-square distribution* χ^2_d.

EXAMPLE 3.1. In the case of a hypersphere in $\mathbb{R}^k$, $j(x) = x$ and $P_j = P_M$. We evaluate the statistic $\|\overline{Z}_{j,n}\|^2 = n\|\Sigma_{j,E}{}^{-1/2}\tan(P_M(\overline{X}) - P_M(\mu))\|^2$. The projection map is $P_M(x) = x/\|x\|$. P_M has the following property: if $v = cx$, then $d_x P_M(v) = 0$; on the other hand, if the restriction of $d_x P_M$ to the orthocomplement of $\mathbb{R}x$ is a conformal map, that is, if $v \cdot x = 0$, then $d_x P_M(v) = \|x\|^{-1}v$. In particular, if we select the coordinate system such that $x = \|x\|e_k$, then one may take $e_a(P_M(x)) = e_a$, and we get

$$d_x P_M(e_b) \cdot e_a(P_M(x)) = \|x\|^{-1}\delta_{ab} \qquad \forall\, a, b = 1, \ldots, k-1, d_x P_M(e_k) = 0.$$

Since $e_k(P_M(\mu))$ points in the direction of μ, $d_\mu P_M(e_b)\cdot\mu = 0$, $\forall\, b = 1, \ldots, k-1$, and we get

$$\Sigma_E = \|\mu\|^{-2}E([\mathbf{X}\cdot e_a(\mu/\|\mu\|)]_{a=1,\ldots,k-1}[\mathbf{X}\cdot e_a(\mu/\|\mu\|)]^t_{a=1,\ldots,k-1}) \tag{3.6}$$

which is the matrix G in formula (A.1) in [19].

REMARK 3.2. The CLT for extrinsic sample means as stated in Proposition 3.1 or Corollary 3.1 cannot be used to construct confidence regions for extrinsic means, since the population extrinsic covariance matrix is unknown. In order to find a consistent estimator of $\Sigma_{j,E}$, note that $\overline{j(X)}$ is a consistent estimator of μ, $d_{\overline{j(X)}}P_j$ converges in probability to $d_\mu P_j$, and $e_a(P_j(\overline{j(X)}))$ converges in probability to $e_a(P_j(\mu))$ and, further,

$$S_{j,n} = n^{-1}\sum(j(X_r) - \overline{j(X)})(j(X_r) - \overline{j(X)})^t$$

is a consistent estimator of Σ. It follows that

$$\begin{aligned}&\left[\sum_{a=1}^{d} d_{\overline{j(X)}}P_j(e_b)\cdot e_a(P_j(\overline{j(X)}))e_a(P_j(\overline{j(X)}))\right]S_{j,n}\\ &\qquad\times\left[\sum_{a=1}^{d} d_{\overline{j(X)}}P_j(e_b)\cdot e_a(P_j(\overline{j(X)}))e_a(P_j(\overline{j(X)}))\right]^t\end{aligned} \tag{3.7}$$

is a consistent estimator of Σ_μ, and $\tan_{P_j(\overline{j(X)})} v$ is a consistent estimator of $\tan(v)$.

If we take the components of the bilinear form associated with the matrix (3.7) w.r.t. $e_1(P_j(\overline{j(X)})), e_2(P_j(\overline{j(X)})), \dots, e_d(P_j(\overline{j(X)}))$, we get a consistent estimator of $\Sigma_{j,E}$ given by

$$\begin{aligned} G(j,X) = {} & \Big[\Big[\sum d_{\overline{j(X)}} P_j(e_b) \cdot e_a(P_j(\overline{j(X)}))\Big]_{a=1,\dots,d}\Big] \cdot S_{j,n} \\ & \times \Big[\Big[\sum d_{\overline{j(X)}} P_j(e_b) \cdot e_a(P_j(\overline{j(X)}))\Big]_{a=1,\dots,d}\Big]^t, \end{aligned} \tag{3.8}$$

and obtain the following results.

THEOREM 3.1. *Assume $j : M \to \mathbb{R}^k$ is a closed embedding of M in $\mathbb{R}^k$. Let $\{X_r\}_{r=1,\dots,n}$ be a random sample from the j-nonfocal distribution Q, and let $\mu = E(j(X_1))$ and assume $j(X_1)$ has finite second-order moments and the extrinsic covariance matrix $\Sigma_{j,E}$ of X_1 is nonsingular. Let $(e_1(p), e_2(p), \dots, e_k(p))$ be an orthonormal frame field adapted to j. If $G(j,X)$ is given by* (3.8), *then for n large enough $G(j,X)$ is nonsingular (with probability converging to* 1) *and* (a) *the statistic*

$$n^{1/2} G(j,X)^{-1/2} \tan(P_j(\overline{j(X)}) - P_j(\mu)) \tag{3.9}$$

converges weakly to $N(0, I_d)$, so that

$$n \| G(j,X)^{-1/2} \tan(P_j(\overline{j(X)}) - P_j(\mu)) \|^2 \tag{3.10}$$

converges weakly to χ^2_d, and (b) *the statistic*

$$n^{1/2} G(j,X)^{-1/2} \tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X)}) - P_j(\mu)) \tag{3.11}$$

converges weakly to $N(0, I_d)$, so that

$$n \| G(j,X)^{-1/2} \tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X)}) - P_j(\mu)) \|^2 \tag{3.12}$$

converges weakly to χ^2_d.

COROLLARY 3.2. *Under the hypothesis of Theorem* 3.1, *a confidence region for μ_E of asymptotic level $1-\alpha$ is given by* (a) $C_{n,\alpha} := j^{-1}(U_{n,\alpha})$, *where* $U_{n,\alpha} = \{\mu \in j(M) : n\|G(j,X)^{-1/2} \tan(P_j(\overline{j(X)}) - P_j(\mu))\|^2 \le \chi^2_{d,1-\alpha}\}$, *or by* (b) $D_{n,\alpha} := j^{-1}(V_{n,\alpha})$, *where* $V_{n,\alpha} = \{\mu \in j(M) : n\|G(j,X)^{-1/2} \times \tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X)}) - P_j(\mu))\|^2 \le \chi^2_{d,1-\alpha}\}$.

Theorem 3.1 and Corollary 3.2 involve pivotal statistics. The advantages of using pivotal statistics in bootstrapping for confidence regions are well known (see, e.g., [1, 2, 5, 9, 24, 25]).

At this point we recall the steps that one takes to obtain a bootstrapped statistic from a pivotal statistic. If $\{X_r\}_{r=1,\dots,n}$ is a random sample from the unknown distribution Q, and $\{X_r^*\}_{r=1,\dots,n}$ is a random sample from the empirical $\hat{Q}_n$, conditionally given $\{X_r\}_{r=1,\dots,n}$, then the statistic

$$T(X,Q) = n\|G(j,X)^{-1/2}\tan(P_j(\overline{j(X)}) - P_j(\mu))\|^2$$

given in Theorem 3.1(a) has the bootstrap analog

$$T(X^*,\hat{Q}_n) = n\|G(j,X^*)^{-1/2}\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)}))\|^2.$$

Here $G(j,X^*)$ is obtained from $G(j,X)$ by substituting $X_1^*,\dots,X_n^*$ for $X_1,\dots,X_n$, and $T(X^*,\hat{Q}_n)$ is obtained from $T(X,Q)$ by substituting $X_1^*,\dots,X_n^*$ for $X_1,\dots,X_n$, $\overline{j(X)})$ for μ and $G(j,X^*)$ for $G(j,X)$.

The same procedure can be used for the vector-valued statistic

$$V(X,Q) = n^{1/2}G(j,X)^{-1/2}\tan(P_j(\overline{j(X)}) - P_j(\mu)),$$

and as a result we get the bootstrapped statistic

$$V^*(X^*,\hat{Q}_n) = n^{1/2}G(j,X^*)^{-1/2}\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)})).$$

For the rest of this section, we will assume that $j(Q)$, when viewed as a measure on the ambient space $\mathbb{R}^k$, *has finite moments of sufficiently high order*. If M is compact, then this is automatic. In the noncompact case finiteness of moments of order 12, along with an assumption of a nonzero absolutely continuous component, is sufficient to ensure an Edgeworth expansion up to order $O(n^{-2})$ of the pivotal statistic $V(X,Q)$ (see [5, 6, 12, 19, 24]). We then obtain the following results:

THEOREM 3.2. *Let $\{X_r\}_{r=1,\dots,n}$ be a random sample from the j-nonfocal distribution Q which has a nonzero absolutely continuous component w.r.t. the volume measure on M induced by j. Let $\mu = E(j(X_1))$ and assume the covariance matrix Σ of $j(X_1)$ is defined and the extrinsic covariance matrix $\Sigma_{j,E}$ is nonsingular and let $(e_1(p), e_2(p),\dots,e_k(p))$ be an orthonormal frame field adapted to j. Then the distribution function of*

$$n\|G(j,X)^{-1/2}\tan(P_j(\overline{j(X)}) - P_j(\mu))\|^2$$

can be approximated by the bootstrap distribution function of

$$n\|G(j,X^*)^{-1/2}\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)}))\|^2$$

with a coverage error $O_p(n^{-2})$.

One may also use nonpivotal bootstrap confidence regions, especially when $G(j,X)$ is difficult to compute. The result in this case is the following (see [4]).

PROPOSITION 3.2. *Under the hypothesis of Proposition 3.1, the distribution function of* $n\|\tan(P_j(\overline{j(X)}) - P_j(\mu))\|^2$ *can be approximated uniformly by the bootstrap distribution of*

$$n\|\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)}))\|^2$$

to provide a confidence region for μ_E *with a coverage error no more than* $O_p(n^{-d/(d+1)})$.

REMARK 3.3. Note that Corollary 3.2(b) provides a computationally simpler scheme than Corollary 3.2(a) for large sample confidence regions; but for bootstrap confidence regions Theorem 3.2, which is the bootstrap analog of Corollary 3.2(a), yields a simpler method. The corresponding $100(1-\alpha)\%$ confidence region is $C^*_{n,\alpha} := j^{-1}(U^*_{n,\alpha})$ with $U^*_{n,\alpha}$ given by

$$U^*_{n,\alpha} = \{\mu \in j(M) : n\|G(j,X)^{-1/2}\tan(P_j(\overline{j(X)}) - P_j(\mu))\|^2 \le c^*_{1-\alpha}\}, \tag{3.13}$$

where $c^*_{1-\alpha}$ is the upper $100(1-\alpha)\%$ point of the values

$$n\|G(j,X^*)^{-1/2}\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)}))\|^2 \tag{3.14}$$

among the bootstrap resamples. One could also use the bootstrap analog of the confidence region given in Corollary 3.2(b) for which the confidence region is $D^*_{n,\alpha} := j^{-1}(V^*_{n,\alpha})$ with $V^*_{n,\alpha}$ given by

$$\begin{aligned} V^*_{n,\alpha} = \{\mu \in j(M) :& \\ & n\|G(j,X)^{-1/2}\tan_{P_j(\overline{j(X)})}(P_j(\overline{j(X)}) - P_j(\mu))\|^2 \le d^*_{1-\alpha}\}, \end{aligned} \tag{3.15}$$

where $d^*_{1-\alpha}$ is the upper $100(1-\alpha)\%$ point of the values

$$n\|G(j,X^*)^{-1/2}\tan_{P_j(\overline{j(X^*)})}(P_j(\overline{j(X^*)}) - P_j(\overline{j(X)}))\|^2 \tag{3.16}$$

among the bootstrap resamples. The region given by (3.13)–(3.14) has coverage error $O_p(n^{-2})$.

4. Asymptotic distributions of sample mean axes, Procrustes mean shapes and extrinsic mean planar projective shapes. In this section we focus on the asymptotic distribution of sample means in axial data analysis and in planar shape data analysis. The axial space is the $(N-1)$-dimensional real projective space $M = \mathbb{R}P^{N-1}$ which can be identified with the sphere $S^{N-1} = \{x \in \mathbb{R}^N | \|x\|^2 = 1\}$ with antipodal points identified (see, e.g., [41]). If $[x] = \{x, -x\} \in \mathbb{R}P^{N-1}$, $\|x\| = 1$, the tangent space at $[x]$ can be described as

$$T_{[x]}\mathbb{R}P^{N-1} = \{([x], v), v \in \mathbb{R}^N | v^t x = 0\}. \tag{4.1}$$

We consider here the general situation when the distribution on $\mathbb{R}P^{N-1}$ may not be concentrated. Note that for N odd, $\mathbb{R}P^{N-1}$ cannot be embedded in $\mathbb{R}^N$, since for any embedding of $\mathbb{R}P^{N-1}$ in $\mathbb{R}^k$ with N odd, the first Stiefel–Whitney class of the normal bundle is not zero ([43], page 51).

The *Veronese–Whitney* embedding is defined for arbitrary N by the formula

$$j([x]) = xx^t, \qquad \|x\| = 1. \tag{4.2}$$

The embedding j maps $\mathbb{R}P^{N-1}$ into a $(\frac{1}{2}N(N+1)-1)$-dimensional Euclidean hypersphere in the space $S(N,\mathbb{R})$ of real $N \times N$ symmetric matrices, where the Euclidean distance d_0 between two symmetric matrices is

$$d_0(A,B) = \mathrm{Tr}((A-B)^2).$$

This embedding, which was already used by Watson [52], is preferred over other embeddings in Euclidean spaces because it is *equivariant* (see [35]). This means that the special orthogonal group $\mathrm{SO}(N)$ of orthogonal matrices with determinant $+1$ acts as a group of isometries on $\mathbb{R}P^{N-1}$ with the metric of constant positive curvature; and it also acts on the left on $S_+(N,\mathbb{R})$, the set of nonnegative definite symmetric matrices with real coefficients, by $T \cdot A = TAT^t$. Also, $j(T \cdot [x]) = T \cdot j([x]), \forall T \in \mathrm{SO}(N), \forall [x] \in \mathbb{R}P^{N-1}$.

Note that $j(\mathbb{R}P^{N-1})$ is the set of all nonnegative definite matrices in $S(N,\mathbb{R})$ of rank 1 and trace 1. The following result appears in [8].

PROPOSITION 4.1. (a) *The set $\mathcal{F}$ of the focal points of $j(\mathbb{R}P^{N-1})$ in $S_+(N,\mathbf{R})$ is the set of matrices in $S_+(N,\mathbf{R})$ whose largest eigenvalues are of multiplicity at least* 2. (b) *The projection $P_j : S_+(N,\mathbb{R}) \backslash \mathcal{F} \to j(\mathbb{R}P^{N-1})$ assigns to each nonnegative definite symmetric matrix A with a highest eigenvalue of multiplicity* 1, *the matrix $j([m])$, where $m(\|m\|=1)$ is an eigenvector of A corresponding to its largest eigenvalue.*

The following result of Prentice [46] is also needed in the sequel.

PROPOSITION 4.2 ([46]). *Assume $[X_r]$, $\|X_r\| = 1$, $r = 1,\dots,n$, is a random sample from a j-nonfocal probability measure Q on $\mathbb{R}P^{N-1}$. Then the j-extrinsic sample covariance matrix $G(j,X)$ is given by*

$$\begin{aligned} G(j,X)_{ab} = {} & n^{-1}(\eta_N - \eta_a)^{-1}(\eta_N - \eta_b)^{-1} \\ & \times \sum_r (m_a \cdot X_r)(m_b \cdot X_r)(m \cdot X_r)^2, \end{aligned} \tag{4.3}$$

where $\eta_a, a = 1,\dots,N$, are eigenvalues of $K := n^{-1}\sum_{r=1}^n X_r X_r^t$ in increasing order and $m_a, a = 1,\dots,N$, are corresponding linearly independent unit eigenvectors.

Here we give a proof of (4.3) based on the equivariance of j to prepare the reader for a similar but more complicated formula of the analogous estimator given later for $\mathbb{C}P^{k-2}$.

Since the map j is equivariant, w.l.o.g. one may assume that $j(\overline{X}_E) = P_j(\overline{j(X)})$ is a diagonal matrix, $\overline{X}_E = [m_N] = [e_N]$ and the other unit eigenvectors of $\overline{j(X)} = D$ are $m_a = e_a, \forall a = 1, \dots, N-1$. We evaluate $d_D P_j$. Based on this description of $T_{[x]}\mathbb{R}P^{N-1}$, one can select in $T_{P_j(D)} j(\mathbb{R}P^{N-1})$ the orthonormal frame $e_a(P_j(D)) = d_{[e_N]} j(e_a)$. Note that $S(N, \mathbf{R})$ has the orthobasis $F_a^b, b \le a$, where, for $a < b$, the matrix F_a^b has all entries zero except for those in the positions $(a, b), (b, a)$ that are equal to $2^{-1/2}$; also $F_a^a = j([e_a])$. A straightforward computation shows that if $\eta_a, a = 1, \dots, N$, are the eigenvalues of D in their increasing order, then $d_D P_j(F_a^b) = 0, \forall b \le a < N$ and $d_D P_j(F_a^N) = (\eta_N - \eta_a)^{-1} e_a(P_j(D))$; from this equation it follows that, if $\overline{j(X)}$ is a diagonal matrix D, then the entry $G(j, X)_{ab}$ is given by

$$G(j, X)_{ab} = n^{-1}(\eta_N - \eta_a)^{-1}(\eta_N - \eta_b)^{-1} \sum_r X_r^a X_r^b (X_r^N)^2.$$

Taking $\overline{j(X)}$ to be a diagonal matrix and $m_a = e_a$, (4.3) follows.

Note that $\mu_{E,j} = [\nu_N]$, where $(\nu_a), a = 1, \dots, N$, are unit eigenvectors of $E(XX^t) = E(j(Q))$ corresponding to eigenvalues in their increasing order. Let $T([\nu]) = n\|G(j, X)^{-1/2} \tan(P_j(\overline{j(X)}) - P_j(E(j(Q))))\|^2$ be the statistic given by (3.10). We can derive now the following theorem as a special case of Theorem 3.1(a).

THEOREM 4.1. *Assume j is the Veronese–Whitney embedding of $\mathbb{R}P^{N-1}$ and $\{[X_r], \|X_r\| = 1, r = 1, \dots, n\}$ is a random sample from a j-nonfocal probability measure Q on $\mathbb{R}P^{N-1}$ that has a nondegenerate j-extrinsic variance. Then $T([\nu])$ is given by*

$$T([\nu]) = n\nu^t[(\nu_a)_{a=1,\dots,N-1}] G(j, X)^{-1} [(\nu_a)_{a=1,\dots,N-1}]^t \nu, \tag{4.4}$$

and, asymptotically, $T([\nu])$ has a χ^2_{N-1} distribution.

PROOF. Since j is an isometric embedding and the tangent space $T_{[\nu_N]}\mathbb{R}P^{N-1}$ has the orthobasis $\nu_1, \dots, \nu_{N-1}$, if we select the first elements of the adapted moving frame in Theorem 3.1 to be $e_a(P_j(\nu_{E,j})) = (d_{[\nu_N]} j)(\nu_a)$, then the ath tangential component of $P_j(\overline{j(X)}) - P_j(\nu)$ w.r.t. this basis of $T_{P_j(E(j(Q)))} j(\mathbb{R}P^{N-1})$ equals up to a sign the ath component of $m - \nu_N$ w.r.t. the orthobasis $\nu_1, \dots, \nu_{N-1}$ in $T_{[\nu_N]}\mathbb{R}R^{N-1}$, namely $\nu_a^t m$. The result follows now from Theorem 3.1(a). □

REMARK 4.1. If we apply Theorem 3.1(b) to the embedding j, we obtain a similar theorem due to Fisher, Hall, Jing and Wood [19], where $T([\nu])$ is replaced by $T([m])$. Similar asymptotic results can be obtained for the large sample distribution of Procrustes means of planar shapes, as we discuss below. Recall that the planar shape space $M = \sum_2^k$ of an ordered set of k points in $\mathbb{C}$ at least two of which are distinct can be identified in different ways with the complex projective space $\mathbb{C}P^{k-2}$ (see, e.g., [8, 31]). Here we regard $\mathbb{C}P^{k-2}$ as a set of equivalence classes $\mathbb{C}P^{k-2} = S^{2k-3}/S^1$ where S^{2k-3} is the space of complex vectors in $\mathbb{C}^{k-1}$ of norm 1, and the equivalence relation on S^{2k-3} is by multiplication with scalars in S^1 (complex numbers of modulus 1). A complex vector $z = (z^1, z^2, \ldots, z^{k-1})$ of norm 1 corresponding to a given configuration of k landmarks, with the identification described in [8], can be displayed in the Euclidean plane (complex line) with the superscripts as labels. If, in addition, r is the largest superscript such that $z^r \neq 0$, then we may assume that $z^r > 0$. Using this representative of the projective point $[z]$ we obtain a unique graphical representation of $[z]$, which will be called the *spherical representation.*

The *Veronese–Whitney* (or simply *Veronese*) *map* is the embedding of $\mathbb{C}P^{k-2}$ in the space of Hermitian matrices $S(k-1, \mathbb{C})$ given in this case by $j([z]) = zz^*$, where, if z is considered as a column vector, z^* is the adjoint of z, that is, the conjugate of the transpose of z. The Euclidean distance in the space of Hermitian matrices $S(k-1, \mathbb{C})$ is $d_0^2(A, B) = \mathrm{Tr}((A-B)(A-B)^*) = \mathrm{Tr}((A-B)^2)$.

