Contributions to Statistics

Barry C. Arnold
Narayanaswamy Balakrishnan
Carlos A. Coelho *Editors*

Methodology and Applications of Statistics

A Volume in Honor of C.R. Rao on the Occasion of his 100th Birthday

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Preface

Professor C. R. Rao has continued his productive research career through his tenth decade, and now begins the eleventh. A celebration of his 100th birthday is completely appropriate. There has been no difficulty in encountering individuals enthusiastic about contributing to this felicitation volume. That it will appear in time for Prof. Rao's 101st birthday is a consequence of the care invested in preparing suitable contributions by the many scholars whose lives have been directly or indirectly influenced by him and his many contributions to Statistics and related fields. We, the editors, consider it an honor to have been able to contribute to the organization and development of this tribute volume. If ever there was a statistician who *needs no introduction*, it is C. R. Rao. This is true even though many students may wonder if his first name is Cramer, or perhaps that his last name might be Blackwell. Be that as it may, they definitely know and respect (as we do) Prof. Rao and his many accomplishments!

We present this volume to Prof. Rao with our best wishes for a continued productive and enjoyable life.

We wish to take this opportunity to thank all those who have contributed papers to this volume. In addition, we express our sincere gratitude to the scholars who provided refereeing services. Their constructive commentaries were, in most cases, much appreciated by the authors.

We also wish to thank our Springer editor, Ms. Veronika Rosteck, who has patiently helped us by guiding us through the necessary steps to bring this project to fruition.

Huntington Beach, CA, USA — Barry C. Arnold
Hamilton, Ontario, Canada — Narayanaswamy Balakrishnan
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May 2021

Dedication

The present volume is intended to honor Prof. Calyampudi Radhakrishna Rao on the occasion of his 100th birthday, which occurred on September 10, 2020.

Professor Calyampudi Radhakrishna Rao is an Eberly Professor Emeritus of Statistics at Pennsylvania State University and before his retirement he also served as Director of the Centre for Multivariate Analysis at Penn State University and as an Adjunct Professor at the University of Pittsburgh.

Calyampudi Radhakrishna Rao was born on September 10, 1920 in Huvvina Hadagalli, then in the integrated Madras Province, now in the state of Karnataka, to C. D. Naidu and A. Laxmikanthamma as their eighth child. If we are allowed to do so, we will hereon address him just as C. R. Rao, for short, and also actually as a statement of friendship and respect.

C. R. Rao's father was a reputed police Inspector at the Criminal Investigation Department, whose job required the family to move from place to place every two or three years. For this reason, C. R. Rao completed his education in classes two and three at Gudur, classes four and five in Nuzvid and the first and second forms in Nandigrama, all nowadays in the state of Andhra Pradesh. After retirement, C. D. Naidu decided to settle in a coastal city in Andhra Pradesh called Visakhapatnam and C. R. Rao finished his high school and obtained his first college degree B.A. (Hons.), with a first class and first rank, in Visakhapatnam. In 1943, C. R. Rao received and MSc in Mathematics from Andhra University and on January 1, 1941, he joined the Indian Statistical Institute (ISI) in Calcutta and a few months later he became a student at Calcutta University, in the newly started MA course in Statistics. He obtained his M.A. degree in Statistics from Calcutta University in 1943 with a first class, first rank, gold medal, and record marks unbeaten till now. Rao has the distinction of standing first in the final examination of all classes where he studied from Primary School to University.

In 1948, C. R. Rao, after working under the direction of R. A. Fisher, obtained his Ph.D. degree from the Cambridge University, King's College, with a Thesis describing new methods for analyzing multivariate data that he developed during his two years stay.

A few years later, Cambridge University awarded him the higher doctorate degree Sc.D., based on peer review of his contributions to statistics and King's College made him a life fellow, a rare honor.

C. R. Rao completed his 100th birthday on September 10, 2020, and along his long and very productive life he gathered, so far, an impressive list of 39 Honorary Doctorate Degrees from nineteen countries in six different continents:

- in Asia: 14 from India (Andhra University, 1967; University of Delhi, 1973; Osmania University, 1977; Indian Statistical Institute, 1989; University of Hyderabad, 1991; Sri Venkateswara University, 1993; Visva Bharati University, 2001; Calcutta University, 2003; University of Madras, 2007; Jawaharlal Nehru Technical University, 2011; Karnataka University, 2012; Rashtriya Sanskrit Vidyapeeth University, 2014; Indian Institute of Technology, Kharagpur, 2014; Jamia Hamdard University, 2018), 1 from the Philippines (University of Philippines, Manila, 1983), 1 from Sri Lanka (University of Colombo, 2012);
- in Australia: 1 (University of Wollongong, 2001);
- in Africa: 1 (University of Pretoria, South Africa, 2004);
- in Europe: 1 from Cyprus (University of Cyprus, Nicosia, 2001), 1 from Finland (University of Tampere, 1985), 1 from Germany (University of Munich, 1995), 2 from Greece (University of Athens, 1976; Athens University of Economics and Business, 1994), 1 from Poland (University of Poznan, 1991), 1 from Portugal (NOVA University of Lisbon, 2006), 1 from Russia (Leningrad University, 1970), 1 from Slovakia (Slovak Academy of Sciences, 1994), 1 from Spain (University of Barcelona, 1995), 1 from Switzerland (University of Neuchatel, 1989);
- in North America: 2 from Canada (University of Guelph, 1996; University of Waterloo, 1997), 6 from U.S.A. (Ohio State University, 1979; Colorado State University, 1990; Kent State University, 2000; Oakland University, Rochester, 2002; University of Rhode Island, 2007; University at Buffalo, State University of New York, 2013);
- in South America: 1 from Brazil (University of Brasilia, 1982), 1 from Peru (Universidad Nacional de San Marcos, Lima, 1982).

C. R. Rao was married to Bhargavi Rao for 69 years. She was a psychologist and professor at Jadavpur University, India. He has a daughter, Tejaswini, a professor of Nutrition and classical Indian dancer, and a son, Veerendra, an electrical engineer and computer scientist whose wife Malini is a speech pathologist. He has two grandchildren: Amar, a computer scientist and Rohith, in business administration.

Some of C. R. Rao's Most Notable Contributions to Statistical Science and Other Areas

C. R. Rao is an extremely prolific author. He is the author of 476 research papers published in prestigious journals and 16 books, one of which, "Statistics and Truth", originally published in English, was translated into French, German, Japanese, Mandarin and Taiwanese, Turkish, and Korean. One other book, "Linear Statistical Inference", which has been in the market for over 50 years, is available, besides English, also in German, Czech, Polish, Chinese, Japanese and Russian.

C. R. Rao has also edited 42 volumes of the "Handbook of Statistics", dealing with the latest methodologies in Statistics.

Some of C. R. Rao's influential papers were the cornerstone for what nowadays are well-known techniques and terms used in Statistics and other areas. His 1945 paper in the Bulletin of the Calcutta Mathematical Society, written at the young age of 25 (Rao, 1945), together with the 1946 book by H. Cramér (Cramér, 1946) established the basis for the well-known "Cramér-Rao lower bound" and the "Cramér-Rao inequality", which set the lower bound for the variance of unbiased estimators. This same paper, together with another paper from Blackwell (Blackwell, 1947) also established the foundations of the well-known Rao-Blackwell Theorem and of the method commonly known as Rao-Blackwellization, through which one may be able to obtain, by conditioning on a sufficient statistic, a much better estimator from what might originally be just a crude estimator, and which combined with some results from the Exponential Family allows for an easy way to obtain UMVU (Uniform Minimum Variance Unbiased) estimators.

This 1945 C. R. Rao paper established yet the basis for what are called the "Fisher-Rao metric" and "Rao distance", which are measures of the change induced in a probability distribution by small changes in its parameters (Aitkinson and Mitchell, 1981). They were introduced in connection with statistical problems of classification and cluster analysis and are based on a differential-geometrical approach, but have found applications in different areas as in some problems in quantum mechanics (Brody and Hughston, 1998) and in the detection of structures in images (Maybank, 2004, 2007). Amari (1985) refers that "It was Rao (1945), in his early twenties, who first noticed the importance of the differential-geometrical approach" in Statistics related problems. This Rao (1945) paper also gave rise to the term "Fisher-Rao metric", which keeps being a topic of research in distribution theory (Brigant et al, 2021).

C. R. Rao's contributions to Multivariate Analysis originated from a study of skeletons from the Jebel Moya archaeological site in Sudan. Jebel Moya is an archaeological site in the southern Gezira Plain in Sudan, approximately 250 km south southeast of Khartoum, where still nowadays the University of Cambridge carries on excavations. The site is one of the largest pastoralist cemeteries in Africa, where thousands of burials have been excavated thus far. In the early 1940's, the Anthropology Department of Cambridge University sent an expedition to *Jebel Moya*, to dig out ancient graves and bring the skeletons of people buried there for study. The

Department wanted to analyze the measurements taken on the skeletons to determine the relationship of the people who lived there with people currently living there or in nearby areas. However, there were no multivariate statistical methods available at that time to treat such problems, involving multiple measurements. C. R. Rao had developed some new multivariate methods for analyzing such multivariate data at the ISI, in Calcutta, together with Prof. Mahalanobis, and had the experience of addressing such problems. In July 1946, Dr. J.C. Trevor, Professor of the Anthropology Department at Cambridge University, sent a telegram to Prof. Mahalanobis asking him to send someone from ISI to analyze the measurements on *Jebel Moya* skeletons using the methodology developed at ISI. C. R. Rao was selected along with R. K. Mukherji, an anthropologist, to go to Cambridge to take measurements on skeletons and analyze the data. They went to Cambridge and worked in the Duckworth Laboratory of the Anthropology Museum for two years (1946–1948) as visiting scholars with pay. Rao had anyway to develop some new multivariate methods to analyze the data. The results based on the analysis of measurements were reported in the book, *Ancient Inhabitants of Jebel Moya*, published by the Cambridge University Press in 1954 under the joint authorship of C. R. Rao and the two anthropologists J.C. Trevor and R. K. Mukherji. At the invitation of the Royal Statistical Society, C. R. Rao presented a discussion paper describing the new multivariate methods he developed in solving the *Jebel Moya* problem. The paper with discussion was published in the Journal of Royal Statistical Society, *Utilization of multiple measurements in problems of biological classification*, *J. Roy. Statist. Soc.* 10: 159–203 (1948). Some new multivariate tests and models that C. R. Rao used in analyzing the Jebel Moya data such as MANOVA (multivariate analysis of variance) are described in his paper *Tests of significance in multivariate analysis, Biometrika*, 35: 58–9 (1948). These two papers are further discussed in Rao's book, *Advanced Statistical Methods*, John Wiley (1952) and they provided some of the foundations of Multivariate Analysis.

Yet in 1948, C. R. Rao published a paper (Rao, 1948) where he works out all the details of what is known as "Rao's Score Test", an alternative to Likelihood Ratio and Wald tests. The three tests are equivalent to the first order of asymptotics, being all three asymptotically optimal, but differ to some extent in the second order properties. Relative to the likelihood ratio test, Rao's score test has the advantage of requiring only the estimation of the likelihood function under the null hypothesis, and, unlike the Wald test, it is invariant to transformations of the parameters. Also, in contrast to most likelihood ratio tests, it may be used when the parameters lie on the boundary of the parameter space. Rao's Score Test found applications in a wide range of areas, from genetics to econometrics (Rao, 1950, 2005; Bera and Ullah, 1991, Anselin, 2011).

But this extraordinarily productive and fruitful era of C. R. Rao has also produced three papers (Rao, 1946, 1947, 1949) which would be the basis for the so-called "Rao's Orthogonal Arrays", a term actually coined in 1950 by Bush (Bush, 1950). Rao's Orthogonal Arrays are "a versatile class of combinational arrangements useful for conducting experiments to determine the optimum mix of a number of factors in a product to maximize the yield, and in the construction of a variety of designs for agricultural, medical and other experiments", as referred by C. R. Rao himself

(Rao, 2009). Orthogonal arrays found applications in several areas including factorial designs in agricultural, medical and other experiments, software testing, being used in situations where the number of inputs is relatively small, but too large to allow for exhaustive testing of every possible input, and it is particularly effective in finding errors associated with faulty logic (Roger and Maxim, 2019), and in quality control, where, associated with the Taguchi methods (Taguchi, 1986; Taguchi et al, 1999), developed during Taguchi's visit to ISI in the early 1950's, and which were largely adopted by the Indian and Japanese industries, and later also by the US industry, are used to improve the quality of manufactured goods, lower their costs and faster their time to market, and also found uses in engineering, biotechnology, marketing and advertising.

In 1954, C. R. Rao received some data from Japan. The aim was to use these data to study the long-term effects of radiation. Since there were some linear relations in the model matrix X, it was necessary to find a replacement for the common inverse of the X'X matrix. As such, C. R. Rao introduced in his 1955 paper (Rao, 1955) the "Pseudo inverse of a singular matrix", or "g-inverse" of a singular matrix, as he himself names it. This was indeed the same year Penrose published his paper on generalized inverses (Penrose, 1955), which would give rise to the well-known Moore-Penrose inverse, giving reference to the previous work of Moore on the topic (Moore, 1920). However, it would be C. R. Rao's paper in 1962 (Rao, 1962) and the monograph he published together with Sujit Kumar Mitra (Rao and Mitra, 1971) that would establish the importance of the generalized inverses in linear models and other areas.

More recently, in a series of three papers published in 1982, C. R. Rao established what is known as "Rao's Quadratic Entropy", a measure of diversity of ecological communities, based on the proportion of the abundance of species present in a community and a measure of dissimilarity among them (Rao, 1982a, b, c). The unified approach provided by Rao's Quadratic Entropy is useful for performing Analysis of Variance type analyses on both qualitative and quantitative data (Zhao, 2010), and "it surpasses other proposed indices" when more than one trait is considered (Zoltán, 2005).

Positions held by C. R. Rao

C. R. Rao retired from active service at the age of 80 from The Pennsylvania State University, PA, USA but he continues to hold an honorary Professorship at The Pennsylvania State University, PA, USA and at the University at Buffalo, SUNY, USA.

Other positions held were:

Indian Statistical Institute, in various capacities 1941–1979
Visiting Professor at University of Illinois 1951–1952
National Professor of India 1987–1992

University Professor, University of Pittsburgh 1979–1988
Eberly Professor of Statistics, The Pennsylvania State University (PSU), PA, USA 1988–2001
Director, Centre for Multivariate Analysis, PSU 2001–2010
Eberly Professor Emeritus (PSU) 2001–
Research Professor, University at Buffalo, SUNY 2010–

C. R. Rao's Fellowships of National Academies and Professional Societies

National Academies

1953—Indian National Science Academy, India
1967—The Royal Society, FRS (U.K. Academy of Sciences)
1974—Indian Academy of Science, India
1975—American Academy of Arts and Science, USA
1983—Third World Academy of Sciences, Trieste, Italy (Founder Fellow)
1988—The National Academy of Sciences, India
1995—National Academy of Sciences, USA
1996—Member of Prometheus Society
1997—Lithuanian Academy of Sciences (Foreign Member)
2009—Honorary Fellow of European Academy of Sciences

Honorary Fellowships

1969—Honorary Fellow Royal Statistical Society, U.K.
1974—Honorary Life Fellow King's College, Cambridge, U.K.
1974—Honorary Member Indian Society of Human Genetics
1983—Honorary Member International Statistics Institute, The Netherlands
1985—Honorary Fellow Calcutta Statistical Association
1986—Honorary Life Member Biometric Society
1990—Honorary Fellow the Finnish Statistical Society
1995—Honorary Fellow the Institute of Combinatorics and its Applications
1998—Honorary Fellow International Indian Statistical Association
2000—Honorary Fellow World Innovation Foundation
2002—Honorary Member Portuguese Statistical Society
2012—Honorary Fellowship Institute of Applied Statistics, Sri Lanka
2012—Honorary Member and Fellow of Indian Society of Probability and Statistics (ISPS)

Fellowships (by Election)

1951—Member International Statistical Institute
1958—Fellow Institute of Mathematical Statistics, U.S.A.
1965—Fellow Andhra Pradesh Academy of Science, India
1972—Fellow American Statistical Association, U.S.A.

1972—Fellow International Econometric Society, U.S.A.
1985—Fellow The Indian Society for Medical Statistics
1994—Fellow American Association for the Advancement of Science (AAAS)
2012—Fellow of the Indian Society of Probability and Statistics

Presidentship of Professional Societies

1971–76 Indian Econometric Society
1973–75 International Biometric Society
1976–77 Institute of Mathematical Statistics, U.S.A. (First person outside the USA to be made president)
1977–79 International Statistical Institute, The Netherlands
1982–84 Forum for Interdisciplinary Mathematics, USA

C. R. Rao's Awards

- **Jerzy Splawa-Neyman Medal**, from the Polish Statistical Association in recognition of "his outstanding contributions to the theory, applications, and teaching of statistics"—2014
- **Guy Medal in Gold** of the Royal Statistical Society, UK "for those who are judged to have merited a significant mark of distinction by reason of their innovative contribution to theory or application of statistics" from the president of the Royal Statistical Society—2011
- **India Science Award**, "for major contributions of a path-breaking nature based on work done in India" from Prime Minister Manmohan Singh—2009
- **The International Mahalanobis Prize**, awarded by International Statistical Institute at the 54th Session held in Berlin for "lifetime achievement"—2003
- **Srinivas Ramanujan Medal** from Indian National Science Association—2003
- **National Medal of Science**—highest award in the US for a scientist honored as "prophet of a better age", from President George W. Bush—2002
- **Desikottama award**, the highest honor bestowed by the University of Visva-Bharati, India, in recognition of his "enormous contributions in the field of statistics and its applications"—2003
- **Padma Vibhushan**, second highest civilian award, from the Government of India for "outstanding contributions to Science and Engineering/Statistics"—2001
- **Army Wilks Medal**, American Statistical Association—2000
- **Mahalanobis Birth Centenary Medal**—1996
- **Fellow of National Academy of Science**, USA,—1995
- **Samuel S. Wilks Medal**, awarded by the American Statistical Association for the great influence he has had on the application of statistical thinking in different disciplines, embodying over a career of more than 40 years in the spirit and ideals of Samuel S. Wilks—1989
- **Founding Fellow of Third World Academy of Science**, Trieste, Italy—1983
- **Jagadish Chandra Bose Medal** of Bose Institute, India—1979

- **Megnad Saha Medal**, of Indian Science Academy, India—1969
- **Padma Bhushan**, one of the civilian awards of a high order of the Government of India, for services in the field of statistical education and research—1968
- **Shanti Swarup Bhatnagar Award**, Council of Scientific and Industrial Research, India, for "notable and outstanding research in statistics" from Pandit Jawaharlal Nehru—1963

In 2000, the Prof. C. R. Rao Young Statistician Award was instituted by the Ministry of Statistics and Programme Implementation, Government of India to be awarded to young statisticians.

Dr. C. R. Rao on his 100th birthday

Dr. C. R. Rao, with his daughter, Dr. Tejaswini Rao, on his 100th birthday
Photos courtesy of Dr. Tejaswini Rao.

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Contents

Applications

General

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Inference

Robust Statistical Inference for One-Shot Devices Based on Density Power Divergences: An Overview

N. Balakrishnan, E. Castilla, and L. Pardo

Abstract In this chapter, we provide a detailed review of divergence-based robust inferential methods for one-shot device testing under different lifetime distributions. Proposed estimators and Wald-type tests are shown to possess a more robust behavior than the classical maximum likelihood estimator (MLE) and Wald test. Some simulation results and real data examples are also presented to illustrate the methods detailed.

Keywords One-shot device testing · Censoring · Reliability · Robust inference · Power-divergence statistics · Wald-type tests

1 Introduction

In this chapter, one-shot device testing data, which is an extreme case of interval censoring, is discussed. One-shot devices can be used only once as they get destroyed immediately after use, and so one can only know whether the failure time is either before or after a specific inspection time. The lifetimes are either left- or right-censored, with the lifetime being less than the inspection time if the test outcome is a failure (resulting in left censoring) and the lifetime being more than the inspection time if the test outcome is a success (resulting in right censoring). Some examples of one-shot devices are nuclear weapons, space shuttles, automobile air bags, fuel injectors, disposable napkins, heat detectors, missiles (Olwell and Sorell 2001) and fire extinguishers (Newby 2008). In survival analysis, these data are called "cur-

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rent status data". For instance, in animal carcinogenicity experiments, one observes whether a tumor has occurred by the examination time for each subject or not.

Due to the advances in manufacturing design and technology, products have now become highly reliable with long lifetimes. This fact would pose a problem in the analysis of data if only a few or no failures are observed. For this reason, accelerated life-tests (ALT) are often used by adjusting a controllable factor, such as temperature or velocity or humidity, in order to induce more failures in the experiment. The study of one-shot devices from ALT data has been developed considerably recently, mainly motivated by the work of Fan et al. (2009). In this work, a Bayesian approach was presented to make inferences on the failure rate and reliability of devices. They found the normal prior to be the best one when the failure observations are rare, that is, when the devices are highly reliable. Balakrishnan and Ling (2012a) developed an expectation–maximization (EM) algorithm for the determination of the MLEs of model parameters under exponential lifetime distribution for devices with a single stress factor. Balakrishnan and Ling (2012b) further extended this work to a model with multiple stress factors. Balakrishnan and Ling (2013) developed more general inferential results for devices with Weibull lifetimes under non-constant shape parameters, while Balakrishnan and Ling (2014) provided inferential work for devices with gamma lifetimes. In Balakrishnan et al. (2015a, b), the problem of one-shot devices under competing risks was considered for the first time.

Most of the results mentioned above are based on MLEs which are well-known to be not only efficient but also non-robust. Therefore, testing procedures based on MLEs face serious robustness problems. Recently, robust inference for one-shot device testing has been developed based on weighted minimum density power divergence (DPD) estimators. These results may be found in several papers (Balakrishnan et al. 2019a, b, 2020a, b, c, d). In this chapter, we present the framework necessary to develop robust estimators and Wald-type tests based on them for different lifetime distributions, and a concise review of the main results in the cited papers.

In this chapter the following data examples will be used to illustrate the methodologies being surveyed.

1. **Electric current data:** These data (see Table 2 in Balakrishnan and Ling 2012b) consist of 120 one-shot devices that were divided into four accelerated conditions with higher-than-normal temperature and electric current, and inspected at three different times. By subjecting the devices to adverse conditions, we shorten the lifetimes, observing more failures in a clear example of an ALT design.
2. **Tumor toxicological data:** These data considered, taken from the National Center for Toxicological Research, were originally reported by Kodell and Nelson (1980) and recently analyzed by Balakrishnan and Ling (2013, 2014) using MLEs under a one-shot device model. These data consisted of 1816 mice, of which 553 had tumors, involving the strain of offspring (F1 or F2), gender (female or male) and concentration of benzidine dihydrochloride (60 ppm, 120 ppm, 200 ppm or 400 ppm) as the stress factors. For each testing condition, the number of mice tested and the number of mice having tumors were all recorded. This is a clear example of current status data.

Table 1 Data on one-shot devices at multiple stress levels and collected at different inspection times

Condition	Inspection time	Devices	Failures	Covariates		
				Stress 1	⋯	Stress J
1	IT_1	K_1	n_1	x_{11}	⋯	x_{1J}
2	IT_2	K_2	n_2	x_{21}	⋯	x_{2J}
⋮	⋮	⋮	⋮	⋮		⋮
I	IT_I	K_I	n_I	x_{I1}	⋯	x_{IJ}

3. **Glass Capacitors data:** These data were presented in Zelen (1959) from a life-test of glass capacitors at higher than usual levels of temperature (in °C), $T = \{170, 180\}$, and voltage $V = \{350, 300, 250, 200\}$. At each of the eight combinations of temperature and voltage, eight items were tested.

The study of these examples, as well as the simulation results presented in this chapter, have been obtained under the R Statistical Software. The *nlm* function has been used for the minimization of the corresponding divergence measure. We suggest the use of the packages *hypergeo* and *expint* for the manipulation of gamma and Weibull distributions, respectively.

1.1 Model Description

Let us suppose that the data are stratified into I testing conditions and that in the ith testing condition, K_i individuals are placed under stress-level combinations with J stress factors, being maintained at certain levels, and the conditions of those units are then observed at pre-specified inspection times IT_i, for $i = 1, \ldots, I$. Then, the number of devices that have failed by time IT_i are recorded as n_i.

In this setting (as summarized in Table 1), we consider that the density and distribution functions of the lifetimes are given, respectively, by $f(t; \boldsymbol{x}_i, \boldsymbol{\theta})$ and $F(t; \boldsymbol{x}_i, \boldsymbol{\theta})$, where $\boldsymbol{x}_i = (1, x_{i1}, \ldots, x_{iJ})^T$ is the vector of stresses associated with the test condition i ($i = 1, \ldots, I$), and $\boldsymbol{\theta} \in \Theta \subseteq \mathbb{R}^S$ is the model parameter vector (S depends on the distribution associated with the model). The reliability function of the lifetimes is denoted by $R(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - F(t; \boldsymbol{x}_i, \boldsymbol{\theta})$.

Assuming independent observations, the likelihood function based on the observed data, presented in Table 1, is given by

$$\mathcal{L}(n_1, \ldots, n_I; \boldsymbol{\theta}) \propto \prod_{i=1}^{I} F^{n_i}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) R^{K_i - n_i}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}), \tag{1}$$

and the corresponding MLE of $\boldsymbol{\theta}$, $\widehat{\boldsymbol{\theta}}$, will be obtained by maximization of (1) or, equivalently, its logarithm, which is

$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}\in\Theta} \log \mathcal{L}(n_1, \ldots, n_I; \boldsymbol{\theta}).$$

We introduce some notation in order to define the MLE on the basis of Kullback–Leibler divergence (Kullback and Leibler 1951). We consider the empirical and theoretical probability vectors

$$\widehat{\boldsymbol{p}}_i = (\widehat{p}_{i1}, \widehat{p}_{i2})^T, \quad i = 1, \ldots, I$$

and

$$\boldsymbol{\pi}_i(\boldsymbol{\theta}) = (\pi_{i1}(\boldsymbol{\theta}), \pi_{i2}(\boldsymbol{\theta}))^T, \quad i = 1, \ldots, I,$$

with $\widehat{p}_{i1} = \frac{n_i}{K_i}$, $\widehat{p}_{i2} = 1 - \frac{n_i}{K_i}$, $\pi_{i1}(\boldsymbol{\theta}) = F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$ and $\pi_{i2}(\boldsymbol{\theta}) = R(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$.

Definition 1 The Kullback–Leibler divergence measure between $\widehat{\boldsymbol{p}}_i$ and $\boldsymbol{\pi}_i(\boldsymbol{\theta})$ is given by

$$d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = \widehat{p}_{i1} \log\left(\frac{\widehat{p}_{i1}}{\pi_{i1}(\boldsymbol{\theta})}\right) + \widehat{p}_{i2} \log\left(\frac{\widehat{p}_{i2}}{\pi_{i2}(\boldsymbol{\theta})}\right),$$

and similarly, the weighted Kullback–Leibler divergence measure for all the units, where $K = \sum_{i=1}^{I} K_i$ is the total number of devices under the life-test, is given by

$$\sum_{i=1}^{I} \frac{K_i}{K} d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = \frac{1}{K} \sum_{i=1}^{I} K_i \left[\widehat{p}_{i1} \log\left(\frac{\widehat{p}_{i1}}{\pi_{i1}(\boldsymbol{\theta})}\right) + \widehat{p}_{i2} \log\left(\frac{\widehat{p}_{i2}}{\pi_{i2}(\boldsymbol{\theta})}\right)\right]. \tag{2}$$

Proposition 1 *The MLE can be obtained as the minimization of the weighted Kullback–Leibler divergence measure in (2), i.e.,*

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\Theta} \sum_{i=1}^{I} \frac{K_i}{K} d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})).$$

1.2 The Weighted Minimum Density Power Divergence

In order to extend the MLE, we define the weighted DPD.

Definition 2 The weighted DPD between the probability vectors $\widehat{\boldsymbol{p}}_i$ and $\boldsymbol{\pi}_i(\boldsymbol{\theta})$ for $\beta > 0$ is given by

$$d_\beta^w(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} d_\beta(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})),$$

where

$$d_\beta(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = \left(\pi_{i1}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i2}^{\beta+1}(\boldsymbol{\theta})\right) - \frac{\beta+1}{\beta}\left(\widehat{p}_{i1}\pi_{i1}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i2}\pi_{i2}^{\beta}(\boldsymbol{\theta})\right) + \frac{1}{\beta}\left(\widehat{p}_{i1}^{\beta+1} + \widehat{p}_{i2}^{\beta+1}\right),$$

and $d_{\beta=0}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = \lim_{\beta\to 0^+} d_\beta(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta}))$, if $\beta = 0$.

The term $\frac{1}{\beta}\left(\widehat{p}_{i1}^{\beta+1} + \widehat{p}_{i2}^{\beta+1}\right)$ does not depend on $\boldsymbol{\theta}$ and so we can define

$$d_\beta^*(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = \left(\pi_{i1}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i2}^{\beta+1}(\boldsymbol{\theta})\right) - \frac{\beta+1}{\beta}\left(\widehat{p}_{i1}\pi_{i1}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i2}\pi_{i2}^{\beta}(\boldsymbol{\theta})\right). \quad (3)$$

Based on (3), we can define the weighted minimum DPD estimator, as follows.

Definition 3 The weighted minimum DPD estimator for $\boldsymbol{\theta}$ is

$$\widehat{\boldsymbol{\theta}}_\beta = \arg\min_{\boldsymbol{\theta}\in\Theta} \sum_{i=1}^{I} \frac{K_i}{K} d_\beta^*(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})), \quad \text{for } \beta > 0,$$

and, in particular, for $\beta = 0$, we have the MLE.

For more details about DPD, see Basu et al. (1998). Now, the estimating equations for obtaining this estimator are given in the following result.

Theorem 1 *For $\beta \geq 0$, the estimating equations are given by*

$$\sum_{i=1}^{I} (K_i F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) - n_i)\left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R^{\beta-1}(t; \boldsymbol{x}_i, \boldsymbol{\theta})\right)\frac{\partial F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \mathbf{0}_S,$$

where $\mathbf{0}_S$ is the null column vector of dimension S.

With regard to the asymptotic distribution of the weighted minimum DPD estimator, $\widehat{\boldsymbol{\theta}}_\beta$, we have the following result.

Theorem 2 *Let $\boldsymbol{\theta}^0$ be the true value of the parameter $\boldsymbol{\theta}$. Then, the asymptotic distribution of the weighted minimum DPD estimator $\widehat{\boldsymbol{\theta}}_\beta$ is given by*

$$\sqrt{K}\left(\widehat{\boldsymbol{\theta}}_\beta - \boldsymbol{\theta}^0\right) \xrightarrow[K\to\infty]{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\boldsymbol{K}_\beta(\boldsymbol{\theta}^0)\boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\right),$$

where the matrices $\boldsymbol{J}_\beta(\boldsymbol{\theta}^0)$ *and* $\boldsymbol{K}_\beta(\boldsymbol{\theta}^0)$ *are given by*

$$\boldsymbol{J}_\beta(\boldsymbol{\theta}) = \sum_{i=1}^{I}\sum_{j=1}^{2}\frac{K_i}{K}\boldsymbol{u}_{ij}(\boldsymbol{\theta})\boldsymbol{u}_{ij}^T(\boldsymbol{\theta})\pi_{ij}^{\beta+1}(\boldsymbol{\theta}), \tag{4}$$

$$\boldsymbol{K}_\beta(\boldsymbol{\theta}) = \sum_{i=1}^{I}\sum_{j=1}^{2}\frac{K_i}{K}\boldsymbol{u}_{ij}(\boldsymbol{\theta})\boldsymbol{u}_{ij}^T(\boldsymbol{\theta})\pi_{ij}^{2\beta+1}(\boldsymbol{\theta}) - \sum_{i=1}^{I}\frac{K_i}{K}\boldsymbol{\xi}_{i,\beta}(\boldsymbol{\theta})\boldsymbol{\xi}_{i,\beta}^T(\boldsymbol{\theta}), \tag{5}$$

with

$$\boldsymbol{u}_{ij}(\boldsymbol{\theta}) = \frac{\partial \log \pi_{ij}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \quad \textit{and} \quad \boldsymbol{\xi}_{i,\beta}(\boldsymbol{\theta}) = \sum_{j=1}^{2}\boldsymbol{u}_{ij}(\boldsymbol{\theta})\pi_{ij}^{\beta+1}(\boldsymbol{\theta}).$$

This result follows from Theorem 3.1 of Ghosh and Basu (2013).

1.3 Wald-Type Tests

Based on the asymptotic distribution of the weighted minimum DPD estimator, we can define Wald-type tests.