Kendall [31] has shown that the Riemannian metric induced on $j(\mathbb{C}P^{k-2})$ by d_0 is a metric of constant holomorphic curvature. The associated Riemannian distance is known as the *Kendall distance* and the full group of isometries on $\mathbb{C}P^{k-2}$ with the Kendall distance is isomorphic to the special unitary group $\mathrm{SU}(k-1)$ of all $(k-1) \times (k-1)$ complex matrices A with $A^*A = I$ and $\det(A) = 1$.

A random variable $X = [Z], \|Z\| = 1$, valued in $\mathbb{C}P^{k-2}$ is j-nonfocal if the highest eigenvalue of $E[ZZ^*]$ is simple, and then the extrinsic mean of X is $\mu_{j,E} = [\nu]$, where $\nu \in \mathbb{C}^{k-1}, \|\nu\| = 1$, is an eigenvector corresponding to this eigenvalue (see [8]). The extrinsic sample mean $\overline{[z]}_{j,E}$ of a random sample $[z_r] = [(z_r^1, \ldots, z_r^{k-1})], \|z_r\| = 1, r = 1, \ldots, n$, from such a nonfocal distribution exists with probability converging to 1 as $n \to \infty$, and is the same as that given by

$$\overline{[z]}_{j,E} = [m], \tag{4.5}$$

where m is a highest unit eigenvector of

$$K := n^{-1} \sum_{r=1}^{n} z_r z_r^*. \tag{4.6}$$

This means that $\overline{[z]}_{j,E}$ is the full Procrustes estimate for parametric families such as Dryden–Mardia distributions or complex Bingham distributions for planar shapes [35, 36]. For this reason, $\mu_{j,E} = [m]$ will be called the *Procrustes* mean of Q.

PROPOSITION 4.3. *Assume $X_r = [Z_r], \|Z_r\| = 1, r = 1, \ldots, n$, is a random sample from a j-nonfocal probability measure Q with a nondegenerate j-extrinsic covariance matrix on $\mathbb{C}P^{k-2}$. Then the j-extrinsic sample covariance matrix $G(j,X)$ as a complex matrix has the entries*

$$G(j,X)_{ab} = n^{-1}(\eta_{k-1} - \eta_a)^{-1}(\eta_{k-1} - \eta_b)^{-1} \times \sum_{r=1}^{n} (m_a \cdot Z_r)(m_b \cdot Z_r)^* |m_{k-1} \cdot Z_r|^2. \tag{4.7}$$

The proof is similar to that given for Proposition 4.2 and is based on the equivariance of the Veronese–Whitney map j w.r.t. the actions of $SU(k-1)$ on $\mathbb{C}P^{k-2}$ and on the set $S_+(k-1,\mathbb{C})$ of nonnegative semidefinite self-adjoint $(k-1)$ by $(k-1)$ complex matrices (see [8]). Without loss of generality we may assume that K in (4.6) is given by $K = \operatorname{diag}\{\eta_a\}_{a=1,\ldots,k-1}$ and the largest eigenvalue of K is a simple root of the characteristic polynomial over $\mathbb{C}$, with $m_{k-1} = e_{k-1}$ as a corresponding complex eigenvector of norm 1. The eigenvectors over $\mathbb{R}$ corresponding to the smaller eigenvalues are given by $m_a = e_a, m'_a = ie_a, a = 1, \ldots, k-2$, and yield an orthobasis for $T_{[m_{k-1}]} j(\mathbb{C}P^{k-2})$. For any $z \in S^{2k-1}$ which is orthogonal to m_{k-1} in $\mathbb{C}^{k-1}$ w.r.t. the real scalar product, we define the path $\gamma_z(t) = [\cos t m_{k-1} + \sin t z]$. Then $T_{P_j(K)} j(\mathbb{C}P^{k-2})$ is generated by the vectors tangent to such paths $\gamma_z(t)$ at $t = 0$. Such a vector, as a matrix in $S(k-1,\mathbb{C})$, has the form $z m^*_{k-1} + m_{k-1} z^*$. In particular, since the eigenvectors of K are orthogonal w.r.t. the complex scalar product, one may take $z = m_a$, $a = 1, \ldots, k-2$, or $z = i m_a$, $a = 1, \ldots, k-2$, and thus get an orthobasis in $T_{P_j(K)} j(M)$. When we norm these vectors to have unit lengths we obtain the orthonormal frame

$$e_a(P_j(K)) = d_{[m_{k-1}]} j(m_a) = 2^{-1/2}(m_a m^*_{k-1} + m_{k-1} m^*_a),$$
$$e'_a(P_j(K)) = d_{[m_{k-1}]} j(i m_a) = i 2^{-1/2}(m_a m^*_{k-1} - m_{k-1} m^*_a).$$

Since the map j is equivariant we may assume that K is diagonal. In this case $m_a = e_a$, $e_a(P_j(K)) = 2^{-1/2} E^{k-1}_a$ and $e'_a(P_j(K)) = 2^{-1/2} F^{k-1}_a$, where E^b_a has all entries zero except for those in the positions (a,b) and (b,a) that are equal to 1, and F^b_a is a matrix with all entries zero except for those in the positions (a,b) and (b,a) that are equal to i, respectively $-i$. Just as in the real case, a straightforward computation shows that $d_K P_j(E^b_a) = d_K P_j(F^b_a) = 0, \forall\, a \le b < k-1$, and

$$d_K P_j(E^{k-1}_a) = (\eta_{k-1} - \eta_a)^{-1} e_a(P_j(K)),$$
$$d_K P_j(F^{k-1}_a) = (\eta_{k-1} - \eta_a)^{-1} e'_a(P_j(K)).$$

We evaluate the extrinsic sample covariance matrix $G(j,X)$ given in (3.8) using the real scalar product in $S(k-1,\mathbb{C})$, namely, $U\cdot V=\operatorname{Re}\operatorname{Tr}(UV^*)$. Note that

$$d_K P_j(E_b^{k-1})\cdot e_a(P_j(K))=(\eta_{k-1}-\eta_a)^{-1}\delta_{ba},$$
$$d_K P_j(E_b^{k-1})\cdot e'_a(P_j(K))=0$$

and

$$d_K P_j(F_b^{k-1})\cdot e'_a(P_j(K))^t=(\eta_{k-1}-\eta_a)^{-1}\delta_{ba},$$
$$d_K P_j(F_b^{k-1})\cdot e_a(P_j(K))=0.$$

Thus we may regard $G(j,X)$ as a complex matrix noting that in this case we get

$$\begin{aligned}G(j,X)_{ab}&=n^{-1}(\eta_{k-1}-\eta_a)^{-1}(\eta_{k-1}-\eta_b)^{-1}\\ &\quad\times\sum_{r=1}^{n}(e_a\cdot Z_r)(e_b\cdot Z_r)^*|e_{k-1}\cdot Z_r|^2,\end{aligned}\tag{4.8}$$

thus proving (4.7) when K is diagonal. The general case follows by equivariance. We consider now the statistic

$$T(\overline{(X)}_E,\mu_E)=n\|G(j,X)^{-1/2}\tan(P_j(\overline{j(X)})-P_j(\mu_E))\|^2$$

given in Theorem 3.1 in the present context of random variables valued in complex projective spaces to get:

THEOREM 4.2. *Let $X_r=[Z_r]$, $\|Z_r\|=1$, $r=1,\dots,n$, be a random sample from a Veronese-nonfocal probability measure Q on $\mathbb{C}P^{k-2}$. Then the quantity (3.10) is given by*

$$T([m],[\nu])=n[(m\cdot\nu_a)_{a=1,\dots,k-2}]G(j,X)^{-1}[(m\cdot\nu_a)_{a=1,\dots,k-2}]^*\tag{4.9}$$

and asymptotically $T([m],[\nu])$ has a χ^2_{2k-4} distribution.

PROOF. The tangent space $T_{[\nu_{k-1}]}\mathbb{C}P^{k-2}$ has the orthobasis $\nu_1,\dots,\nu_{k-2},\nu_1^*,\dots,\nu_{k-2}^*$. Note that since j is an isometric embedding, we may select the first elements of the adapted moving frame in Corollary 3.1 to be $e_a(P_j(\mu))=(d_{[\nu_{k-1}]}j)(\nu_a)$, followed by $e_a^*(P_j(\mu))=(d_{[\nu_{k-1}]}j)(\nu_a^*)$. Then the ath tangential component of $P_j(\overline{j(X)})-P_j(\mu)$ w.r.t. this basis of $T_{P_j(\mu)}j(\mathbb{C}P^{k-2})$ equals up to a sign the component of $m-\nu_{k-1}$ w.r.t. the orthobasis $\nu_1,\dots,\nu_{k-2}$ in $T_{[\nu_{k-1}]}\mathbb{C}P^{k-2}$, which is $\nu_a^t m$; and the a^*th tangential components are given by $\nu_a^{*t}m$, and together (in complex multiplication) they yield the complex vector $[(m\cdot\nu_a)_{a=1,\dots,k-2}]$. The claim follows from this and from (4.3), as a particular case of Corollary 3.1. □

We may derive from this the following large sample confidence regions.

COROLLARY 4.1. *Assume $X_r = [Z_r]$, $\|Z_r\| = 1$, $r = 1, \ldots, n$, is a random sample from a j-nonfocal probability measure Q on $\mathbb{C}P^{k-2}$. An asymptotic $(1-\alpha)$-confidence region for $\mu_E^j(Q) = [\nu]$ is given by $R_\alpha(\mathbf{X}) = \{[\nu] : T([m],[\nu]) \leq \chi^2_{2k-4,\alpha}\}$, where $T([m],[\nu])$ is given in (4.9). If Q has a nonzero absolutely continuous component w.r.t. the volume measure on $\mathbb{C}P^{k-2}$, then the coverage error of $R_\alpha(\mathbf{X})$ is of order $O(n^{-1})$.*

For small samples the coverage error could be quite large, and a bootstrap analogue of Theorem 4.2 is preferable.

THEOREM 4.3. *Let j be the Veronese embedding of $\mathbb{C}P^{k-2}$, and let $X_r = [Z_r]$, $\|Z_r\| = 1$, $r = 1, \ldots, n$, be a random sample from a j-nonfocal distribution Q on $\mathbb{C}P^{k-2}$ having a nonzero absolutely continuous component w.r.t. the volume measure on $\mathbb{C}P^{k-2}$. Assume in addition that the restriction of the covariance matrix of $j(Q)$ to $T_{[\nu]}j(\mathbb{C}P^{k-2})$ is nondegenerate. Let $\mu_E(Q) = [\nu]$ be the extrinsic mean of Q. For a resample $\{Z_r^*\}_{r=1,\ldots,n}$ from the sample consider the matrix $K^* := n^{-1}\sum Z_r^* Z_r^{*^*}$. Let $(\eta_a^*)_{a=1,\ldots,k-1}$ be the eigenvalues of K^* in their increasing order, and let $(m_a^*)_{a=1,\ldots,k-1}$ be the corresponding unit complex eigenvectors. Let $G^*(j,X)^*$ be the matrix obtained from $G(j,X)$ by substituting all the entries with *-entries. Then the bootstrap distribution function of*

$$T([m]^*,[m]) := n[(m_{k-1}^* \cdot m_a^*)_{a=1,\ldots,k-2}]G^*((j,X)^*)^{-1}[(m_{k-1} \cdot m_a^*)_{a=1,\ldots,k-2}]^*$$

approximates the true distribution function of $T([m],[\nu])$ given in Theorem 4.2 with an error of order $O_p(n^{-2})$.

REMARK 4.2. For distributions that are reasonably concentrated one may determine a nonpivotal bootstrap confidence region using Corollary 3.1(a). The chart used here features affine coordinates in $\mathbb{C}P^{k-2}$. Recall that the complex space $\mathbb{C}^{k-2}$ can be embedded in $\mathbb{C}P^{k-2}$, preserving collinearity. Such a standard *affine* embedding, missing only a hyperplane at infinity, is $(z^1, \ldots, z^{k-2}) \to [z^1 : \cdots : z^{k-1} : 1]$. This leads to the notion of *affine* coordinates of a point

$$p = [z^1 : \cdots : z^m : z^{k-1}], \qquad z^{k-1} \neq 0,$$

to be defined as

$$(w^1, w^2, \ldots, w^{k-2}) = \left(\frac{z^1}{z^{k-1}}, \ldots, \frac{z^{k-2}}{z^{k-1}}\right).$$

To simplify the notation the simultaneous confidence intervals used in the next section can be expressed in terms of simultaneous *complex confidence intervals*. If $z = x + iy, w = u + iv, x < u, y < v$, then we define the complex interval $(z, w) = \{c = a + ib | a \in (x, u), b \in (y, v)\}$.

5. Applications. In this last section we consider three applications.

APPLICATION 1. Here we consider the data set of $n = 50$ South magnetic pole positions (latitudes and longitudes), determined from a paleomagnetic study of New Caledonian laterities ([20], page 278). As an example of application of Section 2, we give a large sample confidence region for the mean location of the South pole based on this data. The sample points to a nonsymmetric distribution on S^2; the extrinsic sample mean and the intrinsic sample mean are given by

$$\overline{X}_E = (0.0105208, 0.199101, 0.979922)^t$$

and, using $\overline{X}_E$ as the initial input of the necessary minimization for constructing $\overline{X}_I$,

$$\overline{X}_I = p = (0.004392, 0.183800, 0.982954)^t.$$

From Examples 2.1 and 2.2, select the orthobasis $e_1(p), e_2(p)$ given in (2.3) and the logarithmic coordinates u^1, u^2 w.r.t. this basis in T_pS^2 defined in (2.4). Then compute the matrix $\hat{\Lambda}$ given in (2.22), to get, using Corollary 2.2, the following 95% asymptotic confidence region for μ_I:

$$\begin{aligned} U = \{&\mathrm{Exp}_p(u^1 e_1(p) + u^2 e_2(p)) | \\ &16.6786(u^1)^2 - 2.9806u^1u^2 + 10.2180(u^1)^2 \le 5.99146\}. \end{aligned}$$

Note that Fisher, Lewis and Embleton ([20], page 112) estimate another location parameter, the *spherical median*. The spherical median here refers to the minimizer of the expected geodesic (or, arc) distance to a given point on the sphere. For this paleomagnetism data, their sample median is at $78.9°, 98.4°$, while the extrinsic sample mean is $78.5°, 89.4°$ and the intrinsic sample mean is $79.4°, 88.6°$. These estimates differ substantially from the current position of the South magnetic pole, a difference accounted for by the phenomenon of migration of the Earth's magnetic poles.

APPLICATION 2. As an application of Section 4, we give a nonpivotal bootstrap confidence region for the mean shape of a group of eight landmarks on the skulls of eight-year-old North American children. The sample used is the University School data ([10], pages 400–405). The data set represents coordinates of anatomical landmarks, whose names and position on the skull are given in [10]. The data are displayed in Figure 1. (The presentation of raw data is similar to other known shape data displays such as in [15], page 46.) The shape variable (in our case, shape of the eight landmarks on the upper mid face) is valued in a planar shape space $\mathbb{C}P^6$ (real dimension = 12). A spherical representation of a shape in this case consists of seven marked

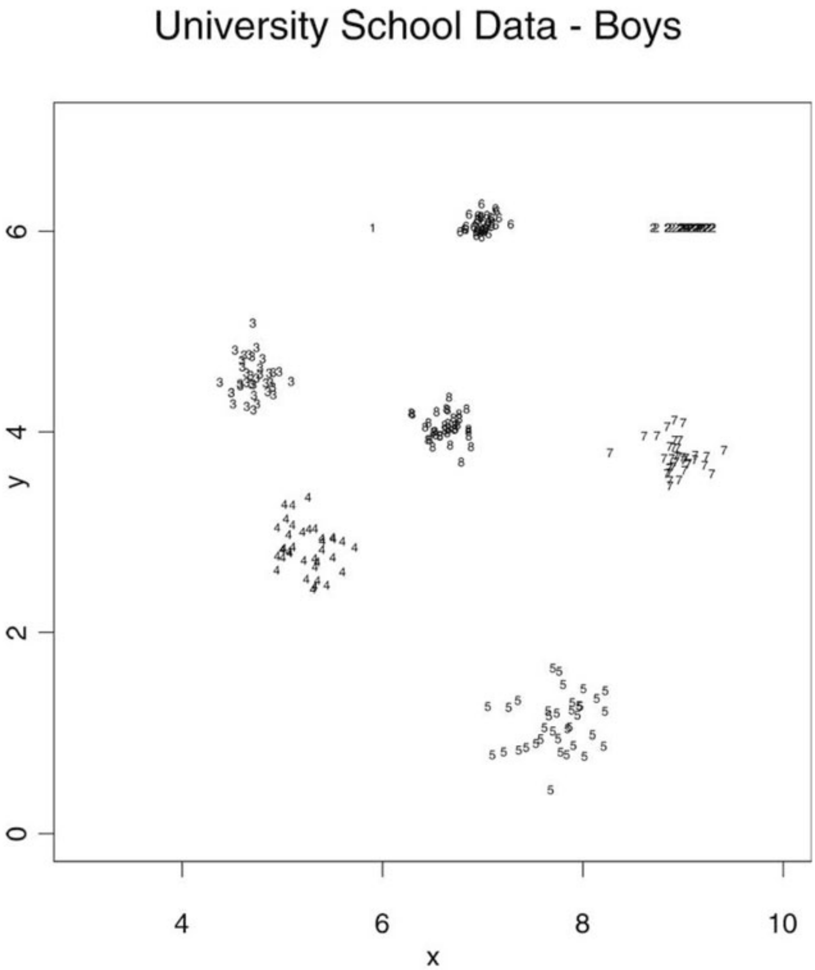

FIG. 1.

points; in Figure 2 we display a spherical representation of this data set. A representative for the extrinsic sample mean (spherical representation) is

$$(-0.67151 + 0.66823i, 0.76939 + 1.05712i, -1.03159 - 0.15998i,$$
$$-0.57776 - 0.87257i, 0.77871 - 1.36178i,$$
$$-0.17489 + 0.82106i, 1.00000 + 0.00000i).$$

We derived the nonpivotal bootstrap distribution using a simple program in S-Plus4.5, that we ran for 500 resamples. A spherical representation of the bootstrap distribution of the extrinsic sample means is displayed in Figure 3. Here we added a representative for the last landmark (the opposite of the sum of the other landmarks since data is centered at 0).

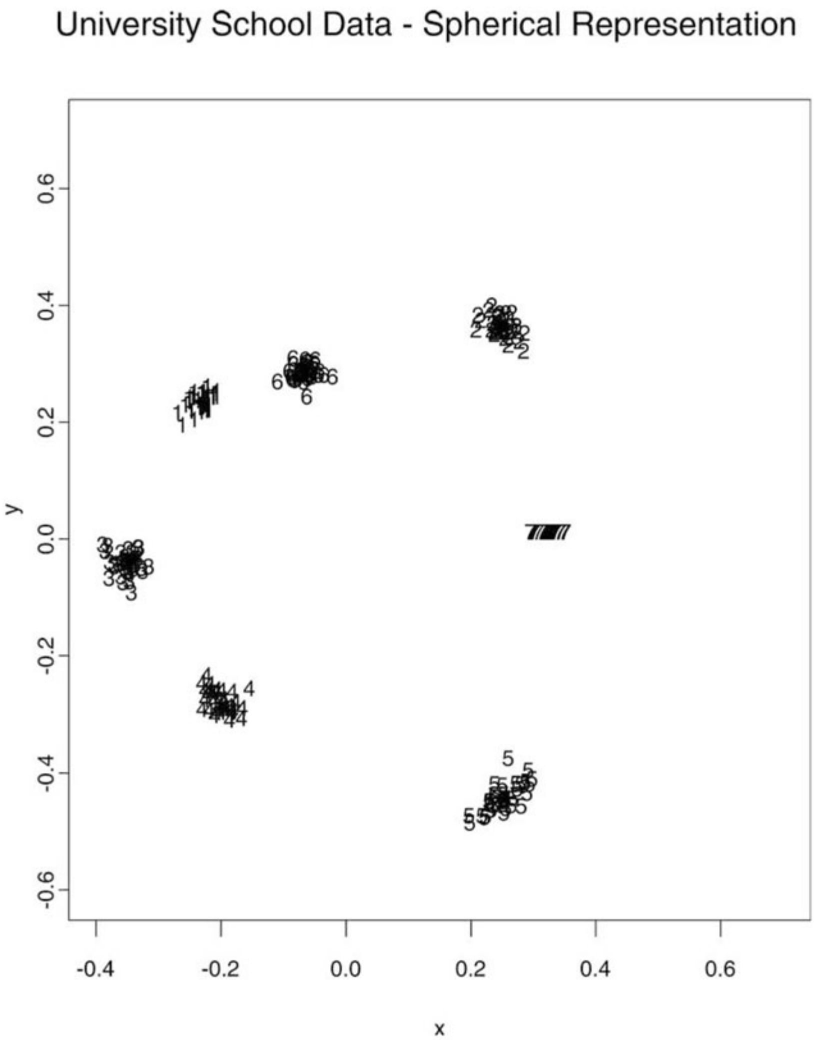

FIG. 2.

Note that the bootstrap distribution of the extrinsic sample mean is very concentrated at each landmark location. This is in agreement with the theory, that predicts in our case a spread of about six times smaller than the spread of the population. It is also an indication of the usefulness of the spherical coordinates. We determined a confidence region for the extrinsic mean using the six 95% simultaneous bootstrap complex intervals for the affine coordinates, as described in Remark 4.2, and found the following complex intervals:

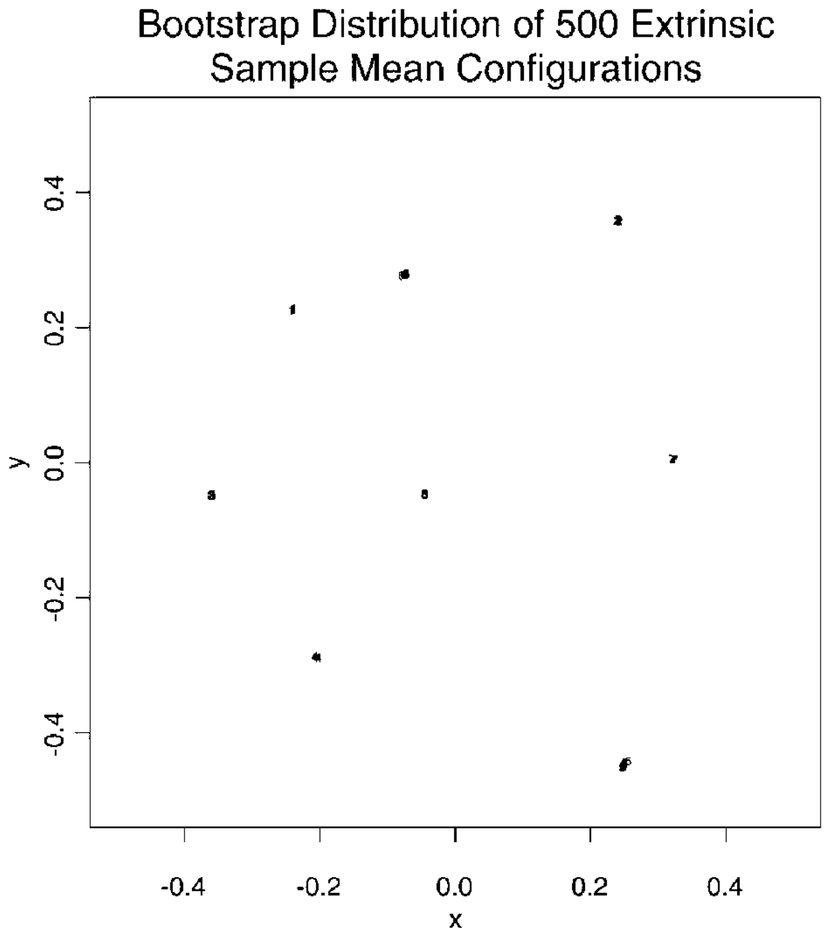

FIG. 3.

for w_1:

$$(-0.677268 + 0.666060i, -0.671425 + 0.672409i),$$

for w_2:

$$(0.767249 + 1.051660i, 0.775592 + 1.058960i),$$

for w_3:

$$(-1.036100 - 0.161467i, -1.029420 - 0.154403i),$$

for w_4:

$$(-0.578941 - 0.875168i, -0.574923 - 0.871553i),$$

for w_5:

$$(0.777688 - 1.366880i, 0.782354 - 1.358390i),$$

for w_6:

$$(-0.177261 + 0.820107i, -0.173465 + 0.824027i).$$

APPLICATION 3. This example is relevant in glaucoma detection. Although it is known that increased intraocular pressure (IOP) may cause a shape change in the eye cup, which is identified with glaucoma, it does not always lead to this shape change. The data analysis presented shows that the device used for measuring the topography of the back of the eye, as reported in [11], is effective in detecting shape change.

We give a nonpivotal bootstrap confidence region for the mean shape change of the eye cup due to IOP. Glaucoma is an eye disorder caused by IOP that is very high. Due to the increased IOP, as the soft spot where the optic nerve enters the eye is pushed backwards, eventually the optic nerve fibers that spread out over the retina to connect to photoreceptors and other retinal neurons can be compressed and damaged. An important diagnostic tool is the ability to detect, in images of the optic nerve head (ONH), increased depth (cupping) of the ONH structures. Two real data-processed images of the ONH cup surface before and after the IOP was increased are shown in Figure 4.

The laser image files are, however, huge-dimensional vectors, and their sizes usually differ. Even if we would restrict the study to a fixed size, there is no direct relationship between the eye cup pictured and the coordinates at a given pixel. A useful data reduction process consists in registration of a number of anatomical landmarks that were identified in each of these images. Assume the position vectors of these landmarks are $X_1, \ldots, X_k, k \geq 4$. Two configurations of landmarks have the same shape if they can be superimposed after a translation, a rotation and a scaling. The shape of the configuration $x = (x_1, \ldots, x_k)$ is labelled $o(x)$ and the space Σ_m^k of shapes

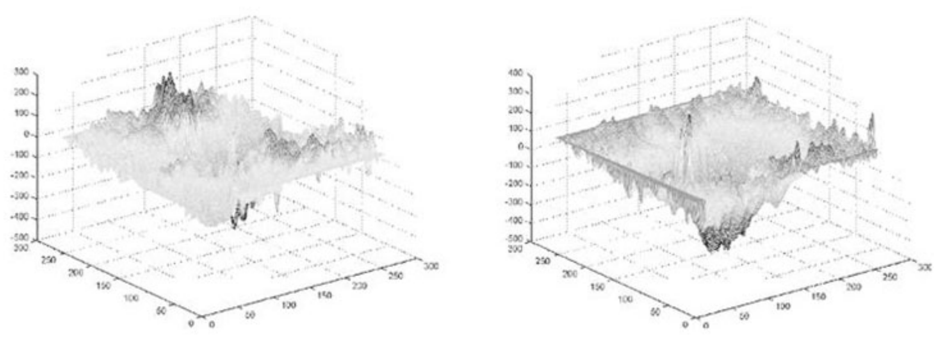

FIG. 4. *Change in the ONH topography from normal* (left) *to glaucomatous* (right).

of configurations of k points in $\mathbb{R}^m$ at least two of which are distinct is the *shape space* introduced by Kendall [31].

We come back to the shape of an ONH cup. This ONH region resembles a "cup" of an ellipsoid and its border has a shape of an ellipse. In this example four landmarks are used. The first three landmarks, denoted by S, T and N, are chosen to be the "top, left and right" points on this ellipse, that is (when referring to the left eye), Superior, Templar and Nose papilla. The last landmark V that we call vertex is the point with the largest "depth" inside the ellipse area that determines the border of the ONH. Therefore, in this example the data analysis is on the shape space of tetrads Σ_3^4, which is topologically a five-dimensional sphere (see [33], page 38); however, the identification with a sphere is nonstandard. On the other hand, it is known that if a probability distribution on Σ_m^k has small support outside a set of singular points, the use of any distance that is compatible with the orbifold topology considered is appropriate in data analysis ([15], page 65) since the data can be linearized. Our choice of the Riemannian metric (5.3) is motivated by considerations of applicability of Theorems 2.2 and 2.3 and computational feasibility. Dryden and Mardia ([15], pages 78–80) have introduced the following five coordinates defined on the generic subset of Σ_3^4 of shapes of a nondegenerate tetrad that they called *Bookstein coordinates*:

$$
\begin{aligned}
v^1 &= (w_{12}w_{13} + w_{22}w_{23} + w_{32}w_{33})/a,\\
v^2 &= ((w_{12}w_{23} - w_{22}w_{13})^2\\
&\qquad + (w_{12}w_{33} - w_{32}w_{13})^2 + (w_{22}w_{33} - w_{23}w_{32})^2)^{1/2}/a,\\
v^3 &= (w_{12}w_{14} + w_{22}w_{24} + w_{32}w_{34})/a,\\
v^4 &= (ab^{1/2})^{-1}(w_{12}^2(w_{23}w_{24} + w_{33}w_{34}) + w_{22}^2(w_{13}w_{14} + w_{33}w_{34})\\
&\qquad + w_{32}^2(w_{13}w_{14} + w_{23}w_{24}) - w_{12}w_{13}(w_{22}w_{24} + w_{32}w_{34})\\
&\qquad - w_{22}w_{32}(w_{23}w_{34} + w_{33}w_{24})\\
&\qquad - w_{12}w_{14}(w_{22}w_{23} + w_{32}w_{33})),\\
v^5 &= (w_{12}w_{23}w_{34} - w_{12}w_{33}w_{24} - w_{13}w_{22}w_{34}\\
&\qquad + w_{13}w_{32}w_{24} + w_{22}w_{33}w_{14} - w_{32}w_{23}w_{14})/(2ab)^{1/2},
\end{aligned}
\tag{5.1}
$$

where

$$
\begin{aligned}
a &= 2(w_{12}^2 + w_{22}^2 + w_{32}^2),\\
b &= w_{12}^2w_{23}^2 + w_{12}^2w_{33}^2 - 2w_{12}w_{13}w_{22}w_{23} + w_{13}^2w_{22}^2 + w_{13}^2w_{32}^2\\
&\quad - 2w_{12}w_{13}w_{32}w_{33} + w_{33}^2w_{22}^2 + w_{23}^2w_{32}^2 - 2w_{22}w_{32}w_{23}w_{33}
\end{aligned}
\tag{5.2}
$$

and

$$w_{ri} = x_i^r - (x_1^r + x_2^r)/2, \qquad r = 2, 3, 4.$$

These coordinates carry useful geometric information on the shape of the 4-ad; v^1 and v^3 give us information on the appearance with respect to the bisector plane of $[X_1X_2]$, v^2 and v^4 give some information about the "flatness" of this 4-ad and v^5 measures the height of the 4-ad (X_1, X_2, X_3, X_4) relative to the distance $\|X_1 - X_2\|$. Assume U is the set of shapes $o(X)$ such that (X_1, X_2, X_3, X_4) is an affine frame in $\mathbb{R}^3$, and $\phi: U \to \mathbb{R}^{3k-7}$ is the map that associates to $o(X)$ its Bookstein coordinates. U is an open dense set in Σ_3^k, with the induced topology. In the particular case $k = 4, \Sigma_3^4$ is topologically a five-dimensional sphere and, from a classical result of Smale [48], Σ_3^4 has a differentiable structure diffeomorphic with the sphere S^5. Moreover, if L is a compact subset of U, there are a finite open covering $U_1 = U, \ldots, U_t$ of Σ_3^4 and a partition of unity $\phi_1, \ldots, \phi_t$, such that $\phi_1(o(X)) = 1, \forall\, o(X) \in L$.

We will use the following Riemannian metric on Σ_3^4: let $(y_1, \ldots, y_5)$ be the Bookstein coordinates of a shape in U_1 and let $g_1 = dy_1^2 + \cdots + dy_5^2$ be a flat Riemannian metric on U_1, and for each $j = 2, \ldots, t$ we consider any fixed Riemannian metric g_j on U_j. Let g be the Riemannian metric given by

$$g = \sum_{j=1}^{t} \phi_j g_j. \tag{5.3}$$

The space (Σ_3^4, d_g) is complete and is flat in a neighborhood of L. In this example the two distributions of shapes of tetrads before and after increase in IOP are close. Hence L, which contains supports of both distributions, consists of shapes of nondegenerate tetrads only.

Computations for the glaucoma data yield the following results. The p-value of the test for equality of the intrinsic means was found to be 0.058, based on the bootstrap distribution of the chi square-like statistic discussed in Remark 2.6. The number of bootstrap resamples for this study was 3000. The chi square-like density histogram is displayed in Figure 5. A matrix plot for the components of the nonpivotal bootstrap distribution of the sample mean differences γ_n^* in Remark 2.6 for this application is displayed in Figure 6. The nonpivotal bootstrap 95% confidence intervals for the mean differences $\gamma_j, j = 1, \ldots, 5$, components of γ in Remark 2.6 associated with the Bookstein coordinates $v_j, j = 1, \ldots, 5$, are: $(-0.0377073, -0.0058545)$ for γ_1, $(0.0014153, 0.0119214)$ for γ_2, $(-0.0303489, 0.0004710)$ for γ_3, $(0.0031686, 0.0205206)$ for γ_4, $(-0.0101761, 0.0496181)$ for γ_5. Note that the individual tests for difference are significant at the 5% level for the first, second and fourth coordinates. However, using the Bonferroni inequality, combining tests for five different shape coordinates each at 5% level leads to a much higher estimated level of significance for the overall shape change.

APPENDIX

The data set in Application 3 consists of a library of scanning confocal laser tomography (SCLT) images of the complicated ONH topography [11].

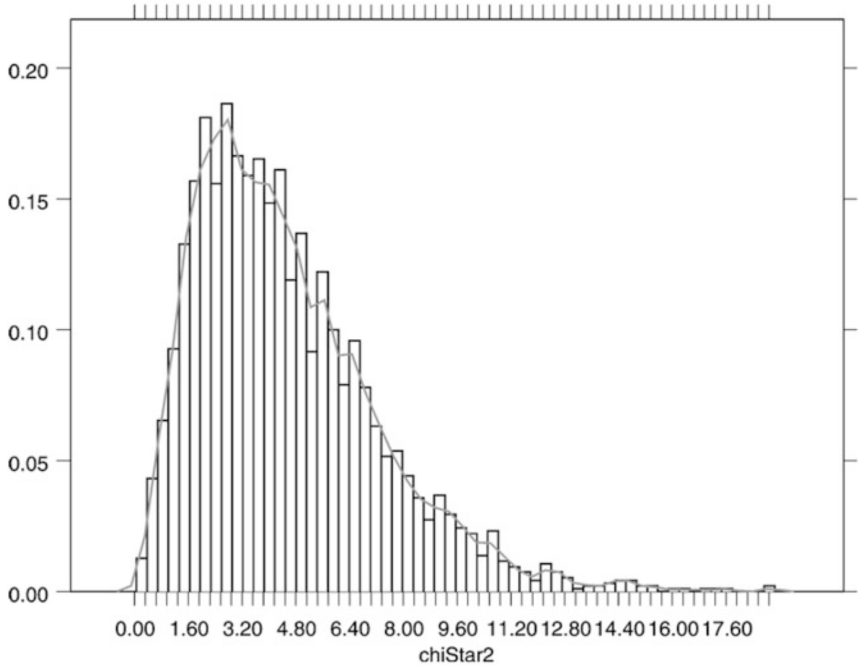

FIG. 5. χ^2-like bootstrap distribution for equality of intrinsic mean shapes from glaucoma data.

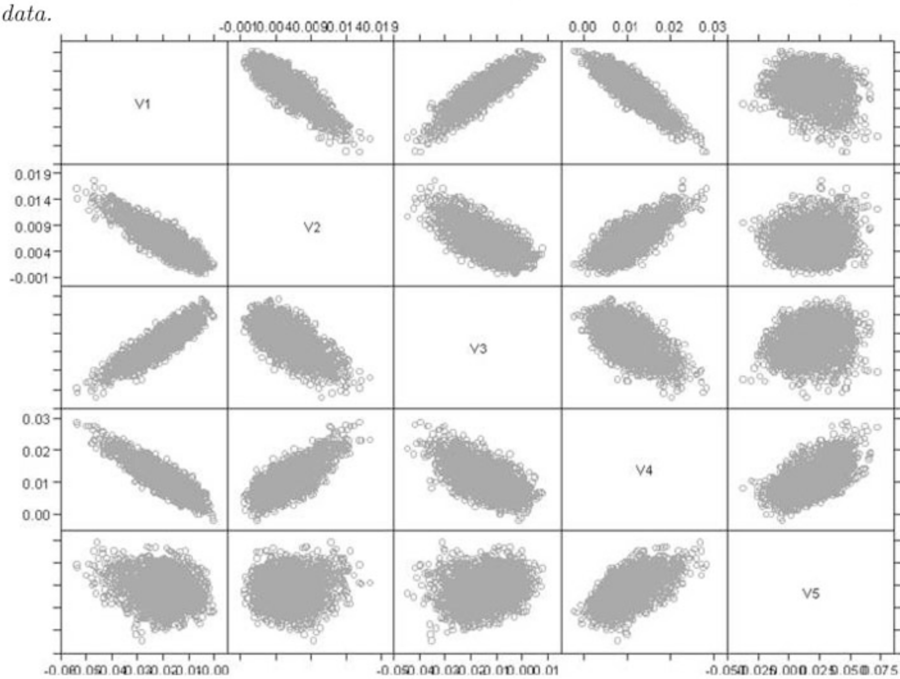

FIG. 6. *Glaucoma data, matrix plot for the bootstrap mean differences associated with Bookstein coordinates due to increased IOP.*

Those images are the so-called *range images*. A range image is, loosely speaking, like a digital camera image, except that each pixel stores a depth rather than a color level. It can also be seen as a set of points in three dimensions. The range data acquired by 3D digitizers such as optical scanners commonly consist of depths sampled on a regular grid. In the mathematical sense, a range image is a 2D array of real numbers which represent those depths. All of the files (observations) are produced by a combination of modules in C++ and SAS that take the raw image output and process it. The 256×256 arrays of height values are the products of this software. Another byproduct is a file which we will refer to as the "abxy" file. This file contain the following information: subject names (denoted by: 1c, 1d, 1e, 1f, 1g, 1i, 1j, 1k, 1l, 1n, 1o, 1p), observation points that distinguish the normal and treated eyes and the $10°$ or $15°$ fields of view for the imaging. The observation point "03" denotes a $10°$ view of the experimental glaucoma eye, "04" denotes a $15°$ view of the experimental glaucoma eye, "11" and "12" denote, respectively, the $10°$ and the $15°$ view of the normal eye. The two-dimensional coordinates of the center (a, b) of the ellipses that bound the ONH region, as well as the sizes of the small and the large axes of the ellipses (x, y), are stored in the so-called "abxy" file. To find out more about the LSU study and the image acquisition, see [11]. File names (each file is one observation) were constructed from the information in the "abxy" file. The list of all the observations is then used as an input for the program (created by G. Derado in C++) which determines the three-dimensional coordinates of the landmarks for each observation considered in our analysis, as well as for determining the fifth Bookstein coordinate for each observation. Each image consists of a 256×256 array of elevation values which represent the "depth" of the ONH. By the "depth" we mean the distance from an imaginary plane, located approximately at the base of the ONH cup, to the "back of the ONH cup."

To reduce the dimensionality of the shape space to 5, out of five landmarks T, S, N, I, V recorded, only four landmarks $(X_1 = T,\ X_2 = S,\ X_3 = N,\ X_4 = V)$ were considered.

The original data were collected in experimental observations on Rhesus monkeys, and after treatment a healthy eye slowly returns to its original shape. For the purpose of IOP increment detection, in this paper only the first set of after-treatment observations of the treated eye is considered.

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19.3 "Statistics on Riemannian manifolds: asymptotic distribution and curvature"

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STATISTICS ON RIEMANNIAN MANIFOLDS: ASYMPTOTIC DISTRIBUTION AND CURVATURE

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(Communicated by Edward C. Waymire)

ABSTRACT. In this article a nonsingular asymptotic distribution is derived for a broad class of underlying distributions on a Riemannian manifold in relation to its curvature. Also, the asymptotic dispersion is explicitly related to curvature. These results are applied and further strengthened for the planar shape space of k-ads.

1. INTRODUCTION

Statistical analysis of a probability measure Q on a differentiable manifold M has diverse applications in directional and axial statistics, morphometrics, medical diagnostics and machine vision ([1, 2, 3, 4, 6, 7, 8, 11, 15]). Most of this analysis focuses on nonintrinsic Fréchet means of Q. In this article we provide a distribution theory for the nonparametric analysis of intrinsic means which can be directly used for the one- and two-sample problems. To be precise, let (M, g) be a Riemannian manifold with metric tensor g and geodesic distance d_g. Define the **Fréchet function** F of Q as

$$F(p) = \int_M d_g^2(p, m) Q(dm), \ p \in M. \tag{1.1}$$

Assume F to be finite. We consider probability measures Q whose support $supp(Q)$ are contained in **geodesic balls** $B(p, r) = \{m : d_g(p, m) < r\}$. If the Fréchet function, restricted to such a ball $B(p, r)$, has a unique minimizer μ_I in $B(p, r)$, we call it the **intrinsic mean of** Q **in** $B(p, r)$. The **sample intrinsic mean** μ_{nI} **in** $B(p, r)$ is the intrinsic mean of $Q_n = \frac{1}{n}\sum_{j=1}^n \delta_{X_j}$ in $B(p, r)$, where $X_1, X_2, \ldots, X_n$ are independent and identically distributed (iid) observations from the underlying distribution Q. Crucial to nonparametric analysis is the asymptotic distribution of μ_{nI}. Our main goals are (i) to derive this asymptotic distribution, assuring its nonsingularity, under as broad a condition on $supp(Q)$ as possible, (ii) to explicitly compute the asymptotic dispersion, and (iii) to apply and refine the general theory to the particularly important **planar shape space** Σ_2^k of k landmarks introduced by Kendall [11].