Let us consider the function $\boldsymbol{m} : \mathbb{R}^S \longrightarrow \mathbb{R}^r$, where $r \leq S$. Then, $\boldsymbol{m}(\boldsymbol{\theta}) = \boldsymbol{0}_r$ represents a composite null hypothesis. We assume that the $S \times r$ matrix

$$\boldsymbol{M}(\boldsymbol{\theta}) = \frac{\partial \boldsymbol{m}^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$$

exists and is continuous in $\boldsymbol{\theta}$, with rank $\boldsymbol{M}(\boldsymbol{\theta}) = r$. For testing

$$H_0 : \boldsymbol{\theta} \in \Theta_0 \text{ against } H_1 : \boldsymbol{\theta} \notin \Theta_0, \tag{6}$$

where $\Theta_0 = \{\boldsymbol{\theta} \in \Theta : \boldsymbol{m}(\boldsymbol{\theta}) = \boldsymbol{0}_r\}$, we can consider the following Wald-type test statistics:

$$W_K(\widehat{\boldsymbol{\theta}}_\beta) = K\boldsymbol{m}^T(\widehat{\boldsymbol{\theta}}_\beta)\left(\boldsymbol{M}^T(\widehat{\boldsymbol{\theta}}_\beta)\boldsymbol{\Sigma}(\widehat{\boldsymbol{\theta}}_\beta)\boldsymbol{M}(\widehat{\boldsymbol{\theta}}_\beta)\right)^{-1}\boldsymbol{m}(\widehat{\boldsymbol{\theta}}_\beta), \tag{7}$$

where $\boldsymbol{\Sigma}_\beta(\widehat{\boldsymbol{\theta}}_\beta) = \boldsymbol{J}_\beta^{-1}(\widehat{\boldsymbol{\theta}}_\beta)\boldsymbol{K}_\beta(\widehat{\boldsymbol{\theta}}_\beta)\boldsymbol{J}_\beta^{-1}(\widehat{\boldsymbol{\theta}}_\beta)$ and $\boldsymbol{J}_\beta(\boldsymbol{\theta})$ and $\boldsymbol{K}_\beta(\boldsymbol{\theta})$ are as given in (4) and (5), respectively.

In the following theorem, we present the asymptotic distribution of $W_K(\widehat{\boldsymbol{\theta}}_\beta)$.

Theorem 3 *The asymptotic null distribution of the proposed Wald-type test statistics, given in Eq. (7), is a chi-squared* (χ^2) *distribution with* r *degrees of freedom, i.e.,*

$$W_K(\widehat{\boldsymbol{\theta}}_\beta) \xrightarrow[K\to\infty]{\mathcal{L}} \chi_r^2.$$

Based on Theorem 3, we will reject the null hypothesis in (6) if

$$W_K(\widehat{\boldsymbol{\theta}}_\beta) > \chi^2_{r,\alpha},$$

where $\chi^2_{r,\alpha}$ is the upper percentage point of order α of χ^2_r distribution.

General results in relation to Wald-type tests based on minimum DPD estimators can be seen in Basu et al. (2016, 2018).

1.4 Influence Function

An important concept in robustness theory is the influence function (Hampel et al. 1986). For any estimator defined in terms of a statistical functional $\boldsymbol{U}(F)$ from the true distribution F, its influence function (IF) is defined as

$$IF(t, \boldsymbol{U}, F) = \lim_{\varepsilon \downarrow 0} \frac{\boldsymbol{U}(F_\varepsilon) - \boldsymbol{U}(F)}{\varepsilon} = \left. \frac{\partial \boldsymbol{U}(F_\varepsilon)}{\partial \varepsilon} \right|_{\varepsilon = 0^+}, \tag{8}$$

where $F_\varepsilon = (1-\varepsilon)F + \varepsilon \Delta_t$, with ε being the contamination proportion and Δ_t being the degenerate distribution at the contamination point t. Thus, the (first-order) IF, as a function of t, measures the standardized asymptotic bias (in its first-order approximation) caused by the infinitesimal contamination at the point t. The maximum of this IF over t indicates the extent of bias due to contamination and so the smaller its value is, the more robust the estimator is.

In this section, we shall present the influence function for the weighted minimum DPD estimator as well as for the Wald-type tests presented in (7).

1.4.1 Robustness of the Weighted Minimum Density Power Divergence Estimators

Let us denote by G_i the true distribution function of a Bernoulli random variable with an unknown probability of success, for the ith group of K_i observations, having mass function g_i. Similarly, let $F_{i,\boldsymbol{\theta}}$ be the distribution function of Bernoulli random variable having a probability of success equal to $\pi_{i1}(\boldsymbol{\theta})$, with probability mass function $f_i(\cdot, \boldsymbol{\theta})$ $(i = 1, ..., I)$, which are related to the model. In vector notation, we consider $\boldsymbol{G} = (G_1 \otimes \mathbf{1}^T_{K_1}, \ldots, G_I \otimes \mathbf{1}^T_{K_I})^T$ and $\boldsymbol{F}_{\boldsymbol{\theta}} = (F_{1,\boldsymbol{\theta}} \otimes \mathbf{1}^T_{K_1}, \ldots, F_{I,\boldsymbol{\theta}} \otimes \mathbf{1}^T_{K_I})^T$.

For any estimator defined in terms of a statistical functional $\boldsymbol{U}(\boldsymbol{G})$ in the set up of data from the true distribution function $\boldsymbol{G}$, its IF in accordance with (8) is defined as

$$IF(\boldsymbol{t}, \boldsymbol{U}, \boldsymbol{G}) = \lim_{\varepsilon \downarrow 0} \frac{\boldsymbol{U}(\boldsymbol{G}_{\varepsilon,\boldsymbol{t}}) - \boldsymbol{U}(\boldsymbol{G})}{\varepsilon} = \left. \frac{\partial \boldsymbol{U}(\boldsymbol{G}_{\varepsilon,\boldsymbol{t}})}{\partial \varepsilon} \right|_{\varepsilon = 0^+},$$

where $\boldsymbol{G}_{\varepsilon,\boldsymbol{t}} = (1-\varepsilon)\boldsymbol{G} + \varepsilon\Delta_{\boldsymbol{t}}$, with ε being the contamination proportion and $\Delta_{\boldsymbol{t}}$ being the distribution function of the degenerate random variable at the contamination point

$$\boldsymbol{t} = (t_{11}, ..., t_{1K_1}, ..., t_{I1}, ..., t_{IK_I})^T \in \mathbb{R}^{IK}.$$

We first need to define the statistical functional $\boldsymbol{U}_\beta(\boldsymbol{G})$ corresponding to the weighted minimum DPD estimator as the minimizer of the weighted sum of DPDs between the true and model densities. This is defined as the minimizer of

$$H_\beta(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \left\{ \sum_{y\in\{0,1\}} \left[f_i^{\beta+1}(y,\boldsymbol{\theta}) - \frac{\beta+1}{\beta} f_i^{\beta}(y,\boldsymbol{\theta}) g_i(y) \right] \right\}, \tag{9}$$

where $g_i(y)$ is the probability mass function associated with G_i and

$$f_i(y,\boldsymbol{\theta}) = y\pi_{i1}(\boldsymbol{\theta}) + (1-y)\pi_{i2}(\boldsymbol{\theta}), \quad y \in \{0,1\}.$$

If we choose $g_i(y) \equiv f_i(y,\boldsymbol{\theta})$, expression (9) gets minimized at $\boldsymbol{\theta} = \boldsymbol{\theta}^0$, implying the Fisher consistency of the weighted minimum DPD estimator functional $\boldsymbol{U}_\beta(\boldsymbol{G})$ in our model.

Under appropriate differentiability conditions, we require the solution of the estimating equations

$$\frac{\partial H_\beta(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \sum_{i=1}^{I} \frac{K_i}{K} \left\{ \sum_{y\in\{0,1\}} \left[f_i^{\beta}(y,\boldsymbol{\theta}) \frac{\partial f_i(y,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} - f_i^{\beta-1}(y,\boldsymbol{\theta}) \frac{\partial f_i(y,\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} g_i(y) \right] \right\} = \mathbf{0}. \tag{10}$$

In order to get the IF of the weighted minimum DPD estimator at $F_{\boldsymbol{\theta}}$ with respect to the kth element of the i_0th group of observations, we replace $\boldsymbol{\theta}$ in (10) by

$$\boldsymbol{\theta}_\varepsilon^{i_0} = \boldsymbol{U}_\beta(G_1 \otimes \mathbf{1}_{K_1}^T, \ldots, G_{i_0-1} \otimes \mathbf{1}_{K_{i_0-1}}^T, G_{i_0,\varepsilon} \otimes \mathbf{1}_{K_{i_0}}^T, G_{i_0+1}, \ldots, G_I \otimes \mathbf{1}_{K_I}^T),$$

where $G_{i_0,\varepsilon}$ is the distribution function associated with the probability mass function

$$g_{i_0,\varepsilon,k}(y) = (1-\varepsilon) f_i(y,\boldsymbol{\theta}^0) + \varepsilon\Delta_{t_{i_0,k}}(y),$$

$\Delta_{t_{i_0,k}}(y) = y\Delta_{t_{i_0,k}}^{(1)} + (1-y)\Delta_{t_{i_0,k}}^{(2)}$, with $\Delta_{t_{i_0,k}}^{(1)}$ being the degenerating function at point $(t_{i_0,k})$, $\Delta_{t_{i_0,k}}^{(2)} = (1 - \Delta_{t_{i_0,k}}^{(1)})$, and

$$g_i(y) = \begin{cases} f_i(y, \boldsymbol{\theta}^0) \text{ if } i \neq i_0, \\ g_{i_0,\varepsilon,k}(y) \text{ if } i = i_0. \end{cases}$$

Differentiating with respect to ε and evaluating this derivative at $\varepsilon = 0$, we obtain the following theorem.

Theorem 4 *Let us consider the one-shot device testing with multiple stress factors defined in (1). The IF with respect to the kth observation of the i_0th group is given by*

$$\begin{aligned} IF(t_{i_0,k}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}) = & \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \frac{K_{i_0}}{K} \left. \frac{\partial \pi_{i_0 1}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^0} \\ & \times \left(\pi_{i_0 1}^{\beta-1}(\boldsymbol{\theta}^0) + \pi_{i_0 2}^{\beta-1}(\boldsymbol{\theta}^0) \right) \left(\pi_{i_0 1}(\boldsymbol{\theta}^0) - \Delta_{i_{0,k}}^{(1)} \right). \end{aligned} \tag{11}$$

In order to get the IF of the weighted minimum DPD estimator at $F_{\boldsymbol{\theta}}$ with respect to all the observations, we replace the parameter $\boldsymbol{\theta}$ in (10) by

$$\boldsymbol{\theta}_\varepsilon^{i_0} = \boldsymbol{U}_\beta(G_{1,\varepsilon} \otimes \mathbf{1}_{K_1}^T, \ldots, G_{i_0-1,\varepsilon} \otimes \mathbf{1}_{K_{i_0-1}}^T, G_{i_0,\varepsilon} \otimes \mathbf{1}_{K_{i_0}}^T, G_{i_0+1,\varepsilon}, \ldots, G_{I,\varepsilon} \otimes \mathbf{1}_{K_I}^T),$$

and the probability mass function $g_i(y)$ by

$$g_{i,\varepsilon,k}(y) = (1-\varepsilon) f_i(y, \boldsymbol{\theta}^0) + \varepsilon \Delta_{t_i,k}(y),$$

in which case we get

$$\begin{aligned} \left. \frac{\partial H_\beta(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_\varepsilon} = & \sum_{i=1}^{I} \frac{K_i}{K} \left\{ \sum_{y \in \{0,1\}} f_i^\beta(y, \boldsymbol{\theta}_\varepsilon) \left. \frac{\partial f_i(y, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_\varepsilon} \right\} \\ & - \sum_{i=1}^{I} \frac{K_i}{K} \left\{ \sum_{y \in \{0,1\}} f_i^{\beta-1}(y, \boldsymbol{\theta}_\varepsilon) \left. \frac{\partial f_i(y, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_\varepsilon} f_i(y, \boldsymbol{\theta}^0) \right\}. \end{aligned}$$

Differentiating with respect to ε and evaluating the expression at $\varepsilon = 0$, we get the following result.

Theorem 5 *Let us consider the one-shot device testing with multiple stress factors defined in (1). The IF with respect to all the observations is given by*

$$\begin{aligned} IF(\boldsymbol{t}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}) = & \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \sum_{i=1}^{I} \frac{K_i}{K} \left. \frac{\partial \pi_{i1}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^0} \\ & \times \left(\pi_{i1}^{\beta-1}(\boldsymbol{\theta}^0) + \pi_{i2}^{\beta-1}(\boldsymbol{\theta}^0) \right) \left(\pi_{i1}(\boldsymbol{\theta}^0) - \Delta_{t_i}^{(1)} \right), \end{aligned} \tag{12}$$

where $\Delta_{t_i}^{(1)} = \sum_{k=1}^{K_i} \Delta_{t_i,k}^{(1)}$.

1.4.2 Robustness of Wald-Type Tests

Next, we study the robustness of the proposed Wald-type test statistics. The IF of a testing procedure, as introduced by Ronchetti and Rousseeuw (1979) for IID data, is also defined as in the case of estimation but with the statistical functional corresponding to the test statistics, and it is studied under the null hypothesis. This concept has been extended to non-homogeneous data, in Aerts and Haesbroeck (2017) and Ghosh and Basu (2018). In the present context, the functional associated with the Wald-type test, evaluated at $\boldsymbol{U}_\beta(\boldsymbol{G})$, is given by

$$W_K(\boldsymbol{U}_\beta(\boldsymbol{G})) = K\boldsymbol{m}^T(\boldsymbol{U}_\beta(\boldsymbol{G}))\left(\boldsymbol{M}^T(\boldsymbol{U}_\beta(\boldsymbol{G}))\boldsymbol{\Sigma}(\boldsymbol{U}_\beta(\boldsymbol{G}))\boldsymbol{M}(\boldsymbol{U}_\beta(\boldsymbol{G}))\right)^{-1}\boldsymbol{m}(\boldsymbol{U}_\beta(\boldsymbol{G})).$$

The IF with respect to the kth observation of the i_0th group of observations, of the functional associated with Wald -type test statistics for testing the composite null hypothesis in (6), is then given by

$$IF(t_{i_0,k}, W_K, F_{\boldsymbol{\theta}^0}) = \left.\frac{\partial W_K(F_{\boldsymbol{\theta}_\varepsilon^{i_0}})}{\partial\varepsilon}\right|_{\varepsilon=0^+} = 0.$$

It, therefore, becomes necessary to consider the second-order IF, as presented in the following result.

Theorem 6 *The second-order IF of the functional associated with Wald-type test statistics, with respect to the kth observation of the i_0th group of observations, is given by*

$$\begin{aligned} IF_2(t_{i_0,k}, W_K, F_{\boldsymbol{\theta}^0}) &= \left.\frac{\partial^2 W_K(F_{\boldsymbol{\theta}_\varepsilon^{i_0}})}{\partial\varepsilon^2}\right|_{\varepsilon=0^+} \\ &= 2\,IF(t_{i_0,k}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0})\boldsymbol{m}^T(\boldsymbol{\theta}^0)\left(\boldsymbol{M}^T(\boldsymbol{\theta}^0)\boldsymbol{\Sigma}(\boldsymbol{\theta}^0)\boldsymbol{M}(\boldsymbol{\theta}^0)\right)^{-1}\boldsymbol{m}(\boldsymbol{\theta}^0)IF(t_{i_0,k}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}), \end{aligned}$$

where $IF(t_{i_0,k}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0})$ is as given in (11).

Similarly, for all the indices, we can state the following result.

Theorem 7 *The second-order IF of the functional associated with Wald-type test statistics, with respect to all the observations, is given by*

$$\begin{aligned} IF_2(\boldsymbol{t}, W_K, F_{\boldsymbol{\theta}^0}) &= \left.\frac{\partial^2 W_K(F_{\boldsymbol{\theta}_\varepsilon})}{\partial\varepsilon^2}\right|_{\varepsilon=0^+} \\ &= 2\,IF(\boldsymbol{t}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0})\boldsymbol{m}^T(\boldsymbol{\theta}^0)\left(\boldsymbol{M}^T(\boldsymbol{\theta}^0)\boldsymbol{\Sigma}(\boldsymbol{\theta}^0)\boldsymbol{M}(\boldsymbol{\theta}^0)\right)^{-1}\boldsymbol{m}(\boldsymbol{\theta}^0)IF(\boldsymbol{t}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}), \end{aligned}$$

where $IF(\boldsymbol{t}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0})$ is as given in (12).

Note that the second-order influence functions of the proposed Wald-type tests are quadratic functions of the corresponding IFs of the weighted minimum DPD estimator for any type of contamination.

2 Robust Inference for One-Shot Device Testing Under Exponential Distribution

Let us consider the problem of one-shot device testing in which the failure time of the devices is assumed to follow an exponential distribution. Some work has been done for the particular case of a single stress model ($J = 1$). Fan et al. (2009) presented a Bayesian approach to develop inference on the failure rate and reliability of devices. They found the normal prior to be the best one when the failure observations are rare, that is, when the devices are highly reliable. Balakrishnan and Ling (2012a) developed an EM algorithm and made a comparative study with the mentioned Bayesian approach, showing that the EM method is more appropriate for products with low and moderate reliability. This work was extended in Balakrishnan and Ling (2012b) for the case of multiple stress factors.

The problem of one-shot device testing under the exponential distribution was also studied on the basis of weighted minimum DPD estimators as well as Wald-type tests based on them. In Balakrishnan et al. (2019b), the case of a single-stress factor was considered, and was subsequently extended to the multiple-stress case in Balakrishnan et al. (2020a). In this section, we present some of the key results obtained in these two papers.

2.1 Inference Under Exponential Distribution

We shall assume that the true lifetime follows an exponential distribution with unknown failure rate $\lambda_i(\boldsymbol{\theta})$, related to the stress factor $\boldsymbol{x}_i$ in a log-linear form as

$$\lambda_i(\boldsymbol{\theta}) = \exp(\boldsymbol{x}_i^T \boldsymbol{\theta}),$$

where $\boldsymbol{x}_i = (x_{i0}, x_{i1}, \ldots, x_{iJ})^T$ and $\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_J)^T$. Thus, here $\Theta = \mathbb{R}^{J+1}$. The corresponding density function and distribution function are, respectively,

$$f(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = \lambda_i(\boldsymbol{\theta}) \exp\{-\lambda_i(\boldsymbol{\theta})t\} = \exp(\boldsymbol{x}_i^T \boldsymbol{\theta}) \exp\{-\exp(\boldsymbol{x}_i^T \boldsymbol{\theta})t\}, \quad t > 0, \quad (13)$$

and

$$F(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - \exp\{-\lambda_i(\boldsymbol{\theta})t\} = 1 - \exp\{-t \exp(\boldsymbol{x}_i^T \boldsymbol{\theta})\}, \quad t > 0. \quad (14)$$

On the other hand, the reliability at time t and the mean lifetime under normal operating conditions $\boldsymbol{x}_i$ are given by

$$R(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - F(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = \exp\left(-t \exp\left(\boldsymbol{x}_i^T \boldsymbol{\theta}\right)\right), \quad t > 0 \quad (15)$$

and

$$E[T_i] = \frac{1}{\lambda_i} = \exp\left(-\boldsymbol{x}_i^T \boldsymbol{\theta}\right).$$

Then, specializing the result given in Theorem 1, for $\beta \geq 0$, the estimating equations are given by

$$\sum_{i=1}^{I} (K_i F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) - n_i) \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R^{\beta-1}(t; \boldsymbol{x}_i, \boldsymbol{\theta})\right) f(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) IT_i \boldsymbol{x}_i = \mathbf{0}_{J+1},$$

where $f(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$, $F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$ and $R(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$ are given, respectively, by (13), (14) and (15).

Following Theorem 2, the asymptotic distribution is given by

$$\sqrt{K}\left(\widehat{\boldsymbol{\theta}}_\beta - \boldsymbol{\theta}^0\right) \xrightarrow[K\to\infty]{\mathcal{L}} \mathcal{N}\left(\mathbf{0}_{J+1}, \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \boldsymbol{K}_\beta(\boldsymbol{\theta}^0) \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\right),$$

where

$$\boldsymbol{J}_\beta(\boldsymbol{\theta}) = \sum_{i}^{I} \frac{K_i}{K} \boldsymbol{x}_i \boldsymbol{x}_i^T f^2(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) IT_i^2 \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})\right), \tag{16}$$

$$\begin{aligned}\boldsymbol{K}_\beta(\boldsymbol{\theta}) = &\sum_{i=1}^{I} \frac{K_i}{K} \boldsymbol{x}_i \boldsymbol{x}_i^T f^2(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) IT_i^2 F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) R(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) \\ &\times \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})\right)^2. \end{aligned} \tag{17}$$

In the context of one-shot device testing under multiple stress factors, we may be interested in checking whether there is a significant relationship between the jth stress factor and the device lifetime. Under the exponential distribution assumption, this can be tested through the Wald-type test given in (7), where $\boldsymbol{m}(\boldsymbol{\theta}) = \theta_j$,

$$\boldsymbol{M}^T(\boldsymbol{\theta}) = (0, \ldots, \overset{(j+1)}{1}, \ldots, \overset{(J+1)}{0})$$

and $\boldsymbol{J}_\beta(\boldsymbol{\theta})$ and $\boldsymbol{K}_\beta(\boldsymbol{\theta})$ are as in (16) and (17), respectively. Some results in relation to the power function of Wald-type tests as well as the asymptotic distribution of $\boldsymbol{W}_K(\widehat{\boldsymbol{\theta}}_\beta)$ under contiguous alternative hypothesis can be found in Balakrishnan et al. (2020a).

The IF with respect to the kth observation of the i_0th group is given by

$$\begin{aligned} IF(t_{i_0,k}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}) = &\boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \frac{K_{i_0}}{K} f(IT_{i_0}; \boldsymbol{x}_{i_0}, \boldsymbol{\theta}^0) IT_{i_0} \boldsymbol{x}_{i_0} \\ &\times \left(F^{\beta-1}(IT_{i_0}; \boldsymbol{x}_{i_0}, \boldsymbol{\theta}^0) + R^{\beta-1}(IT_{i_0}; \boldsymbol{x}_{i_0}, \boldsymbol{\theta}^0)\right) \left(F(IT_{i_0}; \boldsymbol{x}_{i_0}, \boldsymbol{\theta}^0) - \Delta_{t_{i_0}}^{(1)}\right). \end{aligned}$$

The IF with respect to all the observations is given by

$$IF(\boldsymbol{t}, \boldsymbol{U}_\beta, F_{\boldsymbol{\theta}^0}) = \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \sum_{i=1}^{I} \frac{K_i}{K} f(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) IT_i \boldsymbol{x}_i$$
$$\times \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) + R^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0)\right) \left(F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) - \Delta_{t_i}^{(1)}\right).$$

In Balakrishnan et al. (2019b), the authors studied the boundedness of the influence functions, for the particular case of only one stress level or with respect to an observation or with respect to all the observations. It was shown that they are bounded on $t_{i_0,k}$ or $\boldsymbol{t}$, but if $\beta = 0$ the norm of the bidimensional influence functions can be very large on (x, IT), in comparison with $\beta > 0$, implying that the proposed weighted minimum DPD estimators with $\beta > 0$ are robust against leverage points, but the classical MLE is evidently non-robust. The same happens for large ITs too, but in accelerated processes inspection times tend not to be large.

2.2 Monte Carlo Simulation Study

In this section, we summarize the main results given in Balakrishnan et al. (2019b, 2020a), where Monte Carlo simulations were carried out to examine the behavior of the weighted minimum DPD estimators of the model parameters under the exponential assumption, for lifetimes.

We consider the devices to have exponential lifetimes subjected to two types of stress factors at two different conditions each, the first one at levels 55 and 70 and the second one at levels 85 and 100, and tested at three different inspection times $IT = \{2, 5, 8\}$. Thus, we can consider a table, such as in Table 1, with $I = 12$ rows corresponding to each of the 12 testing conditions. To evaluate the robustness of the weighted minimum DPD estimators, we have studied the behavior of this model under the consideration of an outlying cell in this table. The model has been examined under $(\theta_0, \theta_1, \theta_2) = (-6.5, 0.03, 0.03)$, different sample sizes and different degrees of contamination. The estimates have been computed with values of the tuning parameter $\beta \in \{0, 0.2, 0.4, 0.6, 0.8\}$.

In the top left of Fig. 1, efficiency of weighted minimum DPD estimators is measured under different sample sizes $K_i \in [40, 200]$ with contaminated data where the observations in the $i = 12$ testing condition have been generated under $(\theta_0, \theta_1, \tilde{\theta}_2) = (-6.5, 0.03, 0.025)$. The best behavior (least RMSE) is obtained for larger values of β. As expected, the RMSEs decrease as the sample size increases. The efficiency is also studied for different degrees of contamination of the parameter θ_1, as displayed in the top right of Fig. 1. Here, $K_i = 100$ and the degree of contamination is given by $4(1 - \frac{\tilde{\theta}_1}{\theta_1}) \in [0, 1]$. We can see how the MLEs and the weighted minimum DPD estimators with small values of tuning parameter β present the smallest RMSEs for weak outliers, i.e., when the degree of contamination is close to 0 ($\tilde{\theta}_1$ is close to θ_1). On the other hand, large values of tuning parameter β result in the weighted minimum DPD estimators having the smallest RMSEs, for medium

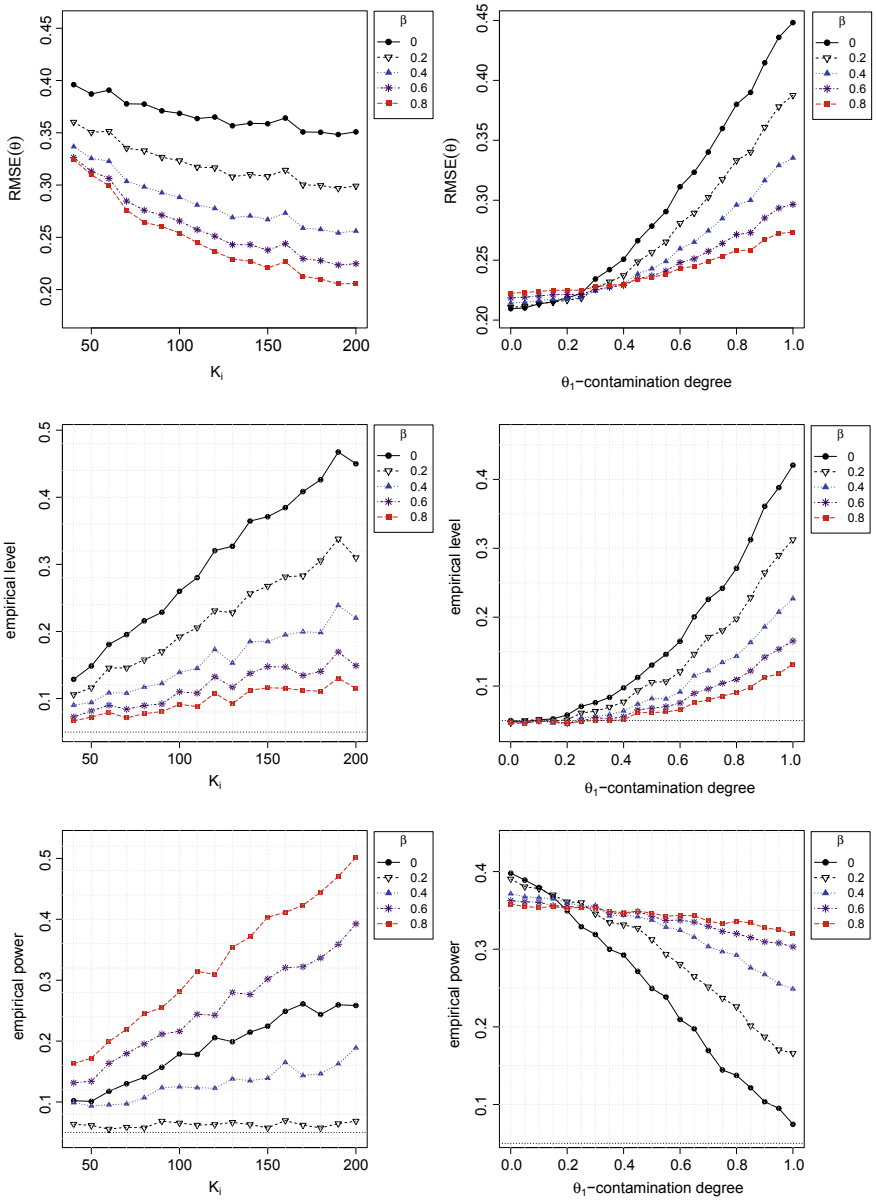

Fig. 1 Exponential distribution at multiple stress levels: RMSEs (top panel) of the weighted minimum DPD estimators of $\boldsymbol{\theta}$, the simulated levels (middle panel) and powers (bottom panel) of Wald-type tests with different sample sizes (left) and different degrees of contamination (right)

and strong outliers, i.e., when the degree of contamination is away from 0 ($\tilde{\theta}_1$ is not close to θ_1).

Let us now empirically evaluate the robustness of the weighted minimum DPD estimator-based Wald-type tests for the model. We first study the observed level (measured as the proportion of test statistics exceeding the corresponding chi-square critical value) of the test under the true null hypothesis $H_0 : \theta_2 = 0.03$ against the alternative $H_1 : \theta_2 \neq 0.03$. As before, these levels are plotted for different values of the sample sizes for contaminated data and for different degrees of contamination of θ_1 with a fixed value of $K_i = 100$ (middle of Fig. 1). Notice that when the pure data are considered, all the observed levels are quite close to the nominal level of 0.05. In the case of contaminated data, the level of the classical Wald test (at $\beta = 0$) as well as the proposed Wald-type tests with small β break down, while the weighted minimum DPD estimator-based Wald-type tests for moderate and large values of β provide greater stability in their levels. To investigate the power robustness of these tests (obtained in a similar manner), we change the true data-generating parameter value to be $\theta_2 = 0.035$; the resulting empirical powers are plotted at the bottom of Fig. 1. Again, the classical Wald test (at $\beta = 0$) presents the best behavior under the pure/low contaminated data, while the weighted minimum DPD estimator-based Wald-type tests with larger $\beta > 0$ lead to better stability in power performance in the case of contaminated samples.

Table 2 Electric current data: Estimated probabilities for different weighted minimum DPD estimators

i	$\frac{n_i}{K_i}$	$\widehat{\pi}_i^{\beta}$										
		$\beta = 0$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
1	0	0.154	0.152	0.150	0.148	0.146	0.144	0.142	0.141	0.139	0.138	**0.137**
2	0.4	0.338	0.340	0.343	0.346	0.348	0.351	0.354	0.356	0.358	0.359	**0.360**
3	0.4	0.371	0.373	0.376	0.378	0.381	0.384	0.387	0.389	0.391	0.393	**0.394**
4	0.7	0.681	0.691	**0.703**	0.715	0.728	0.740	0.752	0.761	0.769	0.776	0.780
5	0.4	**0.342**	0.338	0.335	0.331	0.327	0.322	0.319	0.315	0.312	0.310	0.309
6	0.7	0.644	0.647	0.650	0.654	0.657	0.661	0.664	0.667	0.669	0.671	**0.672**
7	0.8	0.686	0.689	0.692	0.695	0.699	0.703	0.706	0.709	0.711	0.713	**0.714**
8	0.8	**0.943**	0.947	0.952	0.957	0.961	0.965	0.969	0.972	0.974	0.976	0.977
9	0.3	0.488	0.484	0.479	0.474	0.469	0.464	0.459	0.454	0.451	0.448	**0.446**
10	0.9	0.808	0.811	0.814	0.817	0.820	0.823	0.825	0.828	0.830	0.831	**0.832**
11	0.9	0.843	0.846	0.848	0.851	0.854	0.856	0.859	0.861	0.863	0.864	**0.865**
12	1	0.990	0.991	0.992	0.993	0.994	0.995	0.996	0.997	0.997	0.997	**0.997**
e_i^{β}		0.082	0.080	0.078	0.077	0.077	0.076	0.076	0.076	0.075	0.075	**0.075**

In bold: estimated probabilities nearest observed probabilities

2.3 A Numerical Example: Electric Current Data

Let us consider the electric current data set introduced in Sect. 1. Table 2 shows the estimated probabilities of the observations computed by means of the weighted minimum DPD estimators with different tuning parameters $\beta \in [0, 1]$, compared with the observed probabilities. Last row in Table 2 shows the estimated mean absolute error of each weighted minimum DPD estimator considered here, e_i^{β}. MLE ($\beta = 0$) seems, in general, to be one of the worst choices to predict each testing condition. In particular, we can say that weighted minimum DPD estimators with a high or moderate value of the tuning parameter β seem to have better behavior than the MLEs when higher-than-normal testing conditions are considered.