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To indicate the role curvature plays in this endeavor, let $r_* = min\{inj(M), \frac{\pi}{\sqrt{\overline{C}}}\}$, where $\overline{C}$ is an upper bound of sectional curvatures of M if this upper bound is positive, and $\overline{C} = 0$ otherwise. Also, $inj(M) \equiv \inf\{d_g(p, C(p)) : p \in M\}$ is the **injectivity radius** of M, where $C(p)$ is the **cut locus** of p, i.e., the set of points of the form $\gamma(t_0)$, where γ is a geodesic and t_0 is the supremum of all $t > 0$ such that the geodesic from p to $\gamma(t)$ is distance minimizing. The **exponential map** exp_p is injective on $\{v \in T_p(M) : |v| < r\}$ if and only if $r \leq r_*$ (Do Carmo [5], p. 271). It follows that a geodesic ball $B(p, r)$ with $r \leq \frac{r_*}{2}$ is **strongly convex**, i.e., for every pair $q, q' \in B(p, r)$ there exists a unique geodesic connecting q, q', entirely contained in $B(p, r)$, this geodesic being distance minimizing. By Proposition 2.1 and Theorem 2.2, if $supp(Q) \subseteq B(p, \frac{r_*}{2})$, then Q has a unique intrinsic mean μ_I in $B(p, \frac{r_*}{2})$. If in addition, $supp(Q) \subseteq B(\mu_I, \frac{r_*}{2})$, then the sample intrinsic mean has asymptotic normal distribution. Further, in the case of manifolds with constant sectional curvature, the asymptotic dispersion can be explicitly expressed in terms of curvature.

It may be noted that our results are not related to those of Pennec [16] who has a number of interesting results on distributions on manifolds, including one that provides an expansion of the density of the (analog of) normal distribution on the manifold in terms of its variance, for the case of small variance.

For background in differential geometry used here, we refer to Do Carmo [5] and Lee [14].

2. Asymptotic distribution and curvature

Let (M, g) be a Riemannian manifold. We continue to use the notation of Section 1. Let Q be a probability measure, $supp(Q) \subseteq B(p, \frac{r_*}{2})$ for some p. Then there is a unique (local) intrinsic mean μ_I in $B(p, \frac{r_*}{2})$ (Kendall [12]). This substantially extends Karchar's result on the existence and uniqueness of a local mean ([9]), but not his important result on the strict convexity of F. We are able to circumvent this difficulty in the case $supp(Q) \subseteq B(\mu_I, \frac{r_*}{2})$. Denote by μ_{nI} the intrinsic mean of Q_n in $B(p, \frac{r_*}{2})$. The inverse of the exponential map $\phi = exp_p^{-1}$ is a diffeomorphism on $B(p, \frac{r_*}{2})$ onto its image, say U, in $T_p(M)$. The image $\tilde{Q} = Q \circ \phi^{-1}$ of Q under ϕ is a probability measure in $T_p(M)$, and the image $\mu = \phi(\mu_I)$ of μ_I is the minimizer of

$$\tilde{F}(x) = \int_U d_g^2(\phi^{-1}x, \phi^{-1}y)\tilde{Q}(dy), \ x \in U. \tag{2.1}$$

Similarly $\mu_n = \phi(\mu_{nI})$ is the corresponding minimizer when $\tilde{Q}$ is replaced by $\tilde{Q}_n = \frac{1}{n}\sum_{j=1}^{n} \delta_{\phi(X_j)}$. As proved in [3], Theorem 2.1, a central limit theorem for the **M-estimator** μ_n may be derived and used to obtain the following result. The **normal coordinates** x, y used here are with respect to a chosen orthonormal basis in T_pM.

Proposition 2.1. *Suppose the support of Q is contained in the geodesic ball $B = B(p, \frac{r_*}{2})$. Let $\phi = exp_p^{-1} : B \longrightarrow \phi(B)$. Define $h(x, y) = d_g^2(\phi^{-1}x, \phi^{-1}y)$; $x, y \in \phi(B)$. Let $((D_rh))_{r=1}^d$ and $((D_rD_sh))_{r,s=1}^d$ be the matrices of first and second order derivatives of $y \mapsto h(x, y)$. Let $\tilde{X}_j = \phi(X_j); j = 1, \ldots, n$, $X_1, \ldots, X_n$ being iid observations from Q. Define*

$$\Lambda = E((D_rD_sh(\tilde{X}_1, \mu)))_{r,s=1}^d, \ \Sigma = Cov((D_rh(\tilde{X}_1, \mu)))_{r=1}^d.$$

If Λ is nonsingular, then

$$\sqrt{n}(\mu_n - \mu) \xrightarrow{\mathcal{L}} N(0, \Lambda^{-1}\Sigma\Lambda^{-1}). \tag{2.2}$$

The natural candidate for p in Proposition 2.1 is the intrinsic mean of Q in $B(p, \frac{r_*}{2})$, namely μ_I. Then we get expressions for Λ and Σ using an orthonormal basis in $T_{\mu_I}M$. Theorem 2.2 below gives a lower bound on Λ and an exact expression when M has constant sectional curvature. The lower bound gives a condition on the nonsingularity of Λ. The nonsingularity of Σ is a milder condition which holds, for example, when Q has a density with respect to the volume measure on M. In the statement of the theorem, the usual partial order $A \geq B$ between $d \times d$ symmetric matrices A, B, means that $A - B$ is nonnegative definite.

Theorem 2.2. *Assume $supp(Q) \subseteq B(p, \frac{r_*}{2})$. Let $\phi = exp_{\mu_I}^{-1} : B(p, \frac{r_*}{2}) \longrightarrow T_{\mu_I}M(\approx \mathbb{R}^d)$, and let C denote an upper bound of all sectional curvatures. Then in normal coordinates with respect to a chosen orthonormal basis in $T_{\mu_I}M$,*

$$D_r h(x, 0) = -2x^r, \quad 1 \leq r \leq d, \tag{2.3}$$

$$[D_r D_s h(x, 0)] \geq \left[2\left(\left(\frac{1 - f(|x|)}{|x|^2}\right) x^r x^s + f(|x|)\delta_{rs}\right)\right]_{1 \leq r,s \leq d}, \tag{2.4}$$

where $|x| = \sqrt{(x^1)^2 + (x^2)^2 + \ldots + (x^d)^2}$,

$$f(x) = \begin{cases} 1 & \text{if } C = 0, \\ \sqrt{C}x\frac{cos(\sqrt{C}x)}{sin(\sqrt{C}x)} & \text{if } C > 0, \\ \sqrt{-C}x\frac{cosh(\sqrt{-C}x)}{sinh(\sqrt{-C}x)} & \text{if } C < 0. \end{cases} \tag{2.5}$$

There is equality in (2.4) when M has constant sectional curvature C, and in this case Λ has the expression

$$\Lambda_{rs} = 2E(\left(\frac{1 - f(|\tilde{X}_1|)}{|\tilde{X}_1|^2}\right) \tilde{X}_1^r \tilde{X}_1^s + (f(|\tilde{X}_1|))\delta_{rs}\ ), \quad 1 \leq r, s \leq d, \tag{2.6}$$

Λ being positive definite if Q has support in $B(\mu_I, \frac{r_*}{2})$.

Proof. Let $\gamma(s)$ be a geodesic, $\gamma(0) = \mu_I$. Define $c(s, t) = exp_m(t exp_m^{-1}\gamma(s))$, $s \in [0, \epsilon]$, $t \in [0, 1]$, as a smooth variation of γ through geodesics lying entirely in $B(p, \frac{r_*}{2})$. Let $T = \frac{\partial}{\partial t}c(s, t)$, $S = \frac{\partial}{\partial s}c(s, t)$. Since $c(s, 0) = m$, $S(s, 0) = 0$, and since $c(s, 1) = \gamma(s)$, $S(s, 1) = \dot{\gamma}(s)$. Also $\langle T, T\rangle = d_g^2(\gamma(s), m)$ is independent of t, and the covariant derivative $D_t T$ vanishes because $t \mapsto c(s, t)$ is a geodesic (for each s). Then

$$d_g^2(\gamma(s), m) = \langle T(s, t), T(s, t)\rangle = \int_0^1 \langle T(s, t), T(s, t)\rangle dt. \tag{2.7}$$

Hence $d_g^2(\gamma(s), m)$ is C^∞ smooth, and using the symmetry of the connection on a parametrized surface (see Lemma 3.4, p. 68 in Do Carmo [5]), we get

$$\begin{aligned} \frac{d}{ds}d_g^2(\gamma(s), m) &= 2\int_0^1 \langle D_s T, T\rangle dt = 2\int_0^1 \frac{d}{dt}\langle T, S\rangle dt \\ &= 2\langle T(s, 1), S(s, 1)\rangle = -2\langle exp_{\gamma(s)}^{-1}m, \dot{\gamma}(s)\rangle. \end{aligned} \tag{2.8}$$

Substituting $s = 0$ in (2.8), we get expressions for $D_r h(x, 0)$ as in (2.3). Also

$$\frac{d^2}{ds^2} d_g^2(\gamma(s), m) = 2\langle D_s T(s,1), S(s,1)\rangle \tag{2.9}$$

$$= 2\langle D_t S(s,1), S(s,1)\rangle = 2\langle D_t J_s(1), J_s(1)\rangle, \tag{2.10}$$

where $J_s(t) = S(s,t)$. Note that J_s is a Jacobi field along $c(s,.)$ with $J_s(0) = 0$, $J_s(1) = \dot\gamma(s)$. Let $J_s^{\perp}$ and J_s^{-} be the normal and tangential components of J_s. The relations (2.13)-(2.15) below may be obtained from Jost [10], p. 197, and Lee [14], Lemma 10.8. For the sake of exposition, we indicate the arguements here. Let η be a unit speed geodesic in M and J a normal Jacobi field along η, $J(0) = 0$. Define

$$u(t) = \begin{cases} t & \text{if } C = 0, \\ \frac{sin(\sqrt{C}t)}{\sqrt{C}} & \text{if } C > 0, \\ \frac{sinh(\sqrt{-C}t)}{\sqrt{-C}} & \text{if } C < 0. \end{cases} \tag{2.11}$$

Then $u''(t) = -Cu(t)$ and

$$(|J|'u - |J|u')'(t) = (|J|'' + C|J|)u(t). \tag{2.12}$$

By exact differentiation and Schwartz inequality, it is easy to show that $|J|'' + C|J| \geq 0$, hence $(|J|'u - |J|u')'(t) \geq 0$ whenever $u(t) \geq 0$. This implies that $|J|'u - |J|u' \geq 0$ if $t \leq t_0$, where u is positive on $(0, t_0)$. Also $|J|' = \frac{\langle J', J\rangle}{|J|}$. Therefore $\langle J(t), D_t J(t)\rangle \geq \frac{u'(t)}{u(t)}|J(t)|^2 \ \forall\ t < t_0$. If we drop the unit speed assumption on η, we get

$$\langle J(1), D_t J(1)\rangle \geq |\dot\eta| \frac{u'(|\dot\eta|)}{u(|\dot\eta|)} |J(1)|^2 \text{ if } |\dot\eta| < t_0. \tag{2.13}$$

Here $t_0 = \infty$ if $C \leq 0$ and equals $\frac{\pi}{\sqrt{C}}$ if $C > 0$. When M has constant sectional curvature C, $J(t) = u(t)E(t)$, where E is a parallel normal vector field along η. Hence

$$\langle J(t), D_t J(t)\rangle = u(t)u'(t)|E(t)|^2 = \frac{u'(t)}{u(t)}|J(t)|^2. \tag{2.14}$$

If we drop the unit speed assumption, we get

$$\langle J(t), D_t J(t)\rangle = |\dot\eta| \frac{u'(|\dot\eta|t)}{u(|\dot\eta|t)} |J(t)|^2. \tag{2.15}$$

Since $J_s^{\perp}$ is a normal Jacobi field along the geodesic $c(s,.)$, from (2.13) and (2.15) it follows that

$$\langle J_s^{\perp}(1), D_t J_s^{\perp}(1)\rangle \geq f(d(\gamma(s), m))|J_s^{\perp}(1)|^2 \tag{2.16}$$

with equality in (2.16) when M has constant sectional curvature C, f being defined in (2.5).

Next suppose J is a Jacobi field along a geodesic η, $J(0) = 0$ and let $J^{-}(t)$ be its tangential component. Then $J^{-}(t) = \lambda t \dot\eta(t)$ where $\lambda t = \frac{\langle J(t), \dot\eta(t)\rangle}{|\dot\eta|^2}$, λ being independent of t. Hence

$$\begin{aligned} (D_t J)^{-}(t) &= \frac{\langle D_t J(t), \dot\eta(t)\rangle}{|\dot\eta|^2} \dot\eta(t) \\ &= \frac{d}{dt}\left(\frac{\langle J(t), \dot\eta(t)\rangle}{|\eta|^2}\right)\dot\eta(t) = \lambda\dot\eta(t) = D_t(J^{-})(t) \end{aligned} \tag{2.17}$$

and

$$D_t|J^-|^2(1) = 2\lambda^2|\dot{\eta}|^2 = 2\frac{\langle J(1),\dot{\eta}(1)\rangle^2}{|\dot{\eta}(1)|^2}$$
$$= D_t\langle J, J^-\rangle(1) = \langle D_tJ(1), J^-(1)\rangle + |J^-(1)|^2$$

which implies

$$\langle D_tJ(1), J^-(1)\rangle = 2\frac{\langle J(1),\dot{\eta}(1)\rangle^2}{|\dot{\eta}(1)|^2} - |J^-(1)|^2 = \frac{\langle J(1),\dot{\eta}(1)\rangle^2}{|\dot{\eta}(1)|^2}. \tag{2.18}$$

Apply (2.17) and (2.18) to the Jacobi field J_s to get

$$D_t(J_s^-)(1) = (D_tJ_s)^-(1) = J_s^-(1) = \frac{\langle J_s(1), T(s,1)\rangle}{|T(s,1)|^2}T(s,1), \tag{2.19}$$

$$\langle D_tJ_s(1), J_s^-(1)\rangle = \frac{\langle J_s(1), T(s,1)\rangle^2}{|T(s,1)|^2}. \tag{2.20}$$

Using (2.16), (2.19) and (2.20), (2.10) becomes

$$\begin{aligned}
\frac{d^2}{ds^2}d_g^2(\gamma(s),m) &= 2\langle D_tJ_s(1), J_s(1)\rangle \\
&= 2\langle D_tJ_s(1), J_s^-(1)\rangle + 2\langle D_tJ_s(1), J_s^\perp(1)\rangle \\
&= 2\langle D_tJ_s(1), J_s^-(1)\rangle + 2\langle D_t(J_s^\perp)(1), J_s^\perp(1)\rangle \\
&\geq 2\frac{\langle J_s(1), T(s,1)\rangle^2}{|T(s,1)|^2} + 2f(|T(s,1)|)|J_s^\perp(1)|^2 \qquad (2.21)\\
&= 2\frac{\langle J_s(1), T(s,1)\rangle^2}{|T(s,1)|^2} + 2f(|T(s,1)|)|J_s(1)|^2 \\
&\quad - 2f(|T(s,1)|)\frac{\langle J_s(1), T(s,1)\rangle^2}{|T(s,1)|^2} \\
&= 2f(d_g(\gamma(s),m))|\dot{\gamma}(s)|^2 + 2(1-f(d_g(\gamma(s),m)))\frac{\langle\dot{\gamma}(s), exp_{\gamma(s)}^{-1}m\rangle^2}{d_g^2(\gamma(s),m)} \qquad (2.22)
\end{aligned}$$

with equality in (2.21) when M has constant sectional curvature C. Substituting $s = 0$ in (2.22), we get a lower bound for $[D_rD_sh(x,0)]$ as in (2.4) and an exact expression for $D_rD_sh(x,0)$ when M has constant sectional curvature. To see this, let $\dot{\gamma}(0) = v$. Then writing $m = \phi^{-1}(x)$, $\gamma(s) = \phi^{-1}(sv)$, one has

$$\begin{aligned}
\frac{d^2}{ds^2}d_g^2(\gamma(s),m)\big|_{s=0} &= \frac{d^2}{ds^2}d_g^2(\phi^{-1}(x),\phi^{-1}(sv))\big|_{s=0} \\
&= \frac{d^2}{ds^2}h(x,sv)\big|_{s=0} = \sum_{r,s=1}^{d} v_rv_sD_rD_sh(x,0). \qquad (2.23)
\end{aligned}$$

Since $d^2(\gamma(s),m)$ is twice continuously differentiable and Q has compact support, using the Lebesgue DCT, we get

$$\frac{d^2}{ds^2}F(\gamma(s))|_{s=0} = \int\frac{d^2}{ds^2}d^2(\gamma(s),m)|_{s=0}Q(dm). \tag{2.24}$$

Then (2.6) follows from (2.22). If $supp(Q) \subseteq B(\mu_I, \frac{r_*}{2})$, then the expression in (2.22) is strictly positive at $s = 0$ for all $m \in supp(Q)$, hence Λ is positive definite. This completes the proof. □

Under the assumptions of Theorem 2.2, it follows that $E(\tilde{X}_1) = 0$ and $\Sigma = 4E(\tilde{X}_1\tilde{X}_1')$. This is also stated in Theorem 2.1 in Bhattacharya [2].

Remark 2.1. It may be noted that the spaces S^d, $\mathbb{R}P^d$ have constant positive curvature. One may also endow the projective shape space with a metric which makes it a space of constant positive curvature, since it is diffeomorphic to a product of real projective spaces ([15]). In the next section we turn to Σ_2^k, whose sectional curvatures range from 1 to 4.

3. Application to the planar shape space Σ_2^k

Consider the planar shape space Σ_2^k of **k-ads** in $\mathbb{R}^2$. An element of Σ_2^k is a set of k landmarks, or points in the plane (not all equal), modulo translation, rotation and scaling. Let S_2^k be the **pre-shape sphere** which is the space of column vectors in $\mathbb{C}^k$ with mean 0 and norm 1. Its tangent space is

$$T_zS_2^k = \{v \in \mathbb{C}^k :\ v'\mathbf{1}_k = Re(z'\bar{v}) = 0\}.$$

Here $\mathbf{1}_k$ denotes the column vector of ones of size k. To apply Proposition 2.1 to carry out nonparametric inference on Σ_2^k, we need to identify the exponential and inverse exponential maps on Σ_2^k. For that we consider their lifts to S_2^k as in Section 4 in Le [13], and Kendall [11]. The map $\pi : S_2^k \to \Sigma_2^k$,

$$z \mapsto \pi(z) = [z] = \{\lambda z : \lambda \in \mathbb{C}, |\lambda| = 1\},$$

is a Riemannian submersion. So the tangent space $T_{[z]}\Sigma_2^k$ is isometric with a subspace of $T_zS_2^k$ called the **horizontal subspace** H_z which is

$$H_z = \{v \in \mathbb{C}^k\ : z'\bar{v} = 0,\ v'\mathbf{1}_k = 0\}.$$

Denote the corresponding isometric mapping by $\chi_{[z]} : T_{[z]}\Sigma_2^k \to H_z$. Then $exp_{[z]} = \pi \circ exp_z \circ \chi_{[z]}$, and

$$\chi_{[z]} \circ exp_{[z]}^{-1} : \Sigma_2^k \setminus C([z]) \to H_z,\ [w] \mapsto \frac{r}{sinr}\{-zcosr + e^{i\theta}w\}, \tag{3.1}$$

$$r = d_g([z],[w]) = arccos(|z'\bar{w}|) \in [0, \frac{\pi}{2}),\ e^{i\theta} = \frac{z'\bar{w}}{|z'\bar{w}|}. \tag{3.2}$$

In (3.1), $C([z])$ is the cut-locus of $[z]$, which is

$$C([z]) = \{[x] \in \Sigma_2^k : d_g([x],[z]) = \frac{\pi}{2}\} = \{[x] : z'\bar{x} = 0\}.$$

Σ_2^k has all sectional curvatures bounded between 1 and 4, and its injectivity radius is $\frac{\pi}{2}$. From a result due to Kendall [12], Q has an intrinsic mean if its support is contained in a geodesic ball of radius $\frac{\pi}{4}$. Suppose $supp(Q) \subseteq B(p, \frac{\pi}{4})$ and let $\mu_I = [\mu]$ be the intrinsic mean of Q in the support, with μ being one of its pre-shapes. The following theorem gives the expression for Λ in Theorem 2.2 and derives a sufficient condition for its nonsingularity.

Theorem 3.1. *Let $\phi : B(p, \frac{\pi}{4}) \to \mathbb{C}^{k-2}(\approx \mathbb{R}^{2k-4})$ be the coodinates of $\chi_{\mu_I} \circ exp_{\mu_I}^{-1} : B(p, \frac{\pi}{4}) \to H_\mu$ with respect to some orthonormal basis $\{v_1, \ldots, v_{k-2}, iv_1, \ldots, iv_{k-2}\}$ for H_μ. Define $h(x,y) = d_g^2(\phi^{-1}x, \phi^{-1}y)$. Let $((D_rh))_{r=1}^{2k-4}$ and $((D_rD_sh))_{r,s=1}^{2k-4}$ be the matrix of first and second order derivatives of $y \mapsto h(x,y)$. Let $\tilde{X}_j = \phi(X_j) = (\tilde{X}_j^1, \ldots, \tilde{X}_j^{k-2})'$; $j = 1, \ldots, n$, $X_1, \ldots, X_n$ being iid observations from Q. Define*

$\Lambda = E((D_r D_s h(\tilde{X}_1, 0)))_{r,s=1}^{2k-4}$. *Then* Λ *is positive definite if the support of* Q *is contained in* $B(\mu_I, R)$, *where* R *is the unique solution of* $tan(x) = 2x$, $x \in (0, \frac{\pi}{2})$.

Proof. For a geodesic γ starting at μ_I, write $\gamma = \pi \circ \tilde{\gamma}$, where $\tilde{\gamma}$ is a geodesic in S_2^k starting at μ. From the proof of Theorem 2.2, for $m = [z] \in B(p, \frac{\pi}{4})$,

$$\frac{d}{ds} d_g^2(\gamma(s), m) = 2\langle T(s,1), \dot{\gamma}(s)\rangle = 2\langle \tilde{T}(s,1), \dot{\tilde{\gamma}}(s)\rangle, \tag{3.3}$$

$$\frac{d^2}{ds^2} d_g^2(\gamma(s), m) = 2\langle D_s T(s,1), \dot{\gamma}(s)\rangle = 2\langle D_s \tilde{T}(s,1), \dot{\tilde{\gamma}}(s)\rangle, \tag{3.4}$$

where $\tilde{T}(s,1) = \chi_{\gamma(s)}(T(s,1))$. From (3.1), this has the expression

$$\tilde{T}(s,1) = -\frac{\rho(s)}{sin(\rho(s))}\left[-cos(\rho(s))\tilde{\gamma}(s) + e^{i\theta(s)}z\right], \tag{3.5}$$

$$\text{where } e^{i\theta(s)} = \frac{z'\tilde{\gamma}(s)}{cos(\rho(s))},\ \rho(s) = d_g(\gamma(s), m).$$

The inner product in (3.3) and (3.4) is the Riemannian metric on TS_2^k which is $\langle v, w\rangle = Re(v'\bar{w})$. Observe that $D_s\tilde{T}(s,1)$ is $\frac{d}{ds}\tilde{T}(s,1)$ projected onto $H_{\tilde{\gamma}(s)}$. Since $\langle \mu, \dot{\tilde{\gamma}}(0)\rangle = 0$,

$$\frac{d^2}{ds^2} d_g^2(\gamma(s), m)|_{s=0} = 2\langle \frac{d}{ds}\tilde{T}(s,1)|_{s=0}, \dot{\tilde{\gamma}}(0)\rangle. \tag{3.6}$$

From (3.5) we have

$$\begin{aligned}\frac{d}{ds}\tilde{T}(s,1)|_{s=0} = {} & \left(\frac{d}{ds}\Big(\frac{\rho(s)cos(\rho(s))}{sin(\rho(s))}\Big)|_{s=0}\right)\mu + \left(\frac{\rho(s)cos(\rho(s))}{sin\rho(s)}|_{s=0}\right)\dot{\tilde{\gamma}}(0) \\ & - \left(\frac{d}{ds}\Big(\frac{\rho(s)}{sin(\rho(s))cos(\rho(s))}\Big)|_{s=0}\right)(\bar{z}'\mu)z \\ & - \left(\frac{\rho(s)}{sin(\rho(s))cos(\rho(s))}|_{s=0}\right)(\bar{z}'\dot{\tilde{\gamma}}(0))z,\end{aligned} \tag{3.7}$$

and along with (3.3), we get

$$\frac{d}{ds}\rho(s)|_{s=0} = \frac{-1}{sin(r)}\langle \dot{\tilde{\gamma}}(0), \frac{\bar{z}'\mu}{cos(r)}z\rangle\ (r := d_g(m, \mu_I)). \tag{3.8}$$

Hence

$$\begin{aligned}\langle \frac{d}{ds}\tilde{T}(s,1)|_{s=0}, \dot{\tilde{\gamma}}(0)\rangle = {} & r\frac{cos(r)}{sin(r)}\|\dot{\tilde{\gamma}}(0)\|^2 - \left(\frac{1}{sin^2 r} - r\frac{cos(r)}{sin^3(r)}\right)(Rex)^2 \\ & + \frac{r}{sin(r)cos(r)}(Imx)^2,\end{aligned} \tag{3.9}$$

where

$$x = e^{i\theta}z'\overline{\dot{\tilde{\gamma}}(0)},\ e^{i\theta} = \frac{z'\mu}{cosr}. \tag{3.10}$$

The value of x in (3.10), and hence the expression in (3.9), depends on z only through $m = [z]$. Also if $\gamma = \pi(\gamma_1) = \pi(\gamma_2)$, γ_1 and γ_2 being two geodesics on S_2^k starting at μ_1 and μ_2 respectively, with $[\mu_1] = [\mu_2] = [\mu]$, then $\gamma_1(t) = \lambda\gamma_2(t)$, where $\mu_2 = \lambda\mu_1$, $\lambda \in \mathbb{C}$. Now it is easy to check that the expression in (3.9) depends on μ only through $[\mu] = \mu_I$. Note that $|x|^2 < 1 - cos^2 r$. So when $|\dot\gamma(0)| = 1$, (3.9) is

$$r\frac{cos(r)}{sin(r)} - \left(\frac{1}{sin^2 r} - r\frac{cos(r)}{sin^3 r}\right)(Rex)^2 + \frac{r}{sinrcosr}(Imx)^2$$
$$> r\frac{cos(r)}{sin(r)} - \left(\frac{1}{sin^2 r} - r\frac{cos(r)}{sin^3 r}\right)sin^2 r = \frac{2r - tanr}{tanr}, \tag{3.11}$$

which is > 0 if $r \leq R$ where $tan(R) = 2R$, $R \in (0, \frac{\pi}{2})$. Thus if $supp(Q) \subseteq B(\mu_I, R)$, then $\frac{d^2}{ds^2} d^2(\gamma(s), m)|_{s=0} > 0$, and hence Λ is positive definite. □

Remark 3.1. It can be shown that $R \in (\frac{\pi}{3}, \frac{2\pi}{5})$. It is approximately 0.37101π.

Remark 3.2. The nonsingularity of Σ defined in Theorem 2.2 is a mild condition which holds in particular if Q has a density (component) with respect to the volume measure on Σ_2^k.

From Proposition 2.1, Theorem 3.1 and Remark 3.2, we conclude that if $supp(Q) \subseteq B(\mu_I, R)$ and if Σ is nonsingular (e.g., if Q is absolutely continuous), then the sample mean from an iid sample has an asymptotically normal distribution with nonsingular dispersion. To get the expressions for Σ and Λ, note that the coordinate ϕ in Theorem 3.1 has the form

$$\phi(m) = (\tilde m^1, \ldots, \tilde m^{k-2})', \ \tilde m^j = \frac{r}{sinr} e^{i\theta} \bar v_j' z.$$

Hence

$$\Sigma_{(2k-4)\times(2k-4)} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}' & \Sigma_{22} \end{bmatrix},$$
$$(\Sigma_{11})_{ij} = 4E(\mathrm{Re}(\tilde X_1^i)\mathrm{Re}(\tilde X_1^j)),\ (\Sigma_{12})_{ij} = 4E(\mathrm{Re}(\tilde X_1^i)\mathrm{Im}(\tilde X_1^j)),$$
$$(\Sigma_{22})_{ij} = 4E(\mathrm{Im}(\tilde X_1^i)\mathrm{Im}(\tilde X_1^j)),\ \ 1 \leq i, j \leq k-2, \tag{3.12}$$

and

$$\Lambda_{(2k-4)\times(2k-4)} = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{12}' & \Lambda_{22} \end{bmatrix}, \tag{3.13}$$

where if $\dot\gamma(0) = \sum_{j=1}^{k-2} x^j v_j + \sum_{j=1}^{k-2} y^j (iv_j)$, $x = [x^1 \ldots x^{k-2}]'$, $y = [y^1 \ldots y^{k-2}]'$, then

$$E\left(\frac{d^2}{ds^2} d_g^2(\gamma(s), X_1)\right)|_{s=0} = x'\Lambda_{11}x + y'\Lambda_{22}y + 2x'\Lambda_{12}y.$$

This gives for $1 \leq r, s \leq k-2$,

$$(\Lambda_{11})_{rs} = 2E\Big[\ d_1 cot(d_1)\delta_{rs} - \frac{(1 - d_1 cot(d_1))}{d_1^2}(\mathrm{Re}\tilde X_1^r)(\mathrm{Re}\tilde X_1^s)$$
$$+ \frac{tan(d_1)}{d_1}(\mathrm{Im}\tilde X_1^r)(\mathrm{Im}\tilde X_1^s)\ \Big],$$
$$(\Lambda_{22})_{rs} = 2E\Big[\ d_1 cot(d_1)\delta_{rs} - \frac{(1 - d_1 cot(d_1))}{d_1^2}(\mathrm{Im}\tilde X_1^r)(\mathrm{Im}\tilde X_1^s)$$
$$+ \frac{tan(d_1)}{d_1}(\mathrm{Re}\tilde X_1^r)(\mathrm{Re}\tilde X_1^s)\ \Big],$$
$$(\Lambda_{12})_{rs} = -2E\Big[\ \frac{(1 - d_1 cot(d_1))}{d_1^2}(\mathrm{Re}\tilde X_1^r)(\mathrm{Im}\tilde X_1^s) + \frac{tan(d_1)}{d_1}(\mathrm{Im}\tilde X_1^r)(\mathrm{Re}\tilde X_1^s)\ \Big],$$

where $d_1 = d_g(X_1, \mu_I)$.

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Statistics on Manifolds with Applications to Shape Spaces

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ABSTRACT. This article provides an exposition of recent developments on the analysis of *landmark based shapes* in which a k-ad, i.e., a set of k points or landmarks on an object or a scene, are observed in 2D or 3D, for purposes of identification, discrimination, or diagnostics. Depending on the way the data are collected or recorded, the appropriate shape of an object is the maximal invariant specified by the space of orbits under a group G of transformations. All these spaces are manifolds, often with natural Riemannian structures. The statistical analysis based on Riemannian structures is said to be *intrinsic*. In other cases, proper distances are sought via an *equivariant embedding* of the manifold M in a vector space E, and the corresponding statistical analysis is called *extrinsic*.

1. Introduction

Statistical analysis of a probability measure Q on a differentiable manifold M has diverse applications in directional and axial statistics, morphometrics, medical diagnostics and machine vision. In this article, we are mostly concerned with the analysis of landmark based data, in which each observation consists of $k > m$ points in m-dimension, representing k locations on an object, called a k-ad. The choice of landmarks is generally made with expert help in the particular field of application. The objects of study can be anything for which two k-ads are equivalent modulo a group of transformations appropriate for the particular problem depending on the method of recording of the observations. For example, one may look at k-ads modulo size and Euclidean rigid body motions of translation and rotation. The analysis of shapes under this invariance was pioneered by Kendall (1977, 1984) and Bookstein (1978). Bookstein's approach is primarily registration-based requiring two or three landmarks to be brought into a standard position by translation, rotation and scaling of the k-ad. For these shapes, we would prefer Kendall's more invariant view of a shape identified with the orbit under rotation (in m-dimension) of the k-ad centered at the origin and scaled to have unit size. The resulting shape space is denoted Σ_k^m. A fairly comprehensive account of parametric inference on these manifolds, with many references to the literature, may be found in Dryden and Mardia (1998). The nonparametric methodology pursued here, along with the geometric and other mathematical issues that accompany it, stems from the earlier

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work of Bhattacharya and Patrangenaru(2002, 2003, 2005).

Recently there has been much emphasis on the statistical analysis of other notions of shapes of k-ads, namely, *affine shapes* invariant under affine transformations, and *projective shapes* invariant under projective transformations. Reconstruction of a scene from two (or more) aerial photographs taken from a plane is one of the research problems in affine shape analysis. Potential applications of projective shape analysis include face recognition and robotics-for robots to visually recognize a scene. (Mardia and Patrangenaru (2005), Bandulasiri et al.(2007)).

Examples of analysis with real data suggest that appropriate nonparametric methods are more powerful than their parametric counterparts in the literature, for distributions that occur in applications (Bhattacharya and Bhattacharya (2008a)).

There is a large literature on registration via landmarks in functional data analysis (see, e.g., Bigot (2006), Xia and Liu (2004), Ramsay and Silverman (2005)), in which proper alignments of curves are necessary for purposes of statistical analysis. However this subject is not closely related to the topics considered in the present article.

The article is organized as follows. Section 2 provides a brief expository description of the geometries of the manifolds that arise in shape analysis. Section 3 introduces the basic notion of the *Fréchet mean* as the unique minimizer of the *Fréchet function* $F(p)$, which is used here to nonparametrically discriminate different distributions. Section 4 outlines the asymptotic theory for *extrinsic mean*, namely, the unique minimizer of the Fréchet function $F(p) = \int_M \rho^2(p,x)Q(dx)$ where ρ is the distance inherited by the manifold M from an equivariant embedding J. In Section 5, we describe the corresponding asymptotic theory for *intrinsic means* on Riemannian manifolds, where ρ is the geodesic distance. In Section 6, we apply the theory of extrinsic and intrinsic analysis to some manifolds including the shape spaces of interest. Finally, Section 7 illustrates the theory with three applications to real data.

2. Geometry of Shape Manifolds

Many differentiable manifolds M naturally occur as submanifolds, or surfaces or hypersurfaces, of an Euclidean space. One example of this is the sphere $S^d = \{p \in \mathbb{R}^{d+1} : \|p\| = 1\}$. The shape spaces of interest here are not of this type. They are generally quotients of a Riemannian manifold N under the action of a transformation group. A number of them are quotient spaces of $N = S^d$ under the action of a compact group G, i.e., the elements of the space are orbits in S^d traced out by the application of G. Among important examples of this kind are axial spaces and Kendall's shape spaces. In some cases the *action of the group is free*, i.e., $gp = p$ only holds for the identity element $g = e$. Then the elements of the orbit $O_p = \{gp \colon g \in G\}$ are in one-one correspondence with elements of G, and one can identify the orbit with the group. The orbit inherits the differential structure of the Lie group G. The tangent space T_pN at a point p may then be decomposed into a *vertical subspace* of dimension that of the group G along the orbit space to which p belongs, and a *horizontal* one which is orthogonal to it. The projection

π, $\pi(p) = O_p$ is a *Riemannian submersion* of N onto the quotient space N/G. In other words, $\langle d\pi(v), d\pi(w)\rangle_{\pi(p)} = \langle v, w\rangle_p$ for horizontal vectors $v, w \in T_pN$, where $d\pi : T_pN \to T_{\pi(p)}N/G$ denotes the differential, or Jacobian, of the projection π. With this metric tensor, N/G has the natural structure of a Riemannian manifold. The intrinsic analysis proposed for these spaces is based on this Riemannian structure (See Section 5).

Often it is simpler both mathematically and computationally to carry out an extrinsic analysis, by embedding M in some Euclidean space $E^k \approx \mathbb{R}^k$, with the distance induced from that of E^k. This is also pursued when an appropriate Riemannian structure on M is not in sight. Among the possible embeddings, one seeks out *equivariant embeddings* which preserve many of the geometric features of M.

DEFINITION 2.1. For a Lie group H acting on a manifold M, an embedding $J : M \to \mathbb{R}^k$ is *H-equivariant* if there exists a group homomorphism $\phi : H \to GL(k, \mathbb{R})$ such that

$$J(hp) = \phi(h)J(p)\ \forall p \in M,\ \forall h \in H. \tag{2.1}$$

Here $GL(k, \mathbb{R})$ is the *general linear group* of all $k \times k$ non-singular matrices.

[Note: Henceforth, BP (...) stands for Bhattacharya and Patrangenaru (...) and BB (...) stands for Bhattacharya and Bhattacharya (...).]

2.1. The Real Projective Space $\mathbb{R}P^d$. This is the axial space comprising axes or lines through the origin in $\mathbb{R}^{d+1}$. Thus elements of $\mathbb{R}P^d$ may be represented as equivalence classes

$$[x] = [x^1 : x^2 : \dots x^{m+1}] = \{\lambda x : \lambda \neq 0\},\ x \in \mathbb{R}^{d+1} \setminus \{0\}. \tag{2.2}$$

One may also identify $\mathbb{R}P^d$ with S^d/G, with G comprising the identity map and the antipodal map $p \mapsto -p$. Its structure as a d-dimensional manifold (with quotient topology) and its Riemannian structure both derive from this identification. Among applications are observations on galaxies, on axes of crystals, or on the line of a geological fissure (Watson (1983), Mardia and Jupp (1999), Fisher et al. (1987), Beran and Fisher (1998), Kendall (1989)).

2.2. Kendall's (Direct Similarity) Shape Spaces Σ_m^k. Kendall's shape spaces are quotient spaces S^d/G, under the action of the *special orthogonal group* $G = SO(m)$ of $m \times m$ orthogonal matrices with determinant $+1$. For the important case $m = 2$, consider the space of all planar k-ads $(z_1, z_2, \dots, z_k)$ $(z_j = (x_j, y_j))$, $k > 2$, excluding those with k identical points. The set of all centered and normed k-ads, say $u = (u_1, u_2, \dots, u_k)$ comprise a unit sphere in a $(2k-2)$-dimensional vector space and is, therefore, a $(2k-3)$-dimensional sphere S^{2k-3}, called the *preshape sphere*. The group $G = SO(2)$ acts on the sphere by rotating each landmark by the same angle. The orbit under G of a point u in the preshape sphere can thus be seen to be a circle S^1, so that Kendall's planer shape space Σ_2^k can be viewed as the quotient space $S^{2k-3}/G \sim S^{2k-3}/S^1$, a $(2k-4)$-dimensional compact manifold. An algebraically simpler representation of Σ_2^k is given by the complex projective space $\mathbb{C}P^{k-2}$, described in Section 6.4. For many applications in archaeology, astronomy, morphometrics, medical diagnosis, etc., see Bookstein (1986, 1997), Kendall (1989), Dryden and Mardia (1998), BP (2003, 2005), BB (2008a) and Small (1996).

2.3. Reflection (Similarity) Shape Spaces $R\Sigma_m^k$. Consider now the *reflection shape* of a k-ad as defined in Section 2.2, but with $SO(m)$ replaced by the larger *orthogonal group* $O(m)$ of all $m \times m$ orthogonal matrices (with determinants either +1 or -1). The reflection shape space $R\Sigma_m^k$ is the space of orbits of the elements u of the preshape sphere whose columns span $\mathbb{R}^m$.

2.4. Affine Shape Spaces $A\Sigma_m^k$. The *affine shape* of a k-ad in $\mathbb{R}^m$ may be defined as the orbit of this k-ad under the group of all *affine transformations* $x \mapsto F(x) = Ax + b$, where A is an arbitrary $m \times m$ non-singular matrix and b is an arbitrary point in $\mathbb{R}^m$. Note that two k-ads $x = (x_1, \ldots, x_k)$ and $y = (y_1, \ldots, y_k)$, (x_j, $y_j \in \mathbb{R}^m$ for all j) have the same affine shape if and only if the centered k-ads $u = (u_1, u_2, \ldots, u_k) = (x_1 - \bar{x}, \ldots, x_k - \bar{x})$ and $v = (v_1, v_2, \ldots, v_k) = (y_1 - \bar{y}, \ldots, y_k - \bar{y})$ are related by a transformation $Au \doteq (Au_1, \ldots, Au_k) = v$. The centered k-ads lie in a linear subspace of $\mathbb{R}^m$ of dimension $m(k-1)$. Assume $k > m+1$. The affine shape space is then defined as the quotient space $H(m,k)/GL(m,R)$, where $H(m,k)$ consists of all centered k-ads whose landmarks span $\mathbb{R}^m$, and $GL(m,\mathbb{R})$ is the general linear group on $\mathbb{R}^m$ (of all $m \times m$ nonsingular matrices) which has the relative topology (and distance) of $\mathbb{R}^{m^2}$ and is a manifold of dimension m^2. It follows that $A\Sigma_m^k$ is a manifold of dimension $m(k-1) - m^2$. For $u, v \in H(m,k)$, since $Au = v$ iff $u'A' = v'$, and as A varies $u'A'$ generates the linear subspace L of $H(m,k)$ spanned by the m rows of u. The affine shape of u, (or of x), is identified with this subspace. Thus $A\Sigma_m^k$ may be identified with the set of all m dimensional subspaces of $\mathbb{R}^{k-1}$, namely, the *Grassmannian* $G_m(k-1)$-a result of Sparr (1995) (Also see Boothby (1986), pp. 63-64, 362-363). Affine shape spaces arise in certain problems of bioinformatics, cartography, machine vision and pattern recognition (Berthilsson and Heyden (1999), Berthilsson and Astrom (1999), Sepiashvili et al. (2003), Sparr (1992, 1996)).