3 Robust Inference for One-Shot Device Testing Under Gamma Distribution

Gamma distribution is commonly used for fitting lifetime data in reliability and survival studies due to its flexibility. Its hazard function can be increasing, decreasing, or constant. When the hazard function of the gamma distribution is a constant, it corresponds to the exponential distribution. In addition to the exponential distribution, the gamma distribution also includes the Chi-square distribution as a special case. The gamma distribution has found a number of applications in different fields. For example, Husak et al. (2007) used it to describe monthly rainfall in Africa for the management of water and agricultural resources, as well as food reserves. Kwon and Frangopol (2010) assessed and predicted bridge fatigue reliabilities of two existing bridges, the Neville Island Bridge and the Birmingham Bridge, based on long-term monitoring data. They made use of log-normal, Weibull and gamma distributions to estimate the mean and standard deviation of the stress range. Tseng et al. (2009) proposed an optimal step-stress accelerated degradation testing plan for assessing the lifetime distribution of products with long lifetimes based on a gamma process.

The problem of one-shot device testing under the gamma distribution was studied on the basis of weighted minimum DPD estimators in Balakrishnan et al. (2019a). This section summarizes some key results presented there.

3.1 Inference Under the Gamma Distribution

Let us denote by $\boldsymbol{\theta} = (a_0, \ldots, a_J, b_0, \ldots, b_J)^T$ the model parameter vector. We shall then assume that the lifetimes of the units, under the testing condition i, follow the gamma distribution with corresponding probability density function and cumulative distribution function as

$$f(t;\boldsymbol{x}_i,\boldsymbol{\theta}) = \frac{t^{\alpha_i-1}}{\lambda_i^{\alpha_i}\Gamma(\alpha_i)}\exp\left(-\frac{t}{\lambda_i}\right),\ t>0,$$

and

$$F(t;\boldsymbol{x}_i,\boldsymbol{\theta}) = \int_0^t \frac{y^{\alpha_i-1}}{\lambda_i^{\alpha_i}\Gamma(\alpha_i)}\exp\left(-\frac{y}{\lambda_i}\right)dy,\ t>0, \tag{18}$$

where $\alpha_i > 0$ and $\lambda_i > 0$ are, respectively, the shape and scale parameters at condition i, which we assume are related to the stress factors in log-linear forms as

$$\alpha_i = \exp\left\{\sum_{j=0}^{J} a_j x_{ij}\right\} \quad \text{and} \quad \lambda_i = \exp\left\{\sum_{j=0}^{J} b_j x_{ij}\right\},$$

with $x_{i0} = 1$ for all i.

For $\beta \geq 0$, the estimating equations are given by

$$\sum_{i=1}^{I}(l_i\boldsymbol{x}_i, s_i\boldsymbol{x}_i)^T\left(K_i F(IT_i;\boldsymbol{x}_i,\boldsymbol{\theta}) - n_i\right) \times\left(F^{\beta-1}(IT_i;\boldsymbol{x}_i,\boldsymbol{\theta}) + (1-F(IT_i;\boldsymbol{x}_i,\boldsymbol{\theta}))^{\beta-1}\right) = \mathbf{0}_{2(J+1)},$$

where

$$l_i = \alpha_i\left\{-\Psi(\alpha_i)\,\pi_{i1}(\boldsymbol{\theta}) + \log\left(\frac{IT_i}{\lambda_i}\right)\pi_{i1}(\boldsymbol{\theta}) - \frac{\left(\frac{IT_i}{\lambda_i}\right)^{\alpha_i}}{\alpha_i^2\Gamma(\alpha_i)}\,{}_2F_2\left(\alpha_i,\alpha_i;1+\alpha_i,1+\alpha_i;-\frac{IT_i}{\lambda_i}\right)\right\} \tag{19}$$

and

$$s_i = -f(IT_i;\boldsymbol{x}_i,\boldsymbol{\theta})\,IT_i, \tag{20}$$

where $F(IT_i;\boldsymbol{x}_i,\boldsymbol{\theta})$ is as given in (18). Here, ${}_nF_m(a_1,\ldots,a_n;b_1,\ldots,b_m;z)$ denotes the Gaussian hypergeometric function. For more details about the Gaussian hypergeometric function, one may refer to Seaborn (1991).

Let $\boldsymbol{\theta}^0$ be the true value of the parameter $\boldsymbol{\theta}$. Then, the asymptotic distribution of the weighted minimum DPD estimator, under the gamma distribution assumption, is given by

$$\sqrt{K}\left(\widehat{\boldsymbol{\theta}}_\beta - \boldsymbol{\theta}^0\right) \xrightarrow[K\to\infty]{\mathcal{L}} \mathcal{N}\left(\mathbf{0}_{2(J+1)}, \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\boldsymbol{K}_\beta(\boldsymbol{\theta}^0)\boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\right),$$

where

$$\boldsymbol{J}_{\beta}(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \boldsymbol{\Psi}_i \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + (1 - F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}))^{\beta-1} \right), \tag{21}$$

$$\boldsymbol{K}_{\beta}(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \boldsymbol{\Psi}_i F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) \left(1 - F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta})\right) \times \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + (1 - F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}))^{\beta-1} \right)^2, \tag{22}$$

and

$$\boldsymbol{\Psi}_i = \begin{pmatrix} l_i^2 \boldsymbol{x}_i \boldsymbol{x}_i^T & l_i s_i \boldsymbol{x}_i \boldsymbol{x}_i^T \\ l_i s_i \boldsymbol{x}_i \boldsymbol{x}_i^T & s_i^2 \boldsymbol{x}_i \boldsymbol{x}_i^T \end{pmatrix},$$

with l_i and s_i as given in (19) and (20), respectively.

If we want to test whether there is a significant relationship between the jth stress factor and the device lifetime, we may use the Wald-type test given in (7), where $\boldsymbol{m}(\boldsymbol{\theta}) = (a_j, b_j)^T$,

$$\boldsymbol{M}^T(\boldsymbol{\theta}) = \begin{pmatrix} 0, \ldots, & \overset{(j+1)}{1}, \ldots, & \overset{(J+j+1)}{0}, \ldots, & \overset{(2(J+1))}{0} \\ 0, \ldots, & 0, \ldots, & 1, \ldots, & 0 \end{pmatrix},$$

and $\boldsymbol{J}_{\beta}(\boldsymbol{\theta})$ and $\boldsymbol{K}_{\beta}(\boldsymbol{\theta})$ are as in (21) and (22), respectively.

The IF with respect to all the observations is given by

$$IF(\boldsymbol{t}, \boldsymbol{U}_{\beta}, F_{\boldsymbol{\theta}^0}) = \boldsymbol{J}_{\beta}^{-1}(\boldsymbol{\theta}^0) \sum_{i=1}^{I} \frac{K_i}{K} (l_i \boldsymbol{x}_i, s_i \boldsymbol{x}_i)^T \times \left(F^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) + R^{\beta-1}(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) \right) \left(F(IT_i; \boldsymbol{x}_i, \boldsymbol{\theta}^0) - \Delta_{t_i}^{(1)} \right),$$

where $\boldsymbol{J}_{\beta}(\boldsymbol{\theta})$ is as given in (21), and l_i and s_i are as in (19) and (20), respectively.

3.2 Monte Carlo Simulation Study

In this section, we summarize the simulation results provided in Balakrishnan et al. (2019a), wherein an extensive Monte Carlo study was carried out to study the performance of the proposed estimators and Wald-type tests under the assumption of gamma lifetime distribution.

We consider the devices to have gamma lifetimes, under 4 different conditions with 2 stress factors at 2 levels, taken to be $\{(30, 40), (40, 40), (30, 50), (40, 50)\}$. The model parameters were set as $(a_0, a_1, a_2, b_0, b_1, b_2) = (6.5, -0.06, -0.06, -0.36, 0.04, -0.01)$ and the inspection times as $IT \in \{5, 10, 15\}$. In order to study the

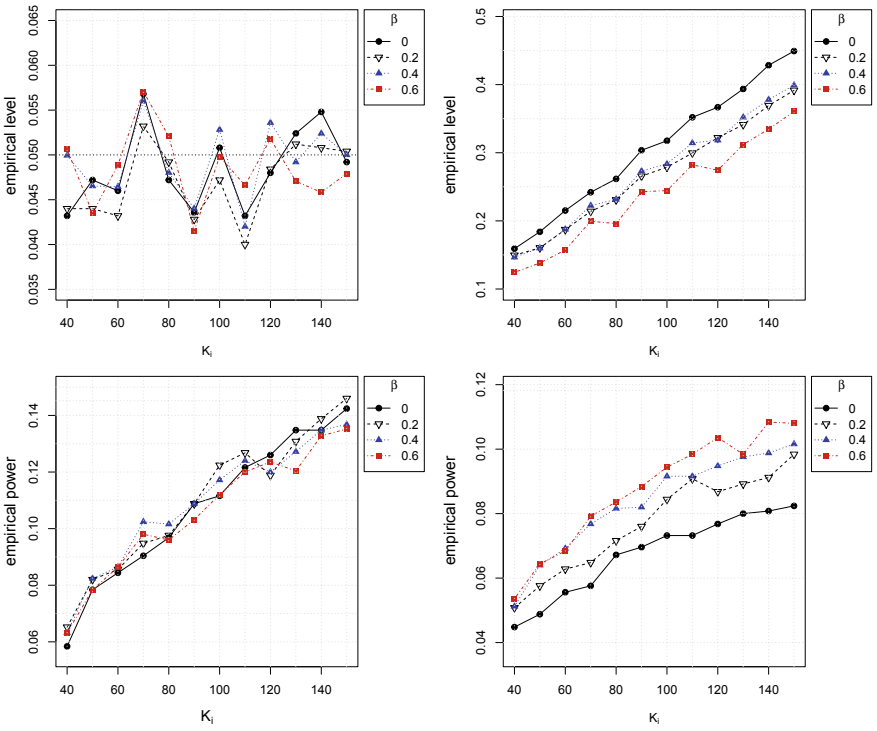

Fig. 2 Gamma distribution at multiple stress levels: Levels and powers for pure (left) and contaminated data (right)

robustness of the proposed Wald-type tests, we consider a contaminated scheme, wherein the first "cell" is generated under $\tilde{a}_1 = -0.035$.

We first study the observed level of the test under the true null hypothesis $H_0 : a_1 = -0.06$ against the alternative $H_1 : a_1 \neq -0.06$. In the top of Fig. 2, these levels are plotted for different values of the sample sizes, pure data (left) and contaminated data ($\tilde{a}_1 = -0.035$, right). Notice that in the case of pure data considered, all the observed levels are close to the nominal level of 0.05. In the case of contaminated data, the level of the classical Wald test (at $\beta = 0$) displays a lack of robustness, while the weighted minimum DPD estimator-based Wald-type tests for moderate and large positive β possess levels closer to the nominal level.

To investigate the power of these tests, we change the true data-generating parameters value to $\boldsymbol{\theta} = (6.5, -0.06, -0.035, -0.36, 0.04, -0.01)$, and $\tilde{a}_1 = -0.45$ in a contaminated scenario, nearer to the null hypothesis. The resulting empirical powers are plotted at the bottom of Fig. 2. When there are no outliers in the data, the classical Wald test (at $\beta = 0$) is quite similar, not even the most powerful one, to other tests. On the other hand, when there are outliers in the data, the Wald-type test with larger $\beta > 0$ provides significantly better power.

Robustness of the proposed weighted minimum DPD estimators is also illustrated in the detailed simulation study in Balakrishnan et al. (2019a).

3.3 A Numerical Example: Application to a Tumor Toxicological Data

Let us apply the proposed procedures to the tumor toxicological data set presented in Sect. 1. Let a_1, a_2 and a_3 denote the parameters corresponding to the covariates of strain of offspring, gender and square root of concentration of the chemical of benzidine dihydrochloride in the shape parameter of the gamma distribution, while b_1, b_2 and b_3 denote similarly for the scale parameter, respectively. The mean time to occurrence of tumors for each group, for different values of $\beta \in \{0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1\}$, are computed and presented in Table 3, where strain $= 0$ for F1 strain of offspring and gender $= 0$ for females.

There is a significant difference between genders, with males having a higher expected lifetime. Also, tumors are induced by an increase in the dosage of benzidine dihydrochloride. Empirical mean absolute error (MAB) and RMSE, measured by comparing predicted probabilities to the observed ones, are also computed. In both cases, MLE is seen to present the maximum error.

Table 3 Gamma distribution at multiple stress levels: weighted minimum DPD estimators of the mean time to the occurrence of tumors (in months), $\widehat{E}[T]$

Strain	Gender	Conc	$\widehat{E}[T]$					
			$\beta = 0$	$\beta = 0.2$	$\beta = 0.4$	$\beta = 0.6$	$\beta = 0.8$	$\beta = 1$
0	0	60	17.461	17.316	17.395	17.433	17.449	17.455
0	1	60	30.103	30.188	30.598	30.712	30.713	30.694
1	0	60	18.438	18.039	18.031	18.029	18.036	18.044
1	1	60	31.787	31.447	31.719	31.762	31.747	31.728
0	0	120	14.676	14.565	14.577	14.594	14.605	14.610
0	1	120	25.301	25.392	25.643	25.710	25.707	25.691
1	0	120	15.496	15.173	15.111	15.092	15.096	15.103
1	1	120	26.715	26.451	26.582	26.588	26.572	26.557
0	0	200	12.348	12.265	12.231	12.231	12.238	12.243
0	1	200	21.288	21.381	21.514	21.547	21.541	21.529
1	0	200	13.039	12.776	12.678	12.649	12.650	12.656
1	1	200	22.478	22.273	22.302	22.283	22.266	22.254
0	0	400	8.991	8.942	8.858	8.840	8.843	8.848
0	1	400	15.500	15.589	15.583	15.574	15.566	15.558
1	0	400	9.493	9.315	9.183	9.142	9.141	9.146
1	1	400	16.366	16.240	16.153	16.106	16.090	16.082

4 Robust Inference for One-Shot Device Testing Under Weibull Distribution

In practice, the Weibull distribution is widely used as a lifetime model in engineering and physical sciences. In fact, the Weibull model is also used extensively in biomedical studies as a proportional hazards model for evaluating the effects of covariates on lifetimes, meaning that the hazard rates of any two products stay in the constant ratio over time; see Meeter and Meeker (1994); Meeker et al. (1998), and the references therein. However, in some situations, the assumption of the constant shape parameter may not be valid; see, for example, Kodell and Nelson (1980), Nogueira et al. (2009) and Vázquez et al. (2010). In such situations, Balakrishnan and Ling (2013) suggested using a log-link of the stress levels to model the unequal shape parameters. Based on this idea, Balakrishnan et al. (2020b) developed robust inference for one-shot device testing under the Weibull distribution with scale and shape parameters varying over stress. In this section, we summarize some of the key results presented in this paper.

4.1 Inference Under the Weibull Distribution

Let us denote by $\boldsymbol{\theta} = (a_0, \ldots, a_J, b_0, \ldots, b_J)^T$ the model parameter vector. We shall then assume that the lifetimes of the units, under the testing condition i, follow Weibull distribution with corresponding probability density function and cumulative distribution function as

$$f_T(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{\eta_i t^{\eta_i - 1}}{\alpha_i^{\eta_i}} e^{-\left(\frac{t}{\alpha_i}\right)^{\eta_i}}, \; t > 0,$$

and

$$F_T(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - e^{-\left(\frac{t}{\alpha_i}\right)^{\eta_i}}, \; t > 0,$$

where $\alpha_i > 0$ and $\eta_i > 0$ are, respectively, the scale and shape parameters at condition i, which we assume are related to the stress factors in log-linear forms as

$$\alpha_i = \exp\left\{\sum_{j=0}^{J} a_j x_{ij}\right\} \quad \text{and} \quad \eta_i = \exp\left\{\sum_{j=0}^{J} b_j x_{ij}\right\},$$

with $x_{i0} = 1$ for all i. Let us denote by $R_T(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - F(t; \boldsymbol{x}_i, \boldsymbol{\theta})$ the reliability function, the probability that the unit lasts lifetime t. The hazard function, given by the ratio of the density function and the reliability function, is

$$h_T(t; \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{\eta_i t^{\eta_i - 1}}{\alpha_i^{\eta_i}},\ t > 0.$$

When $\eta_i = 1$, the hazard rate is constant and the Weibull distribution in this case is simply exponential distribution. When $\eta_i > 1$, the unit suffers an increasing rate of failure as it ages, while the opposite is the case when $\eta_i < 1$. This last case is less common in practice, unless we only consider the early part of lifetimes of devices.

Notice that, as suggested in the literature (see, for example, Meeter and Meeker 1994 and Ng et al. 2002), it is often more convenient to work with the extreme value distribution for the log-lifetimes, as it belongs to the location–scale family rather than the Weibull distribution belonging to the scale–shape family. For this reason, we will also consider here the extreme value distribution with the corresponding probability density, distribution and reliability functions as

$$f_W(\omega; \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{1}{\sigma_i} e^{\frac{\omega-\mu_i}{\sigma_i}} e^{-e^{\frac{\omega-\mu_i}{\sigma_i}}} = \frac{1}{\sigma_i} \xi_i e^{-\xi_i},\ -\infty < \omega < \infty, \tag{23}$$

$$F_W(\omega; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - e^{-e^{\frac{\omega-\mu_i}{\sigma_i}}} = 1 - e^{-\xi_i},\ -\infty < \omega < \infty, \tag{24}$$

$$R_W(\omega; \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - F_W(\omega; \boldsymbol{x}_i, \boldsymbol{\theta}) = e^{-e^{\frac{\omega-\mu_i}{\sigma_i}}} = e^{-\xi_i},\ -\infty < \omega < \infty, \tag{25}$$

where $\omega = \log(t)$, $\xi_i = e^{\frac{\omega-\mu_i}{\sigma_i}}$, the location parameter $\mu_i = log(\alpha_i) = \sum_{j=0}^{J} a_j x_{ij}$ and the scale parameter $\sigma_i = \eta_i^{-1} = \exp\{-\sum_{j=0}^{J} b_j x_{ij}\}$.

Following this notation, for $\beta \geq 0$, the estimating equations are given by

$$\sum_{i=1}^{I} (l_i \boldsymbol{x}_i, s_i \boldsymbol{x}_i)^T \left(K_i F_W\left(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}\right) - n_i\right) \times \left(F_W^{\beta-1}\left(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}\right) + R_W^{\beta-1}\left(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}\right)\right) = \mathbf{0}_{2(J+1)},$$

where $F_W(lIT_i; S_i, \boldsymbol{\theta})$, $F_W(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$ and $R_W(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta})$ are as given in (23), (24) and (25), respectively, and

$$l_i = -\{\xi_i e^{-\xi_i}\}/\sigma_i, \quad s_i = \xi_i e^{-\xi_i} log(\xi_i), \quad i = 1, \ldots, I.$$

Let $\boldsymbol{\theta}^0$ be the true value of the parameter. The asymptotic distribution of the weighted minimum DPD estimator, $\widehat{\boldsymbol{\theta}}_\beta$, is given by

$$\sqrt{K}(\widehat{\boldsymbol{\theta}}_\beta - \boldsymbol{\theta}^0) \xrightarrow[K\to\infty]{\mathcal{L}} \mathcal{N}\left(\mathbf{0}_{2(J+1)}, \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0) \boldsymbol{K}_\beta(\boldsymbol{\theta}^0) \boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\right),$$

where $\boldsymbol{J}_\beta(\boldsymbol{\theta})$ and $\boldsymbol{K}_\beta(\boldsymbol{\theta})$ are given by

$$\boldsymbol{J}_\beta(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \boldsymbol{\Psi}_i \left(F_W^{\beta-1}(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R_W^{\beta-1}(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) \right), \tag{26}$$

$$\boldsymbol{K}_\beta(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \boldsymbol{\Psi}_i F_W(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) R_W(lIT_i; S_I, \boldsymbol{\theta}) \times \left(F_W^{\beta-1}(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) + R_W^{\beta-1}(lIT_i; \boldsymbol{x}_i, \boldsymbol{\theta}) \right)^2, \tag{27}$$

with

$$\boldsymbol{\Psi}_i = \begin{pmatrix} l_i^2 \boldsymbol{x}_i \boldsymbol{x}_i^T & l_i s_i \boldsymbol{x}_i \boldsymbol{x}_i^T \\ l_i s_i \boldsymbol{x}_i \boldsymbol{x}_i^T & s_i^2 \boldsymbol{x}_i \boldsymbol{x}_i^T \end{pmatrix}.$$

For testing $\boldsymbol{m}(\boldsymbol{\theta}) = \boldsymbol{0}_r$, with $\boldsymbol{m} : \mathbb{R}^{2(J+1)} \longrightarrow \mathbb{R}^r$, $r \leq 2(J+1)$, we consider Wald-type tests defined in (7). The $2(J+1) \times r$ matrix $\boldsymbol{M}$ appearing in (7) is given by

$$\boldsymbol{M}(\boldsymbol{\theta}) = \frac{\partial \boldsymbol{m}^T(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}},$$

and $\boldsymbol{J}_\beta(\boldsymbol{\theta})$ and $\boldsymbol{K}_\beta(\boldsymbol{\theta})$ are as given in (26) and (27), respectively.

4.2 Monte Carlo Simulation Study

An extensive simulation study was carried out in Balakrishnan et al. (2020b) to illustrate the robustness of the weighted minimum DPD estimators and the Wald-type tests under the assumption of the Weibull distribution for lifetimes. In this section, we summarize the main results presented there.

Let us consider unbalanced data, which does not have an equal sample size for all the groups. This data consists of a total of $K = 300$ observations, and is as presented in Table 4. The lifetimes of devices are simulated from the Weibull distribution with $\boldsymbol{\theta}^T = (5.3, -0.025, -0.6, 0.03)$ (moderate reliability). To examine the robustness in this ALT plan, we increase each one of the parameters of the outlying first cell, denoted by $\tilde{a}_0$, $\tilde{a}_1$, $\tilde{b}_0$ and $\tilde{b}_1$.

We compute empirical Wald-type test levels for the testing problem

$$H_0 : a_1 = -0.05 \quad \text{vs.} \quad H_1 : a_1 \neq -0.05.$$

Results, presented in Fig. 3, illustrate again the lack of robustness of MLE in the presence of medium and strong outliers.

Table 4 Weibull distribution at multiple stress levels: ALT plan, unbalanced data

i	x_i	IT_i	K_i
1	30	8	60
2	40	8	40
3	50	8	20
4	30	16	60
5	40	16	20
6	50	16	20
7	30	24	40
8	40	24	20
9	50	24	20

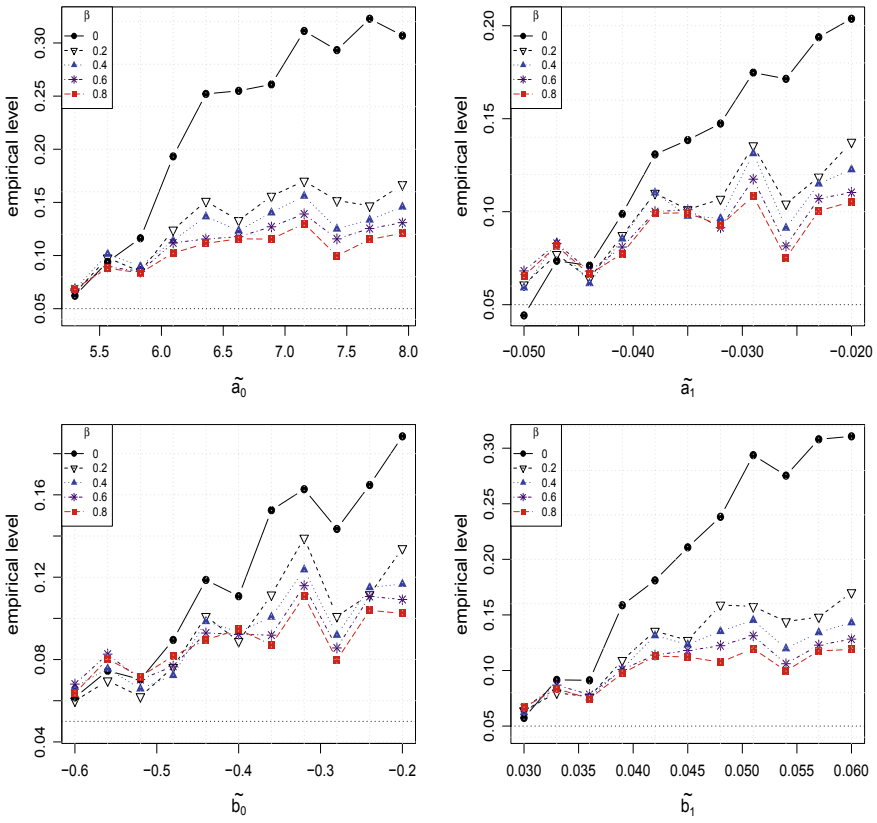

Fig. 3 Weibull distribution at multiple stress levels: empirical levels for unbalanced data

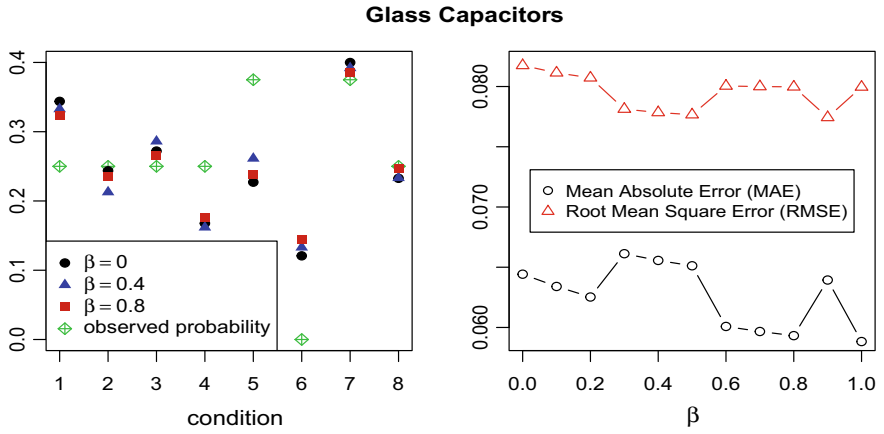

Fig. 4 Glass Capacitors example. Left: estimated versus observed probabilities. Right: RMSEs and MAEs of the estimated probabilities

4.3 A Numerical Example: Glass Capacitors

Let us consider the glass capacitors data set presented in Sect. 1. We adapt these data to the one-shot device model taking the inspection times to be $IT = \{258, 315, 455, 1065\}$, respectively. Logically, higher inspection times are needed when applying less extreme voltages. These data and their relation with the Weibull distribution have been widely studied in the literature; see, for example, Meeker et al. (1998) and Rigdon et al. (2012). As suggested in these papers, we have used the predictors as $\log(V)$ and $1/T_K$, where T_K is the temperature in degrees Kelvin.

Weighted minimum DPD estimators are computed for different values of the tuning parameter, β, and predicted probabilities are compared to the observed ones (Fig. 4). The MAEs and RMSEs are presented in this figure as well. It is easily seen that the MLE seems to be either the worst, or one of the worst estimators in this case.

5 Robust Inference for One-Shot Device Testing Under Proportional Hazards Model

Under the classical parametric setup, product lifetimes are assumed to be fully described by a probability distribution involving some model parameters. This has been done with some common lifetime distributions such as exponential (Balakrishnan and Ling 2012b), gamma or Weibull (Balakrishnan and Ling 2013), as described in the preceding sections. However, because data from one-shot devices do not contain actual lifetimes, parametric inferential methods can be very sensitive to violations of the model assumption. Ling et al. (2015) proposed a semi-

parametric model, in which, under the proportional hazards assumption, the hazard rate is allowed to change in a non-parametric way. The simulation study carried out in Ling et al. (2015) shows that their proposed method works very well. However, this method suffers again from lack of robustness, as it is based on the (non-robust) MLEs of model parameters.

The problem of developing weighted minimum DPD estimators for one-shot device testing under the proportional hazards model was dealt with in Balakrishnan et al. (2020c). In this section, we summarize some key results presented there.

5.1 Model Description

Consider S constant-stress accelerated life-tests and I inspection times. For the ith life-test, K_s devices are placed under stress-level combinations with J stress factors, $\boldsymbol{x}_s = (x_{s1}, \ldots, x_{sJ})$, of which K_{is} are tested at the ith inspection time IT_i, where $K_s = \sum_{i=1}^{I} K_{is}$ and $0 < IT_1 < \cdots < IT_I$. Then, the number of devices that have failed by time IT_i at stress $\boldsymbol{x}_s$ are recorded as n_{is}. One-shot device testing data obtained from such a life-test can then be represented as $(n_{is}, K_{is}, \boldsymbol{x}_s, IT_i)$, for $i = 1, 2, \ldots, I$ and $s = 1, 2, \ldots, S$.

Instead of assuming that the true lifetimes of devices follow a specific parametric distribution such as exponential, gamma and Weibull, we assume here that the cumulative hazard function of the lifetimes of devices is of the proportional form

$$H(t, \boldsymbol{x}; \boldsymbol{\eta}, \boldsymbol{\alpha}) = H_0(t; \boldsymbol{\eta})\lambda(\boldsymbol{x}; \boldsymbol{\alpha}), \tag{28}$$

where $H_0(t; \boldsymbol{\eta})$ is the baseline cumulative hazard function with $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_I)$, and $\boldsymbol{\alpha} = (\alpha_1 \ldots, \alpha_J)$ is a vector of coefficients for stress factors. The model in (28) is thus composed of two independent components, with one measuring the changes in the baseline ($H_0(t; \boldsymbol{\eta})$) and the other influencing the stress factors ($\lambda(\boldsymbol{x}; \boldsymbol{\alpha})$).

The corresponding reliability function is given by

$$R(t, \boldsymbol{x}; \boldsymbol{\eta}, \boldsymbol{\alpha}) = \exp\left(-H(t, \boldsymbol{x}; \boldsymbol{\eta}, \boldsymbol{\alpha})\right) = R_0(t; \boldsymbol{\eta})^{\lambda(\boldsymbol{x}; \boldsymbol{\alpha})},$$

where $R_0(t; \boldsymbol{\eta}) = \exp(-H_0(t; \boldsymbol{\eta}))$ is the baseline reliability function, with $0 < R_0(IT_I; \boldsymbol{\eta}) < R_0(IT_{I-1}; \boldsymbol{\eta}) < \cdots < R_0(IT_1; \boldsymbol{\eta}) < 1$. Therefore, we let

$$\gamma(\eta_i) = \begin{cases} 1 - R_0(IT_I; \boldsymbol{\eta}) = 1 - \exp(-\exp(\eta_I)), & i = I, \\ \dfrac{1 - R_0(IT_i; \boldsymbol{\eta})}{1 - R_0(IT_{i+1}; \boldsymbol{\eta})} = 1 - \exp(-\exp(\eta_i)), & i = 1, \ldots, I-1. \end{cases}$$

We then have

$$R_0(IT_i;\boldsymbol{\eta}) = 1 - \prod_{m=i}^{I}\{1-\exp(-\exp(\eta_m))\} = 1 - G_i,$$

where $G_i = \prod_{m=i}^{I}\{1-\exp(-\exp(\eta_m))\}$.

We now assume a log-linear link function for relating the stress levels to the failure times of the units in the cumulative hazard function in (28) as

$$\lambda(\boldsymbol{x}_s;\boldsymbol{\alpha}) = \exp(\boldsymbol{\alpha}^T\boldsymbol{x}_s) = \exp\left(\sum_{j=1}^{J}\alpha_j x_{sj}\right).$$

5.1.1 Maximum Likelihood Estimator and Weighted Minimum DPD Estimators

Consider the proportional hazards model for one-shot devices in (28). The log-likelihood function based on these data is then given by

$$\begin{aligned}\ell(n_{11},\ldots,n_{IS};\boldsymbol{\eta},\boldsymbol{\alpha}) &= \sum_{i=1}^{I}\sum_{s=1}^{S} n_{is}\log\left[1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right] \\ &\quad + (K_{is}-n_{is})\log\left[R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right] + C \\ &= \sum_{i=1}^{I}\sum_{s=1}^{S} n_{is}\log\left[1-(1-G_i)^{\exp\left(\sum_{j=1}^{J}\alpha_j x_{sj}\right)}\right] \\ &\quad + (K_{is}-n_{is})\log(1-G_i)\exp\left(\sum_{j=1}^{J}\alpha_j x_{sj}\right) + C, \quad (29)\end{aligned}$$

where C is a constant not depending on $\boldsymbol{\eta}$ and $\boldsymbol{\alpha}$.