2.5. Projective Shape Spaces $P\Sigma_m^k$. For purposes of machine vision, if images are taken from a great distance, such as a scene on the ground photographed from an airplane, affine shape analysis is appropriate. Otherwise, *projective shape* is a more appropriate choice. If one thinks of images or photographs obtained through a central projection (a pinhole camera is an example of this), a ray is received as a point on the image plane (e.g., the film of the camera). Since axes in 3D comprise the projective space $\mathbb{R}P^2$, k-ads in this view are valued in $\mathbb{R}P^2$. Note that for a 3D k-ad to represent a k-ad in $\mathbb{R}P^2$, the corresponding axes must all be distinct. To have invariance with regard to camera angles, one may first look at the original noncollinear (centered) 3D k-ad u and achieve affine invariance by its affine shape (i.e., by the equivalence class Au, $A \in GL(3,\mathbb{R})$), and finally take the corresponding equivalence class of axes in $\mathbb{R}P^2$ to define the projective shape of the k-ad as the equivalence class, or orbit, with respect to projective transformations on $\mathbb{R}P^2$. A projective shape (of a k-ad) is singular if the k axes lie on a vector plane ($\mathbb{R}P^1$). For $k > 4$, the space of all non-singular shapes is the 2D projective shape space, denoted $P_0\Sigma_2^k$.

In general, a projective (general linear) transformation α on $\mathbb{R}P^m$ is defined in terms of an $(m+1) \times (m+1)$ nonsingular matrix $A \in GL(m+1,\mathbb{R})$ by

$$\alpha([x]) = \alpha([x^1 : \ldots : x^{m+1}]) = [A(x^1, \ldots, x^{m+1})'], \tag{2.3}$$

where $x = (x^1, \ldots, x^{m+1}) \in \mathbb{R}^{m+1} \setminus \{0\}$. The group of all projective transformations on $\mathbb{R}P^m$ is denoted by $PGL(m)$. Now consider a k-ad $(y_1, \ldots, y_k)$ in $\mathbb{R}P^m$, say $y_j = [x_j]$ $(j = 1, \ldots, k)$, $k > m + 2$. The projective shape of this k-ad is its orbit under $PGL(m)$, i.e., $\{(\alpha y_1, \ldots, \alpha y_k)\colon \alpha \in PGL(m)\}$. To exclude singular shapes, define a k-ad $(y_1, \ldots, y_k) = ([x_1], \ldots, [x_k])$ to be in *general position* if the linear span of $\{y_1, \ldots, y_k\}$ is $\mathbb{R}P^m$, i.e., if the linear span of the set of k representative points $\{x_1, \ldots, x_k\}$ in $\mathbb{R}^{m+1}$ is $\mathbb{R}^{m+1}$. The space of shapes of all k-ads in general position is the projective shape space $P_0\Sigma_m^k$. Define a projective frame in $\mathbb{R}P^m$ to be an ordered system of $m+2$ points in general position. Let $I = i_1 < \ldots < i_{m+2}$ be an ordered subset of $\{1, \ldots, k\}$. A manifold structure on $P_I\Sigma_m^k$, the open dense subset of $P_0\Sigma_m^k$, of k-ads for which $(y_{i1}, \ldots, y_{i_{m+2}})$ is a projective frame in $\mathbb{R}P^m$, was derived in Mardia and Patrangenaru (2005) as follows. The standard frame is defined to be $([e_1], \ldots, [e_{m+1}], [e_1 + e_2 + \ldots + e_{m+1}])$, where $e_j \in \mathbb{R}^{m+1}$ has 1 in the j-th coordinate and zeros elsewhere. Given two projective frames $(p_1, \ldots, p_{m+2})$ and $(q_1, \ldots, q_{m+2})$, there exists a unique $\alpha \in PGL(m)$ such that $\alpha(p_j) = q_j$ $(j = 1, \ldots, k)$. By ordering the points in a k-ad such that the first $m + 2$ points are in general position, one may bring this ordered set, say, $(p_1, \ldots, p_{m+2})$, to the standard form by a unique $\alpha \in PGL(m)$. Then the ordered set of remaining $k - m - 2$ points is transformed to a point in $(\mathbb{R}P^m)^{k-m-2}$. This provides a diffeomorphism between $P_I\Sigma_m^k$ and the product of $k - m - 2$ copies of the real projective space $\mathbb{R}P^m$.

We will return to these manifolds again in Section 6. Now we turn to nonparametric inference on general manifolds.

3. Fréchet Means on Metric Spaces

Let (M, ρ) be a metric space, ρ being the distance, and let $f \geq 0$ be a given continuous increasing function on $[0, \infty)$. For a given probability measure Q on (the Borel sigmafield of) M, define the *Fréchet function* of Q as

$$F(p) = \int_M f(\rho(p, x))Q(dx), \quad p \in M. \tag{3.1}$$

DEFINITION 3.1. Suppose $F(p) < \infty$ for some $p \in M$. Then the set of all p for which $F(p)$ is the minimum value of F on M is called the *Fréchet Mean set* of Q, denoted by C_Q. If this set is a singleton, say $\{\mu_F\}$, then μ_F is called the *Fréchet Mean* of Q. If $X_1, X_2, \ldots, X_n$ are independent and identically distributed (iid) M-valued random variables defined on some probability space $(\Omega, \mathcal{F}, P)$ with common distribution Q, and $Q_n \doteq \frac{1}{n}\sum_{j=1}^n \delta_{X_j}$ is the corresponding empirical distribution, then the Fréchet mean set of Q_n is called the *sample Fréchet mean set*, denoted by C_{Q_n}. If this set is a singleton, say $\{\mu_{F_n}\}$, then μ_{F_n} is called the *sample Fréchet mean*.

Proposition 3.1 proves the consistency of the sample Fréchet mean as an estimator of the Fréchet mean of Q.

PROPOSITION 3.1. *Let M be a compact metric space. Consider the Fréchet function F of a probability measure given by (3.1). Given any $\epsilon > 0$, there exists an integer-valued random variable $N = N(\omega, \epsilon)$ and a P-null set $A(\omega, \epsilon)$ such that*

$$C_{Q_n} \subset C_Q^\epsilon \equiv \{p \in M : \rho(p, C_Q) < \epsilon\}, \ \forall n \geq N \tag{3.2}$$

outside of $A(\omega,\epsilon)$. In particular, if $C_Q = \{\mu_F\}$, then every measurable selection, μ_{F_n} from C_{Q_n} is a strongly consistent estimator of μ_F.

PROOF. For simplicity of notation, we write $C = C_Q$, $C_n = C_{Q_n}$, $\mu = \mu_F$ and $\mu_n = \mu_{F_n}$. Choose $\epsilon > 0$ arbitrarily. If $C^\epsilon = M$, then (3.2) holds with $N = 1$. If $D = M \setminus C^\epsilon$ is nonempty, write

$$\begin{aligned} l &= \min\{F(p) : p \in M\} = F(q)\ \forall q \in C, \\ l + \delta(\epsilon) &= \min\{F(p) : p \in D\},\ \delta(\epsilon) > 0. \end{aligned} \tag{3.3}$$

It is enough to show that

$$\max\{|F_n(p) - F(p)| : p \in M\} \longrightarrow 0 \text{ a.s., as } n \to \infty. \tag{3.4}$$

For if (3.4) holds, then there exists $N \geq 1$ such that, outside a P-null set $A(\omega,\epsilon)$,

$$\begin{aligned} \min\{F_n(p) : p \in C\} &\leq l + \frac{\delta(\epsilon)}{3}, \\ \min\{F_n(p) : p \in D\} &\geq l + \frac{\delta(\epsilon)}{2},\ \forall n \geq N. \end{aligned} \tag{3.5}$$

Clearly (3.5) implies (3.2).

To prove (3.4), choose and fix $\epsilon' > 0$, however small. Note that $\forall p, p', x \in M$,

$$|\rho(p,x) - \rho(p',x)| \leq \rho(p,p').$$

Hence

$$\begin{aligned} |F(p) - F(p')| &\leq \max\{|f(\rho(p,x)) - f(\rho(p',x))| : x \in M\} \\ &\leq \max\{|f(u) - f(u')| : |u - u'| \leq \rho(p,p')\}, \\ |F_n(p) - F_n(p')| &\leq \max\{|f(u) - f(u')| : |u - u'| \leq \rho(p,p')\}. \end{aligned} \tag{3.6}$$

Since f is uniformly continuous on $[0, R]$ where R is the diameter of M, so are F and F_n on M, and there exists $\delta(\epsilon') > 0$ such that

$$|F(p) - F(p')| \leq \frac{\epsilon'}{4},\ |F_n(p) - F_n(p')| \leq \frac{\epsilon'}{4} \tag{3.7}$$

if $\rho(p,p') < \delta(\epsilon')$. Let $\{q_1, \ldots, q_k\}$ be a $\delta(\epsilon')-$net of M, i.e., $\forall\ p \in M$ there exists $q(p) \in \{q_1, \ldots, q_k\}$ such that $\rho(p, q(p)) < \delta(\epsilon')$. By the strong law of large numbers, there exists an integer-valued random variable $N(\omega,\epsilon')$ such that outside of a P-null set $A(\omega,\epsilon')$, one has

$$|F_n(q_i) - F(q_i)| \leq \frac{\epsilon'}{4}\ \forall i = 1, 2, \ldots, k;\ \text{if } n \geq N(\omega,\epsilon'). \tag{3.8}$$

From (3.7) and (3.8) we get

$$\begin{aligned} |F(p) - F_n(p)| &\leq |F(p) - F(q(p))| + |F(q(p)) - F_n(q(p))| + |F_n(q(p)) - F_n(p)| \\ &\leq \frac{3\epsilon'}{4} < \epsilon',\ \forall p \in M, \end{aligned}$$

if $n \geq N(\omega,\epsilon')$ outside of $A(\omega,\epsilon')$. This proves (3.4). □

REMARK 3.1. Under an additional assumption guaranteeing the existence of a minimizer of F, Proposition 3.1 can be extended to all metric spaces whose closed and bounded subsets are all compact. We will consider such an extension elsewhere, thereby generalizing Theorem 2.3 in BP (2003). For statistical analysis on shape spaces which are compact manifolds, Proposition 3.1 suffices.

REMARK 3.2. One can show that the reverse of (3.2) that is "$C_Q \subset C^{\epsilon}_{Q_n}$ $\forall$ $n \geq N(\omega, \epsilon)$" does not hold in general. See for example Remark 2.6 in BP (2003).

REMARK 3.3. In view of Proposition 3.1, if the Fréchet mean μ_F of Q exists as a unique minimizer of F, then every measurable selection of a sequence $\mu_{F_n} \in C_{Q_n}$ $(n \geq 1)$ converges to μ_F with probability one. In the rest of the paper it therefore suffices to define the sample Fréchet mean as a measurable selection from C_{Q_n} $(n \geq 1)$.

Next we consider the asymptotic distribution of μ_{F_n}. For Theorem 3.2, we assume M to be a differentiable manifold of dimension d. Let ρ be a distance metrizing the topology of M. The proof of the theorem is similar to that of Theorem 2.1 in BP (2005). Denote by D_r the partial derivative w.r.t. the r^{th} coordinate. $(r = 1, \ldots, d)$.

THEOREM 3.2. *Suppose the following assumptions hold:*
A1 *Q has support in a single coordinate patch, (U, ϕ). [$\phi : U \longrightarrow \mathbb{R}^d$ smooth.] Let $Y_j = \phi(X_j)$, $j = 1, \ldots, n$.*
A2 *Fréchet mean μ_F of Q is unique.*
A3 *$\forall x, y \to h(x, y) = (\rho^{\phi})^2(x, y) = \rho^2(\phi^{-1}x, \phi^{-1}y)$ is twice continuously differentiable in a neighborhood of $\phi(\mu_F) = \mu$.*
A4 $\mathrm{E}\{\mathrm{D}_r h(Y, \mu)\}^2 < \infty$ $\forall r$.
A5 $\mathrm{E}\{\sup_{|u-v|\leq\epsilon} |\mathrm{D}_s\mathrm{D}_r h(Y, v) - \mathrm{D}_s\mathrm{D}_r h(Y, u)|\} \to 0$ *as* $\epsilon \to 0$ $\forall$ r, s.
A6 $\Lambda = ((\ \mathrm{E}\{\mathrm{D}_s\mathrm{D}_r h(Y, \mu)\}\ ))$ *is nonsingular.*
A7 $\Sigma = \mathrm{Cov}[\mathrm{grad}\ h(Y_1, \mu)]$ *is nonsingular.*
Let $\mu_{F,n}$ be a measurable selection from the sample Frechet mean set. Then under the assumptions ***A1-A7***,

$$\sqrt{n}(\mu_n - \mu) \xrightarrow{\mathcal{L}} N(0, \Lambda^{-1}\Sigma(\Lambda')^{-1}). \tag{3.9}$$

4. Extrinsic Means on Manifolds

From now on, we assume that M is a Riemannian manifold of dimension d. Let G be a Lie group acting on M and let $J : M \to \mathbb{E}^N$ be a H-equivariant embedding of M into some euclidean space $\mathbb{E}^N$ of dimension N. For all our applications, H is compact. Then J induces the metric

$$\rho(x, y) = \|J(x) - J(y)\| \tag{4.1}$$

on M, where $\|.\|$ denotes Euclidean norm ($\|u\|^2 = \sum_{i=1}^N {u_i}^2$ $\forall u = (u_1, u_2, .., u_N)$). This is called the *extrinsic distance* on M.

For the Fréchet function F in (3.1), let $f(r) = r^2$ on $[0, \infty)$. This choice of the Fréchet function makes the Frechet mean computable in a number of important examples using Proposition 4.1. Assume $J(M) = \tilde{M}$ is a closed subset of $\mathbb{E}^N$.Then for every $u \in \mathbb{E}^N$ there exists a compact set of points in $\tilde{M}$ whose distance from u is the smallest among all points in $\tilde{M}$. We denote this set by

$$P_{\tilde{M}}u = \{x \in \tilde{M} : \|x - u\| \leq \|y - u\|\ \forall y \in \tilde{M}\}. \tag{4.2}$$

If this set is a singleton, u is said to be a *nonfocal point* of $\mathbb{E}^N$ (w.r.t. $\tilde{M}$), otherwise it is said to be a *focal point* of $\mathbb{E}^N$.

DEFINITION 4.1. Let $(M, \rho), J$ be as above. Let Q be a probability measure on M such that the Fréchet function

$$F(x) = \int \rho^2(x, y) Q(dy) \tag{4.3}$$

is finite. The Fréchet mean (set) of Q is called the *extrinsic mean (set)* of Q. If X_i, $i = 1, \ldots, n$ are iid observations from Q and $Q_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$, then the Fréchet mean(set) of Q_n is called the *extrinsic sample mean(set)*.

Let $\tilde{Q}$ and $\tilde{Q}_n$ be the images of Q and Q_n respectively in $\mathbb{E}^N$: $\tilde{Q} = Q \circ J^{-1}$, $\tilde{Q}_n = Q_n \circ J^{-1}$.

PROPOSITION 4.1. *(a) If $\tilde{\mu} = \int_{\mathbb{E}^N} u\tilde{Q}(du)$ is the mean of $\tilde{Q}$, then the extrinsic mean set of Q is given by $J^{-1}(P_{\tilde{M}}\tilde{\mu})$. (b) If $\tilde{\mu}$ is a nonfocal point of $\mathbb{E}^N$ then the extrinsic mean of Q exists (as a unique minimizer of F).*

PROOF. See Proposition 3.1, BP (2003). □

COROLLARY 4.2. *If $\tilde{\mu} = \int_{\mathbb{E}^N} u\tilde{Q}(du)$ is a nonfocal point of $\mathbb{E}^N$ then the extrinsic sample mean μ_n (any measurable selection from the extrinsic sample mean set) is a strongly consistent estimator of the extrinsic mean μ of Q.*

PROOF. Follows from Proposition 3.1 for compact M. For the more general case, see BP (2003). □

4.1. Asymptotic Distribution of the Extrinsic Sample Mean. Although one can apply Theorem 3.2 here, we prefer a different, and more widely applicable approach, which does not require that the support of Q be contained in a coordinate patch. Let $\bar{Y} = \frac{1}{n}\sum_{j=1}^{n} Y_j$ be the (sample) mean of $Y_j = P(X_j)$. In a neighborhood of a nonfocal point such as $\tilde{\mu}$, $P(.)$ is smooth. Hence it can be shown that

$$\sqrt{n}[P(\bar{Y}) - P(\tilde{\mu})] = \sqrt{n}(d_{\tilde{\mu}}P)(\bar{Y} - \tilde{\mu}) + o_P(1) \tag{4.4}$$

where $d_{\tilde{\mu}}P$ is the differential (map) of the projection $P(.)$, which takes vectors in the tangent space of $\mathbb{E}^N$ at $\tilde{\mu}$ to tangent vectors of $\tilde{M}$ at $P(\tilde{\mu})$. Let $f_1, f_2, \ldots, f_d$ be an orthonormal basis of $T_{P(\tilde{\mu})}J(M)$ and $e_1, e_2, \ldots, e_N$ be an orthonormal basis (frame) for $T\mathbb{E}^N \approx \mathbb{E}^N$. One has

$$\sqrt{n}(Y - \tilde{\mu}) = \sum_{j=1}^{N} \langle \sqrt{n}(Y - \tilde{\mu}), e_j \rangle e_j,$$

$$\begin{aligned} d_{\tilde{\mu}}P(\sqrt{n}(Y - \tilde{\mu})) &= \sum_{j=1}^{N} \langle \sqrt{n}(Y - \tilde{\mu}), e_j \rangle d_{\tilde{\mu}}P(e_j) \\ &= \sum_{j=1}^{N} \langle \sqrt{n}(Y - \tilde{\mu}), e_j \rangle \sum_{r=1}^{d} \langle d_{\tilde{\mu}}P(e_j), f_r \rangle f_r \\ &= \sum_{r=1}^{d} [\sum_{j=1}^{N} \langle d_{\tilde{\mu}}P(e_j), f_r \rangle \langle \sqrt{n}(Y - \tilde{\mu}), e_j \rangle] f_r. \end{aligned} \tag{4.5}$$

Hence $\sqrt{n}[P(\bar{Y}) - P(\tilde{\mu})]$ has an asymptotic Gaussian distribution on the tangent space of $J(M)$ at $P(\tilde{\mu})$, with mean vector zero and a dispersion matrix (w.r.t. the basis vector $\{f_r : 1 \leq r \leq d\}$)

$$\Sigma = A'VA$$

where

$$A \equiv A(\tilde{\mu}) = (((d_{\tilde{\mu}}P(e_j), f_r\rangle))_{1\leq j\leq N, 1\leq r\leq d}$$

and V is the $N \times N$ covariance matrix of $\tilde{Q} = Q \circ J^{-1}$ (w.r.t. the basis $\{e_j : 1 \leq j \leq N\}$). In matrix notation,

$$\sqrt{n}\bar{T} \xrightarrow{\mathcal{L}} N(0, \Sigma) \text{ as } n \to \infty, \tag{4.6}$$

where

$$T_j(\tilde{\mu}) = A'[\langle(Y_j - \tilde{\mu}), e_1\rangle \ldots \langle(Y_j - \tilde{\mu}), e_N\rangle]', \; j = 1, \ldots, n$$

and

$$\bar{T} \equiv \bar{T}(\tilde{\mu}) = \frac{1}{n}\sum_{j=1}^{n} T_j(\tilde{\mu}).$$

This implies, writing $\mathcal{X}_d^2$ for the chisquare distribution with d degrees of freedom,

$$n\bar{T}'\Sigma^{-1}\bar{T} \xrightarrow{\mathcal{L}} \mathcal{X}_d^2, \text{ as } n \to \infty. \tag{4.7}$$

A confidence region for $P(\tilde{\mu})$ with asymptotic confidence level $1 - \alpha$ is then given by

$$\{P(\tilde{\mu}) : nT'\hat{\Sigma}^{-1}T \leq \mathcal{X}_d^2(1 - \alpha)\} \tag{4.8}$$

where $\hat{\Sigma} \equiv \hat{\Sigma}(\tilde{\mu})$ is the sample covariance matrix of $\{T_j(\tilde{\mu})\}_{j=1}^n$. The corresponding bootstrapped confidence region is given by

$$\{P(\tilde{\mu}) : n\bar{T}'\hat{\Sigma}^{-1}\bar{T} \leq c^*_{(1-\alpha)}\} \tag{4.9}$$

where $c^*_{(1-\alpha)}$ is the upper $(1 - \alpha)$-quantile of the bootstrapped values U^*, $U^* = n\bar{T}^{*\prime}\hat{\Sigma}^{*-1}\bar{T}^*$ and $\bar{T}^*$, $\hat{\Sigma}^*$ being the sample mean and covariance respectively of the bootstrap sample $\{T_j^*(\bar{Y})\}_{j=1}^n$.

5. Intrinsic Means on Manifolds

Let (M, g) be a complete connected Riemannian manifold with metric tensor g. Then the natural choice for the distance metric ρ in Section 3 is the geodesic distance d_g on M. Unless otherwise stated, we consider the function $f(r) = r^2$ in (3.1) throughout this section and later sections. However one may take more general f. For example one may consider $f(r) = r^a$, for suitable $a \geq 1$.

Let Q be a probability distribution on M with finite Fréchet function

$$F(p) = \int_M d_g^2(p, m)Q(dm). \tag{5.1}$$

Let $X_1, \ldots, X_n$ be an iid sample from Q.

Definition 5.1. The Fréchet mean set of Q under $\rho = d_g$ is called the *intrinsic mean set* of Q. The Fréchet mean set of the empirical distribution Q_n is called the *sample intrinsic mean set.*

Before proceeding further, let us define a few technical terms related to Riemannian manifolds which we will use extensively in this section. For details on Riemannian Manifolds, see DoCarmo (1992), Gallot et al. (1990) or Lee (1997).