Let $\boldsymbol{\theta} = (\boldsymbol{\eta},\boldsymbol{\alpha})$. The MLE, $\widehat{\boldsymbol{\theta}}$, of $\boldsymbol{\theta}$, is obtained by the maximization of (29), i.e.,

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \ell(n_{11},\ldots,n_{IS};\boldsymbol{\eta},\boldsymbol{\alpha}).$$

In order to study the relation between the MLE, $\widehat{\boldsymbol{\theta}}$, with the Kullback–Leibler divergence measure, we introduce the empirical and theoretical probability vectors, as follows:

$$\widehat{\boldsymbol{p}}_{is} = (\widehat{p}_{is1},\widehat{p}_{is2})^T = \left(\frac{n_{is}}{K_{is}}, \frac{K_{is}-n_{is}}{K_{is}}\right)^T, \quad i=1,\ldots,I,\ s=1,\ldots,S,$$

$$\boldsymbol{\pi}_{is}(\boldsymbol{\eta},\boldsymbol{\alpha}) = (\pi_{is1}(\boldsymbol{\eta},\boldsymbol{\alpha}),\pi_{is2}(\boldsymbol{\eta},\boldsymbol{\alpha}))^T, \quad i=1,\ldots,I,\ s=1,\ldots,S,$$

where $\pi_{is1}(\boldsymbol{\eta}, \boldsymbol{\alpha}) = 1 - R(IT_i, \boldsymbol{x}_s; \boldsymbol{\eta}, \boldsymbol{\alpha})$ and $\pi_{is2}(\boldsymbol{\eta}, \boldsymbol{\alpha}) = R(IT_i, \boldsymbol{x}_s; \boldsymbol{\eta}, \boldsymbol{\alpha})$.

It can be shown that the log-likelihood function $\ell(n_{11}, \ldots, n_{IS}; \boldsymbol{\eta}, \boldsymbol{\alpha})$, given in (29), is related to the weighted Kullback–Leibler divergence measure through

$$\sum_{i=1}^{I}\sum_{s=1}^{S} \frac{K_{is}}{K} d_{KL}(\widehat{\boldsymbol{p}}_{is}, \boldsymbol{\pi}_{is}(\boldsymbol{\eta}, \boldsymbol{\alpha})) = c - \frac{1}{K}\ell(n_{11}, \ldots, n_{IS}; \boldsymbol{\eta}, \boldsymbol{\alpha}),$$

with c being a constant not dependent on $\boldsymbol{\eta}$ and $\boldsymbol{\alpha}$. Therefore, the MLE, $\widehat{\boldsymbol{\theta}}$, of $\boldsymbol{\theta}$, can then be defined as

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{I}\sum_{s=1}^{S} \frac{K_{is}}{K} d_{KL}(\widehat{\boldsymbol{p}}_{is}, \boldsymbol{\pi}_{is}(\boldsymbol{\eta}, \boldsymbol{\alpha})). \tag{30}$$

As an extension of this, the weighted minimum DPD estimator for $\boldsymbol{\theta}$ is given by

$$\widehat{\boldsymbol{\theta}}_{\beta} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{I}\sum_{s=1}^{S} \frac{K_{is}}{K} d^{*}_{\beta}(\widehat{\boldsymbol{p}}_{is}, \boldsymbol{\pi}_{is}(\boldsymbol{\eta}, \boldsymbol{\alpha})), \quad \text{for } \beta > 0,$$

and for $\beta = 0$, we have the MLE, $\widehat{\boldsymbol{\theta}}$, as given in (30).

Remark 1 Suppose the lifetimes of one-shot devices under test follow the Weibull distribution with the same shape parameter $\tau = exp(b)$ and scale parameters related to the stress levels, $a_s = exp(\sum_{j=1}^{J} c_j x_{sj}), s = 1, \ldots, S$. The cumulative distribution function of the Weibull distribution is then given by

$$F_T(t; a_s, \tau) = 1 - exp\left(-\left(\frac{t}{a_s}\right)^{\tau}\right), \quad t > 0.$$

If the proportional hazards assumption holds, then the baseline reliability and the coefficients of stress factors are given by

$$R_0(t; \beta) = exp(-t^{\tau} exp(-\tau c_0))$$

and $\alpha_s = -\tau c_s, \quad s = 1, \ldots, S$. Furthermore, we have

$$\eta_i = log\left(-log\left(1 - \frac{1 - R_0(IT_i)}{1 - R_0(IT_{i+1})}\right)\right),$$
$$\eta_I = \tau(log(IT_I) - c_0).$$

5.2 Inference Under Proportional Hazards Model

In the same way, as done in previous models, the estimating equations for the weighted minimum DPD estimator in the proportional hazards model and its asymptotic distribution can be derived and are presented in the following theorems.

Theorem 8 *For $\beta \geq 0$, the estimating equations are given by*

$$\sum_{i=1}^{I}\sum_{s=1}^{S}\delta_{is}(\boldsymbol{\eta})\left(K_{is}(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))-n_{is}\right) \times\left[(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))^{\beta-1}+R^{\beta-1}(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right]=\mathbf{0}_I,$$

$$\sum_{i=1}^{I}\sum_{s=1}^{S}\delta_{is}(\boldsymbol{\alpha})\left(K_{is}(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))-n_{is}\right) \times\left[(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))^{\beta-1}+R^{\beta-1}(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right]=\mathbf{0}_J,$$

where

$$\delta_{is}(\boldsymbol{\eta})=\frac{\partial R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})}{\partial\boldsymbol{\eta}}=-(1-G_i)^{\lambda(\boldsymbol{x}_s;\boldsymbol{\alpha})-1}\lambda(\boldsymbol{x}_s;\boldsymbol{\alpha})\frac{\partial G_i}{\partial\boldsymbol{\eta}}, \tag{31}$$

$$\delta_{is}(\boldsymbol{\alpha})=\frac{\partial R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})}{\partial\boldsymbol{\alpha}}=(1-G_i)^{\lambda(\boldsymbol{x}_s;\boldsymbol{\alpha})}log(1-G_i)\lambda(\boldsymbol{x}_s;\boldsymbol{\alpha})\boldsymbol{x}_s, \tag{32}$$

with

$$\frac{\partial G_i}{\partial\eta_u}=\begin{cases}\exp(\eta_u)\exp(-\exp(\eta_u))G_i/\gamma(\eta_u) & ,i\leq u,\\ 0 & ,i>u.\end{cases}$$

Theorem 9 *Let $\boldsymbol{\theta}^0$ be the true value of the parameter $\boldsymbol{\theta}$. Then, the asymptotic distribution of the weighted minimum DPD estimator, $\widehat{\boldsymbol{\theta}}_\beta$, is given by*

$$\sqrt{K}(\widehat{\boldsymbol{\theta}}_\beta-\boldsymbol{\theta}^0)\xrightarrow[K\to\infty]{\mathcal{L}}\mathcal{N}\left(\mathbf{0}_{I+J},\boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\boldsymbol{K}_\beta(\boldsymbol{\theta}^0)\boldsymbol{J}_\beta^{-1}(\boldsymbol{\theta}^0)\right),$$

where $\boldsymbol{J}_\beta(\boldsymbol{\theta})$ and $\boldsymbol{K}_\beta(\boldsymbol{\theta})$ are given by

$$\boldsymbol{J}_\beta(\boldsymbol{\theta})=\sum_{i=1}^{I}\sum_{s=1}^{S}\frac{K_{is}}{K}\Delta_{is}(\boldsymbol{\eta},\boldsymbol{\alpha})\left[(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))^{\beta-1}+R^{\beta-1}(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right]$$

$$\boldsymbol{K}_\beta(\boldsymbol{\theta})=\sum_{i=1}^{I}\sum_{s=1}^{S}\frac{K_{is}}{K}\Delta_{is}(\boldsymbol{\eta},\boldsymbol{\alpha})(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}), \times\left[(1-R(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha}))^{\beta-1}+R^{\beta-1}(IT_i,\boldsymbol{x}_s;\boldsymbol{\eta},\boldsymbol{\alpha})\right]^2,$$

with

$$\Delta_{is}(\boldsymbol{\eta}, \boldsymbol{\alpha}) = \begin{pmatrix} \delta_{is}(\boldsymbol{\eta})\delta_{is}^{T}(\boldsymbol{\eta}) & \delta_{is}(\boldsymbol{\eta})\delta_{is}^{T}(\boldsymbol{\alpha}) \\ \delta_{is}(\boldsymbol{\alpha})\delta_{is}^{T}(\boldsymbol{\eta}) & \delta_{is}(\boldsymbol{\alpha})\delta_{is}^{T}(\boldsymbol{\alpha}) \end{pmatrix},$$

and $\delta_{is}(\boldsymbol{\eta})$ *and* $\delta_{is}(\boldsymbol{\alpha})$ *being as given in (31) and (32), respectively.*

Following similar steps as in the previous sections, Wald-type tests can be developed for testing composite null hypotheses here in this situation as well.

5.3 Monte Carlo Simulation Study

In Balakrishnan et al. (2020c), an extensive simulation study has been carried out to illustrate the robustness of the proposed estimators and tests in the proportional hazards model. Here, we present some illustrative results in relation to weighted minimum DPD estimators.

Suppose the lifetimes of test units follow a Weibull distribution (see Remark 1). All the test units were divided into $S = 4$ groups, subject to different acceleration conditions with $J = 2$ stress factors at two elevated stress levels each, that is, $(x_1, x_2) = \{(55, 70), (55, 100), (85, 70), (85, 100)\}$, and were inspected at $I = 3$ different times, $(IT_1, IT_2, IT_3) = (2, 5, 8)$.

We assume $(c_0, c_1, c_2) = (6.5, -0.03, -0.03)$, for $b = 0.5$. The outlying cell (taken to be $i = 3$, $s = 4$) is generated under the parameters $(\tilde{c}_1, \tilde{c}_2) = (-0.027, -0.027)$ and $\tilde{b} = 0.45$.

Bias of the estimates are then computed for different (equal) sample sizes $K_{is} \in \{50, 70, 100\}$ and tuning parameters $\beta \in \{0, 0.2, 0.4, 0.6\}$ for pure as well as contaminated data. The obtained results are presented in Table 5. As expected, when the sample size increases, errors tend to decrease, while in the contaminated data set, these errors are generally greater than in the case of uncontaminated data. Weighted minimum DPD estimators with $\beta > 0$ present a better behavior than the MLEs in terms of robustness. Note that reliabilities are underestimated and that the estimates are quite precise in all the cases.

In Balakrishnan et al. (2020c), a numerical example was presented to illustrate the proposed methods. In this example, it has been shown that the proportional hazards assumption fits the data at least as well as the Weibull model (Sect. 4). The problem of choosing the optimal tuning parameter is also considered in Balakrishnan et al. (2020c). Both a discrepancy measure and the method of Warwick and Jones (2005) are discussed and applied to the example, concluding that the optimal tuning parameter is $\beta \approx 0.5$.

Table 5 Bias for the semi-parametric model with $b = 0.5$ and $c_0 = 6.5$

$K_{is} = 50$	True value	Pure data				Contaminated data			
		0	0.2	0.4	0.6	0	0.2	0.4	0.6
η_1	−1.3884	−0.0029	−0.0263	−0.0696	−0.1044	0.2856	0.1916	0.1329	0.0742
η_2	−0.4817	−0.0001	−0.0145	−0.0391	−0.0882	0.1818	0.12322	0.1240	0.1247
η_3	−7.2883	−0.0846	−0.1506	−0.3402	−0.9790	1.2143	0.814	0.1485	0.3355
α_1	0.0495	0.0006	0.0010	0.0024	−0.0821	−0.0089	−0.0059	−0.0012	−0.3268
α_2	0.0495	0.0006	0.0011	0.0025	−0.1015	−0.0089	−0.0059	−0.0011	−0.3991
$R(15, \boldsymbol{x}_0)$	0.9632	−0.0016	−0.0018	−0.0014	0.0016	−0.0278	−0.0198	−0.0106	−0.0015
$K_{is} = 70$	True value	Pure data				Contaminated data			
		0	0.2	0.4	0.6	0	0.2	0.4	0.6
η_1	−1.3884	−0.0151	−0.0356	−0.0563	−0.0844	0.2868	0.1890	0.0329	0.0220
η_2	−0.4817	−0.0088	−0.0207	−0.0325	−0.1191	0.1830	0.1204	0.0256	0.0454
η_3	−7.2883	−0.0612	−0.1564	−0.2244	−0.9998	1.2465	0.8760	0.1449	−0.0141
α_1	0.0495	0.0004	0.0011	0.0015	−0.0160	−0.0092	−0.0064	−0.0010	−0.1577
α_2	0.0495	0.0005	0.0011	0.0017	−0.0207	−0.0091	−0.0063	−0.0011	−0.1933
$R(15, \boldsymbol{x}_0)$	0.9632	−0.0012	−0.0010	−0.0008	0.0015	−0.0280	−0.0198	−0.0098	−0.0012
$K_{is} = 100$	True value	Pure data				Contaminated data			
		0	0.2	0.4	0.6	0	0.2	0.4	0.6
η_1	−1.3884	−0.0090	−0.0110	−0.0592	−0.2306	0.2862	0.1993	0.0564	0.0376
η_2	−0.4817	−0.0053	−0.0063	−0.0337	−0.1231	0.1817	0.12619	0.03911	−0.01015
η_3	−7.2883	−0.0689	−0.0758	−0.2944	−0.9665	1.2240	0.8742	0.2192	−0.3851
α_1	0.0495	0.0005	0.0005	0.0020	−0.0088	−0.0090	−0.00635	−0.0017	−0.0940
α_2	0.0495	0.0004	0.0005	0.0021	−0.0120	−0.0090	−0.00642	−0.00164	−0.11596
$R(15, \boldsymbol{x}_0)$	0.9632	−0.0001	−0.0002	0.0002	0.0024	−0.0260	−0.0181	−0.0088	−0.0005

6 Robust Inference for One-Shot Device Testing Under Exponential Distribution and Competing Risks

In lifetime data analysis, it is often the case that the products under study can experience one of the different types of failure. For example, in the context of survival analysis, we can have several different types of failure (death, relapse, opportunistic infection, etc.) that are of interest to us, leading to the so-called "competing risks" scenario. A competing risk is an event whose occurrence precludes the occurrence of the primary event of interest. In a study examining time to death attributable, for instance, to cardiovascular causes, death attributable to non-cardiovascular causes would be a competing risk. Crowder (2006) has presented a review of this competing risks problem for which one needs to estimate the failure rates for each cause. Balakrishnan et al. (2015a, b) and So (2016) have discussed the problem of one-shot devices under competing risks for the first time. A robust extension, based on weighted minimum DPD estimators, and assuming exponential lifetimes, has been done in Balakrishnan et al. (2020d). Some of the key results developed in Balakrishnan et al. (2020d) are presented in this section.

6.1 Model Description

The setting for an accelerated life-test for one-shot devices under competing risks scenario considered here is stratified in I testing conditions as follows:

1. The tests are checked at inspection times IT_i, for $i = 1, \ldots, I$.
2. The devices are tested under J different stress levels, $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{iJ})^T$, for $i = 1, \ldots, I$.
3. K_i devices are tested in the ith test condition, for $i = 1, \ldots, I$.
4. The number of devices failed due to the rth cause under the ith test condition is denoted by n_{ir}, for $i = 1, \ldots I,\ r = 1, \ldots, R$.
5. The number of devices that survive under the ith test condition is denoted by $n_{i0} = K_i - \sum_{r=1}^{R} n_{ir}$.

This setting is summarized in Table 6. For simplicity, and as considered in Balakrishnan et al. (2015a), we will limit the number of stress levels to $J = 1$ and the number of competing causes to $R = 2$, even though inference for the general case when $J > 1$ and $R > 2$ can be presented in an analogous manner.

Let us denote the random variable for the failure time due to causes 1 and 2 as T_{irk}, for $r = 1, 2$, $i = 1, \ldots, I$, and $k = 1, \ldots, K_i$, respectively. We now assume that T_{irk} follows an exponential distribution with failure rate parameter $\lambda_{ir}(\boldsymbol{\theta})$ and its probability density function

Table 6 One-shot device testing under competing risks

Condition	Times	Devices	Survivals	Failures			Stress levels		
				Cause 1	⋯	Cause R	Stress 1	⋯	Stress J
1	IT_1	K_1	n_{10}	n_{11}	⋯	n_{1R}	x_{11}	⋯	x_{1J}
2	IT_2	K_2	n_{20}	n_{21}	⋯	n_{2R}	x_{21}	⋯	x_{2J}
⋮	⋮	⋮		⋮		⋮		⋮	⋮
I	IT_I	K_I	n_{I0}	n_{I1}	⋯	n_{IR}	x_{I1}	⋯	x_{IJ}

$$
\begin{aligned}
f_r(t; x_i, \boldsymbol{\theta}) &= \lambda_{ir}(\boldsymbol{\theta}) e^{-\lambda_{ir}(\boldsymbol{\theta})t}, \quad t > 0, \\
\lambda_{ir}(\boldsymbol{\theta}) &= \theta_{r0} \exp(\theta_{r1} x_i), \\
\boldsymbol{\theta} &= (\theta_{10}, \theta_{11}, \theta_{20}, \theta_{21})^T, \quad \theta_{r0}, \theta_{r1} > 0, \quad r = 1, 2,
\end{aligned}
$$

where x_i is the stress factor of the condition i and $\boldsymbol{\theta}$ is the model parameter vector, with $\boldsymbol{\theta} \in \mathbb{R}^4$.

We shall use $\pi_{i0}(\boldsymbol{\theta})$, $\pi_{i1}(\boldsymbol{\theta})$ and $\pi_{i2}(\boldsymbol{\theta})$ for the survival probability, failure probability due to cause 1 and failure probability due to cause 2, respectively. Their expressions are

$$
\begin{aligned}
\pi_{i0}(\boldsymbol{\theta}) &= (1 - F_1(IT_i; x_i, \boldsymbol{\theta}))(1 - F_2(IT_i; x_i, \boldsymbol{\theta})) = \exp(-(\lambda_{i1} + \lambda_{i2}) IT_i), \\
\pi_{i1}(\boldsymbol{\theta}) &= \frac{\lambda_{i1}}{\lambda_{i1} + \lambda_{i2}} (1 - \exp(-(\lambda_{i1} + \lambda_{i2}) IT_i)), \\
\pi_{i2}(\boldsymbol{\theta}) &= \frac{\lambda_{i2}}{\lambda_{i1} + \lambda_{i2}} (1 - \exp(-(\lambda_{i1} + \lambda_{i2}) IT_i)),
\end{aligned}
$$

where $\lambda_{ir} = \lambda_{ir}(\boldsymbol{\theta})$, $r = 1, 2$. Derivations of these expressions can be found in So (2016) (p. 151).

6.1.1 Maximum Likelihood Estimator and Weighted Minimum DPD Estimator

The likelihood function is given by

$$
\mathcal{L}(n_{01}, \ldots, n_{I2}; \boldsymbol{\theta}) \propto \prod_{i=1}^{I} \pi_{i0}(\boldsymbol{\theta})^{n_{i0}} \pi_{i1}(\boldsymbol{\theta})^{n_{i1}} \pi_{i2}(\boldsymbol{\theta})^{n_{i2}}, \tag{33}
$$

where $n_{0i} + n_{1i} + n_{2i} = K_i$, $i = 1, \ldots, I$.

The maximum likelihood estimator (MLE) of $\boldsymbol{\theta}$, denoted by $\widehat{\boldsymbol{\theta}}$, is obtained by maximizing the likelihood function in (33) or, equivalently, its logarithm. Let us introduce the following probability vectors:

$$\widehat{\boldsymbol{p}}_i = (\widehat{p}_{i0}, \widehat{p}_{i1}, \widehat{p}_{i2})^T = \frac{1}{K_i}(n_{i0}, n_{i1}, n_{i2})^T, \quad i = 1, \ldots, I, \tag{34}$$

$$\boldsymbol{\pi}_i(\boldsymbol{\theta}) = (\pi_{i0}(\boldsymbol{\theta}), \pi_{i1}(\boldsymbol{\theta}), \pi_{i2}(\boldsymbol{\theta}))^T, \quad i = 1, \ldots, I. \tag{35}$$

The Kullback–Leibler divergence measure, between $\widehat{\boldsymbol{p}}_i$ and $\boldsymbol{\pi}_i(\boldsymbol{\theta})$, is given by

$$\begin{aligned} d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) &= \sum_{r=0}^{2} \widehat{p}_{ir} \log\left(\frac{\widehat{p}_{ir}}{\pi_{ir}(\boldsymbol{\theta})}\right) \\ &= \frac{1}{K_i}\left\{n_{i0}\log\left(\frac{n_{i0}/K_i}{\pi_{i0}(\boldsymbol{\theta})}\right) + n_{i1}\log\left(\frac{n_{i1}/K_i}{\pi_{i1}(\boldsymbol{\theta})}\right) + n_{i2}\log\left(\frac{n_{i2}/K_i}{\pi_{i2}(\boldsymbol{\theta})}\right)\right\}, \end{aligned}$$

and the weighted Kullback–Leibler divergence measure is given by

$$\begin{aligned} d_{KL}^{W}(\boldsymbol{\theta}) &= \sum_{i=1}^{I} \frac{K_i}{K} d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) \\ &= \frac{1}{K}\sum_{i=1}^{I}\left\{n_{i0}\log\left(\frac{n_{i0}/K_i}{\pi_{i0}(\boldsymbol{\theta})}\right) + n_{i1}\log\left(\frac{n_{i1}/K_i}{\pi_{i1}(\boldsymbol{\theta})}\right) + n_{i2}\log\left(\frac{n_{i2}/K_i}{\pi_{i2}(\boldsymbol{\theta})}\right)\right\}, \end{aligned}$$

with $K = K_1 + \cdots + K_I$. The likelihood function $\mathcal{L}(n_{01}, \ldots, n_{I2}; \boldsymbol{\theta})$, given in (33), is related to the weighted Kullback–Leibler divergence measure through

$$d_{KL}^{W}(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} d_{KL}(\widehat{\boldsymbol{p}}_i, \boldsymbol{\pi}_i(\boldsymbol{\theta})) = c - \frac{1}{K}\log \mathcal{L}(n_{01}, \ldots, n_{I2}; \boldsymbol{\theta}), \tag{36}$$

with c being a constant, not dependent on $\boldsymbol{\theta}$.

Then, the MLE of $\boldsymbol{\theta}$, $\widehat{\boldsymbol{\theta}}$, can be obtained by the minimization of the weighted Kullback–Leibler divergence measure given in (36).

Given the probability vectors $\widehat{\boldsymbol{p}}_i$ and $\boldsymbol{\pi}_i(\boldsymbol{\theta})$, defined in (34) and (35), respectively, the weighted DPD between the two probability vectors is given by

$$\begin{aligned} d_{\beta}^{W}(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \Big[&\left(\pi_{i0}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i1}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i2}^{\beta+1}(\boldsymbol{\theta})\right) \\ &- \frac{\beta+1}{\beta}\left(\widehat{p}_{i0}\pi_{i0}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i1}\pi_{i1}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i2}\pi_{i2}^{\beta}(\boldsymbol{\theta})\right) + \frac{1}{\beta}\left(\widehat{p}_{i0}^{\beta+1} + \widehat{p}_{i1}^{\beta+1} + \widehat{p}_{i2}^{\beta+1}\right)\Big], \end{aligned}$$

but the term $\frac{1}{\beta}\left(\widehat{p}_{i0}^{\beta+1} + \widehat{p}_{i1}^{\beta+1} + \widehat{p}_{i2}^{\beta+1}\right)$, $i = 1, ..., I$, does not have any role in the minimization with respect to $\boldsymbol{\theta}$. Therefore, in order to minimize $d_{\beta}^{W}(\boldsymbol{\theta})$, we can consider the equivalent measure

$$
{}^{*}d_{\beta}^{W}(\boldsymbol{\theta}) = \sum_{i=1}^{I} \frac{K_i}{K} \left[\left(\pi_{i0}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i1}^{\beta+1}(\boldsymbol{\theta}) + \pi_{i2}^{\beta+1}(\boldsymbol{\theta}) \right) - \frac{\beta+1}{\beta} \left(\widehat{p}_{i0} \pi_{i0}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i1} \pi_{i1}^{\beta}(\boldsymbol{\theta}) + \widehat{p}_{i2} \pi_{i2}^{\beta}(\boldsymbol{\theta}) \right) \right].
$$

We can define the weighted minimum DPD estimator of $\boldsymbol{\theta}$ as

$$
\widehat{\boldsymbol{\theta}}_{\beta} = \arg\min_{\boldsymbol{\theta} \in \Theta} {}^{*}d_{\beta}^{W}(\boldsymbol{\theta}), \quad \text{for } \beta > 0
$$

and for $\beta = 0$, we obtain the weighted maximum likelihood estimator.

6.2 Inference Under Exponential Distribution and Competing Risks

Theorem 10 *The weighted minimum DPD estimator of $\boldsymbol{\theta}$, with tuning parameter $\beta \geq 0$, $\widehat{\boldsymbol{\theta}}_{\beta}$, can be obtained as the solution of the following system of four equations:*

$$
\sum_{i=1}^{I} K_i \left\{ -\pi_{i0}(\boldsymbol{\theta}) I T_i \left[\pi_{i0}(\boldsymbol{\theta})^{\beta-1} (\pi_{i0}(\boldsymbol{\theta}) - p_{i0}) - (1 - \pi_{i0}(\boldsymbol{\theta}))^{\beta-1} \Gamma_{i,\beta} \right] \boldsymbol{l}_i + (1 - \pi_{i0}(\boldsymbol{\theta}))^{\beta} \Gamma_{i,\beta}^{*} \right\} = \mathbf{0}_4,
$$

where

$$
\Gamma_{i,\beta} = \frac{\lambda_{i1}^{\beta} \left[\frac{\lambda_{i1}}{\lambda_{i1}+\lambda_{i2}} (1 - \pi_{i0}(\boldsymbol{\theta})) - p_{i1} \right] + \lambda_{i2}^{\beta} \left[\frac{\lambda_{i2}}{\lambda_{i1}+\lambda_{i2}} (1 - \pi_{i0}(\boldsymbol{\theta})) - p_{i2} \right]}{(\lambda_{i1} + \lambda_{i2})^{\beta}},
$$

$$
\Gamma_{i,\beta}^{*} = \frac{\lambda_{i1}^{\beta-1} \left[\frac{\lambda_{i1}}{\lambda_{i1}+\lambda_{i2}} (1 - \pi_{i0}(\boldsymbol{\theta})) - p_{i1} \right] - \lambda_{i2}^{\beta-1} \left[\frac{\lambda_{i2}}{\lambda_{i1}+\lambda_{i2}} (1 - \pi_{i0}(\boldsymbol{\theta})) - p_{i2} \right]}{(\lambda_{i1} + \lambda_{i2})^{\beta-1}},
$$

$\boldsymbol{l}_i = (\lambda_{i1}/\theta_{10}, \lambda_{i1} x_i, \lambda_{i2}/\theta_{20}, \lambda_{i2} x_i)^T$ *and* $\boldsymbol{r}_i = \frac{\lambda_{i1}\lambda_{i2}}{(\lambda_{i1}+\lambda_{i2})^2} (1/\theta_{10}, x_i, -1/\theta_{20}, -x_i)^T$.

Now, by using Theorem 3.1 in Ghosh and Basu (2013), we can obtain the asymptotic distribution of the above weighted minimum DPD estimator.

Theorem 11 *Let $\boldsymbol{\theta}^0$ be the true value of the parameter $\boldsymbol{\theta}$. Then, the asymptotic distribution of the weighted minimum DPD estimator of $\boldsymbol{\theta}$, $\widehat{\boldsymbol{\theta}}_{\beta}$, is given by*

$$
\sqrt{K} \left(\widehat{\boldsymbol{\theta}}_{\beta} - \boldsymbol{\theta}^0 \right) \xrightarrow[K \to \infty]{\mathcal{L}} \mathcal{N} \left(\mathbf{0}_4, \boldsymbol{J}_{\beta}^{-1}(\boldsymbol{\theta}^0) \boldsymbol{K}_{\beta}(\boldsymbol{\theta}^0) \boldsymbol{J}_{\beta}^{-1}(\boldsymbol{\theta}^0) \right),
$$

where

$$\boldsymbol{J}_{\beta}(\boldsymbol{\theta}) = \sum_{i=1}^{I}\sum_{r=0}^{2}\frac{K_i}{K}\boldsymbol{u}_{ir}^{*}(\boldsymbol{\theta})\boldsymbol{u}_{ir}^{*T}(\boldsymbol{\theta})\pi_{ir}^{\beta-1}(\boldsymbol{\theta}),$$

$$\boldsymbol{K}_{\beta}(\boldsymbol{\theta}) = \sum_{i=1}^{I}\sum_{r=0}^{2}\frac{K_i}{K}\boldsymbol{u}_{ir}^{*}(\boldsymbol{\theta})\boldsymbol{u}_{ir}^{*T}(\boldsymbol{\theta})\pi_{ir}^{2\beta-1}(\boldsymbol{\theta}) - \sum_{i=1}^{I}\frac{K_i}{K}\boldsymbol{\xi}_{i,\beta}(\boldsymbol{\theta})\boldsymbol{\xi}_{i,\beta}^{T}(\boldsymbol{\theta}),$$

with $\boldsymbol{\xi}_{i,\beta}(\boldsymbol{\theta}) = \sum_{r=0}^{2}\boldsymbol{u}_{ir}^{*}(\boldsymbol{\theta})\pi_{ir}^{\beta}(\boldsymbol{\theta})$, $\boldsymbol{u}_{ir}^{*}(\boldsymbol{\theta}) = \frac{\partial\pi_{ir}(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}^{T}}$, *and*

$$\begin{aligned}
\frac{\partial\pi_{i0}(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}} &= -IT_i\pi_{i0}(\boldsymbol{\theta})\boldsymbol{l}_i,\\
\frac{\partial\pi_{i1}(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}} &= \frac{\lambda_{i1}}{\lambda_{i1}+\lambda_{i2}}IT_i\pi_{i0}(\boldsymbol{\theta})\boldsymbol{l}_i + (1-\pi_{i0}(\boldsymbol{\theta}))\boldsymbol{r}_i,\\
\frac{\partial\pi_{i2}(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}} &= \frac{\lambda_{i2}}{\lambda_{i1}+\lambda_{i2}}IT_i\pi_{i0}(\boldsymbol{\theta})\boldsymbol{l}_i - (1-\pi_{i0}(\boldsymbol{\theta}))\boldsymbol{r}_i,
\end{aligned}$$

$\boldsymbol{l}_i = (\lambda_{i1}/\theta_{10}, \lambda_{i1}x_i, \lambda_{i2}/\theta_{20}, \lambda_{i2}x_i)^T$ *and* $\boldsymbol{r}_i = \frac{\lambda_{i1}\lambda_{i2}}{(\lambda_{i1}+\lambda_{i2})^2}(1/\theta_{10}, x_i, -1/\theta_{20}, -x_i)^T$.

6.3 Monte Carlo Simulation Study

We consider unbalanced data with unequal sample sizes for the test conditions. This data set, which consists a total of $K = 300$ devices, is presented in Table 7. A competing risks model, with two different causes of failure, was generated with parameters $\boldsymbol{\theta} = (0.001, 0.05, 0.0001, 0.08)^T$. To examine the robustness in this ALT

Table 7 ALT plan, unbalanced data

i	x_i	IT_i	K_i
1	35	10	50
2	45	10	40
3	55	10	20
4	65	10	40
5	35	20	20
6	45	20	20
7	55	20	30
8	65	20	20
9	35	30	20
10	45	30	20
11	55	30	10
12	65	30	10

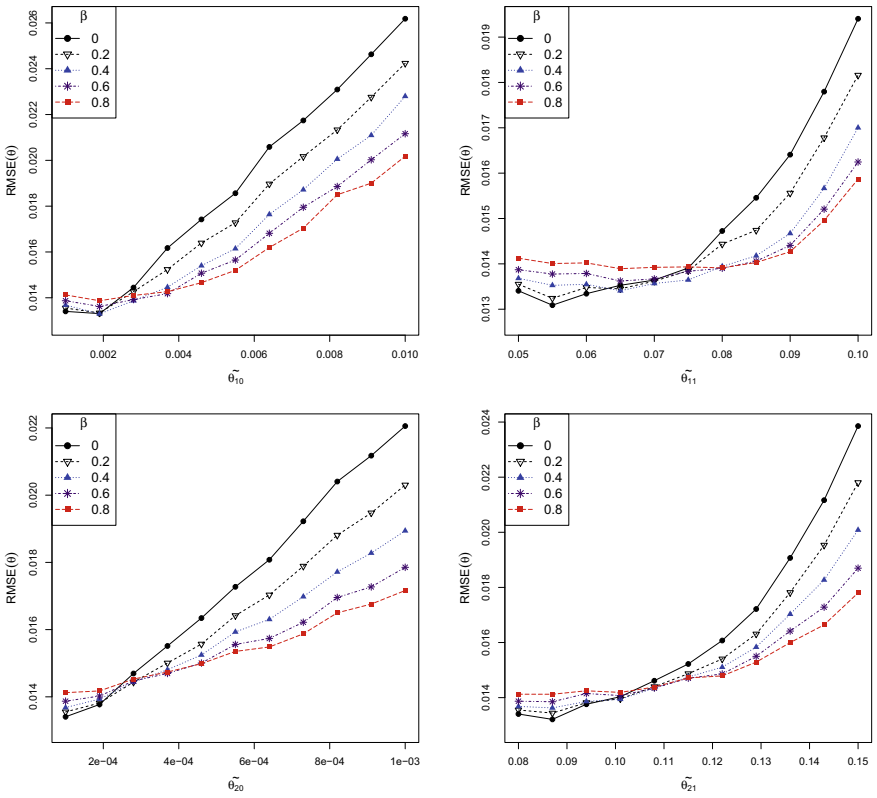

Fig. 5 RMSEs of the weighted minimum density power divergence estimators of $\boldsymbol{\theta}$ for different contamination parameter values. Unbalanced data

plan (in which the devices are tested under high stress levels, so that more failures can be observed), we increased each of the parameters of the outlying first cell (Fig. 5). The contaminated parameters are expressed by $\tilde{\theta}_{10}, \tilde{\theta}_{11}, \tilde{\theta}_{20}$ and $\tilde{\theta}_{21}$, respectively.

When there is no contamination in the cell or the degree of contamination is very low, and in concordance with results obtained in the previous scenario, MLE is observed to be the most efficient estimator. However, when the degree of contamination increases, there is an increase in the error for all the estimators, but weighted minimum DPD estimators are shown to be much more robust. This was also the case for whatever choice of the contamination parameters we considered.

7 Notes and Comments

A one-shot device is a unit that performs its function only once and, after use, the device either gets destroyed or must be rebuilt. To evaluate the reliability of such products, an ALT plan is usually employed by increasing the levels of stress factors and then extrapolating the life characteristics from high stress conditions to normal operating conditions. The study of a one-shot device from ALT data has been developed considerably recently, mainly motivated by the work of Fan et al. (2009), which was followed by other interesting papers (see, for example, Balakrishnan and Ling 2012a, b, 2013). All these papers are based on MLE, although it's lack of robustness is well-known.

In this chapter, an overview of the divergence-based methodology for one-shot device testing is provided. The use of DPDs allows the development of robust estimators and Wald-type tests, which are shown to be an interesting alternative to the classical MLE and Wald test, although a slight loss in efficiency is unavoidable. This robustness is proved with the study of the influence functions and illustrated with simulation studies and numerical examples. Different lifetime distributions, such as exponential, gamma and Weibull, are considered for the case of multiple stress levels and one cause of failure, while a competing risks extension is also discussed under the exponential assumption. Sections 2, 3 and 4 summarize results presented in Balakrishnan et al. (2020a, b, 2019a), respectively, while Sects. 5 and 6 present the results in Balakrishnan et al. (2020c, d).

For further work, we can develop robust inference for one-shot devices with competing risks under gamma and Weibull distributions. We can also consider a generalized gamma distribution for lifetime and develop the corresponding inference and model discrimination between exponential, gamma, Weibull and log-normal distributions within this family, as the generalized gamma contains all these distributions as special cases. Finally, we may consider the model with dependent components, as the independence assumption may not be a realistic setting in many practical cases. This could be done, for example, by modeling the dependence structure by a uniform or a Gaussian or Archimedean copula. Work on these problems is currently in progress, and we hope to report these findings in a future paper.

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Statistical Meaning of Mean Functions: A Novel Matrix Mean Derived from Fisher Information

Abram M. Kagan and Paul J. Smith

Abstract C. R. Rao has contributed to a broad variety of statistics, including linear models, Fisher information, multivariate analysis and matrix theory. This article extends a line of Rao's research, which exploits properties of Fisher information to derive or rederive analytic inequalities. In this article, properties of Fisher information are applied to mixed Gaussian distributions to yield a matrix mean function which lies between the arithmetic and harmonic means, analogous to the geometric mean. Fisher information also yields a generalized weighted arithmetic–harmonic mean inequality.

Keywords Matrix inequalities · Fisher information · Scale mixtures of Gaussians

1 Introduction

Fisher information is a fundamental concept in statistics because it quantifies the efficiency of point estimators in finite samples and the asymptotic behavior of maximum likelihood estimators. The importance of Fisher information is derived from two properties:

- *Monotonicity*: The Fisher information in a statistic (a reduction of a set of data) is never greater than the information in the complete data set.
- *Additivity*: The total Fisher information in a set of independent observations is the sum of the Fisher information of each of its components.

This article applies the Fisher information to develop analytic inequalities involving both scalars and matrices. The monotonicity and additivity of Fisher information are key tools in deriving or reproving analytic inequalities, as shown below. The

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general approach is to formulate a probability model, specialize it to Gaussian distributions and use information-theoretic properties of the model to derive inequalities based on statistical principles.

Kagan and Smith (2001) used the Fisher information to create statistical proofs of the monotonicity and convexity of the matrix function $\mathbf{A}^{-1}$ for Hermitian matrices. That is,

$$\mathbf{A} \geq \mathbf{B} \Rightarrow \mathbf{B}^{-1} \geq \mathbf{A}^{-1}$$

and, given weights $w_1, \ldots, w_n$ such that $w_j \geq 0$ and $\sum w_j = 1$,

$$(w_1\mathbf{A}_1 + \cdots + w_n\mathbf{A}_n)^{-1} \leq w_1\mathbf{A}_1^{-1} + \cdots + w_n\mathbf{A}_n^{-1}.$$

(Here and throughout the paper, for any pair of Hermitian matrices, $\mathbf{A} \geq \mathbf{B}$ means $\mathbf{A} - \mathbf{B}$ is nonnegative definite.) Similarly, the matrix function $\mathbf{A}^2$ is shown to be convex using statistical methods.

The convexity result above was extended to a notion of matrix-weighted averages in Kagan and Smith (1999). The scalar weights in $w_1\mathbf{A}_1 + \cdots + w_n\mathbf{A}_n$ are replaced by matrix weights as follows:

$$\mathbf{B}_1^T\mathbf{A}_1\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{A}_n\mathbf{B}_n$$

where $\mathbf{B}_1^T\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{B}_n = \mathbf{I}$. It was shown that $\mathbf{A}^2$ and $\mathbf{A}^{-1}$ are *hyperconvex* functions, meaning that

$$(\mathbf{B}_1^T\mathbf{A}_1\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{A}_n\mathbf{B}_n)^2 \leq \mathbf{B}_1^T\mathbf{A}_1^2\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{A}_n^2\mathbf{B}_n$$

and

$$(\mathbf{B}_1^T\mathbf{A}_1\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{A}_n\mathbf{B}_n)^{-1} \leq \mathbf{B}_1^T\mathbf{A}_1^{-1}\mathbf{B}_1 + \cdots + \mathbf{B}_n^T\mathbf{A}_n^{-1}\mathbf{B}_n.$$

As before, these results were derived by making use of the properties of the Fisher information.

The results described above are similar to the use of properties of entropy and related informational quantities to derive and extend classical inequalities. See Dembo et al. (1991) for an exposition of that work.

2 Properties of Fisher Information

Basic results concerning Fisher information are given in standard textbooks on mathematical statistics, for example, Rao (1973) and Bickel and Doksum (2015). Let $\mathbf{X}$ be a random vector with density $p(\mathbf{x}; \boldsymbol{\theta})$ depending on a parameter $\boldsymbol{\theta}$. We assume the score function

$$J(\mathbf{x}; \boldsymbol{\theta}) = (\partial/\partial\boldsymbol{\theta}) \log p(\mathbf{x}; \boldsymbol{\theta})$$

is well defined. Then $\mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta})$, the Fisher information on $\boldsymbol{\theta}$ contained in $\mathbf{X}$, is defined as

$$\mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta}) = \text{Var-Cov}[J(\mathbf{X};\boldsymbol{\theta})] = E_{\boldsymbol{\theta}}[J(\mathbf{X};\boldsymbol{\theta})J(\mathbf{X};\boldsymbol{\theta})^T].$$

Under further regularity conditions,

$$\mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta}) = E_{\boldsymbol{\theta}}\left[-\frac{\partial}{\partial\boldsymbol{\theta}}\frac{\partial}{\partial\boldsymbol{\theta}^T}\log p(\mathbf{x};\boldsymbol{\theta})\right].$$

The fundamental information inequality (or Cramér–Rao inequality) states that if $\mathbf{T}$ is an unbiased estimator of $\boldsymbol{\theta}$, then

$$\text{Var-Cov}_{\boldsymbol{\theta}}[\mathbf{T}] \geq \mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta})^{-1}.$$

When $\boldsymbol{\theta}$ is a location parameter, $\mathbf{X}$ has density $p(\mathbf{x}-\boldsymbol{\theta})$. The Fisher information on a location parameter becomes

$$\mathbf{I}_{\mathbf{X}} = \int (\partial \log p(\mathbf{x})/\partial\mathbf{x})(\partial \log p(\mathbf{x})/\partial\mathbf{x}^T)\,p(\mathbf{x})d\mathbf{x}.$$

Plainly, $\mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta}) = \mathbf{I}_{\mathbf{X}}$ is constant in $\boldsymbol{\theta}$. (The notation $\mathbf{I}_{\mathbf{X}}$ by default denotes the information on a location parameter $\boldsymbol{\theta}$ throughout this paper.)

If $\mathbf{X}_\sigma$ is distributed as $\sigma\mathbf{X}$, the density of $\mathbf{X}_\sigma$ is $(1/\sigma)p((\mathbf{x}-\boldsymbol{\theta})/\sigma)$ and plainly $\mathbf{I}_{\mathbf{X}_\sigma} = \mathbf{I}_{\mathbf{X}}/\sigma^2$.

For a scalar Gaussian random variable $X \sim N(\theta, \sigma^2)$, one has $I_X = 1/\sigma^2$, and for any X with $E[X] = \theta$ and $\text{Var}(X) = \sigma^2$, $I_X \geq 1/\sigma^2$. This is a consequence of the Cramér–Rao inequality.

3 Mixtures, Mean Functions and Inequalities

Consider an experiment consisting of observing a pair (Δ, X), where Δ is a discrete random variable with $P(\Delta = i) = w_i$ and the conditional distribution of X given $\Delta = i$ is $N(\theta, \sigma_i^2)$, $i = 1, \ldots, n$.

The marginal distribution of X is a scale mixture of Gaussian distributions $N(\theta, \sigma_1^2), \ldots, N(\theta, \sigma_n^2)$ with mixture parameter $\mathbf{w} = (w_1, \ldots, w_n)$. Its density is

$$p(x-\theta) = w_1\varphi_{\sigma_1}(x-\theta) + \cdots + w_n\varphi_{\sigma_n}(x-\theta). \tag{1}$$

Here, $\varphi(x)$ is the density of the standard normal $Z \sim N(0,1)$ and $\varphi_\sigma(w) = \sigma^{-1}\varphi(w/\sigma)$. The variance σ^2 of X with density (1) is

$$\sigma^2 = w_1\sigma_1^2 + \cdots + w_n\sigma_n^2. \tag{2}$$

The Fisher information on θ contained in the pair (Δ, X) is

$$I_{(\Delta,X)} = w_1/\sigma_1^2 + \cdots + w_n/\sigma_n^2. \tag{3}$$

Monotonicity of the Fisher information (the information in the whole data set is never less than in any part of it; in the present case, X is a part of (Δ, X)) implies

$$I_X \le I_{\Delta,X}.$$

For any Y with $E[Y] = \theta$ and finite variance, $I_Y \ge 1/\mathrm{Var}(Y)$. Hence, one gets a two-sided inequality for I_X with density $p(x-\theta)$:

$$\left[\sum_1^n w_i\sigma_i^2\right]^{-1} \le I_X \le \sum_1^n w_i/\sigma_i^2. \tag{4}$$

Since $p(x-\theta)$ in (1) is completely determined by the weights $w_1, \ldots, w_n$ and variances $\sigma_1^2, \ldots, \sigma_n^2$, so is I_X. On setting $a_1 = 1/\sigma_1^2, \ldots, a_n = 1/\sigma_n^2$, the inequality (4) takes the form

$$\left[\sum_1^n w_i/a_i\right]^{-1} \le I_X(a_1, \ldots, a_n; w_1, \ldots, w_n) \le \sum_1^n w_i a_i. \tag{5}$$

4 An Information-Based Mean Function

Recall that a function $M(a_1, \ldots, a_n)$ is called a *mean function* if for all $a_1 \ge 0, \ldots, a_n \ge 0$:

(i) $\min(a_1, \ldots, a_n) \le M(a_1, \ldots, a_n) \le \max(a_1, \ldots, a_n)$;
(ii) for any $\lambda > 0$, $M(\lambda a_1, \ldots, \lambda a_n) = \lambda M(a_1, \ldots, a_n)$.

Classical examples of mean functions are arithmetic, geometric and harmonic means.

From (5), the Fisher information $I_X(a_1, \ldots, a_n; w_1, \ldots, w_n)$ satisfies (i). Furthermore, for any $\lambda > 0$, $I_X(\lambda a_1, \ldots, \lambda a_n; w_1, \ldots, w_n)$ is the Fisher information in X_λ with density

$$p_\lambda(x-\theta) = w_1\varphi_{\sigma_1/\lambda} + \ldots + w_n\varphi_{\sigma_n/\lambda} = \sqrt{\lambda}p(\sqrt{\lambda}(x-\theta))$$

and due to the well-known property of the Fisher information mentioned above,

$$I_X(\lambda a_1, \ldots, \lambda a_n; w_1, \ldots, w_n) = \lambda I_X(a_1, \ldots, a_n; w_1, \ldots, w_n)$$

so that $I_X(a_1, \ldots, a_n; w_1, \ldots, w_n)$ satisfies (ii). Thus, $I_X(a_1, \ldots, a_n; w_1, \ldots, w_n)$ is a mean function. We suggest calling it the *infomean*.

Inequalities (4) and (5) have a statistical interpretation. Their right-hand sides are the Fisher information on θ in the pair (Δ, X) with

$$P(\Delta = i) = w_i, \quad X|\{\Delta = i\} \sim N(\theta, a_i = 1/\sigma_i^2), \quad i = 1, \ldots, n. \tag{6}$$

The left-hand sides are the Fisher information on θ in a Gaussian $X \sim N(\theta, \sigma^2)$ with σ^2 given by (2).

Turn now to the case when $a_1, \ldots, a_n$ are replaced by positive definite Hermitian matrices $\mathbf{A}_1, \ldots, \mathbf{A}_n$. As is well known, the inequality between the arithmetic and harmonic means still holds:

$$[w_1\mathbf{A}_1^{-1} + \cdots + w_n\mathbf{A}_n^{-1}]^{-1} \leq w_1\mathbf{A}_1 + \cdots + w_n\mathbf{A}_n. \tag{7}$$

The matrices are not assumed to commute, so their geometric mean is not defined. (See Sect. 6 for a discussion of geometric means of matrices.)

Suppose that $\mathbf{X}$ is a d-dimensional random vector with distribution given by a density $p(\mathbf{x} - \boldsymbol{\theta})$, where $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_d]^T$ is a d-dimensional parameter. Then the vector score

$$\mathbf{J} = \mathbf{J}(\mathbf{X} - \boldsymbol{\theta}) = [\partial \log p/\partial\theta_1, \ldots, \partial \log p/\partial\theta_d]^T$$

is well defined, and $E_{\boldsymbol{\theta}}\|\mathbf{J}(\mathbf{X} - \boldsymbol{\theta})\|^2 < \infty$. The $d \times d$ matrix $E_{\boldsymbol{\theta}}(\mathbf{J}\mathbf{J}^T) = \mathbf{I}_{\mathbf{X}}(\boldsymbol{\theta})$ is called the matrix of the Fisher information on $\boldsymbol{\theta}$ contained in $\mathbf{X}$. (The superscript T denotes transposition.)

For any Gaussian $\mathbf{Y} \sim N_d(\boldsymbol{\theta}, \mathbf{V})$ with mean vector $\boldsymbol{\theta}$ and non-degenerate covariance matrix $\mathbf{V}$, $\mathbf{I}_{\mathbf{Y}} = \mathbf{V}^{-1}$. For any $\mathbf{Y} \sim p(\mathbf{y} - \boldsymbol{\theta})$ with covariance matrix $\mathbf{V}$, the information matrix is evidently constant with respect to $\boldsymbol{\theta}$ and $\mathbf{I}_{\mathbf{X}} \geq \mathbf{V}^{-1}$.

Let $(\Delta, \mathbf{X})$ be a pair of random elements whose distribution is given by

$$P(\Delta = i) = w_i, \quad \mathbf{X}|\{\Delta = i\} \sim N_d(\boldsymbol{\theta}, \mathbf{V}_i), \quad i = 1, \ldots, n. \tag{8}$$

The marginal density $p(\mathbf{x} - \boldsymbol{\theta})$ of $\mathbf{X}$ is the mixture of the $N_d(\boldsymbol{\theta}, \mathbf{V}_1), \ldots, N_d(\boldsymbol{\theta}, \mathbf{V}_n)$ densities with mixture weights $w_1, \ldots, w_n$. Similar to (2), the covariance matrix $\mathbf{V}$ of $\mathbf{X}$ is

$$\mathbf{V} = w_1\mathbf{V}_1 + \cdots + w_n\mathbf{V}_n \tag{9}$$

and the matrix of Fisher information on $\boldsymbol{\theta}$ in the pair $(\Delta, \mathbf{X})$ is

$$I_{\Delta,\mathbf{X}} = w_1\mathbf{V}_1^{-1} + \cdots + w_n\mathbf{V}_n^{-1}, \tag{10}$$

which is constant in $\boldsymbol{\theta}$.

As in the case of a scalar-valued θ, when $\boldsymbol{\theta}$ is vector-valued, the matrix of the Fisher information is monotone. In this case, $I_{\mathbf{X}} \leq I_{\Delta,\mathbf{X}}$.

On setting $\mathbf{A}_1 = \mathbf{V}_1^{-1}, \ldots, \mathbf{A}_n = \mathbf{V}_n^{-1}$, $I_{\mathbf{X}}$ becomes a function of $\mathbf{A}_1, \ldots, \mathbf{A}_n$ and the mixing probabilities $w_1, \ldots, w_n$. Comparing it with $I_{\Delta,\mathbf{X}}$ on one side and with the matrix of the Fisher information in a Gaussian $Z \sim N_d(\boldsymbol{\theta}, V)$ on the other leads to

$$(w_1\mathbf{A}_1^{-1} + \ldots + w_n\mathbf{A}_n^{-1})^{-1} \le I_{\mathbf{X}}(\mathbf{A}_1, \ldots, \mathbf{A}_n; w_1, \ldots, w_n) \le w_1\mathbf{A}_1 + \ldots + w_n\mathbf{A}_n. \tag{11}$$

We want to emphasize that the matrices $\mathbf{A}_1, \ldots, \mathbf{A}_n$ are not assumed to commute.

As a function of $\mathbf{A}_1, \ldots, \mathbf{A}_n$, $I_{\mathbf{X}}$ satisfies the above condition (ii) and the following version of (i): if a matrix $\bar{\mathbf{A}}$ and a positive matrix $\underline{\mathbf{A}}$ are such that $\underline{\mathbf{A}} \le A_i \le \bar{\mathbf{A}}$, $i = 1, \ldots, n$, then $\underline{A} \le I_{\mathbf{X}} \le \bar{A}$. The statistical interpretation of (11) is the same as that of (4) and (5).

5 An Inequality for Fisher Information in Sums of Random Variables

In the previous section, we considered the Fisher information in a scale mixture of Gaussian densities to obtain analytic inequalities of mean functions. In this section, we follow a different approach by examining the Fisher information on weighted location parameters in an independent sample of n observations. The model is as follows.

For independent $X_1, \ldots, X_n$ with finite Fisher information and $w_1 > 0, \ldots, w_n > 0$, $w_1 + \cdots + w_n = 1$, set

$$U_i = X_i + w_i^{\alpha}\theta, \quad i = 1, \ldots, n. \tag{12}$$

The information in U_i on θ equals $I_{U_i} = w_i^{2\alpha} I_{X_i}$. Observe that for any constant $c > 0$, the information on θ in U_i equals that in cU_i. (This model may be regarded as a version of regression through the origin.)

Multiplying both sides of (12) by w_i^{β}, where $\beta = 1 - \alpha$, and taking the sum of the results gives

$$U = \sum_1^n w_i^{\beta} U_i = \sum_1^n w_i^{\beta} X_i + \theta$$

whence

$$I_U = I_{\sum_1^n w_i^{\beta} X_i}. \tag{13}$$

The information about θ in the vector $(w_1^{\beta}U_1, \ldots, w_n^{\beta}U_n)$ with independent components is the same as in the vector $(U_1, \ldots, U_n)$. Due to monotonicity and additivity of the Fisher information,

$$I_U = I_{\sum_1^n w_i^{\beta} U_i} \le \sum_1^n I_{U_i} \tag{14}$$

whence

$$I_{\sum_1^n w_i^\beta X_i} \leq \sum_1^n w_i^{2\alpha} I_{X_i} \tag{15}$$

for $\alpha + \beta = 1$. For $n = 2$, $\alpha = \beta = 1/2$, this inequality is known (e.g., see Dembo et al. 1991, Theorem 13).

When the X_i are independent Gaussian variables with variances $\sigma_i^2 = 1/a_i$, the sum $\sum w_i^\beta X_i$ has a Gaussian distribution with variance $\sum w_i^{2\beta}/a_i$ and (15) takes the form

$$\sum_1^n w_i^{2\alpha} a_i \geq \frac{1}{\sum w_i^{2\beta}/a_i} \tag{16}$$

for α, β subject to $\alpha + \beta = 1$.

Replacing $2\alpha, 2\beta$ with α, β subject to $\alpha + \beta = 2$ gives a generalization, in a sense, of the classical inequality between the arithmetic and harmonic means:

$$\sum_1^n w_i^{\alpha} a_i \geq \frac{1}{\sum w_i^{\beta}/a_i} \tag{17}$$

for $\alpha + \beta = 2$.

In the d-dimensional Gaussian case, $\mathbf{X}_i$ has variance–covariance matrices $\mathbf{V}_i = \mathbf{A}_i^{-1}$ and $I_{\mathbf{X}_i} = \mathbf{A}_i$. The above derivation yields the inequality

$$\sum_1^n w_i^{\alpha} \mathbf{A}_i \geq \left(\sum w_i^{\beta} \mathbf{A}_i^{-1} \right)^{-1} \tag{18}$$

for $\alpha + \beta = 2$.

6 General Comments

The paper reveals the statistical meaning of classical mean functions (see in this connection Rao 2000a, b; Kagan and Smith 2001; Kagan 2003; Kagan and Rao 2003) and introduces a matrix mean of purely statistical origin, called the infomean. It leads to a new inequality similar to the classical inequality among the arithmetic, geometric and harmonic means and holds when the arguments of the mean functions are Hermitian positive definite matrices, not necessarily commuting, in which case the geometric mean is not uniquely defined.

Several definitions of a matrix geometric mean have been proposed, of which the most plausible is $\mathbf{A}\#\mathbf{B} = \mathbf{A}^{1/2} \left(\mathbf{A}^{-1/2} \mathbf{B} \mathbf{A}^{-1/2} \right)^{1/2} \mathbf{A}^{1/2}$, where $\mathbf{A}$ and $\mathbf{B}$ are positive definite matrices. The concept extends to geometric means of several matrices. See Bhatia (2013) for an exposition.

The material of the paper can be used as a part of the chapter on the Fisher information in graduate courses in Statistics.

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The Legend of the Equality of OLSE and BLUE: Highlighted by C. R. Rao in 1967

Augustyn Markiewicz, Simo Puntanen, and George P. H. Styan

Abstract In this article, we go through some crucial developments regarding the equality of the ordinary least squares estimator and the best linear unbiased estimator in the general linear model. C. R. Rao (Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. University of California Press, Berkeley, pp. 355–372, 1967) appears to be the first to provide necessary and sufficient conditions for the general case when both the model matrix and the random error term's covariance matrix are possibly deficient in rank. We describe the background of the problem area and provide some examples. We also consider some personal CRR-related glimpses of our research careers and provide a rather generous list of references.

Keywords Best linear unbiased estimator · BLUE · Efficiency of ordinary least squares · Estimability · Generalized inverse · Ordinary least squares estimator · OLSE · Linear model · Löwner ordering

1 Introduction and Background

Let us begin by quoting the beginning of Chap. 10, entitled "BLUE", of the *Matrix Tricks Book* by Puntanen et al. (2011):

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> Over the years, one of our favourite research topics in linear models has been the equality between OLSE and BLUE of $\mathbf{X}\boldsymbol{\beta}$. In Proposition 10.1 [in the present article Theorem 4] we collect together some necessary and sufficient conditions for their equality. We find this collection very useful and we believe it includes several interesting linear algebraic problems.
>
> While preparing this book, for a long time the title of this chapter was "OLSE versus BLUE", but the simpler version "BLUE" describes better the matrix tricks under consideration. In the sections of this chapter we consider, for example, the best unbiased linear predictors, BLUPs, and mixed models.

We will closely follow the article "The equality of the ordinary least squares estimator and the best linear unbiased estimator" in *The American Statistician* by Puntanen and Styan (1989), the most cited joint paper by these authors, as well as the articles by Baksalary et al. (1990b) and by Puntanen and Styan (1996): "A brief biography and appreciation of Calyampudi Radhakrishna Rao, with a bibliography of books and papers". Our aim is to give an easy-to-read review for a non-expert of the area and illustrate the role of C. R. Rao in its development. This article contains no new technical results, makes no claim at completeness; this is a brief survey—but we believe that the years after 1989 have matured our insight into this area. Browsing again through the old material was very interesting. Hopefully we can express this in what follows.

To give some perspective, we start by going through some background in the spirit of Puntanen and Styan (1996).

In 1954, C. R. Rao received some data collected in Japan in order to study the long-term effects of radiation on atom bomb casualties in Hiroshima and Nagasaki. The statistical analysis involved finding a matrix to replace the inverse of $\mathbf{X}'\mathbf{X}$, where $\mathbf{X}$ is the model matrix in the linear model and $\mathbf{X}'$ stands for its transpose; here the matrix $\mathbf{X}'\mathbf{X}$ was singular. This led to a *pseudoinverse* which was introduced by Rao (1955) in *Sankhyā*. This was the same year that Penrose (1955) published his paper on generalized inverses. Rao then discovered that the key condition for a generalized inverse $\mathbf{G}$ of a matrix $\mathbf{A}$ was the equation $\mathbf{AGA} = \mathbf{A}$, introducing the notation $\mathbf{G} = \mathbf{A}^-$. The calculus of generalized inverses and the unified theory of linear estimation were then presented by Rao (1962), in the *Journal of the Royal Statistical Society, Ser. B*. The subject of generalized inverses was further developed leading to the monograph (Rao and Mitra 1971a) with Sujit Kumar Mitra entitled *Generalized Inverse of Matrices and its Applications*.

As a sidetrack, below is an excerpt from S.K. Mitra's interview, carried out in February 1993 in the Indian Statistical Institute, New Delhi, see Puntanen and Styan (2012). Professor Mitra was replying to the following question: When was the decision made that you will start writing that book with Professor Rao?

> In 1967 we had a summer school at the ISI, with a lot of students participating. Often new areas of statistics and mathematics were exposed to the students during these six weeks of summer. I was in fact once the programme director of such a summer school.
>
> As a member of the summer school, I was able to get the best of C. R. Rao's papers and manuscripts. So I taught a course in the summer school and then by the time I had completed the course, I myself had some new results. In fact my first two papers on generalized inverses, which appeared in 1968, were essentially papers that appeared in their first form in these summer schools.

> Professor C. R. Rao had at that time already decided to write a book on generalized inverses all by himself. It was also announced as a forthcoming publication of the Statistical Publishing Society in Calcutta. He must have seen my new results and in a few days he invited me be a coauthor. That is how that book started.

Using the concept of generalized inverse, Rao (1971, 1973a), further developed a unified theory for linear estimation, noting that generalized inverses were particularly helpful with explicit expressions for projectors. We wish to cite a few words from the Appendix of the article by Rao (1971). The title of the Appendix was "The Atom Bomb and Generalized Inverse". Below the first and last paragraph of the Appendix are quoted.

> The author was first led to the definition of a pseudoinverse (now called generalized inverse or g-inverse) of a singular matrix in 1945–1955 when he undertook to carry out multivariate analysis of anthropometric data obtained on families of Hiroshima and Nagasaki to study the effects of radiation due atom bomb explosions, on request from Dr. W. J. Schull of the University of Michigan. The computation and use of a pseudoinverse are given in a statistical report prepared by the author, which is incorporated in Publication No. 461 of the National Academy of Sciences, U.S.A., by Neel and Schull (1956). It may be of interest to the audience to know the circumstances under which the pseudoinverse had to be introduced.
>
> It is hard to believe that scientists have found in what has been described as the greatest tragedy a source for providing material and simulation for research in many directions.

2 What Is OLSE, What Is BLUE?

Let us quickly recall the definition of the ordinary least squares estimator, OLSE, and the best linear unbiased estimator, BLUE, and before that, the linear statistical model under discussion. We will consider the general linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}\,, \quad \text{or shortly the triplet } \mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}\,, \tag{1}$$

where $\mathbf{X}$ is a known $n \times p$ model matrix, $\mathbf{y}$ is an observable n-dimensional random vector, $\boldsymbol{\beta}$ is p-dimensional vector of unknown but fixed parameters, and $\boldsymbol{\varepsilon}$ is an unobservable vector of random errors with expectation $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$, and covariance matrix $\mathrm{cov}(\boldsymbol{\varepsilon}) = \mathbf{V}$. We will denote $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ so that $\mathrm{E}(\mathbf{y}) = \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$. Often the covariance matrix is of the type $\sigma^2\mathbf{V}$, where σ^2 is an unknown positive constant. However, in our considerations σ^2 has no role. The nonnegative definite matrix $\mathbf{V}$ is known and can be singular. If $\mathbf{V}$ is not known things get much more complicated; for the so-called empirical best linear unbiased predictors in the linear mixed model, see, for example, Haslett and Welsh (2019).

Then some words about the notation. The symbols $\mathbf{A}^-$, $\mathbf{A}^+$, $\mathbf{A}'$, $\mathscr{C}(\mathbf{A})$, and $\mathscr{C}(\mathbf{A})^\perp$, denote, respectively, a generalized inverse, the (unique) Moore–Penrose inverse, the transpose, the column space, and the orthogonal complement of the column space of the matrix $\mathbf{A}$. Notation $\mathbf{A}^-$ refers to any matrix satisfying $\mathbf{A}\mathbf{A}^-\mathbf{A} = \mathbf{A}$ and $\mathbf{A}^+$ satisfies the four Moore–Penrose conditions. By $(\mathbf{A} : \mathbf{B})$ we denote the partitioned

matrix with $\mathbf{A}_{a\times b}$ and $\mathbf{B}_{a\times c}$ as submatrices. The symbol $\mathbf{A}^{\perp}$ stands for any matrix satisfying $\mathscr{C}(\mathbf{A}^{\perp}) = \mathscr{C}(\mathbf{A})^{\perp}$. Furthermore, we will use $\mathbf{P}_{\mathbf{A}} = \mathbf{A}\mathbf{A}^{+} = \mathbf{A}(\mathbf{A}'\mathbf{A})^{-}\mathbf{A}'$ to denote the orthogonal projector (with respect to the standard inner product) onto the column space $\mathscr{C}(\mathbf{A})$, and $\mathbf{Q}_{\mathbf{A}} = \mathbf{I} - \mathbf{P}_{\mathbf{A}}$, where $\mathbf{I}$ refers to the identity matrix of appropriate order. In particular, we denote shortly

$$\mathbf{H} = \mathbf{P}_{\mathbf{X}}\,, \quad \mathbf{M} = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}}\,. \tag{2}$$

A linear statistic $\mathbf{By}$ is said to be a linear unbiased estimator, LUE, for the parametric function $\mathbf{K}\boldsymbol{\beta}$, where $\mathbf{K} \in \mathbb{R}^{q\times p}$, if its expectation is equal to $\mathbf{K}\boldsymbol{\beta}$, i.e.

$$\mathrm{E}(\mathbf{By}) = \mathbf{BX}\boldsymbol{\beta} = \mathbf{K}\boldsymbol{\beta} \quad \text{for all } \boldsymbol{\beta} \in \mathbb{R}^{p}, \quad \text{i.e., } \mathbf{BX} = \mathbf{K}\,. \tag{3}$$

When $\mathscr{C}(\mathbf{K}') \subseteq \mathscr{C}(\mathbf{X}')$ holds, $\mathbf{K}\boldsymbol{\beta}$ is said to be estimable.

Definition 1 The linear unbiased estimator $\mathbf{By}$ is the best linear unbiased estimator, BLUE, of estimable $\mathbf{K}\boldsymbol{\beta}$ if $\mathbf{By}$ has the smallest covariance matrix in the Löwner sense among all linear unbiased estimators of $\mathbf{K}\boldsymbol{\beta}$:

$$\mathrm{cov}(\mathbf{By}) \le_{\mathrm{L}} \mathrm{cov}(\mathbf{B}_{\#}\mathbf{y}) \quad \text{for all } \mathbf{B}_{\#} : \mathbf{B}_{\#}\mathbf{X} = \mathbf{K}\,, \tag{4}$$

that is, $\mathrm{cov}(\mathbf{B}_{\#}\mathbf{y}) - \mathrm{cov}(\mathbf{By})$ is nonnegative definite for all $\mathbf{B}_{\#} : \mathbf{B}_{\#}\mathbf{X} = \mathbf{K}$.