(1) *Geodesic*: These are curves γ on the manifold with zero acceleration. They are locally length minimizing curves. For example, consider great circles on the sphere or straight lines in $\mathbb{R}^d$.
(2) *Exponential map*: For $p \in M$, $v \in T_pM$, we define $\exp_p v = \gamma(1)$, where γ is a geodesic with $\gamma(0) = p$ and $\dot\gamma(0) = v$.
(3) *Cut locus*: For a point $p \in M$, define the cut locus $C(p)$ of p as the set of points of the form $\gamma(t_0)$, where γ is a unit speed geodesic starting at p and t_0 is the supremum of all $t > 0$ such that γ is distance minimizing from p to $\gamma(t)$. For example, $C(p) = \{-p\}$ on the sphere.
(4) *Sectional Curvature*: Recall the notion of Gaussian curvature of two dimensional surfaces. On a Riemannian manifold M, choose a pair of linearly independent vectors $u, v \in T_pM$. A two dimensional submanifold of M is swept out by the set of all geodesics starting at p and with initial velocities lying in the two-dimensional section π spanned be u, v. The Gaussian curvature of this submanifold is called the sectional curvature at p of the section π.
(5) *Injectivity Radius*: Define the injectivity radius of M as

$$\mathrm{inj}(M) = \inf\{d_g(p, C(p)) : p \in M\}.$$

For example the sphere of radius 1 has injectivity radius equal to π.

Also let $r_* = \min\{\mathrm{inj}(M), \frac{\pi}{\sqrt{\overline{C}}}\}$, where $\overline{C}$ is the least upper bound of sectional curvatures of M if this upper bound is positive, and $\overline{C} = 0$ otherwise. The exponential map at p is injective on $\{v \in T_p(M) : |v| < r_*\}$. By $B(p, r)$ we will denote an open ball with center $p \in M$ and radius r, and $\bar{B}(p, r)$ will denote its closure.

In case Q has a unique intrinsic mean μ_I, it follows from Proposition 3.1 and Remark 3.1 that the sample intrinsic mean μ_{nI} (a measurable selection from the sample intrinsic mean set) is a consistent estimator of μ_I. Broad conditions for the existence of a unique intrinsic mean are not known. From results due to Karchar (1997) and Le (2001), it follows that if the support of Q is in a geodesic ball of radius $\frac{r_*}{4}$, i.e. $\mathrm{supp}(Q) \subseteq B(p, \frac{r_*}{4})$, then Q has a unique intrinsic mean. This result has been substantially extended by Kendall (1990) which shows that if $\mathrm{supp}(Q) \subseteq B(p, \frac{r_*}{2})$, then there is a unique local minimum of the Fréchet function F in that ball. Then we redefine the (local) intrinsic mean of Q as that unique minimizer in the ball. In that case one can show that the (local) sample intrinsic mean is a consistent estimator of the intrinsic mean of Q. This is stated in Proposition 5.1.

PROPOSITION 5.1. *Let Q have support in $B(p, \frac{r_*}{2})$ for some $p \in M$. Then (a) Q has a unique (local) intrinsic mean μ_I in $B(p, \frac{r_*}{2})$ and (b) the sample intrinsic mean μ_{nI} in $B(p, \frac{r_*}{2})$ is a strongly consistent estimator of μ_I.*

PROOF. (a) Follows from Kendall (1990).
(b) Since $\mathrm{supp}(Q)$ is compact, $\mathrm{supp}(Q) \subseteq B(p, r)$ for some $r < \frac{r_*}{2}$. From Lemma 1, Le (2001), it follows that $\mu_I \in B(p, r)$ and μ_I is the unique intrinsic mean of Q restricted to $\bar{B}(p, r)$. Now take the compact metric space in Proposition 3.1 to be $\bar{B}(p, r)$ and the result follows. □

For the asymptotic distribution of the sample intrinsic mean, we may use Theorem 3.2. For that we need to verify assumptions A1-A7. Theorem 5.2 gives sufficient conditions for that. In the statement of the theorem, the usual partial order $A \geq B$ between $d \times d$ symmetric matrices A, B, means that $A - B$ is nonnegative definite.

THEOREM 5.2. *Assume* $\mathrm{supp}(Q) \subseteq B(p, \frac{r_*}{2})$. *Let* $\phi = \exp_{\mu_I}^{-1} : B(p, \frac{r_*}{2}) \longrightarrow T_{\mu_I}M(\approx \mathbb{R}^d)$. *Then the map* $y \to h(x,y) = d_g^2(\phi^{-1}x, \phi^{-1}y)$ *is twice continuously differentiable in a neighborhood of* 0 *and in terms of normal coordinates with respect to a chosen orthonaormal basis for* $T_{\mu_I}M$,

$$\mathrm{D}_r h(x,0) = -2x^r, \quad 1 \leq r \leq d, \tag{5.2}$$

$$[\mathrm{D}_r\mathrm{D}_s h(x,0)] \geq \left[2\{\left(\frac{1-f(|x|)}{|x|^2}\right) x^r x^s + f(|x|)\delta_{rs}\}\right]_{1\leq r,s\leq d}. \tag{5.3}$$

Here $x = (x^1, \ldots, x^d)'$, $|x| = \sqrt{(x^1)^2 + (x^2)^2 + \ldots (x^d)^2}$ *and*

$$f(y) = \begin{cases} 1 \text{ if } \overline{C} = 0 \\ \sqrt{\overline{C}}y\frac{\cos(\sqrt{\overline{C}}y)}{\sin(\sqrt{\overline{C}}y)} \text{ if } \overline{C} > 0 \\ \sqrt{-\overline{C}}y\frac{\cosh(\sqrt{-\overline{C}}y)}{\sinh(\sqrt{-\overline{C}}y)} \text{ if } \overline{C} < 0 \end{cases} \tag{5.4}$$

There is equality in (5.3) *when* M *has constant sectional curvature* $\overline{C}$, *and in this case* Λ *has the expression:*

$$\Lambda_{rs} = 2\mathrm{E}\{\left(\frac{1-f(|\tilde{X}_1|)}{|\tilde{X}_1|^2}\right)\tilde{X}_1^r\tilde{X}_1^s + f(|\tilde{X}_1|)\delta_{rs}\}, \quad 1 \leq r,s \leq d. \tag{5.5}$$

Λ *is positive definite if* $\mathrm{supp}(Q) \in B(\mu_I, \frac{r_*}{2})$.

PROOF. See Theorem 2.2., BB (2008b). ☐

From Theorem 5.2 it follows that $\Sigma = 4\mathrm{Cov}(Y_1)$ where $Y_j = \phi(X_j)$, $j = 1, \ldots, n$ are the normal coorinates of the sample $X_1, \ldots, X_n$ from Q. It is nonsingular if $Q \circ \phi^{-1}$ has support in no smaller dimensional subspace of $\mathbb{R}^d$. That holds if for example Q has a density with respect to the volume measure on M.

6. Applications

In this section we apply the results of the earlier sections to some important manifolds. We start with the unit sphere S^d in $\mathbb{R}^{d+1}$.

6.1. S^d**.** Consider the space of all directions in $\mathbb{R}^{d+1}$ which can be identified with the unit sphere

$$S^d = \{x \in \mathbb{R}^{d+1} : \|x\| = 1\}.$$

Statistics on S^2, often called *directional statistics*, have been among the earliest and most widely used statistics on manifolds. (See, e.g., Watson (1983), Fisher et al. (1996), Mardia and Jupp (1999)). Among important applications, we cite paleomagnetism, where one may detect and/or study the shifting of magnetic poles on earth over geological times. Another application is the estimation of the direction of a signal.

6.1.1. ***Extrinsic Mean on*** S^d. The inclusion map $i : S^d \to \mathbb{R}^{d+1}$, $i(x) = x$ provides a natural embedding for S^d into $\mathbb{R}^{d+1}$. The extrinsic mean set of a probability distribution Q on S^d is then the set $P_{S^d}\tilde{\mu}$ on S^d closest to $\tilde{\mu} = \int_{\mathbb{R}^{d+1}} x\tilde{Q}(dx)$, where $\tilde{Q}$ is Q regarded as a probability measure on $\mathbb{R}^{d+1}$. Note that $\tilde{\mu}$ is non-focal iff $\tilde{\mu} \neq 0$ and then Q has a unique extrinsic mean $\mu = \frac{\tilde{\mu}}{\|\tilde{\mu}\|}$.

6.1.2. ***Intrinsic Mean on*** S^d. At each $p \in S^d$, endow the tangent space $T_pS^d = \{v \in \mathbb{R}^{d+1} : v.p = 0\}$ with the metric tensor $g_p : T_p \times T_p \to \mathbb{R}$ as the restriction of the scaler product at p of the tangent space of $\mathbb{R}^{d+1}$: $g_p(v_1, v_2) = v_1.v_2$. The geodesics are the big circles,

$$\gamma_{p,v}(t) = (\cos t|v|)p + (\sin t|v|)\frac{v}{|v|}. \tag{6.1}$$

The exponential map, $exp_p : T_pS^d \to S^d$ is

$$exp_p(v) = \cos(|v|)p + \sin(|v|)\frac{v}{|v|}, \tag{6.2}$$

and the geodesic distance is

$$d_g(p, q) = \arccos(p.q) \in [0, \pi]. \tag{6.3}$$

This space has constant sectional curvature 1 and injectivity radius π. Hence if Q has support in an open ball of radius $\frac{\pi}{2}$, then it has a unique intrinsic mean in that ball.

6.2. $\mathbb{R}P^d$**.** Consider the real projective space $\mathbb{R}P^d$ of all lines through the origin in $\mathbb{R}^{d+1}$. The elements of $\mathbb{R}P^d$ may be represented as $[u] = \{-u, u\}$ $(u \in S^d)$.

6.2.1. ***Extrinsic Mean on*** $\mathbb{R}P^d$. $\mathbb{R}P^d$ can be embedded into the space of $k \times k$ real symmetric matrices $S(k, \mathbb{R})$, $k = d + 1$ via the *Veronese-Whitney embedding* $J : \mathbb{R}P^d \to S(k, \mathbb{R})$ which is given by

$$J([u]) = uu' = ((u_iu_j))_{1\le i,j\le k} \ (u = (u_1, .., u_k)' \in S^d). \tag{6.4}$$

As a linear subspace of $\mathbb{R}^{k^2}$, $S(k, \mathbb{R})$ has the Euclidean distance

$$\|A - B\|^2 \equiv \sum_{1\le i,j\le k} (a_{ij} - b_{ij})^2 = \text{Trace}(A - B)(A - B)'. \tag{6.5}$$

This endows $\mathbb{R}P^d$ with the extrinsic distance ρ given by

$$\rho^2([u], [v]) = \|uu' - vv'\|^2 = 2(1 - (u'v)^2). \tag{6.6}$$

Let Q be a probability distribution on $\mathbb{R}P^d$ and let $\tilde{\mu}$ be the mean of $\tilde{Q} = Q \circ J^{-1}$ considered as a probability measure on $S(k, \mathbb{R})$. Then $\tilde{\mu} \in S^+(k, \mathbb{R})$-the space of $k \times k$ real symmetric nonnegative definite matices, and the projection of $\tilde{\mu}$ into $J(\mathbb{R}P^d)$ is given by the set of all uu' where u is a unit eigenvector of $\tilde{\mu}$ corresponding to the largest eigenvalue. Hence the projection is unique, i.e. $\tilde{\mu}$ is nonfocal iff its largest eigenvalue is simple, i.e., if the eigenspace corresponding to the largest eigenvalue is one dimensional. In that case the extrinsic mean of Q is $[u]$, u being a unit eigenvector in the eigenspace of the largest eigenvalue..

6.2.2. ***Intrinsic Mean on*** $\mathbb{R}P^d$. $\mathbb{R}P^d$ is a complete Riemannian manifold with geodesic distance

$$d_g([p], [q]) = \arccos(|p.q|) \in [0, \frac{\pi}{2}]. \tag{6.7}$$

It has constant sectional curvature 4 and injectivity radius $\frac{\pi}{2}$. Hence if the support of Q is contained in an open geodesic ball of radius $\frac{\pi}{4}$, it has a unique intrinsic mean in that ball.

6.3. Σ_m^k**.** Consider a set of k points in $\mathbb{R}^m$, not all points being the same. Such a set is called a k-ad or a configuration of k landmarks. We will denote a k-ad by the $m \times k$ matrix, $x = [x_1 \dots x_k]$ where x_i, $i = 1, \dots, k$ are the k landmarks from the object of interest. Assume $k > m$. The *direct similarity shape* of the k-ad is what remains after we remove the effects of translation, rotation and scaling. To remove translation, we substract the mean $x = \frac{1}{k}\sum_{i=1}^k x_i$ from each landmark to get the centered k-ad $w = [x_1 - \bar{x} \dots x_k - \bar{x}]$. We remove the effect of scaling by dividing w by its euclidean norm to get

$$u = [\frac{x_1 - \bar{x}}{\|w\|} \dots \frac{x_k - \bar{x}}{\|w\|}] = [u_1 u_2 \dots u_k]. \tag{6.8}$$

This u is called the *preshape* of the k-ad x and it lies in the unit sphere S_m^k in the hyperplane

$$H_m^k = \{u \in \mathbb{R}^{km} \colon \sum_{j=1}^k u_j = 0\}. \tag{6.9}$$

Thus the preshape space S_m^k may be identified with the sphere S^{km-m-1}. Then the shape of the k-ad x is the orbit of z under left multiplication by $m \times m$ rotation matrices. In other words $\Sigma_m^k = S^{km-m-1}/SO(m)$. The cases of importance are $m = 2, 3$. Next we turn to the case $m = 2$.

6.4. Σ_2^k**.** As pointed out in Sections 2.2 and 6.3, $\Sigma_2^k = S^{2k-3}/SO(2)$. For a simpler representation, we denote a k-ad in the plane by a set of k complex numbers. The preshape of this complex k-vector x is $z = \frac{x-\bar{x}}{\|x-\bar{x}\|}$, $x = (x_1, \dots, x_k) \in \mathbb{C}^k$, $\bar{x} = \frac{1}{k}\sum_{i=1}^k x_i$. z lies in the complex sphere

$$S_2^k = \{z \in \mathbb{C}^k \colon \sum_{j=1}^k |z_j|^2 = 1, \sum_{j=1}^k z_j = 0\} \tag{6.10}$$

which may be identified with the real sphere of dimension $2k - 3$. Then the shape of x can be represented as the orbit

$$\sigma(x) = \sigma(z) = \{e^{i\theta} z \colon -\pi < \theta \leq \pi\} \tag{6.11}$$

and

$$\Sigma_2^k = \{\sigma(z) \colon z \in S_2^k\}. \tag{6.12}$$

Thus Σ_2^k has the structure of the complex projective space $\mathbb{C}P^{k-2}$ of all complex lines through the origin in $\mathbb{C}^{k-1}$, an important and well studied manifold in differential geometry (See Gallot et al. (1993), pp. 63-65, 97-100, BB (2008b)).

6.4.1. ***Extrinsic Mean on*** Σ_2^k. Σ_2^k can be embedded into $S(k, \mathbb{C})$-the space of $k \times k$ complex Hermitian matrices, via the *Veronese-Whitney embedding*

$$J \colon \Sigma_2^k \to S(k, \mathbb{C}),\ J(\sigma(z)) = zz^*. \tag{6.13}$$

J is equivariant under the action of $SU(k)$-the group of $k \times k$ complex matrices Γ such that $\Gamma^*\Gamma = I$, $\det(\Gamma) = 1$. To see this, let $\Gamma \in SU(k)$. Then Γ defines a diffeormorphism,

$$\Gamma : \Sigma_2^k \to \Sigma_2^k,\ \Gamma(\sigma(z)) = \sigma(\Gamma(z)). \tag{6.14}$$

The map ϕ_Γ on $S(k, \mathbb{C})$ defined by

$$\phi_\Gamma(A) = \Gamma A \Gamma^* \tag{6.15}$$

preserves distances and has the property

$$(\phi_\Gamma)^{-1} = \phi_{\Gamma^{-1}},\ \phi_{\Gamma_1\Gamma_2} = \phi_{\Gamma_1} \circ \phi_{\Gamma_2}. \tag{6.16}$$

That is (6.15) defines a group homomorphism from $SU(k)$ into a group of isometries of $S(k, \mathbb{C})$. Finally note that $J(\Gamma(\sigma(z))) = \phi_\Gamma(J(\sigma(z)))$. Informally, the symmetries $SU(k)$ of Σ_2^k are preserved by the embedding J.

$S(k, \mathbb{C})$ is a (real) vector space of dimension k^2. It has the Euclidean distance,

$$\|A - B\|^2 = \sum_{i,j} |a_{ij} - b_{ij}\|^2 = \text{Trace}(A - B)^2. \tag{6.17}$$

Thus the extrinsic distance ρ on Σ_2^k induced from the Veronese-Whitney embedding is given by

$$\rho^2(\sigma(x), \sigma(y)) = \|uu^* - vv^*\|^2 = 2(1 - |u^*v|^2), \tag{6.18}$$

where x and y are two k-ads, u and v are their preshapes respectively.

Let Q be a probability distribution on Σ_2^k and let $\tilde{\mu}$ be the mean of $\tilde{Q} = Q \circ J^{-1}$, regarded as a probability measure on $\mathbb{C}^{k^2}$. Then $\tilde{\mu} \in S_+(k, \mathbb{C})$: the space of $k \times k$ complex positive semidefinite matrices. Its projection into $J(\Sigma_2^k)$ is given by $P(\tilde{\mu}) = \{uu^*\}$ where u is a unit eigenvector of $\tilde{\mu}$ corresponding to its largest eigenvalue. The projection is unique, i.e. $\tilde{\mu}$ is nonfocal, and Q has a unique extrinsic mean μ_E, iff the eigenspace for the largest eigenvalue of $\tilde{\mu}$ is (complex) one dimensional, and then $\mu_E = \sigma(u)$, $u(\neq 0) \in$ eigenspace of the largest eigenvalue of $\tilde{\mu}$. Let $X_1, \ldots X_n$ be an iid sample from Q. If $\tilde{\mu}$ is nonfocal, the sample extrinsic mean μ_{nE} is a consistent estimator of μ_E and $J(\mu_{nE})$ has an assymptotic Gaussian distribution on the tangent space $T_{P(\tilde{\mu})}J(\Sigma_2^k)$ (see Section 4),

$$\sqrt{n}(J(\mu_{nE}) - J(\mu_E)) = \sqrt{n} d_{\tilde{\mu}} P(\overline{\tilde{X}} - \tilde{\mu}) + o_P(1) \xrightarrow{\mathcal{L}} N(0, \Sigma). \tag{6.19}$$

Here $\tilde{X}_j = J(X_j)$, $j = 1, \ldots, n$. In (6.19), $d_{\tilde{\mu}} P(\overline{\tilde{X}} - \tilde{\mu})$ has coordinates

$$T(\tilde{\mu}) = (\sqrt{2}\text{Re}(U_a^* \tilde{X} U_k), \sqrt{2}\text{Im}(U_a^* \tilde{X} U_k))_{a=2}^{k-1} \tag{6.20}$$

with respect to the basis

$$\{(\lambda_k - \lambda_a)^{-1} U v_k^a U^*, (\lambda_k - \lambda_a)^{-1} U w_k^a U^*\}_{a=2}^{k-1} \tag{6.21}$$

for $T_{P(\tilde{\mu})}J(\Sigma_2^k)$ (see Section 3.3, BB (2008a)). Here $U = [U_1 \ldots U_k] \in SO(k)$ is such that $U^* \tilde{\mu} U = D \equiv \text{Diag}(\lambda_1, \ldots, \lambda_k)$, $\lambda_1 \leq \ldots \leq \lambda_{k-1} < \lambda_k$ being the eigenvalues of $\tilde{\mu}$. $\{v_b^a : 1 \leq a \leq b \leq k\}$ and $\{w_b^a : 1 \leq a < b \leq k\}$ is the canonical orthonormal basis frame for $S(k, \mathbb{C})$, defined as

$$v_b^a = \begin{cases} \frac{1}{\sqrt{2}}(e_a e_b^t + e_b e_a^t), & a < b \\ e_a e_a^t, & a = b \end{cases}$$

$$w_b^a = \frac{i}{\sqrt{2}}(e_a e_b^t - e_b e_a^t),\ a < b \tag{6.22}$$

where $\{e_a : 1 \leq a \leq k\}$ is the standard canonical basis for $\mathbb{R}^k$.

Given two independent samples $X_1, \ldots X_n$ iid Q_1 and $Y_1, \ldots Y_m$ iid Q_2 on Σ_2^k, we may like to test if $Q_1 = Q_2$ by comparing their extrinsic mean shapes. Let μ_{iE} denote the extrinsic mean of Q_i and let μ_i be the mean of $Q_i \circ J^{-1}$ $i = 1, 2$.