Under the model $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$, the ordinary least squares estimator, OLSE, for $\boldsymbol{\beta}$ is the solution minimizing the quantity $\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$ with respect to $\boldsymbol{\beta}$ yielding to the normal equation $\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{y}$. Thus, if $\mathbf{X}$ has full column rank, the OLSE of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{X}^{+}\mathbf{y}$. In the general case, the set of *all* vectors $\hat{\boldsymbol{\beta}}$ satisfying $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$, can be written as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y} + [\mathbf{I}_p - (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}]\mathbf{t}\,, \tag{5}$$

where $(\mathbf{X}'\mathbf{X})^{-}$ is an arbitrary (but fixed) generalized inverse of $\mathbf{X}'\mathbf{X}$ and $\mathbf{t} \in \mathbb{R}^{p}$ is free to vary. On the other hand, every solution to the normal equations can be written as $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}$ for some $(\mathbf{X}'\mathbf{X})^{-}$.

Of course, it is questionable whether it is quite correct to call $\hat{\boldsymbol{\beta}}$ an estimator when it is not unique (after $\mathbf{y}$ is being observed); it is merely a *solution* to the normal equations; "This point cannot be overemphasized", as stated by Searle (1971, p. 169). In this context, we wish to cite also the following from Searle (2000, p. 26):

> One of the greatest contributions to understanding the apparent quirkiness of normal equations of non-full rank (as is customary with linear models), which have an infinity of solutions, is due to Rao (1962). Using the work of Moore (1920) and Penrose (1955), he showed how a generalized inverse matrix yields a solution to the normal equations and how that solution can be used to establish estimable functions and their estimators—and these results are invariant to whatever generalized inverse is being used. Although the arithmetic of generalized inverses is scarcely any less than that of regular inverses, the use of generalized inverses is of enormous help in understanding estimability and its consequences.

If $\mathbf{K}\boldsymbol{\beta}$ is estimable, then $\mathbf{K}\hat{\boldsymbol{\beta}} = \mathbf{K}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}$, i.e. the OLSE of $\mathbf{K}\boldsymbol{\beta}$ is unique whatever choice of $\hat{\boldsymbol{\beta}}$, i.e. whatever $(\mathbf{X}'\mathbf{X})^{-}$ we use. This can be seen from Lemma 2.2.4 of Rao and Mitra (1971a) which states that for nonnull matrices $\mathbf{A}$ and $\mathbf{C}$ the following holds:

$$\mathbf{A}\mathbf{B}^{-}\mathbf{C} = \mathbf{A}\mathbf{B}^{+}\mathbf{C} \text{ for all } \mathbf{B}^{-} \iff \mathscr{C}(\mathbf{C}) \subseteq \mathscr{C}(\mathbf{B}) \,\&\, \mathscr{C}(\mathbf{A}') \subseteq \mathscr{C}(\mathbf{B}') \,. \tag{6}$$

In particular, choosing $(\mathbf{X}'\mathbf{X})^{-}$ as $(\mathbf{X}'\mathbf{X})^{+}$ and using $\mathbf{X}^{+} = (\mathbf{X}'\mathbf{X})^{+}\mathbf{X}'$, we can write $\mathbf{K}\hat{\boldsymbol{\beta}} = \mathbf{K}(\mathbf{X}'\mathbf{X})^{+}\mathbf{X}'\mathbf{y} = \mathbf{K}\mathbf{X}^{+}\mathbf{y}$.

For $\mathbf{K} = \mathbf{X}$, we have

$$\mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta}) = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y} = \mathbf{X}\mathbf{X}^{+}\mathbf{y} = \mathbf{P}_{\mathbf{X}}\mathbf{y} = \mathbf{H}\mathbf{y} = \hat{\boldsymbol{\mu}} \,. \tag{7}$$

Obviously $\hat{\boldsymbol{\mu}} = \mathbf{H}\mathbf{y}$ is a LUE for $\mathbf{X}\boldsymbol{\beta}$. Let $\mathbf{B}\mathbf{y}$ be another LUE of $\mathbf{X}\boldsymbol{\beta}$, i.e. $\mathbf{B}$ satisfies $\mathbf{B}\mathbf{X} = \mathbf{X}$ and thereby $\mathbf{B}\mathbf{H} = \mathbf{H} = \mathbf{H}\mathbf{B}'$. Thus, under the model $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{I}_n\}$:

$$\mathrm{cov}(\mathbf{B}\mathbf{y}) = \mathrm{cov}[\mathbf{H}\mathbf{y} - (\mathbf{H} - \mathbf{B})\mathbf{y}] = \mathrm{cov}(\mathbf{H}\mathbf{y}) + \mathrm{cov}[(\mathbf{H} - \mathbf{B})\mathbf{y}] \geq_{\mathrm{L}} \mathrm{cov}(\mathbf{H}\mathbf{y}) \,, \tag{8}$$

and so we have proved a simple version of the *Gauss–Markov theorem*:

Theorem 1 *Under the model* $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{I}_n\}$*, the* OLSE *of* $\mathbf{X}\boldsymbol{\beta}$ *is the* BLUE *of* $\mathbf{X}\boldsymbol{\beta}$*, or shortly*

$$\hat{\boldsymbol{\mu}} = \mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta}) = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta}) = \tilde{\boldsymbol{\mu}} \,, \tag{9}$$

and for any estimable $\mathbf{K}\boldsymbol{\beta}$*,* $\mathrm{OLSE}(\mathbf{K}\boldsymbol{\beta}) = \mathrm{BLUE}(\mathbf{K}\boldsymbol{\beta})$.

When (9) holds, we will use phrases like "OLSE is BLUE". The claim concerning estimable $\mathbf{K}\boldsymbol{\beta}$ in Theorem 1 can be confirmed by observing that due to estimability, $\mathbf{K}\boldsymbol{\beta} = \mathbf{L}\mathbf{X}\boldsymbol{\beta}$ for some $\mathbf{L}$ and thereby $\mathrm{OLSE}(\mathbf{K}\boldsymbol{\beta}) = \mathbf{L}\,\mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta}) = \mathbf{L}\mathbf{H}\mathbf{y}$. Actually, under $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$, the statements $\mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta}) = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta})$ and $\mathrm{OLSE}(\mathbf{K}\boldsymbol{\beta}) = \mathrm{BLUE}(\mathbf{K}\boldsymbol{\beta})$ for *all* estimable $\mathbf{K}\boldsymbol{\beta}$ are equivalent. It is clear that $\boldsymbol{\beta}$ is estimable if and only if $\mathbf{X}$ has full column rank.

Consider now the model $\mathscr{M}$ where $\mathbf{V}$ is positive definite, and suppose that $\mathbf{V}^{1/2}$ is the positive definite square root of $\mathbf{V}$. Premultiplying $\mathscr{M}$ by $\mathbf{V}^{-1/2}$ gives the transformed model $\mathscr{M}_{\#} = \{\mathbf{V}^{-1/2}\mathbf{y},\ \mathbf{V}^{-1/2}\mathbf{X}\boldsymbol{\beta},\ \mathbf{I}_n\}$. In light of Theorem 1, the BLUE of $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{M}_{\#}$ equals the OLSE under $\mathscr{M}_{\#}$ and thus

$$\mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}_{\#}) = \tilde{\boldsymbol{\mu}}(\mathscr{M}_{\#}) = \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} = \mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}}\mathbf{y} \,, \tag{10}$$

where $\mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}}$ is the orthogonal projector onto $\mathscr{C}(\mathbf{X})$ when the inner product matrix is $\mathbf{V}^{-1}$. Here is a crucial question: is the BLUE of $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{M}_{\#}$ the same as under $\mathscr{M}$, in other words, has the transformation done via $\mathbf{V}^{-1/2}$ any effect on the BLUE of $\mathbf{X}\boldsymbol{\beta}$? The answer is that there is no effect and that

$$\mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}}\mathbf{y} = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}) = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}_{\#}) = \mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta} \mid \mathscr{M}_{\#}) \,. \tag{11}$$

The result (11), sometimes referred to as the Aitken-approach, see Aitken (1935), Farebrother (1990, 1997) and Searle (1996), is well known in statistical textbooks. Farebrother (1990) points out that Aitken's contribution to the subject was to show that a least squares estimator of $\boldsymbol{\beta}$ minimizing $(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})'\mathbf{V}^{-1}(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})$ could be obtained by premultiplying the model $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$ by an $n \times n$ matrix $\mathbf{D}$ satisfying $\mathbf{DVD}' = \mathbf{I}_n$. However, Aitken did not show that this estimator was the best linear unbiased estimator.

The property that the transformation via $\mathbf{V}^{-1/2}$ has no effect on the BLUE is phrased as "$\mathbf{V}^{-1/2}\mathbf{y}$ is linearly sufficient for $\mathbf{X}\boldsymbol{\beta}$"; see, e.g. Baksalary and Kala (1981a, 1986) and Haslett et al. (2020).

Example 1 (*Very simple model*) Let us consider a linear model $\mathbf{y} = \mathbf{x}\beta + \boldsymbol{\varepsilon}$, where $\operatorname{cov}(\mathbf{y}) = \mathbf{V}$. Then

$$\text{OLSE}(\beta) = \hat{\beta} = (\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}'\mathbf{y}\,, \qquad \operatorname{var}(\hat{\beta}) = (\mathbf{x}'\mathbf{x})^{-2}\mathbf{x}'\mathbf{V}\mathbf{x}\,, \tag{12a}$$

$$\text{BLUE}(\beta) = \tilde{\beta} = (\mathbf{x}'\mathbf{V}^{-1}\mathbf{x})^{-1}\mathbf{x}'\mathbf{V}^{-1}\mathbf{y}, \qquad \operatorname{var}(\tilde{\beta}) = (\mathbf{x}'\mathbf{V}^{-1}\mathbf{x})^{-1}, \tag{12b}$$

where "var" refers to the variance. Now we have $\operatorname{var}(\tilde{\beta}) \le \operatorname{var}(\hat{\beta})$, i.e.

$$(\mathbf{x}'\mathbf{V}^{-1}\mathbf{x})^{-1} \le (\mathbf{x}'\mathbf{x})^{-2}\mathbf{x}'\mathbf{V}\mathbf{x}\,, \quad \text{i,e.,} \quad (\mathbf{x}'\mathbf{x})^2 \le \mathbf{x}'\mathbf{V}^{-1}\mathbf{x}\cdot\mathbf{x}'\mathbf{V}\mathbf{x}\,, \tag{13}$$

which is a special case of the famous Cauchy–Schwarz inequality. It is well known that the equality in (13) holds if and only if

$$\mathbf{V}\mathbf{x} = \lambda\mathbf{x}\,, \quad \text{for some } \lambda \in \mathbb{R}\,, \tag{14}$$

and hence $\mathbf{x}$ is an eigenvector of $\mathbf{V}$ corresponding to eigenvalue λ. Condition (14) is just a version of Anderson's (1948) condition for the equality of OLSE and BLUE; see the beginning of Sect. 3 below. Notice that putting $\mathbf{x} = \mathbf{1}$, a vector of ones, shows that the arithmetic mean $\bar{y}$ is BLUE whenever $\mathbf{V}$ has its row totals equal, i.e. $\mathbf{V1} = \lambda\mathbf{1}$ for some scalar λ.

We might ask how "bad" the OLSE could be with respect to the BLUE. One natural measure for the relative efficiency of OLSE is the ratio of their variances:

$$\phi = \text{eff}(\hat{\beta}) = \frac{\operatorname{var}(\tilde{\beta})}{\operatorname{var}(\hat{\beta})} = \frac{(\mathbf{x}'\mathbf{V}^{-1}\mathbf{x})^{-1}}{(\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}'\mathbf{V}\mathbf{x}(\mathbf{x}'\mathbf{x})^{-1}} = \frac{(\mathbf{x}'\mathbf{x})^2}{\mathbf{x}'\mathbf{V}\mathbf{x}\cdot\mathbf{x}'\mathbf{V}^{-1}\mathbf{x}}\,. \tag{15}$$

Clearly, we have $0 < \phi \le 1$, where the upper bound is obtained if and only if OLSE equals BLUE. The lower bound of ϕ can be obtained from the Kantorovich inequality; see, e.g. Watson et al. (1997),

$$\tau_1^2 := \frac{4\lambda_1\lambda_n}{(\lambda_1+\lambda_n)^2} \le \frac{(\mathbf{x}'\mathbf{x})^2}{\mathbf{x}'\mathbf{V}\mathbf{x}\cdot\mathbf{x}'\mathbf{V}^{-1}\mathbf{x}} = \text{eff}(\hat{\beta}) = \phi\,, \tag{16}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$ are the eigenvalues of $\mathbf{V}$. The lower bound is obtained when $\mathbf{x}$ is proportional either to $\mathbf{t}_1 + \mathbf{t}_n$ or to $\mathbf{t}_1 - \mathbf{t}_n$; in short, $\mathbf{x}$ is proportional to $\mathbf{x}_{\text{bad}} = \mathbf{t}_1 \pm \mathbf{t}_n$, where $\mathbf{T} = (\mathbf{t}_1 : \mathbf{t}_2 : \ldots : \mathbf{t}_n)$ is the matrix with $\mathbf{t}_i$ being the orthonormal eigenvectors of $\mathbf{V}$ corresponding to eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. □

Consider then the covariance matrices of OLSE and BLUE when $\mathbf{X}$ has a full column rank and $\mathbf{V}$ is positive definite. Then under $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$,

$$\text{cov}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}, \quad \text{cov}(\tilde{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}, \tag{17}$$

and we have the Löwner ordering

$$(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} \leq_{\text{L}} (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}. \tag{18}$$

If $\mathbf{X}$ does not have a full column rank then $\mathbf{X}\tilde{\boldsymbol{\beta}} = \tilde{\boldsymbol{\mu}} = \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$ and

$$\text{cov}(\tilde{\boldsymbol{\mu}}) = \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}' \leq_{\text{L}} \mathbf{H}\mathbf{V}\mathbf{H} = \text{cov}(\hat{\boldsymbol{\mu}})\,. \tag{19}$$

What is now interesting is that the difference $\text{cov}(\hat{\boldsymbol{\beta}}) - \text{cov}(\tilde{\boldsymbol{\beta}})$ has an alternative representation, expressed in Theorem 2 below. Among the first places where Theorem 2 occurs are probably the papers by Khatri (1966, Lemma 1) and Rao (1967, Lemmas 2a–2c); see also Rao (1973a, Problem 33, p. 77).

Theorem 2 *Consider the linear model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$*, where* $\mathbf{X}$ *has full column rank and* $\mathbf{V}$ *is positive definite, and denote* $\mathbf{H} = \mathbf{P}_{\mathbf{X}}$, $\mathbf{M} = \mathbf{I}_n - \mathbf{H}$. *Then*

(a) $\text{cov}(\tilde{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} = (\mathbf{X}'\mathbf{X})^{-1}[\mathbf{X}'\mathbf{V}\mathbf{X} - \mathbf{X}'\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}\mathbf{X}](\mathbf{X}'\mathbf{X})^{-1}$
$= \mathbf{X}^{+}[\mathbf{V} - \mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}](\mathbf{X}^{+})'$
$= \text{cov}(\hat{\boldsymbol{\beta}}) - (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$,

(b) $\text{cov}(\hat{\boldsymbol{\beta}}) - \text{cov}(\tilde{\boldsymbol{\beta}}) = \mathbf{X}^{+}\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}(\mathbf{X}^{+})'$,

(c) $\text{cov}(\hat{\boldsymbol{\mu}}) - \text{cov}(\tilde{\boldsymbol{\mu}}) = \mathbf{H}\mathbf{V}\mathbf{H} - \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}' = \mathbf{H}\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}\mathbf{H}$,

(d) $\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1} = \mathbf{I}_n - \mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M} = \mathbf{H} - \mathbf{H}\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}$.

In (c) *and* (d) *the matrix* $\mathbf{X}$ *does not need to have full column rank.*

Actually, instead of $\mathbf{M}$, Rao (1967, Lemmas 2a–2c) used a full column rank matrix $\mathbf{Z}$ spanning $\mathscr{C}(\mathbf{X})^{\perp}$. Thus, for example,

$$(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1} = \mathbf{X}^{+} - \mathbf{X}^{+}\mathbf{V}\mathbf{Z}(\mathbf{Z}'\mathbf{V}\mathbf{Z})^{-1}\mathbf{Z}'. \tag{20}$$

It is noteworthy that for a positive definite $\mathbf{V}$ we have

$$\begin{aligned}\dot{\mathbf{M}} :&= \mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M} = \mathbf{V}^{-1/2}\mathbf{P}_{\mathbf{V}^{1/2}\mathbf{M}}\mathbf{V}^{-1/2} \\ &= \mathbf{V}^{-1/2}(\mathbf{I}_n - \mathbf{P}_{\mathbf{V}^{-1/2}\mathbf{X}})\mathbf{V}^{-1/2} = \mathbf{V}^{-1}(\mathbf{I}_n - \mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}})\,.\end{aligned} \tag{21}$$

Thus, the BLUE's residual can be expressed as $\mathbf{y} - \tilde{\boldsymbol{\mu}} = \mathbf{V}\dot{\mathbf{M}}\mathbf{y}$ and the "weighted sum of squares of errors" is

$$\mathrm{SSE}(\mathbf{V}) = (\mathbf{y} - \tilde{\boldsymbol{\mu}})'\mathbf{V}^{-1}(\mathbf{y} - \tilde{\boldsymbol{\mu}}) = \mathbf{y}'\dot{\mathbf{M}}\mathbf{y}\,, \tag{22}$$

while the corresponding quantity in model $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{I}_n\}$ is $\mathrm{SSE}(\mathbf{I}) = \mathbf{y}'\mathbf{M}\mathbf{y}$.

What does it mean to have the equality OLSE = BLUE? There is no problem if this equality is interpreted as a short version of the phrase "**Hy** has the minimal covariance matrix in the sense of Definition 1". On the other hand, for example, in the full rank model, we might ask what is the "real meaning" of the equality

$$\mathbf{H}\mathbf{y} = \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} = \mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}}\mathbf{y}\,? \tag{23}$$

Estimator $\mathbf{H}\mathbf{y}$ is a random vector as is $\mathbf{P}_{\mathbf{X};\mathbf{V}^{-1}}\mathbf{y}$; this is so before observing $\mathbf{y}$. The equality of two random vectors requires a specific definition and the essential matter is how the set of possible realized values of the response variable $\mathbf{y}$ is defined. Notice that we do not make a notational difference between the random vector $\mathbf{y}$ and its realized value.

The model $\mathscr{M}$ is said to be *consistent* if the observed value of $\mathbf{y}$ lies in $\mathscr{C}(\mathbf{X} : \mathbf{V})$:

$$\mathbf{y} \in \mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathscr{C}(\mathbf{X} : \mathbf{V}\mathbf{X}^{\perp}) = \mathscr{C}(\mathbf{X} : \mathbf{V}\mathbf{M}) = \mathscr{C}(\mathbf{X}) \oplus \mathscr{C}(\mathbf{V}\mathbf{M})\,, \tag{24}$$

where $\oplus$ refers to the direct sum. For the equality $\mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathscr{C}(\mathbf{X} : \mathbf{V}\mathbf{M})$, see, e.g. Rao (1974, Lemma 2.1). Let $\mathbf{A}$ and $\mathbf{B}$ be $m \times n$ matrices. Then, in the consistent model $\mathscr{M}$, the estimators $\mathbf{A}\mathbf{y}$ and $\mathbf{B}\mathbf{y}$ are said to be equal with probability 1 if

$$\mathbf{A}\mathbf{y} = \mathbf{B}\mathbf{y} \quad \text{for all } \mathbf{y} \in \mathscr{C}(\mathbf{X} : \mathbf{V})\,, \quad \text{i.e.,} \quad \mathbf{A}(\mathbf{X} : \mathbf{V}) = \mathbf{B}(\mathbf{X} : \mathbf{V})\,, \tag{25}$$

which further can be written as $\mathbf{A}(\mathbf{X} : \mathbf{V}\mathbf{M}) = \mathbf{B}(\mathbf{X} : \mathbf{V}\mathbf{M})$. Often we drop off the phrase "with probability 1". In (23) the vector $\mathbf{y}$ varies through $\mathscr{C}(\mathbf{X} : \mathbf{V}) = \mathbb{R}^n$ and thus (23) becomes the equality between the multipliers $\mathbf{H}$ and $\mathbf{P}_{\mathbf{X},\mathbf{V}^{-1}}$. For the consistency of the linear model, see, e.g. Rao (1973a, p. 297), and Baksalary et al. (1992).

We will use short notations like $\mathbf{A}\mathbf{y} = \mathrm{BLUE}(\boldsymbol{\mu} \mid \mathscr{M}) = \tilde{\boldsymbol{\mu}} = \tilde{\boldsymbol{\mu}}(\mathscr{M})$. Thus, the equality $\mathrm{OLSE}(\boldsymbol{\mu}) = \mathrm{BLUE}(\boldsymbol{\mu})$, i.e. $\hat{\boldsymbol{\mu}} = \tilde{\boldsymbol{\mu}}$ means that

$$\mathbf{H}\mathbf{y} = \mathbf{A}\mathbf{y} \quad \text{for all } \mathbf{y} \in \mathscr{C}(\mathbf{X} : \mathbf{V})\,, \tag{26}$$

where $\mathbf{A}$ is a matrix providing the $\tilde{\boldsymbol{\mu}}$. There is an infinite number of such matrices $\mathbf{A}$ when $\mathrm{rank}(\mathbf{X} : \mathbf{V}) < n$, but under a consistent model the realized value of $\mathbf{A}\mathbf{y}$ is unique.

Example 2 (*Equality of OLSE and* $\mathbf{P}_{\mathbf{X};\mathbf{V}^{+}}\mathbf{y}$) Denoting $\mathbf{P}_{\mathbf{X};\mathbf{V}^{+}} = \mathbf{X}(\mathbf{X}'\mathbf{V}^{+}\mathbf{X})^{+}\mathbf{X}'\mathbf{V}^{+}$, one might be curious to know under which condition $\mathbf{P}_{\mathbf{X};\mathbf{V}^{+}}\mathbf{y}$ equals $\hat{\boldsymbol{\mu}}$ (w.p. 1). This happens if and only if $\mathbf{X}(\mathbf{X}'\mathbf{V}^{+}\mathbf{X})^{+}\mathbf{X}'\mathbf{V}^{+}(\mathbf{X} : \mathbf{V}) = \mathbf{H}(\mathbf{X} : \mathbf{V})$, i.e.

$$\text{(i)}\ \ \mathbf{X}(\mathbf{X}'\mathbf{V}^{+}\mathbf{X})^{+}\mathbf{X}'\mathbf{V}^{+}\mathbf{X} = \mathbf{X}\,, \quad \text{and} \quad \text{(ii)}\ \ \mathbf{X}(\mathbf{X}'\mathbf{V}^{+}\mathbf{X})^{+}\,\mathbf{X}'\mathbf{P}_{\mathbf{V}} = \mathbf{H}\mathbf{V}. \tag{27}$$

Postmultiplying (ii) in (27) by $\mathbf{V}^{+}\mathbf{X}$ and using (i) yields $\mathbf{X} = \mathbf{H}\mathbf{P}_{\mathbf{V}}\mathbf{X}$ and thereby $\mathbf{X}'\mathbf{X} = \mathbf{X}'\mathbf{P}_{\mathbf{V}}\mathbf{X}$, i.e. $\mathbf{X}'\mathbf{Q}_{\mathbf{V}}\mathbf{X} = \mathbf{0}$, so that $\mathscr{C}(\mathbf{X}) \subseteq \mathscr{C}(\mathbf{V})$. This is the result obtained by Baksalary and Kala (1983). It becomes particularly interesting if we utilize the following fact, see Zyskind and Martin (1969) and Mitra and Rao (1968, p. 286):

$$\mathbf{X}(\mathbf{X}'\mathbf{V}^{+}\mathbf{X})^{+}\mathbf{X}'\mathbf{V}^{+}\mathbf{y} = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta}) \iff \mathscr{C}(\mathbf{X}) \subseteq \mathscr{C}(\mathbf{V})\,. \tag{28}$$

This means that $\mathbf{P}_{\mathbf{X};\mathbf{V}^{+}}\mathbf{y}$ equals $\hat{\boldsymbol{\mu}}$ only if they equal $\tilde{\boldsymbol{\mu}}$. The model where $\mathscr{C}(\mathbf{X}) \subseteq \mathscr{C}(\mathbf{V})$, is often called a *weakly singular* linear model. Actually then $\mathbf{P}_{\mathbf{X};\mathbf{V}^{+}}\mathbf{y}$ is invariant for any choice of generalized inverses involved. □

3 Year 1967: a Good One for the OLSE = BLUE

As noted by Puntanen and Styan (1989, p. 154), the first condition for the equality between OLSE and BLUE of $\mathbf{X}\boldsymbol{\beta}$ was obtained by Anderson (1948, p. 92):

> Let $\mathbf{X}$ and $\mathbf{V}$ have full rank. If the p columns of the $n \times p$ matrix $\mathbf{X}$ are linear combinations of p of the eigenvectors of $\mathbf{V}$, then OLSE is BLUE.

Anderson's result was published in *Skandinavisk Aktuarietidskrift* (from 1973: *Scandinavian Actuarial Journal*), and as Anderson says in his interview in *Statistical Science* (DeGroot 1986, p. 102): "As a result it did not get a great deal of attention … So from time to time people discover that paper."

That Anderson's condition is also necessary may be deduced from results obtained by Watson (1951, 1955). Watson was discussing the efficiency of OLSE showing the necessity of Anderson's condition for $p = 1$.

Magness and McGuire (1962) appear to be the first to show that this condition is both necessary and sufficient, though Anderson (1972, p. 472) mentioned that sufficiency was essentially given in his (Anderson 1948) paper. Interestingly, Magness and McGuire (1963) published the following "Acknowledgment of priority":

> Theorem 2 of the authors' paper (Magness and McGuire 1962) is a special case of Eq. (3.5) of Watson (1955). Also, the fact that least squares and minimum variance estimates are equally efficient when the regression vectors are eigenvectors of the noise covariance matrix is apparently known and is referred to by Watson. The authors regret having overlooked Professor Watson's outstanding prior contribution.

It seems that Zyskind, in an invited paper presented at the 1962 Institute of Mathematical Statistics Annual Meeting, was the first author to consider the equality of the OLSE and BLUE when $\mathbf{X}$ has rank less than p, see Zyskind (1962) which is an abstract of his talk. The covariance matrix was still assumed positive definite.

Goldman and Zelen (1964) allowed the covariance matrix $\mathbf{V}$ to be possibly singular; they obtained a similar eigenvector condition to that of Anderson (1948), namely $\mathscr{C}(\mathbf{X}) = \mathscr{C}(\mathbf{T}_{[r]})$ where $\mathbf{T}_{[r]}$ is an $n \times r$ matrix whose columns are the r eigenvectors corresponding to r nonzero eigenvalues of $\mathbf{V}$ with $r = \mathrm{rank}(\mathbf{X})$. As shown later by Zyskind (1967, p. 1098), the nonzero requirement is not needed.

Rao (1967, 1968) appears to be the first to provide further necessary and sufficient conditions for the general case when both $\mathbf{X}$ and $\mathbf{V}$ are possibly deficient in rank. In 1965 at the Fifth Berkeley Symposium, Rao (1967, p. 364) presented the following two conditions, each of which is both necessary and sufficient for the equality of the OLSE($\mathbf{X}\boldsymbol{\beta}$) and the BLUE($\mathbf{X}\boldsymbol{\beta}$):

$$\text{(i)}\ \ \mathbf{X}'\mathbf{V}\mathbf{X}^{\perp} = \mathbf{0}\,,\ \text{i.e.,}\ \mathbf{HVM} = \mathbf{0}\,,\quad \text{(ii)}\ \ \mathbf{V} = \alpha\mathbf{I}_n + \mathbf{X}\mathbf{A}\mathbf{X}' + \mathbf{X}^{\perp}\mathbf{B}(\mathbf{X}^{\perp})'\,, \tag{29}$$

for some scalar α and some symmetric $\mathbf{A}$ and $\mathbf{B}$ so that $\mathbf{V}$ is nonnegative definite. It is clear that (i) is equivalent to $\mathscr{C}(\mathbf{V}\mathbf{X}) \subseteq \mathscr{C}(\mathbf{X})$, which becomes equality if $\mathbf{V}$ is positive definite. Rao (1968, p. 68) emphasized that "the basis of the proof is the following: the necessary and sufficient condition that a statistic is a minimum variance unbiased estimator is that it has zero covariance with statistics whose expectation is identically zero (Rao 1965, pp. 185, 257) [referring to the first edition of Rao 1973a]."

Notice that the case (ii) of (29), which is sometimes called "Rao's structure", occurs in the mixed linear model, where $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{X}\mathbf{u} + \mathbf{X}^{\perp}\mathbf{v} + \mathbf{e}$, and $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{e}$ are uncorrelated random vectors with zero expectations and covariance matrices $\boldsymbol{\Gamma}$, $\boldsymbol{\Theta}$, and $\sigma^2\mathbf{I}_n$, respectively. See also Mitra and Rao (1969) for properties of specific structures of V.

Zyskind (1967, Theorem 2) who referred to Rao (1967), gave, without any restrictive rank assumptions, eight necessary and sufficient conditions under which OLSE is BLUE, thus extending the results he gave in Zyskind (1962). Kempthorne (1975), in the obituary for Zyskind (1929–1974), writes:

> Zyskind's interest in the method of least squares led to a rather remarkable set of papers. …A subsequent (Zyskind 1967) paper laid out the bulk of the story with respect to equality of OLSE and BLUE. …The importance of this whole line of work is underscored by the occurrence of related work by W. H. Kruskal, C. R. Rao and G. S. Watson, as well as others.

Because Rao gave his paper in 1965 and Zyskind (1967) refers to it, we credit Rao as the first author to have established $\mathbf{HVM} = \mathbf{0}$; see Baksalary and Kala (1983, pp. 119 and 240) and Kempthorne (1976, p. 217). In his Acknowledgements Zyskind (1967) writes: "I wish to thank Professor C. R. Rao for permitting me to see a copy of the final version of his manuscript (Rao 1967) before its publication."

We might cite an interesting piece from Rao's interview by DeGroot (1987, p. 59):

> RAO: There was another incident recently in which somebody claimed priority because he had mentioned a result slightly less general than mine in an abstract in the *Annals*. You can say anything in an abstract. If it is right, you can claim credit and priority.
>
> DEGROOT: Yes. Take a chance; maybe it will be right. There is no serious screening of abstracts. I think that's OK, as long as everyone realizes that the results are not necessarily correct or original.
>
> RAO: Actually when that person wrote the full paper on the basis of the abstract, I was a referee and it turned out that this result was also not correct as stated.

Rao (1968, p. 259) further commented on Zyskind (1967) and Watson (1967) in the following way (in our notation):

> In my previous paper (Rao 1967), I gave details of the proof of (29) when $\mathbf{V}$ and $\mathbf{X}'\mathbf{X}$ are nonsingular and mentioned that the same proof holds more generally for singular $\mathbf{V}$ and $\mathbf{X}'\mathbf{X}$. I omitted the details in the latter as the extension was extremely simple, and not relevant to the main theme of the paper.
>
> In a recent paper, Zyskind (1967) thought that there may be some difficulty in proving the condition (29) in its widest generality when $\mathbf{V}$ is singular. Watson (1967) writes that, "Rao (1965) [referring to the Fifth Berkeley Symposium] remarks that his result is true for $\mathbf{V}$ singular and rank of $\mathbf{X}$ is below p. Some skill with generalized inverses might show the proof is still valid." In view of these remarks and other statements it seems necessary to elaborate the earlier proof.

An early description of the coordinate-free approach to linear models was made by Kruskal (1961, 1968). Watson (1967, p. 1682) wrote:

> In some 1962 correspondence with Dr. M. E. Muller and the author, Professor W. Kruskal indicated a coordinate-free proof of the necessity and sufficiency when $\mathbf{X}$, but not $\mathbf{V}$, is possibly not of full rank. This result is particularly simple to prove because, instead of working with $\hat{\boldsymbol{\beta}}$ and $\tilde{\boldsymbol{\beta}}$ he uses $\hat{\boldsymbol{\mu}} = \mathbf{X}\hat{\boldsymbol{\beta}}$ and $\tilde{\boldsymbol{\mu}} = \mathbf{X}\tilde{\boldsymbol{\beta}}$. He states that "$\hat{\boldsymbol{\mu}} = \tilde{\boldsymbol{\mu}}$ if and only if $\mathscr{C}(\mathbf{VX}) = \mathscr{C}(\mathbf{X})$". The author hopes that Professor Kruskal's result will appear in the near future.

In an interview by Zabell (1994, p. 294), Kruskal mentions, referring to his (Kruskal 1968) paper: "That started out as an exercise, an exam exercise in the course I was giving, and then Geoff Watson came along with much the same material; he encouraged me to try for publication."

Herr (1980, p. 46), in an interesting article "On the history of the use of geometry in the general linear model", commented on various approaches to handle linear models. About Kruskal he writes the following:

> These two papers. Kruskal (1968, 1975), are elegant examples of the analytic geometric approach to linear models. In Kruskal (1968), the question of equality of simple least squares and best linear unbiased estimates, which was considered in Zyskind (1967) and Watson (1967), is treated using a coordinate-free approach. The comparison of the parts of the three papers dealing with this question is very instructive. The simplicity and beauty of the coordinate-free approach is clearly demonstrated by such a comparison.
>
> In Kruskal (1975), an analytic geometric approach is used with such skill and grace that the paper ought to be required reading for anyone who might be tempted to deal with generalized inverses.

Eaton, also a great promoter of the coordinate-free approach, see his papers (Eaton 1970, 1978), wrote in Eaton (2007, p. 265):

> The direct effect of Kruskal (1968), a marvelous paper, is relatively easy to describe. In coordinate-free language, here is a statement of the main result of that paper:
>
> The Gauss–Markov and least squares estimators are the same if and only if the linear manifold of the mean vector is an invariant subspace of the covariance.
>
> [$\mathscr{C}(\mathbf{VX}) \subseteq \mathscr{C}(\mathbf{X})$, in our notation.]

Anderson (1971, p. 563) gave a quite different rank criterion for the equality of OLSE and BLUE in the form of rank-additivity, assuming $\mathbf{V}$ and $\mathbf{X}$ be of full rank. George Styan (1973) extended this criterion by removing the restriction on the

rank of $\mathbf{X}$. Below is George's description (in our notation) on this development, see Baksalary and Styan (2005, p. 16).

> I think that the first paper by Jerzy Baksalary I read was Baksalary and Kala (1977), which I reviewed for *Mathematical Reviews*. In that paper it is shown that in the linear model $\{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$ the best linear unbiased estimator of $\mathbf{X}\boldsymbol{\beta}$ equals the ordinary least-squares estimator if and only if
>
> $$\operatorname{rank}(\mathbf{X}'\mathbf{T}_1) + \operatorname{rank}(\mathbf{X}'\mathbf{T}_2) \cdots + \operatorname{rank}(\mathbf{X}'\mathbf{T}_s) = \operatorname{rank}(\mathbf{X}), \tag{30}$$
>
> where $\mathbf{V}$ has s distinct eigenvalues and $\mathbf{T}_1, \mathbf{T}_2, \ldots, \mathbf{T}_s$ are matrices of corresponding orthonormalized eigenvectors. Here $\mathbf{X}$ can be less than full column rank and $\mathbf{V}$ may be singular. The result for $\mathbf{X}$ possibly of less than full column rank but with $\mathbf{V}$ positive definite was established by me in Styan (1973), extending the earlier result with $\mathbf{X}$ of full column rank and $\mathbf{V}$ positive definite due to Anderson (1971, p. 561).
>
> The paper by Baksalary and Kala (1977) prompted me to read further papers by Baksalary and Kala, and [*…old reminiscences …*] on 27 August 1980 both Jerzy Baksalary and Radoslaw Kala met me at the main railway station in Poznań.

A very different modification of the problem of when the OLSE is the BLUE originates from McElroy (1967). We present it here in a generalized version due to Zyskind (1969) and Baksalary and van Eijnsbergen (1988): Given a matrix $\mathbf{U}$, such that $\operatorname{rank}(\mathbf{U}) \leq n - 1$, when does $\hat{\boldsymbol{\mu}} = \tilde{\boldsymbol{\mu}}$ hold for every model matrix $\mathbf{X}$ satisfying $\mathscr{C}(\mathbf{U}) \subseteq \mathscr{C}(\mathbf{X})$.

We have now more or less covered the development of the OLSE versus BLUE saga up till the end of the 1970s, having the role of Professor Rao in mind. There is a lot of interesting literature after that (as well as before) that we have no space to discuss. However, ‘

- Gouriéroux and Monfort (1980), Baltagi (1989), McAleer (1992) and Larocca (2005) providing econometric examples and references;
- Chapter 8 of Rao and Mitra (1971a), and Mathew and Bhimasankaram (1983a, b) reviewing conditions for optimality and validity of least squares theory;
- Baksalary and Kala (1978, 1980) and Haberman (1975) who studied the Euclidean distance between OLSE and BLUE.

We may also mention Yongge Tian who in numerous papers has studied OLSE versus BLUE matters using so-called matrix rank methods; see, e.g. Tian (2013), Tian and Zhang (2016) and Puntanen et al. (2005).

The model $\mathscr{M}$ can be extended to the case when we wish to predict a “new future” value of $\mathbf{y}_*$, assumed to be coming from $\mathbf{y}_* = \mathbf{X}_*\boldsymbol{\beta} + \boldsymbol{\varepsilon}_*$, where $\mathbf{X}_*$ is a known $q \times p$ matrix and $\boldsymbol{\varepsilon}_*$ is a q-dimensional random error vector. We assume that $\operatorname{cov}(\mathbf{y}, \mathbf{y}_*) = \mathbf{V}_{12}$ is known. For conditions of $\mathbf{A}\mathbf{y}$ being the best linear unbiased predictor, BLUP, for $\mathbf{y}_*$, minimizing the covariance matrix of the prediction error, see, e.g. Goldberger (1962), Christensen (2011, p. 294), and Isotalo and Puntanen (2006, p. 1015). For relations between OLSE, BLUE and BLUP, see, e.g. Watson (1972), Baksalary and Kala (1981b) and Haslett et al. (2014).

We feel it appropriate, though not fully related to OLSE versus BLUE, to complete this section (where the main year was 1967), by mentioning that on 5 April 1967, C. R.

Rao left Calcutta for London and attended the induction ceremony to the Fellowship of the Royal Society, on 6 April 1967. This prompted Professor P. C. Mahalanobis to use the following words in his speech on 12 February 1968, see Mahalanobis (1969, p. 239):

> I should now like to say, briefly, how proud I feel that C. R. Rao was elected a Fellow of the Royal Society last year. He came to the Institute in January 1941 to learn statistics. I feel proud that my direct pupil is now in the Royal Society. In India, we have a saying *Putrat ichhyet parajayam*. One wishes for defeat by his son. I have no children. In India there is also the alternative version *Sishyat ichhyet parajayam*. One wishes for defeat by his pupil. It is my great happiness to admit defeat by my pupil.

4 OLSE = BLUE: Conditions

Theorem 3 *Consider the general linear model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$. *Then* $\mathrm{OLSE}(\mathbf{X}\boldsymbol{\beta}) = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta})$ *if and only if any of the following equivalent conditions holds.* (*Note:* $\mathbf{V}$ *is replaceable with* $\mathbf{V}^+$ *and* $\mathbf{H}$ *and* $\mathbf{M}$ *can be interchanged.*)

(i) $\mathbf{HV} = \mathbf{VH}$, (ii) $\mathbf{HV} = \mathbf{HVH}$, (iii) $\mathbf{HVM} = \mathbf{0}$,
(ii) $\mathbf{X}'\mathbf{V}\mathbf{X}^\perp = \mathbf{0}$, (v) $\mathscr{C}(\mathbf{VX}) \subseteq \mathscr{C}(\mathbf{X})$, (vi) $\mathscr{C}(\mathbf{VX}) = \mathscr{C}(\mathbf{X}) \cap \mathscr{C}(\mathbf{V})$,
(vii) $\mathbf{HVH} \le_{\mathrm{L}} \mathbf{V}$, *i.e.* $\mathbf{V} - \mathbf{HVH}$ *is nonnegative definite,*
(viii) $\mathbf{HVH} \le_{\mathrm{rs}} \mathbf{V}$, *i.e.* $\mathrm{rank}(\mathbf{V} - \mathbf{HVH}) = \mathrm{rank}(\mathbf{V}) - \mathrm{rank}(\mathbf{HVH})$, *i.e.* $\mathbf{HVH}$ *and* $\mathbf{V}$ *are rank-subtractive,*
(ix) $\mathscr{C}(\mathbf{X})$ *has a basis consisting of* r *eigenvectors of* $\mathbf{V}$, *where* $r = \mathrm{rank}(\mathbf{X})$,
(x) $\mathrm{rank}(\mathbf{T}_1'\mathbf{X}) + \cdots + \mathrm{rank}(\mathbf{T}_s'\mathbf{X}) = \mathrm{rank}(\mathbf{X})$, *where* $\mathbf{T}_i$ *is a matrix consisting of the orthogonal eigenvectors w.r.t. the* i*th largest eigenvalue* $\lambda_{(i)}$ *of* $\mathbf{V}$; $\lambda_{(1)} > \cdots > \lambda_{(s)}$,
(xi) $\mathbf{T}_i'\mathbf{H}\mathbf{T}_i = (\mathbf{T}_i'\mathbf{H}\mathbf{T}_i)^2$ *for all* $i = 1, 2, \ldots, s$,
(xii) $\mathbf{T}_i'\mathbf{H}\mathbf{T}_j = \mathbf{0}$ *for all* $i, j = 1, 2, \ldots, s$, $i \neq j$,
(xiii) $\mathscr{C}(\mathbf{T}_i) = \mathscr{C}(\mathbf{T}_i) \cap \mathscr{C}(\mathbf{X}) \oplus \mathscr{C}(\mathbf{T}_i) \cap \mathscr{C}(\mathbf{M})$ *for all* $i = 1, \ldots, s$,
(xiv) *the squared nonzero canonical correlations between* $\mathbf{y}$ *and* $\mathbf{Hy}$ *are the nonzero eigenvalues of* $\mathbf{V}^-\mathbf{HVH}$ *for all* $\mathbf{V}^-$,
(xv) $\mathbf{V} \in \mathcal{V}_1 = \{\, \mathbf{V} \ge_{\mathrm{L}} \mathbf{0} : \mathbf{V} = \mathbf{HAH} + \mathbf{MBM}\,,\ \mathbf{A} \ge_{\mathrm{L}} \mathbf{0}\,,\ \mathbf{B} \ge_{\mathrm{L}} \mathbf{0} \,\}$,
(xvi) $\mathbf{V} \in \mathcal{V}_2 = \{\, \mathbf{V} \ge_{\mathrm{L}} \mathbf{0} : \mathbf{V} = \mathbf{XCX}' + \mathbf{X}^\perp\mathbf{D}(\mathbf{X}^\perp)',\ \mathbf{C} \ge_{\mathrm{L}} \mathbf{0}\,,\ \mathbf{D} \ge_{\mathrm{L}} \mathbf{0} \,\}$,
(xvii) $\mathbf{V} \in \mathcal{V}_3 = \{\, \mathbf{V} \ge_{\mathrm{L}} \mathbf{0} : \mathbf{V} = \alpha\mathbf{I} + \mathbf{XKX}' + \mathbf{X}^\perp\mathbf{L}(\mathbf{X}^\perp)',\ \alpha \in \mathbb{R}\,,\ \mathbf{K} = \mathbf{K}',\ \mathbf{L} = \mathbf{L}' \,\}$.

Some sources for the above statements are given in Sect. 3. For collections of the proofs, see Alalouf and Styan (1984) and Puntanen et al. (2011, Chap. 10). Notice the somewhat peculiar statements (vii), (viii) and (xiv); they appear in Baksalary and Puntanen (1989, 1990a, b). Some further conditions are given by Baksalary et al. (2013, Theorem 5).

Example 3 (*Centering the model*) Consider the partitioned linear model

$$\mathscr{M}_{12} = \{\mathbf{y},\ \mathbf{1}\alpha + \mathbf{X}_0\boldsymbol{\beta}_{\mathbf{x}}\,,\ \mathbf{I}_n\}\,, \quad \text{where } \mathbf{X}_0 \in \mathbb{R}^{n\times k}, \tag{31}$$

and $\mathbf{1} \in \mathbb{R}^n$ is a vector of ones. Assume that $\mathbf{X} = (\mathbf{1} : \mathbf{X}_0)$ has full column rank. Premultiplying $\mathscr{M}_{12}$ by the centering matrix $\mathbf{C} = \mathbf{I}_n - \mathbf{P}_{\mathbf{1}}$ yields the centered model

$$\mathscr{M}_{12\cdot 1} = \{\mathbf{C}\mathbf{y},\ \mathbf{C}\mathbf{X}_0\boldsymbol{\beta}_{\mathbf{x}}\,,\ \mathbf{C}\}\,. \tag{32}$$

In this centered model, we have a singular covariance matrix and hence it may seem that finding a BLUE would be problematic. However, corresponding to condition (v) of Theorem 3 we have now $\mathscr{C}(\mathbf{C}\cdot\mathbf{C}\mathbf{X}_0) \subseteq \mathscr{C}(\mathbf{C}\mathbf{X}_0)$ and thus

$$\text{BLUE}(\boldsymbol{\beta}_{\mathbf{x}} \mid \mathscr{M}_{12\cdot 1}) = \text{OLSE}(\boldsymbol{\beta}_{\mathbf{x}} \mid \mathscr{M}_{12\cdot 1}) = (\mathbf{X}_0'\mathbf{C}\mathbf{X}_0)^{-1}\mathbf{X}_0'\mathbf{C}\mathbf{y} := \hat{\boldsymbol{\beta}}_{\mathbf{x}}\,. \tag{33}$$

On the other hand, it is standard textbook material that $\hat{\boldsymbol{\beta}}_{\mathbf{x}}$ is the BLUE for $\boldsymbol{\beta}_{\mathbf{x}}$ in the partitioned model $\mathscr{M}_{12}$. Thus centering has no effect on the BLUE of $\boldsymbol{\beta}_{\mathbf{x}}$, and so $\mathbf{C}\mathbf{y}$ is a linearly sufficient statistic for $\boldsymbol{\beta}_{\mathbf{x}}$ in $\mathscr{M}_{12}$. Centering is a simple example of the model reduction, i.e. premultiplying $\mathscr{M}_{12} = \{\mathbf{y}, \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2, \mathbf{V}\}$ by $\mathbf{M}_1 = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}_1}$, yielding to

$$\mathscr{M}_{12\cdot 1} = \{\mathbf{M}_1\mathbf{y},\ \mathbf{M}_1\mathbf{X}_2\boldsymbol{\beta}_2,\ \mathbf{M}_1\mathbf{V}\mathbf{M}_1\}\,, \tag{34}$$

see, e.g. Groß and Puntanen (2000) and Chu et al. (2004, 2005). □

Example 4 (*Intraclass correlation*) Consider $\mathbf{V}$ which has the intraclass correlation structure (of which the centering matrix $\mathbf{C}$ is an example), that is, $\mathbf{V}$ is of the type $\mathbf{V} = (1-\varrho)\mathbf{I}_n + \varrho\mathbf{1}\mathbf{1}'$, where $-\frac{1}{n-1} \le \varrho \le 1$. In this situation $\mathbf{H}\mathbf{V} = (1-\varrho)\mathbf{H} + \varrho\mathbf{H}\mathbf{1}\mathbf{1}'$, and thereby $\mathbf{H}\mathbf{V} = \mathbf{V}\mathbf{H}$ if and only if

$$\mathbf{H}\mathbf{1}\mathbf{1}' = \mathbf{1}\mathbf{1}'\mathbf{H}\,. \tag{35}$$

We can conclude that (35) holds if and only if $\mathbf{1}$ is an eigenvector of $\mathbf{H}$, i.e. $\mathbf{H}\mathbf{1} = \lambda\mathbf{1}$. The eigenvalues of $\mathbf{H}$ are 0 and 1, with multiplicities $n - \text{rank}(\mathbf{X})$ and $\text{rank}(\mathbf{X})$, respectively. Hence (35) holds, i.e. OLSE = BLUE, if and only if $\mathbf{1} \in \mathscr{C}(\mathbf{X})$ or $\mathbf{1} \in \mathscr{C}(\mathbf{X})^{\perp}$. □

5 The Fundamental BLUE Equation

Theorem 4 below provides so-called fundamental BLUE equations.

Theorem 4 *Consider the linear model* $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$. *Then the linear estimator* $\mathbf{G}\mathbf{y}$ *is the* BLUE *for* $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ *if and only if* $\mathbf{G} \in \mathbb{R}^{n\times n}$ *satisfies the equation*

$$\mathbf{G}(\mathbf{X} : \mathbf{V}\mathbf{X}^{\perp}) = (\mathbf{X} : \mathbf{0})\,. \tag{36}$$

Moreover, let $\mathbf{K}\boldsymbol{\beta}$*, where* $\mathbf{K} \in \mathbb{R}^{q\times p}$*, be estimable so that* $\mathscr{C}(\mathbf{K}') \subseteq \mathscr{C}(\mathbf{X}')$*. Then* $\mathbf{By}$ *is the* BLUE *of* $\mathbf{K}\boldsymbol{\beta}$ *if and only if* $\mathbf{B} \in \mathbb{R}^{q\times n}$ *satisfies the equation*

$$\mathbf{B}(\mathbf{X} : \mathbf{V}\mathbf{X}^{\perp}) = (\mathbf{K} : \mathbf{0})\,. \tag{37}$$

For the proofs, see, e.g. Rao (1973b, p. 282) and for coordinate-free approach Drygas (1970, p. 55) and Zmyślony (1980). For further proofs see, for example, Groß (2004), Kala (1981, Theorem 3.1), Puntanen et al. (2011), and Puntanen et al. (2011, Theorem 10). Baksalary (2004) provides a proof which he describes as follows: "From the algebraic point of view, the present development seems to be the simplest from among all accessible in the literature till now".

Of course, in (37) and (36) we can replace $\mathbf{X}^{\perp}$ with $\mathbf{M} = \mathbf{I}_n - \mathbf{P}_{\mathbf{X}}$. Equation (36) is always solvable for $\mathbf{G}$ while (37) is solvable whenever $\mathbf{K}\boldsymbol{\beta}$ is estimable. Solutions are unique if and only if $\mathrm{rank}(\mathbf{X} : \mathbf{V}) = n$. The solution for $\mathbf{G}$ satisfying $\mathbf{G}(\mathbf{X} : \mathbf{VM}) = (\mathbf{X} : \mathbf{0})$ can be expressed, for example, in the following ways:

$$\mathbf{G}_1 = (\mathbf{X} : \mathbf{0})(\mathbf{X} : \mathbf{VM})^{-}, \qquad \mathbf{G}_2 = \mathbf{I}_n - \mathbf{VM}(\mathbf{MVM})^{-}\mathbf{M}\,, \tag{38a}$$

$$\mathbf{G}_3 = \mathbf{H} - \mathbf{HVM}(\mathbf{MVM})^{-}\mathbf{M}\,, \qquad \mathbf{G}_4 = \mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}'\mathbf{W}^{-}, \tag{38b}$$

where $\mathbf{W}$ belongs to the class of matrices

$$\mathscr{W} = \{\mathbf{W} \in \mathbb{R}^{n\times n} : \mathbf{W} = \mathbf{V} + \mathbf{XUX}',\ \mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{X} : \mathbf{V})\}\,. \tag{39}$$

In (39), $\mathbf{U}$ can be any $p \times p$ matrix as long as $\mathscr{C}(\mathbf{W}) = \mathscr{C}(\mathbf{X} : \mathbf{V})$ is satisfied; see, e.g. Baksalary et al. (1990a, Theorem 2), Baksalary and Mathew (1990, Theorem 2) and Harville (1997, p. 468). The *general* solution to (36) can be expressed as $\mathbf{G}_i + \mathbf{N}_i\mathbf{Q}_{\mathbf{W}}$ where $\mathbf{N}_i \in \mathbb{R}^{n\times n}$ are free to vary. For the relations between the representations of the BLUEs, see, e.g. Albert (1973), Rao (1978, 1979), Rao and Mitra (1971b) and Searle (1994).

The covariance matrix of the $\tilde{\boldsymbol{\mu}} = \mathrm{BLUE}(\mathbf{X}\boldsymbol{\beta})$ can be expressed as

$$\begin{aligned}\mathrm{cov}(\tilde{\boldsymbol{\mu}}) &= \mathbf{HVH} - \mathbf{HVM}(\mathbf{MVM})^{-}\mathbf{MVH} = \mathbf{V} - \mathbf{VM}(\mathbf{MVM})^{-}\mathbf{MV}\\ &= \mathbf{X}(\mathbf{X}'\mathbf{W}^{-}\mathbf{X})^{-}\mathbf{X}' - \mathbf{XUX}',\end{aligned} \tag{40}$$

where $\mathbf{W} = \mathbf{V} + \mathbf{XUX}' \in \mathscr{W}$; see, e.g. Baksalary et al. (1990a) and Isotalo et al. (2008a, b). Notice that

$$\mathrm{cov}(\hat{\boldsymbol{\mu}} - \tilde{\boldsymbol{\mu}}) = \mathrm{cov}(\hat{\boldsymbol{\mu}}) - \mathrm{cov}(\tilde{\boldsymbol{\mu}}) = \mathbf{HVM}(\mathbf{MVM})^{-}\mathbf{MVH}\,. \tag{41}$$

Corresponding to (22), the weighted sum of squares of errors in the general case is

$$\mathrm{SSE}(\mathbf{W}) = (\mathbf{y} - \tilde{\boldsymbol{\mu}})'\mathbf{V}^{-}(\mathbf{y} - \tilde{\boldsymbol{\mu}}) = \mathbf{y}'\dot{\mathbf{M}}\mathbf{y}\,, \quad \text{where } \dot{\mathbf{M}} = \mathbf{M}(\mathbf{MVM})^{-}\mathbf{M}. \tag{42}$$

Suppose that we have two models $\mathscr{A}_1 = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}_1\}$ and $\mathscr{A}_2 = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}_2\}$, which have different covariance matrices. Then we can ask, for example, what is needed that every representation of the BLUE of $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{A}_1$ remains BLUE under $\mathscr{A}_2$. Mitra and Moore (1973) give a very clear description of the different problems occurring. Let $\mathbf{G}$ be such a matrix that $\mathbf{Gy}$ is the BLUE for $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{A}_1$, Then we say that $\mathbf{Gy}$ remains BLUE under $\mathscr{A}_2$ if the following implication holds:

$$\mathbf{G}(\mathbf{X} : \mathbf{V}_1\mathbf{M}) = (\mathbf{X} : \mathbf{0}) \implies \mathbf{G}(\mathbf{X} : \mathbf{V}_2\mathbf{M}) = (\mathbf{X} : \mathbf{0}) . \tag{43}$$

It appears that every representation of the BLUE for $\mathbf{X}\boldsymbol{\beta}$ under $\mathscr{A}_1$ remains BLUE under $\mathscr{A}_2$ and only if any of the following equivalent conditions hold:

$$\text{(i) } \mathscr{C}(\mathbf{V}_2\mathbf{M}) \subseteq \mathscr{C}(\mathbf{V}_1\mathbf{M}) , \quad \text{(ii) } \mathbf{V}_2 = \alpha\mathbf{V}_1 + \mathbf{X}\mathbf{A}\mathbf{X}' + \mathbf{V}_1\mathbf{M}\mathbf{B}\mathbf{M}\mathbf{V}_1 , \tag{44}$$

for some $\alpha \in \mathbb{R}$, and $\mathbf{A}$ and $\mathbf{B}$ such that $\mathbf{V}_2$ is nonnegative definite. It is clear that even if (44) holds, the covariance matrices of $\mathbf{Gy}$ under $\mathscr{A}_1$ and $\mathscr{A}_2$ may be different; see, e.g. Rao and Mitra (1971b, Chap. 8). For the proof of (44) and related discussion, see, e.g. Mitra and Moore (1973, Theorems 4.1–4.2), and Rao (1968, Lemma 5) and Rao (1971, Theorems 5.2, 5.5). For a special note on the interpretation of (i) for $\mathbf{V}_2 = \mathbf{I}_n$, see Markiewicz et al. (2010).

6 The Relative Efficiency of OLSE

In this section, we follow closely Puntanen et al. (2011, Sect. 10.8) to take a brief look at the relative efficiency of OLSE with respect to the BLUE. Consider the linear model $\mathscr{M} = \{\mathbf{y}, \mathbf{X}\boldsymbol{\beta}, \mathbf{V}\}$, where $\mathbf{X}$ has full column rank and $\mathbf{V}$ is positive definite. Then by Theorem 2,

$$\operatorname{cov}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}, \quad \operatorname{cov}(\tilde{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}, \tag{45a}$$

$$\operatorname{cov}(\hat{\boldsymbol{\beta}}) - \operatorname{cov}(\tilde{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} := \mathbf{D} . \tag{45b}$$

The relative efficiency, so-called Watson efficiency, see Watson (1955, p. 330), of OLSE versus BLUE is defined as the ratio of the determinants of the covariance matrices:

$$\operatorname{eff}(\hat{\boldsymbol{\beta}}) = \frac{|\operatorname{cov}(\tilde{\boldsymbol{\beta}})|}{|\operatorname{cov}(\hat{\boldsymbol{\beta}})|} = \frac{|\mathbf{X}'\mathbf{X}|^2}{|\mathbf{X}'\mathbf{V}\mathbf{X}| \cdot |\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}|} = \frac{|\operatorname{cov}(\hat{\boldsymbol{\beta}}) - \mathbf{D}|}{|\operatorname{cov}(\hat{\boldsymbol{\beta}})|} . \tag{46}$$

We have $0 < \operatorname{eff}(\hat{\boldsymbol{\beta}}) \leq 1$, with $\operatorname{eff}(\hat{\boldsymbol{\beta}}) = 1$ if and only if $\hat{\boldsymbol{\beta}} = \tilde{\boldsymbol{\beta}}$. Moreover, the efficiency can be expressed as

$$\begin{aligned}\text{eff}(\hat{\boldsymbol{\beta}}) &= |\mathbf{I}_p - \mathbf{X}'\mathbf{V}\mathbf{M}(\mathbf{M}\mathbf{V}\mathbf{M})^{-}\mathbf{M}\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{V}\mathbf{X})^{-1}| = |[\text{cov}(\hat{\boldsymbol{\beta}})]^{-1} \cdot \text{cov}(\tilde{\boldsymbol{\beta}})| \\ &= (1-\kappa_1^2)\cdots(1-\kappa_p^2) = \theta_1^2 \cdots \theta_p^2\,, \end{aligned} \tag{47}$$

where $\kappa_1 \geq \kappa_2 \geq \cdots \geq \kappa_p \geq 0$ and $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_p > 0$ are the canonical correlations between $\mathbf{X}'\mathbf{y}$ and $\mathbf{M}\mathbf{y}$, and $\hat{\boldsymbol{\beta}}$ and $\tilde{\boldsymbol{\beta}}$, respectively. Notice that

$$\text{cov}\begin{pmatrix}\hat{\boldsymbol{\beta}} \\ \tilde{\boldsymbol{\beta}}\end{pmatrix} = \begin{pmatrix}\text{cov}(\hat{\boldsymbol{\beta}}) & \text{cov}(\tilde{\boldsymbol{\beta}}) \\ \text{cov}(\tilde{\boldsymbol{\beta}}) & \text{cov}(\tilde{\boldsymbol{\beta}})\end{pmatrix} = \begin{pmatrix}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} & (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} \\ (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} & (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\end{pmatrix}, \tag{48}$$

and thus the squared canonical correlations between $\hat{\boldsymbol{\beta}}$ and $\tilde{\boldsymbol{\beta}}$ are the eigenvalues of the matrix product $[\text{cov}(\hat{\boldsymbol{\beta}})]^{-1}\,\text{cov}(\tilde{\boldsymbol{\beta}})[\text{cov}(\tilde{\boldsymbol{\beta}})]^{-1}\,\text{cov}(\tilde{\boldsymbol{\beta}})$:

$$\{\theta_1^2, \ldots, \theta_p^2\} = \text{ch}\big[[\text{cov}(\hat{\boldsymbol{\beta}})]^{-1}\,\text{cov}(\tilde{\boldsymbol{\beta}})\big]\,, \tag{49}$$

where $\text{ch}(\cdot)$ denotes the set of the eigenvalues of the matrix argument. On account of (49), we see, as claimed in (47), that indeed

$$\theta_1^2 \cdots \theta_p^2 = |[\text{cov}(\hat{\boldsymbol{\beta}})]^{-1} \cdot \text{cov}(\tilde{\boldsymbol{\beta}})|\,. \tag{50}$$

The efficiency formulas (47) in terms of κ_i's and θ_i's were first introduced by Watson (1967, p. 1686) and by Bartmann and Bloomfield (1981), respectively. It can be shown that the nonzero canonical correlations between $\mathbf{X}'\mathbf{y}$ and $\mathbf{M}\mathbf{y}$ are the same as those between $\mathbf{H}\mathbf{y}$ and $\mathbf{M}\mathbf{y}$. For further references on the relative efficiency and canonical correlations, see, e.g. Chu et al. (2004, 2005) and Drury et al. (2002).

As regards the lower bound of the OLSE's efficiency, Bloomfield and Watson (1975) and Knott (1975) proved the following inequality:

$$\text{eff}(\hat{\boldsymbol{\beta}}) \geq \frac{4\lambda_1\lambda_n}{(\lambda_1+\lambda_n)^2} \cdot \frac{4\lambda_2\lambda_{n-1}}{(\lambda_2+\lambda_{n-1})^2} \cdots \frac{4\lambda_p\lambda_{n-p+1}}{(\lambda_p+\lambda_{n-p+1})^2} = \tau_1^2\,\tau_2^2 \cdots \tau_p^2\,, \tag{51}$$

where $\lambda_i = \text{ch}_i(\mathbf{V}) = i$th largest eigenvalue and $\tau_i = i$th *antieigenvalue* of $\mathbf{V}$; it is assumed that $p \leq n/2$. The concept of antieigenvalue was introduced by Gustafson (1972); see also Gustafson (2006, 2012) and Rao (2007).

Assuming that $p \leq n/2$, the minimum of ϕ is attained when $\mathbf{X}$ is chosen as $(\mathbf{t}_1 \pm \mathbf{t}_n : \mathbf{t}_2 \pm \mathbf{t}_{n-1} : \ldots : \mathbf{t}_p \pm \mathbf{t}_{n-p+1})$, where $\mathbf{t}_i$ are the orthonormal eigenvectors of $\mathbf{V}$ with respect to λ_i. The inequality (51) was originally conjectured in 1955 by Durbin (see Watson 1955, p. 331), but first established (for $p > 1$) only twenty years later by Bloomfield and Watson (1975) and Knott (1975). For further proofs (and related considerations), see Khatri and Rao (1981, 1982).

Another measure of efficiency of OLSE, introduced by Bloomfield and Watson (1975), is based on the Frobenius norm of the commutator $\mathbf{H}\mathbf{V} - \mathbf{V}\mathbf{H}$:

$$\psi = \tfrac{1}{2}\|\mathbf{H}\mathbf{V} - \mathbf{V}\mathbf{H}\|_F^2 = \tfrac{1}{2}\,\text{trace}(\mathbf{H}\mathbf{V} - \mathbf{V}\mathbf{H})(\mathbf{H}\mathbf{V} - \mathbf{V}\mathbf{H})' = \|\mathbf{H}\mathbf{V}\mathbf{M}\|_F^2\,. \tag{52}$$

Bloomfield and Watson (1975) proved that $\psi \leq \frac{1}{4}\sum_{i=1}^{p}(\lambda_i - \lambda_{n-i-1})^2$, and that the equality is attained in the same situation as the minimum of ϕ.

Rao (1985a) studied the trace of the difference between the covariance matrices of the OLSE and BLUE of $\mathbf{X}\boldsymbol{\beta}$:

$$\eta = \text{trace}[\text{cov}(\mathbf{X}\hat{\boldsymbol{\beta}}) - \text{cov}(\mathbf{X}\tilde{\boldsymbol{\beta}})] = \text{trace}[\mathbf{HVH} - \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}']\,. \tag{53}$$

Styan (1983) considered (53) when $p = 1$ and Liski et al. (1992) considered the upper bound of the trace of $\mathbf{HVM}(\mathbf{MVM})^{-}\mathbf{MVH}$.

We can now conveniently complete this section with a somewhat curious remark. Namely, in the references of Rao (1985a, p. 255), it is said: "Simo Puntanen, Personal communication, 1982." The story behind is that Simo indeed was communicating with Professor Rao about the upperbound of (53) explaining it to be a tough problem. So, Professor Rao conveniently decided to solve the problem.

7 Personal Glimpses and Conclusions

The matrix algebra related to matters like the equality of OLSE and BLUE is not apparently everybody's cup of tea and some discussion in the literature appears to be rather critical. One of the most critical is by Kempthorne (1989) writing as his comment on Puntanen and Styan (1989): "I suggest that Zyskind and Rao gave the bulk of the story and that the flood of papers since their work has added only trivially, arcanely, and (usually) uselessly." Sengupta and Jammalamadaka (2003, p. 311) agreed with Kempthorne's criticism. Searle (1989), however, gives some supporting remarks on the importance of the OLSE versus BLUE topic and according to Harville (1990), "Puntanen and Styan's (1989) article should be very useful to anyone with an interest in linear-model theory". Baksalary (1988, p. 98) states that "The importance of this problem is due to the fact that such conditions characterize which (unknown) dispersion structures can be ignored without consequence to best linear unbiased estimation."