Then $\mu_{iE} = J^{-1}P(\mu_i)$, and we wish to test $H_0 : P(\mu_1) = P(\mu_2)$. Let $\tilde{X}_j = J(X_j)$, $j = 1, \dots, n$ and $\tilde{Y}_j = J(Y_j)$, $j = 1, \dots, m$. Let T_j, S_j denote the asymptotic coordinates for $\tilde{X}_j, \tilde{Y}_j$ respectively in $T_{P(\hat{\mu})}J(\Sigma_2^k)$ as defined in (6.20). Here $\hat{\mu} = \frac{n\overline{X}+m\overline{Y}}{m+n}$ is the pooled sample mean. We use the two sample test statistic

$$T_{nm} = (T - S)'(\frac{1}{n}\hat{\Sigma}_1 + \frac{1}{m}\hat{\Sigma}_2)^{-1}(T - S). \tag{6.23}$$

Here $\hat{\Sigma}_1, \hat{\Sigma}_2$ denote the sample covariances of T_j, S_j respectively. Under H_0, $T_{nm} \xrightarrow{\mathcal{L}} \mathcal{X}^2_{2k-4}$ (see Section 3.4, BB (2008a)). Hence given level α, we reject H_0 if $T_{nm} > \mathcal{X}^2_{2k-4}(1-\alpha)$.

6.4.2. ***Intrinsic Mean on*** Σ_2^k. Identified with $\mathbb{C}P^{k-2}$, Σ_2^k is a complete connected Riemannian manifold. It has all sectional curvatures bounded between 1 and 4 and injectivity radius of $\frac{\pi}{2}$ (see Gallot et al. (1990), pp. 97-100, 134). Hence if *supp*$(Q) \in B(p, \frac{\pi}{4})$, $p \in \Sigma_2^k$, it has a unique intrinsic mean μ_I in the ball.

Let $X_1, \dots X_n$ be iid Q and let μ_{nI} denote the sample intrinsic mean. Under the hypothesis of Theorem 5.2,

$$\sqrt{n}(\phi(\mu_{nI}) - \phi(\mu_I)) \xrightarrow{\mathcal{L}} N(0, \Lambda^{-1}\Sigma\Lambda^{-1}). \tag{6.24}$$

However Theorem 5.2 does not provide an analytic computation of Λ, since Σ_2^k does not have constant sectional curvature. Proposition 6.1 below gives the precise expression for Λ. It also relaxes the support condition required for Λ to be positive definite.

PROPOSITION 6.1. *With respect to normal coordinates,* $\phi : B(p, \frac{\pi}{4}) \to \mathbb{C}^{k-2} (\approx \mathbb{R}^{2k-4})$, Λ *as defined in Theorem 3.2 has the following expression:*

$$\Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{12}' & \Lambda_{22} \end{bmatrix} \tag{6.25}$$

where for $1 \le r, s \le k-2$,

$$(\Lambda_{11})_{rs} = 2\mathrm{E}\Big[\, d_1 \cot(d_1)\delta_{rs} - \frac{\{1 - d_1\cot(d_1)\}}{d_1^2}(\mathrm{Re}\tilde{X}_{1,r})(\mathrm{Re}\tilde{X}_{1,s}) + \frac{\tan(d_1)}{d_1}(\mathrm{Im}\tilde{X}_{1,r})(\mathrm{Im}\tilde{X}_{1,s})\,\Big],$$

$$(\Lambda_{22})_{rs} = 2\mathrm{E}\Big[\, d_1 \cot(d_1)\delta_{rs} - \frac{\{1 - d_1\cot(d_1)\}}{d_1^2}(\mathrm{Im}\tilde{X}_{1,r})(\mathrm{Im}\tilde{X}_{1,s}) + \frac{\tan(d_1)}{d_1}(\mathrm{Re}\tilde{X}_{1,r})(\mathrm{Re}\tilde{X}_{1,s})\,\Big],$$

$$(\Lambda_{12})_{rs} = -2\mathrm{E}\Big[\, \frac{\{1 - d_1 cot(d_1)\}}{d_1^2}(\mathrm{Re}\tilde{X}_{1,r})(\mathrm{Im}\tilde{X}_{1,s}) + \frac{\tan(d_1)}{d_1}(\mathrm{Im}\tilde{X}_{1,r})(\mathrm{Re}\tilde{X}_{1,s})\,\Big]$$

where $d_1 = d_g(X_1, \mu_I)$ *and* $\tilde{X}_j \equiv (\tilde{X}_{j,1}, \dots, \tilde{X}_{j,k-2}) = \phi(X_j)$, $j = 1, \dots, n$. Λ *is positive definite if* $\mathrm{supp}(Q) \in B(\mu_I, 0.37\pi)$.

PROOF. See Theorem 3.1, BB (2008b). ☐

Note that with respect to a chosen orthonormal basis $\{v_1, \dots, v_{k-2}\}$ for $T_{\mu_I}\Sigma_2^k$, ϕ has the expression

$$\phi(m) = (\tilde{m}_1, \dots, \tilde{m}_{k-2})'$$

where

$$\tilde{m}_j = \frac{r}{\sin r} e^{i\theta} \bar{v}_j' z,\ r = d_g(m, \mu_I) = \arccos(|z_0' \bar{z}|),\ e^{i\theta} = \frac{z_0' \bar{z}}{|z_0' \bar{z}|}. \tag{6.26}$$

Here z, z_0 are the preshapes of m, μ_I respectively (see Section 3, BB (2008b)).

Given two independent samples $X_1, \ldots X_n$ iid Q_1 and $Y_1, \ldots Y_m$ iid Q_2, one may test if Q_1 and Q_2 have the same intrinsic mean μ_I. The test statistic used is

$$T_{nm} = (n-m)(\hat{\phi}(\mu_{nI}) - \hat{\phi}(\mu_{mI}))' \hat{\Sigma}^{-1} (\hat{\phi}(\mu_{nI}) - \hat{\phi}(\mu_{mI})). \tag{6.27}$$

Here μ_{nI} and μ_{mI} are the sample intrinsic means for the X and Y samples respectively and $\hat{\mu}$ is the pooled sample intrinsic mean. Then $\hat{\phi} = \exp_{\hat{\mu}}^{-1}$ gives normal coordinates on the tangent space at $\hat{\mu}$, and $\hat{\Sigma} = (m+n)\left(\frac{1}{n}\hat{\Lambda}_1^{-1}\hat{\Sigma}_1\hat{\Lambda}_1^{-1} + \frac{1}{m}\hat{\Lambda}_2^{-1}\hat{\Sigma}_2\hat{\Lambda}_2^{-1}\right)$, where (Λ_1, Σ_1) and (Λ_2, Σ_2) are the parameters in the asymptotic distribution of $\sqrt{n}(\phi(\mu_{nI}) - \phi(\mu_I))$ and $\sqrt{m}(\phi(\mu_{mI} - \phi(\mu_I))$ respectively, as defined in Theorem 3.2., and $(\hat{\Lambda}_1, \hat{\Sigma}_1)$ and $(\hat{\Lambda}_2, \hat{\Sigma}_2)$ are consistent sample estimates. Assuming H_0 to be true, $T_{nm} \xrightarrow{\mathcal{L}} \mathcal{X}^2_{2k-4}$ (see Section 4.1, BB (2008a)). Hence we reject H_0 at asymptotic level $1-\alpha$ if $T_{nm} > \mathcal{X}^2_{2k-4}(1-\alpha)$.

6.5. $R\Sigma_m^k$**.** For $m > 2$, the direct similarity shape space Σ_m^k fails to be a manifold. That is because the action of $SO(m)$ is not in general free (see, e.g., Kendall et al. (1999) and Small (1996)). To avoid that one may consider the shape of only those k-ads whose preshapes have rank at least $m-1$. This subset is a manifold but not complete (in its geodesic distance). Alternatively one may also remove the effect of reflection and redefine shape of a k-ad x as

$$\sigma(x) = \sigma(z) = \{Az \colon A \in O(m)\} \tag{6.28}$$

where z is the preshape. Then $R\Sigma_m^k$ is the space of all such shapes where rank of z is m. In other words

$$R\Sigma_m^k = \{\sigma(z) \colon z \in S_m^k,\ \mathrm{rank}(z) = m\}. \tag{6.29}$$

This is a manifold. It has been shown that the map

$$J : R\Sigma_m^k \to S(k, \mathbb{R}),\ J(\sigma(z)) = z'z \tag{6.30}$$

is an embedding of the reflection shape space into $S(k, \mathbb{R})$ (see Bandulasiri and Patrangenaru (2005), Bandulasiri et al. (2007), and Dryden et al. (2007)) and is H-equivariant where $H = O(k)$ acts on the right: $A\sigma(z) \doteq \sigma(zA')$, $A \in O(k)$.

Let Q be a probability distribution on $R\Sigma_m^k$ and let $\tilde{\mu}$ be the mean of $Q \circ J^{-1}$ regarded as a probability measure on $S(k, \mathbb{R})$. Then $\tilde{\mu}$ is positive semi-definite with rank atleast m. Let $\tilde{\mu} = UDU'$ be the singular value decomposition of $\tilde{\mu}$, where $D = \mathrm{Diag}(\lambda_1, \ldots, \lambda_k)$ consists of ordered eigen values $\lambda_1 \geq \ldots \geq \lambda_m \geq \ldots \geq \lambda_k \geq 0$ of $\tilde{\mu}$, and $U = [U_1 \ldots U_k]$ is a matrix in $SO(k)$ whose columns are the corresponding orthonormal eigen vectors. Then we may define the mean reflection shape set of Q as the set

$$\{\mu \in R\Sigma_m^k \colon J(\mu) = \frac{\sum_{j=1}^m \lambda_j U_j U_j'}{\sum_{j=1}^m \lambda_j}\} \tag{6.31}$$

The set in (6.31) is a singleton, and hence Q has a unique mean reflection shape μ iff $\lambda_m > \lambda_{m+1}$. Then $\mu = \sigma(u)$ where

$$u = [\sqrt{\frac{\lambda_1}{\sum_{j=1}^{m} \lambda_j}}U_1 \ldots \sqrt{\frac{\lambda_m}{\sum_{j=1}^{m} \lambda_j}}U_m]'. \tag{6.32}$$

6.6. $A\Sigma_m^k$. Let z be a centered k-ad in $H(m,k)$, and let $\sigma(z)$ denote its affine shape, as defined in Section 2.4. Consider the map

$$J : A\Sigma_m^k \to S(k,\mathbb{R}),\ J(\sigma(z)) \equiv P = FF' \tag{6.33}$$

where $F = [f_1 f_2 \ldots f_m]$ is an orthonormal basis for the row space of z. This is an embedding of $A\Sigma_m^k$ into $S(k,\mathbb{R})$ with the image

$$J(A\Sigma_m^k) = \{A \in S(k,\mathbb{R}) : A^2 = A,\ \mathrm{Trace}(A) = m,\ A\mathbf{1} = 0\}. \tag{6.34}$$

It is equivariant under the action of $O(k)$ (see Dimitric (1996)).

Proposition 6.2. *Let Q be a probability distribution on $A\Sigma_m^k$ and let $\tilde{\mu}$ be the mean of $Q \circ J^{-1}$ in $S(k,\mathbb{R})$. The projection of $\tilde{\mu}$ into $J(A\Sigma_m^k)$ is given by*

$$P(\tilde{\mu}) = \{\sum_{j=1}^{m} U_j U_j'\} \tag{6.35}$$

where $U = [U_1 \ldots U_k] \in SO(k)$ is such that $U'\tilde{\mu}U = D \equiv \mathrm{Diag}(\lambda_1, \ldots, \lambda_k)$, $\lambda_1 \geq \ldots \geq \lambda_m \geq \ldots \geq \lambda_k$. $\tilde{\mu}$ is nonfocal and Q has a unique extrinsic mean μ_E iff $\lambda_m > \lambda_{m+1}$. Then $\mu_E = \sigma(F')$ where $F = [U_1 \ldots U_m]$.

Proof. See Sughatadasa (2006). □

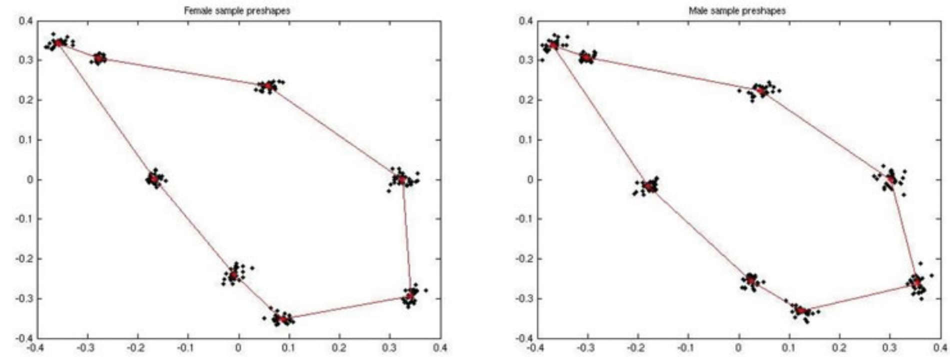
6.7. $P_0\Sigma_m^k$. Consider the diffeomorphism between $P_I\Sigma_m^k$ and $(\mathbb{R}P^m)^{k-m-2}$ as defined in Section 2.5. Using that one can embedd $P_I\Sigma_m^k$ into $S(m+1,\mathbb{R})^{k-m-2}$ via the Veronese Whitney embedding of Section 6.2 and perform extrinsic analysis in a dense open subset of $P_0\Sigma_m^k$.

7. Examples

7.1. Example 1: Gorilla Skulls. To test the difference in the shapes of skulls of male and female gorillas, eight landmarks were chosen on the midline plane of the skulls of 29 male and 30 female gorillas. The data can be found in Dryden and Mardia (1998), pp. 317-318. Thus we have two iid samples in Σ_2^k, $k = 8$. The sample extrinsic mean shapes for the female and male samples are denoted by $\hat{\mu}_{1E}$ and $\hat{\mu}_{2E}$ where

$$\hat{\mu}_{1E} = \sigma[-0.3586 + 0.3425i, 0.3421 - 0.2943i, 0.0851 - 0.3519i, -0.0085 - 0.2388i,$$
$$-0.1675 + 0.0021i, -0.2766 + 0.3050i, 0.0587 + 0.2353i, 0.3253],$$
$$\hat{\mu}_{2E} = \sigma[-0.3692 + 0.3386i, 0.3548 - 0.2641i, 0.1246 - 0.3320i, 0.0245 - 0.2562i,$$
$$-0.1792 - 0.0179i, -0.3016 + 0.3072i, 0.0438 + 0.2245i, 0.3022]$$

The corresponding intrinsic mean shapes are denoted by $\hat{\mu}_{1I}$ and $\hat{\mu}_{2I}$. They are very close to the extrinsic means ($d_g(\hat{\mu}_{1E}, \hat{\mu}_{1I}) = 5.5395 \times 10^{-7}$, $d_g(\hat{\mu}_{2E}, \hat{\mu}_{2I}) = 1.9609 \times 10^{-6}$). Figure 1 shows the preshapes of the sample k-ads along with that of the extrinsic mean. The sample preshapes have been rotated appropriately so as to minimize the Euclidean distance from the mean preshape. Figure 2 shows the preshapes of the extrinsic means for the two samples along with that of the



(a) (b)

FIGURE 1. 1a and 1b show 8 landmarks from skulls of 30 female and 29 male gorillas, respectively, along with the mean shapes. * correspond to the mean shapes' landmarks.

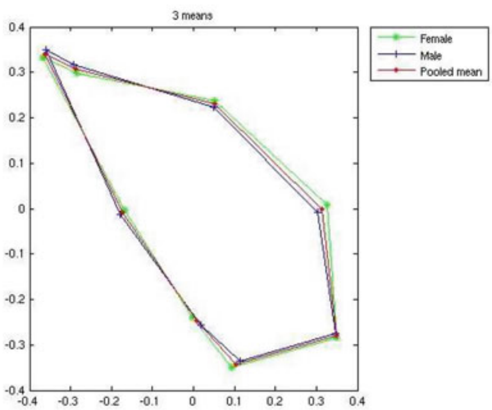
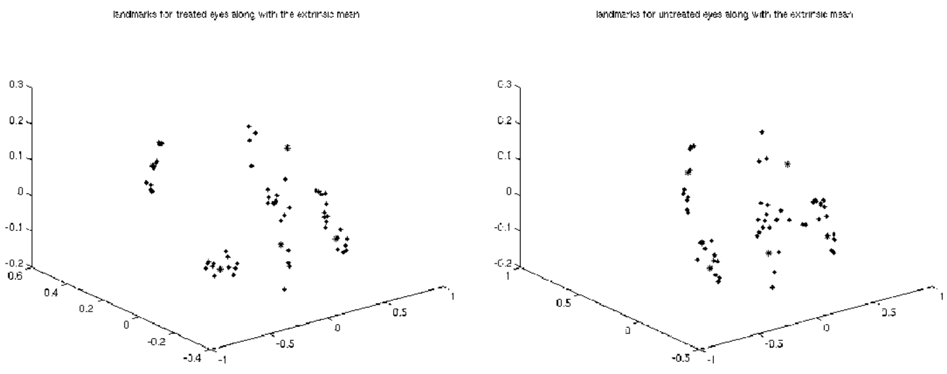


FIGURE 2. The sample extrinsic means for the 2 groups along with the pooled sample mean, corresponding to Figure 1.

pooled sample extrinsic mean. In BB (2008a), nonparametric two sample tests are performed to compare the mean shapes. The statistics (6.23) and (6.27) yield the following values:

$$\text{Extrinsic: } T_{nm} = 392.6, \text{ p-value} = P(\mathcal{X}^2_{12} > 392.6) < 10^{-16}.$$
$$\text{Intrinsic: } T_{nm} = 391.63, \text{ p-value} = P(\mathcal{X}^2_{12} > 391.63) < 10^{-16}.$$

A parametric F-test (Dryden and Mardia (1998), pp. 154) yields $F = 26.47$, p-value $= P(F_{12,46} > 26.47) = 0.0001$. A parametric (Normal) model for Bookstein coordinates leads to the Hotelling's T^2 test (Dryden and Mardia (1998), pp. 170-172) yields the p-value 0.0001.



(a) (b)

FIGURE 3. 3a and 3b show 5 landmarks from treated and untreated eyes of 12 monkeys, respectively, along with the mean shapes. * correspond to the mean shapes' landmarks.

7.2. Example 2: Schizophrenic Children. In this example from Bookstein (1991), 13 landmarks are recorded on a midsagittal two-dimensional slice from a Magnetic Resonance brain scan of each of 14 schizophrenic children and 14 normal children. In BB (2008a), nonparametric two sample tests are performed to compare the extrinsic and intrinsic mean shapes of the two samples. The values of the two-sample test statistics (6.23), (6.27), along with the p-values are as follows.

Extrinsic: $T_{nm} = 95.5476$, p-value $= P(\mathcal{X}^2_{22} > 95.5476) = 3.8 \times 10^{-11}$.
Intrinsic: $T_{nm} = 95.4587$, p-value $= P(\mathcal{X}^2_{22} > 95.4587) = 3.97 \times 10^{-11}$.

The value of the likelihood ratio test statistic, using the so-called *offset normal shape distribution* (Dryden and Mardia (1998), pp. 145-146) is $-2\log\Lambda = 43.124$, p-value $= P(\mathcal{X}^2_{22} > 43.124) = 0.005$. The corresponding values of Goodall's F-statistic and Bookstein's Monte Carlo test (Dryden and Mardia (1998), pp. 145-146) are $F_{22,572} = 1.89$, p-value $= P(F_{22,572} > 1.89) = 0.01$. The p-value for Bookstein's test $= 0.04$.

7.3. Example 3: Glaucoma detection. To detect any shape change due to Glaucoma, 3D images of the Optic Nerve Head (ONH) of both eyes of 12 rhesus monkeys were collected. One of the eyes was treated while the other was left untreated. 5 landmarks were recorded on each eye and their reflection shape was considered in $R\Sigma^k_3$, $k = 5$. For details on landmark registration, see Derado et al. (2004). The landmark coordinates can be found in BP (2005). Figure 3 shows the preshapes of the sample k-ads along with that of the mean shapes. The sample points have been rotated and (or) reflected so as to minimize their Euclidean distance from the mean preshapes. Figure 4 shows the preshapes of the mean shapes for the two eyes along with that of the pooled sample mean shape. In Bandulasari et al. (2007), 4 landmarks are selected and the sample mean shapes of the two eyes are compared. Five local coordinates are used in the neighborhood of the mean to compute Bonferroni type Bootstrap Confidence Intervals for the difference between

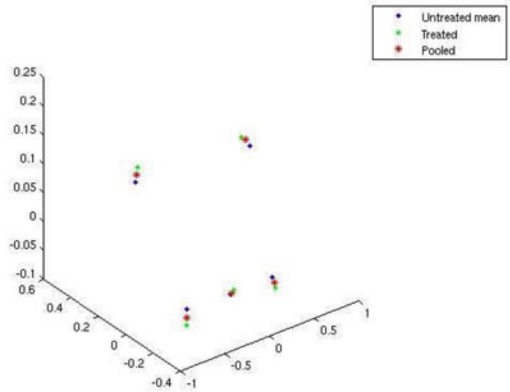


FIGURE 4. The sample means for the 2 eyes along with the pooled sample mean, corresponding to Figure 3.

the local reflection similarity shape coordinates of the paired glaucomatous versus control eye (see Section 6.1, Bandulasari et al. (2007) for details). It is found that the means are different at 1% level of significance.

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