In any event, we still find this area offering unexpected and interesting matrix problems. Over the years, in our teaching (not only in research) we have attempted to make our students familiar with the matrix algebra related to OLSE and BLUE matters: we have found it very educational. One evidence of our interest is the book *Formulas Useful for Linear Regression Analysis and Related Matrix Theory: It's Only Formulas But We Like Them*, by Puntanen et al. (2013).

When DeGroot (1987, p. 60) asked Professor Rao for his favourite publications, part of the answer was the following:

> Rao: …A second set of papers I like are mostly in the analysis of repeated measurements and in singular linear models, i.e., when the design and covariance matrices are deficient in rank. I developed generalized inverses of matrices for dealing with such problems. …

There is some important interesting personal history between the authors and Professor Rao that we briefly wish to mention. First, while spending his sabbatical in Finland from September 1975 to August 1976, the third author, George, visited C. R. Rao in spring 1976 in New Delhi. He sent a postcard to Simo:

> En route, Calcutta – Bombay, 27 March 1976. Unbelievable that we've been gone six weeks already & will be back in two. Spent a hectic month in Delhi; wrote two papers. Hope C. R. Rao will visit Helsinki in mid-June. Relaxed for three days in Kathmandu, …Greetings, George.

C. R. Rao did not come to Finland in 1976 but indeed he did so in 1983, 1985, 1987 (twice), and 1990. He attended three conferences organized in Tampere and in 1985 received an Honorary Ph.D. In June 1987 he attended a conference but in January he was an opponent on the thesis defence of Simo. The thesis was entitled "On the Relative Goodness of Ordinary Least Squares Estimation in the General Linear Model"; see Puntanen (1987).

Actually Simo met C. R. Rao for the first time in Sheffield, UK, in August 1982, at the first ICOTS Conference (see the website), which George also attended. During this conference Simo invited C. R. Rao to be a keynote speaker in a statistical conference in Tampere in 1983. Rao replied: "I'll come if you George will come too." So they both certainly came—and wrote papers for the *Proceedings*, see Rao (1985b) and Styan (1985).

The first author of the present paper, Augustyn Markiewicz, has two joint articles with C. R. Rao, published in Baksalary et al. (1992, 1995). The third coauthor of those papers was Jerzy K. Baksalary (1944–2005), a prolific Polish linear algebra and linear models lover. Those papers deal with the admissibility concept and the consistency of the linear model; see also C. R. Rao's comments on Jerzy's career in Baksalary and Styan (2005, p. 16).

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Comparison of Local Powers of Some Exact Tests for a Common Normal Mean with Unequal Variances

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Abstract The inferential problem of drawing inference about a common mean μ of several independent normal populations with unequal variances has drawn universal attention, and there are many exact and asymptotic tests for testing a null hypothesis $H_0 : \mu = \mu_0$ against two-sided alternatives. In this paper we provide a review of some of these exact and asymptotic tests and present theoretical expressions of local powers of the exact tests and a comparison. It turns out that, in the case of equal sample size, a uniform comparison and ordering of the exact tests based on their local power can be carried out even when the variances are unknown. Our observation is that both modified F and modified t tests based on a suitable combination of component F and t statistics perform the best in terms of local power among all exact tests under consideration. An exact test based on inverse normal method of combination of P-values also performs reasonably well.

Keywords Common mean · Exact test · Local power · Meta-analysis · P-value

Disclaimer: This article is released to inform interested parties of ongoing research and to encourage discussion. The views expressed are those of the authors and not those of the U.S. Census Bureau.

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Table 1 Percentage of albumin in plasma protein of four different experiments

Experiment	n_i	Mean	Variance
A	12	62.3	12.99
B	15	60.3	7.84
C	7	59.5	33.43
D	16	61.5	18.51

Table 2 Selenium content in nonfat milk powder using four methods

Method	n_i	Mean	Variance
Atomic absorption spectrometry	8	105.0	85.71
Neutron activation: instrumental	12	109.8	20.75
Neutron activation: radiochemical	14	109.5	2.73
Isotope dilution mass spectrometry	8	113.3	33.64

1 Introduction

The inferential problem of drawing inference about a common mean μ of several independent normal populations with unequal variances has drawn universal attention, and there are many exact tests for testing a null hypothesis $H_0 : \mu = \mu_0$ against two-sided alternatives $H_1 : \mu \neq \mu_0$. In this paper we provide a review of their local powers and a comparison.

A well-known context of this problem occurred when Meier (1953) was approached to draw inference about the mean of albumin in plasma protein in human subjects based on results from four experiments, reproduced below (Table 1).

Another scenario happened when Eberhardt et al. (1989) had results from four experiments about nonfat milk powder and the problem was to draw inference about the mean Selenium in nonfat milk powder by combining the results from four methods (Table 2).

A similar situation arises in the context of environmental data analysis when upon identifying a hot-spot in a contaminated area, samples are drawn and sent to several labs simultaneously and then the resulting data are combined for eventual analysis. This parallel data analysis is especially important for subsequent adoption of remedial actions in case the mean contamination level at the site is found to exceed a certain threshold.

A possible application scenario at the Census Bureau may arise if there is a need to draw inference about average wage of college graduates in a specified age group in a certain state. County level information can be collected from each county via simple random sampling. Then under a model-based approach with a common overall mean wage across the state and heterogeneous county level variances, the results developed in this paper can be useful. Of course, in case of complex surveys involving survey weights, our current formulation of the inference problem will not be applicable.

A general formulation of the problem can be stated as follows. There are k normal populations with a common mean μ and different variances $\sigma_1^2, \cdots, \sigma_k^2$. Based on a sample of size n_i from the i^{th} population, we want to test $H_0 : \mu = \mu_0$ versus $H_1 : \mu \neq \mu_0$. Obviously, there exist k independent t-tests based on $t_i = \frac{\sqrt{n_i}(\bar{X}_i - \mu_0)}{S_i}$ that follows central t distribution with ν_i degrees of freedom. Note that the assumption of normality is crucial in our subsequent discussion. Most meta-analysis applications are based on this assumption (Hartung et al. 2008).

The natural meta-analysis question now is: how to combine the results from the k independent t-tests? As one can expect, there are many ways of accomplishing this task based on some exact and some asymptotic procedures. Let us first briefly review the asymptotic procedures for testing hypothesis about common mean μ.

In the trivial case when the k population variances are completely known, the common mean μ can easily be estimated using the maximum likelihood estimator $\hat{\mu} = [\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} \bar{X}_i][\sum_{j=1}^{k} \frac{n_j}{\sigma_j^2}]^{-1}$ with $Var(\hat{\mu}) = \left[\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2}\right]^{-1}$. This estimator $\hat{\mu}$ is the minimum variance unbiased estimator under normality as well as the best linear unbiased estimator without normality for estimating μ. A simple test based on standard normal z is obvious in this case.

However, in most cases, the population variances are unknown and a familiar estimate, known as the Graybill–Deal estimate can be used (Graybill and Deal 1959). This unbiased estimator $\hat{\mu}_{GD}$ together with its variance are given as

$$\hat{\mu}_{GD} = \frac{\sum_{i=1}^{k} \frac{n_i}{S_i^2} \bar{X}_i}{\sum_{j=1}^{k} \frac{n_j}{S_j^2}} \quad \text{with} \quad Var(\hat{\mu}_{GD}) = E\left[\left(\sum_{i=1}^{k} \frac{n_i \sigma_i^2}{S_i^4}\right) \Big/ \left(\sum_{i=1}^{k} \frac{n_i}{S_i^2}\right)^2\right].$$

Khatri and Shah (1974) proposed exact variance expression for $\hat{\mu}_{GD}$, which is complicated and cannot be easily implemented. To address this inferential problem, Meier (1953) derived a first-order approximation of the variance of $\hat{\mu}_{GD}$ as

$$Var(\hat{\mu}_{GD}) = \left[\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2}\right]^{-1} \left[1 + 2\sum_{i=1}^{k} \frac{1}{n_i - 1} c_i(1 - c_i) + O\left(\sum_{i=1}^{k} \frac{1}{(n_i - 1)^2}\right)\right]; c_i = \frac{n_i/\sigma_i^2}{\sum_{j=1}^{k} n_j/\sigma_j^2}.$$

Sinha (1985) in the same spirit derived an unbiased estimator of the variance of $\hat{\mu}_{GD}$ that is a convergent series. A first-order approximation of this estimator is

$$\widehat{Var}_{(1)}(\hat{\mu}_{GD}) = \frac{1}{\sum_{i=1}^{k} \frac{n_i}{S_i^2}} \left[1 + \sum_{i=1}^{k} \frac{4}{n_i + 1} \left(\frac{n_i/S_i^2}{\sum_{j=1}^{k} n_j/S_j^2} - \frac{n_i^2/S_i^4}{(\sum_{j=1}^{k}(n_j/S_j^2)^2} \right) \right].$$

The above estimator is comparable to Meier's (1953) approximate estimator

$$\widehat{Var}_{(2)}(\hat{\mu}_{GD}) = \frac{1}{\sum_{i=1}^{k} \frac{n_i}{S_i^2}} \left[1 + \sum_{i=1}^{k} \frac{4}{n_i - 1} \left(\frac{n_i/S_i^2}{\sum_{j=1}^{k} n_j/S_j^2} - \frac{n_i^2/S_i^4}{(\sum_{j=1}^{k}(n_j/S_j^2)^2} \right) \right].$$

The "classical" meta-analysis variance estimator, $\widehat{Var}_{(3)}(\hat{\mu}_{GD})$, and approximate variance estimator proposed by Hartung (1999) $\widehat{Var}_{(4)}(\hat{\mu}_{GD})$ are the two other variance estimators of $\hat{\mu}_{GD}$ which are given by

$$\widehat{Var}_{(3)}(\hat{\mu}_{GD}) = \frac{1}{\sum_{i=1}^{k} \frac{n_i}{S_i^2}} \quad \& \quad \widehat{Var}_{(4)}(\hat{\mu}_{GD}) = \frac{1}{k-1} \sum_{i=1}^{k} \left(\frac{n_i/S_i^2}{\sum_{j=1}^{k} n_j/S_j^2} \right) (\bar{X}_i - \hat{\mu}_{GD})^2.$$

We should mention that a parametric bootstrap approach based on Graybill–Deal estimate was suggested in Malekzadeh and Kharrati-Kopaei (2018) to draw inference about μ which works quite well in large samples. Likewise, inference based on the MLE of μ suggested in Chang and Pal (2008) is also asymptotic in nature. As mentioned earlier, the central focus of this paper is to critically examine some exact tests for the common mean. A power comparison of these available exact tests is then a natural desire. In this paper this is precisely what we accomplish by comparing six exact tests based on their local powers.

The organization of the paper is as follows. In Sect. 2 we provide a brief description of the six exact tests with their references. The pdf of non-central t which naturally plays a pivotal role for studying power of t tests is given along with its local expansion (in terms of its non-centrality parameter). Section 3, a core section of the paper, provides expressions of local powers of all the proposed tests. Appendix I at the end contains proofs of all technical results. Section 4 contains some numerical (power) comparisons in the case of equal sample sizes and also in the case of one specific unequal sample sizes. We conclude this paper with some remarks in Sect. 5.

2 Review of Six Exact Tests for H_0 Versus H_1

Consider k independent normal populations where the i^{th} population follows a normal distribution with mean $\mu \in \mathbb{R}$ and variance $\sigma_i^2 > 0$. Let $\bar{X}_i$ denote the sample mean, S_i^2 the (unbiased) sample variance, and n_i the sample size of the i^{th} population. Then, we have $\bar{X}_i \sim \mathcal{N}(\mu, \frac{\sigma_i^2}{n_i})$ and $\frac{(n_i-1)S_i^2}{\sigma_i^2} \sim \chi^2_{\nu_i}$, where $\nu_i = (n_i - 1)$ and $i = 1, \cdots, k$. Note that the statistics $\{\bar{X}_i, S_i^2, i = 1, \cdots, k\}$ are all mutually independent.

A generic notation for a t statistic based on a sample of size n is $t_{obs} = \sqrt{n}(\bar{x} - \mu_0)/s$. We can refer to this t computed from a given data set as the observed value of our test statistic, and reject H_0 when $|t_{obs}| > t_{\nu;\alpha/2}$, where ν is the degrees of freedom and α is Type I error level. A test for H_0 based on a P-value on the other hand is based on $P_{obs} = P[|t_\nu| > |t_{obs}|]$, and we reject H_0 at level α if $P_{obs} < \alpha$. Here t_ν stands for the central t variable with ν degrees of freedom and $t_{\nu;\alpha/2}$ stands for the upper $\alpha/2$ percentile of t_ν. It is easy to check that the two approaches are obviously equivalent.

A random P-value which has a $Uniform(0, 1)$ distribution under H_0 is defined as $P_{ran} = P[|t_\nu| > |t_{ran}|]$, where $t_{ran} = \sqrt{n}(\bar{X} - \mu_0)/S$. All suggested tests for H_0 are based on P_{obs} and t_{obs} values and their properties, including size and power, are studied under P_{ran} and t_{ran}. To simplify notations, we will denote P_{obs} by small p and P_{ran} by large P. Six exact tests based on t_{obs} and p values from k independent studies as available in the literature are listed below.

2.1 P-Value Based Exact Tests

2.1.1 Tippett's Test

This minimum P-value test was proposed by Tippett et al. (1931), who noted that, if $P_1, \cdots, P_k$ are independent p-values from continuous test statistics, then each has a uniform distribution under H_0. Suppose that $P_{(1)}, \cdots, P_{(k)}$ are ordered p-values. According to this method, the common mean null hypothesis $H_0 : \mu = \mu_0$ is rejected at α level of significance if $P_{(1)} < \left[1 - (1 - \alpha)^{\frac{1}{k}}\right]$. Incidentally, this test is equivalent to the test based on $M_t = max_{1 \le i \le k}|t_i|$ suggested by Cohen and Sackrowitz (1984).

2.1.2 Wilkinson's Test

This test statistic proposed by Wilkinson (1951) is a generalization of Tippett's test that uses not just the smallest but the r^{th} smallest p-value ($P_{(r)}$) as a test statistic. The common mean null hypothesis $H_0 : \mu = \mu_0$ will be rejected if $P_{(r)} < d_{r,\alpha}$, where $P_{(r)}$ follows a *Beta* distribution with parameters r and $(k - r + 1)$ under H_0 and $d_{r,\alpha}$ satisfies $Pr\{P_{(r)} < d_{r,\alpha}|H_0\} = \alpha$. Obviously, this procedure generates a sequence of tests for different values of $r = 1, 2, \cdots, k$. And an attempt has been made to identify the best choice of r (Table 4).

2.1.3 Inverse Normal Test

This exact test procedure which involves transforming each p-value to the corresponding normal score was proposed independently by Stouffer et al. (1949) and Lipták (1958). Using this inverse normal method, hypothesis about the common μ will be rejected at α level of significance if $\left[\sum_{i=1}^{k} \Phi^{-1}(P_i)\right]\left[\sqrt{k}\right]^{-1} < -z_\alpha$, where Φ^{-1} denotes the inverse of the cdf of a standard normal distribution and z_α stands for the upper α level cutoff point of a standard normal distribution.

2.1.4 Fisher's Inverse χ^2-Test

This inverse χ^2-test is one of the most widely used exact test procedures for combining k independent p-values (Fisher 1932). This procedure uses the $\prod_{i=1}^{k} P_i$ to combine the k independent p-values. Then, using the connection between uniform and χ^2 distributions, the hypothesis about the common μ will be rejected if $-2\sum_{i=1}^{k} \ln(P_i) > \chi^2_{2k,\alpha}$, where $\chi^2_{2k,\alpha}$ denotes the upper α critical value of a χ^2-distribution with $2k$ degrees of freedom.

2.2 Exact Test Based on a Modified t

Fairweather (1972) consider a test based on a weighted linear combination of the t_i's. In this paper, we consider a variation of this test based on a weighted linear combination of $|t_i|$ as we are testing a non-directional alternative. Our test statistic T_1 is given as $\sum_{i=1}^{k} w_{1i}|t_i|$, where $w_{1i} \propto [Var(|t_i|)]^{-1}$ with $Var(|t_i|) = \left[[\nu_i(\nu_i - 2)^{-1}] - \left([\Gamma(\frac{\nu_i-1}{2})\sqrt{\nu_i}][\Gamma(\frac{\nu_i}{2})\sqrt{\pi}]^{-1}\right)^2\right]$. The null hypothesis $H_0 : \mu = \mu_0$ will be rejected if $T_1 > d_{1\alpha}$, where $Pr\{T_1 > d_{1\alpha}|H_0\} = \alpha$. In applications $d_{1\alpha}$ is computed by simulation.

2.3 Exact Test Based on a Modified F

Jordan and Krishnamoorthy (1996) considered a weighted linear combination of the F-test statistics F_i, namely, T_2, which is given as $\sum_{i=1}^{k} w_{2i} F_i$, $F_i = t_i^2 \sim F(1, \nu_i)$, and $w_{2i} \propto [Var(F_i)]^{-1}$ with $Var(F_i) = [2\nu_i^2(\nu_i - 1)][(\nu_i - 2)^2(\nu_i - 4)]^{-1}$ for $\nu_i > 4$. The null hypothesis $H_0 : \mu = \mu_0$ will be rejected if $T_2 > d_{2\alpha}$, where $Pr\{T_2 > d_{2\alpha} | H_0\} = \alpha$. In applications $d_{2\alpha}$ is computed by simulation.

We mention in passing that Philip et al. (1999) studied some properties of the confidence interval for the common mean μ based on Fisher's test and inverse normal test.

The pdfs of t statistic under the null and alternative hypotheses which will be required in the sequel are given below. $\delta = \sqrt{n}(\mu_1 - \mu_0)/\sigma$ below stands for the non-centrality parameter when μ_1 is chosen as an alternative value. Later, we will denote $(\mu_1 - \mu_0)$ by Δ.

$$f_\nu(t) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi}\,\Gamma(\frac{\nu}{2})}\left(1 + \frac{t^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

$$f_{\nu;\delta}(t) = \frac{\nu^{\frac{\nu}{2}} \exp\left(\frac{-\nu\delta^2}{2(t^2+\nu)}\right)}{\sqrt{\pi}\,\Gamma(\frac{\nu}{2}) 2^{\frac{\nu-1}{2}} \left(t^2 + \nu\right)^{\frac{\nu+1}{2}}} \int_0^\infty y^\nu \exp\left[-\frac{1}{2}\left(y - \frac{\delta t}{\sqrt{t^2+\nu}}\right)^2\right] dy$$

First and second derivatives of $f_{\nu;\delta}(t)$ evaluated at $\delta = 0$ (equivalently, $\Delta = 0$) which will play a pivotal role in the study of local powers of the proposed tests appear below.

$$\frac{\partial f_{\nu;\delta}(t)}{\partial \delta}\Big|_{\delta=0} = \frac{t}{\sqrt{2\pi}\left(\frac{t^2}{\nu} + 1\right)^{\frac{\nu+2}{2}}}$$

$$\frac{\partial^2 f_{\nu;\delta}(t)}{\partial \delta^2}\Big|_{\delta=0} = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}}\left[\frac{t^2 - 1}{(\frac{t^2}{\nu} + 1)^{\frac{\nu+3}{2}}}\right]$$

3 Expressions of Local Powers of the Six Proposed Tests

In this section we provide the expressions of local powers of the suggested exact tests. A common premise is that we derive an expression of the power of a test under $\Delta \neq 0$, and carry out its Taylor expansion around $\Delta = 0$. It turns out that due to two-sided nature of our tests, the first term vanishes, and we retain terms of order $O(\Delta^2)$.

The final expressions of the local powers of the proposed tests are given below in the general case and also in the special case when $n_1 = \cdots = n_k = n$, and $\nu_1 = \cdots = \nu_k = \nu = n - 1$. All throughout, we write $\Psi = \sum_{i=1}^{k} \frac{1}{\sigma_i^2}$ which is relevant in the special case. For detailed proofs of all technical results below we refer to the Appendix section of this paper.

3.1 Local Power of Tippett's Test $[LP(T)]$

$$LP(T) \approx \alpha + (1-\alpha)^{\frac{k-1}{k}} \frac{\Delta^2}{2} \left(\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} |\xi_{\nu_i T}(a_\alpha)| \right) \tag{1}$$

$$= \alpha + \left[\frac{n\Delta^2}{2} \Psi \right] \left[(1-\alpha)^{\frac{k-1}{k}} \right] |\xi_{\nu T}(a_\alpha)| \qquad \text{[special case]}$$

where $\xi_{\nu T}(a_\alpha) = \int_{-t_\nu(\frac{a_\alpha}{2})}^{t_\nu(\frac{a_\alpha}{2})} \frac{\partial^2 f_{\nu;\delta}(t)}{\partial \delta^2}\Big|_{\delta=0} dt$; $a_\alpha = [1-(1-\alpha)^{\frac{1}{k}}]$. It turns out that $\xi_{\nu T}(a_\alpha) < 0$.

3.2 Local Power of Wilkinson's Test $[LP(W_r)]$

$$LP(W_r) \approx \alpha + \binom{k-1}{r-1} d_{r;\alpha}^{r-1} (1-d_{r;\alpha})^{k-r} \frac{\Delta^2}{2} \left[\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} |\xi_{iW}(d_{r,\alpha})| \right] \tag{2}$$

$$= \alpha + \left[\frac{n\Delta^2}{2} \Psi \right] \binom{k-1}{r-1} |\xi_{\nu W}(d_{r;\alpha})| d_{r;\alpha}^{r-1} (1-d_{r;\alpha})^{k-r} \qquad \text{[special case]}$$

where $\xi_{\nu W}(d_{r;\alpha})$ is equivalent to $\xi_{\nu T}(a_\alpha)$ with $a_\alpha = d_{r;\alpha}$. It turns out that $\xi_{\nu W}(d_{r;\alpha}) < 0$.

Remark: For the special case $r = 1$, $LP(W_r) = LP(T)$, as expected, because $d_{1;\alpha} = [1-(1-\alpha)^{\frac{1}{k}}]$, implying $(1-d_{1;\alpha})^{k-1} = (1-\alpha)^{\frac{k-1}{k}}$.

3.3 Local Power of Inverse Normal Test $[LP(INN)]$

$$LP(INN) \approx \alpha + \frac{\Delta^2}{2\sqrt{k}} \phi(z_\alpha) \sum_{i=1}^{k} \frac{n_i \nu_i}{\sigma_i^2} \left[\frac{z_\alpha [B_{\nu_i} - C_{\nu_i}]}{2\sqrt{k}} - A_{\nu_i} \right] \tag{3}$$

$$= \alpha + \left[\frac{n\Delta^2}{2} \Psi \right] \frac{\nu}{\sqrt{k}} \phi(z_\alpha) \left[\frac{z_\alpha [B_\nu - C_\nu]}{2\sqrt{k}} - A_\nu \right] \qquad \text{[special case]}$$

where $A_\nu = \int_{-\infty}^{\infty} u\phi(u)Q_\nu(u)du$; $B_\nu = \int_{-\infty}^{\infty} u^2\phi(u)Q_\nu(u)du$; $C_\nu = \int_{-\infty}^{\infty} \phi(u)Q_\nu(u)du$; $Q_\nu(u) = \left[\frac{x^2-1}{x^2+\nu}\right]_{x=t_\nu(\frac{c}{2}),\ c=\Phi(u)}$; $\phi(u)$ is standard normal pdf and $\Phi(u)$ is standard normal cdf.

3.4 Local Power of Fisher's Test $[LP(F)]$

$$LP(F) \approx \alpha + \frac{\Delta^2}{2}\left[\sum_{i=1}^{k}\frac{n_i\nu_i}{2\sigma_i^2}D_{\nu_i}\right]\left[E\left\{\{\ln(T/2)\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right] \tag{4}$$

$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]\frac{\nu D_\nu}{2}\left[E\left\{\{\ln(T/2)\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right] \quad [\text{special case}]$$

where $D_0 = E\big[\log(q)\big]$; $D_\nu = E\big[U\psi_\nu(U)\big]$; $U \sim$exp[2]; $q \sim$gamma$[1,k]$; $T \sim$gamma$[2,k]$; $\psi_\nu(u) = \left[\frac{x^2-1}{x^2+\nu}\right]_{x=t_\nu(\frac{c}{2}),\ c=\exp(-\frac{u}{2})}$.

3.5 Local Power of a Modified t Test $[LP(T_1)]$

$$LP(T_1) \approx \alpha + \frac{\Delta^2}{2}\left(\sum_{j=1}^{k}\frac{n_j}{\sigma_j^2}E_{H_0}\left[\left\{\frac{(t_j^2-1)\nu_j}{t_j^2+\nu_j}\right\}I_{\{\sum_{i=1}^{k} w_{1i}|t_i|>d_1\alpha\}}\right]\right) \tag{5}$$

$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]E_{H_0}\left[\left\{\frac{(t_1^2-1)\nu}{t_1^2+\nu}\right\}I_{\{\sum_{i=1}^{k}|t_i|>d_{1\alpha}\}}\right] \quad [\text{special case}]$$

3.6 Local Power of a Modified F Test $[LP(T_2)]$

$$LP(T_2) \approx \alpha + \frac{\Delta^2}{2}\left(\sum_{j=1}^{k}\frac{n_j}{\sigma_j^2}E_{H_0}\left[\left\{\frac{[F_j-1]\nu_j}{F_j+\nu_j}\right\}I_{\{\sum_{i=1}^{k} w_{2i}F_i>d_{2\alpha}\}}\right]\right) \tag{6}$$

$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]E_{H_0}\left[\left\{\frac{[F_1-1]\nu}{F_1+\nu}\right\}I_{\{\sum_{i=1}^{k}F_i>d_{2\alpha}\}}\right] \quad [\text{special case}]$$

4 Comparison of Local Powers

It is interesting to observe from the above expressions that in the special case of equal sample size, local powers can be readily compared, irrespective of the values

Table 3 Comparison of the 2^{nd} term of local powers [without $n\Delta^2\Psi/2$] of six exact tests for different values of k and n (equal sample size)

Exact test	k = 5			k = 10			k = 15		
	n = 15	n = 25	n = 40	n = 15	n = 25	n = 40	n = 15	n = 25	n = 40
Tippett	0.0575	0.0633	0.0667	0.0322	0.0361	0.0383	0.0227	0.0257	0.0275
Wilkinson	0.0633	0.0664	0.0681	0.0412	0.0430	0.0441	0.0324	0.0338	0.0346
Inverse normal	**0.0667**	**0.0683**	**0.0699**	**0.0438**	**0.0454**	**0.0462**	**0.0349**	**0.0355**	**0.0369**
Fisher	0.0575	0.0579	0.0602	0.0421	0.0429	0.0441	0.0321	0.0343	0.0363
Modified t	**0.0737**	**0.0759**	**0.0768**	**0.0486**	**0.0511**	**0.0516**	**0.0391**	**0.0409**	**0.0412**
Modified F	**0.0752**	**0.0784**	**0.0807**	**0.0495**	**0.0527**	**0.0533**	**0.0388**	**0.0401**	**0.0411**

Table 4 Comparison of the 2^{nd} term of local powers [without $n\Delta^2\Psi/2$] of Wilkinson's test for $n = 15$ (equal sample size) and different values of k and r ($\leq k$)

r	k = 5	k = 10	k = 15	k = 20	k = 30	k = 40
1	0.0575	0.0322	0.0227	0.0177	0.0124	0.0096
2	**0.0633**	0.0395	0.0292	0.0234	0.0169	0.0134
3	0.0587	**0.0412**	0.0317	0.0259	0.0193	0.0155
4	0.0494	0.0404	**0.0324**	0.0271	0.0206	0.0168
5	0.0359	0.0384	0.0322	**0.0275**	0.0214	0.0176
6		0.0355	0.0314	0.0274	0.0214	0.0181
7		0.0320	0.0302	0.0270	**0.0220**	0.0185
8		0.0279	0.0287	0.0264	0.0219	0.0187
9		0.0230	0.0270	0.0256	0.0218	**0.0188**
10		0.0168	0.0250	0.0246	0.0215	0.0187
11			0.0229	0.0235	0.0212	0.0186
12			0.0205	0.0224	0.0208	0.0185
13			0.0178	0.0211	0.0203	0.0184
14			0.0147	0.0197	0.0198	0.0181
15			0.0108	0.0182	0.0192	0.0179

of the unknown variances (involved through Ψ, which is a common factor in all the expressions of local power).

Table 3 represents values of the 2^{nd} term of local power given above in Eqs. 1–6, apart from the common term $\left[\frac{n\Delta^2}{2}\Psi\right]$ for different values of k, n and choices of r ($\leq k$) with maximum local power. A comparison of the 2^{nd} term of local power of Wilkinson's test for different values of r ($\leq k$) is provided in Table 4 for $n = 15$ and $k \in \{5, 10, 15, 20, 30, 40\}$. All throughout we have used $\alpha = 5\%$.

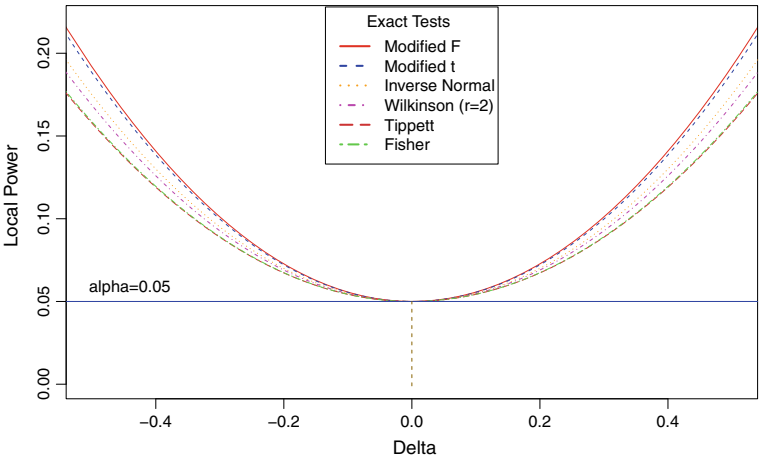

Fig. 1 Comparison of local powers of six exact tests for $n = 15$, $k = 5$ and $\Psi = 1$

Here are some interesting observations: comparing Tippett's and Wilkinson's tests, we note that Wilkinson's test for some $r > 1$ always outperforms Tippett's test, and the optimal choice of r seems to increase with k (Table 4 and Fig. 2), it is just above $\sqrt{k}$. Among the other tests, Fig. 1 with $\Psi = 1$ reveals that both modified F and modified t tests fare the best uniformly in the design parameters n and k. Inverse normal-based exact test also performs reasonably well in the case of equal sample size for all values of k and n (Table 3). Another advantage of this test is that its cutoff point can be readily obtained without any simulation.

Some limited local power computations in case of unequal sample sizes are reported in Table 5. It again follows that both modified F and modified t tests have an edge over all other tests. Our recommendation based on the local power comparison of the available exact tests is to advocate the use of these modified exact tests in all scenarios.

Following the suggestion of first reviewer, we have added a table (Table 6) that shows a comparison of modified t and modified F local powers and Monte Carlo simulated powers for different values of n, Δ^2, $k = 5$ and $\sigma_i^2 \in \{1.0, 1.5, 2.0, 0.5, 0.3\}$. It turns out that for smaller values of Δ^2 the accuracies are fairly good even for small value of n. Following the suggestion of second reviewer, we have added two figures (Figs. 3 and 4) displaying approximate pdf of U for small values of Δ^2 and simulated pdf of U for the same small values of Δ^2 (Fig. 3), and approximate pdf of U for small values of Δ^2 and approximate normal pdf of U for the same small values of Δ^2 (Fig. 4). The figures attest testimony to our assumption that the pdf of U for local alternatives can be approximated by a normal distribution.

Table 5 Coefficients of $\Delta^2/2$ in the 2^{nd} term of local powers of six exact tests for different values of k, n (unequal sample sizes) and σ^2

Exact test	k = 2	k = 3	k = 4
	$n_1 = 10, \sigma_1^2 = 1$ $n_2 = 20, \sigma_2^2 = 2$	$n_1 = 10, \sigma_1^2 = 1$ $n_2 = 20, \sigma_2^2 = 2$ $n_3 = 30, \sigma_3^2 = 3$	$n_1 = 10, \sigma_1^2 = 1$ $n_2 = 20, \sigma_2^2 = 2$ $n_3 = 30, \sigma_3^2 = 3$ $n_4 = 40, \sigma_4^2 = 4$
Tippett	2.3332	2.6606	2.9108
Inv normal	2.3603	2.7753	3.1284
Fisher	1.7280	2.1528	2.5140
Modified t	2.4524	2.9990	3.4404
Modified F	**2.5011**	**3.0077**	**3.5252**
Wilkinson ($r = 1$)	2.3332	2.6606	2.9108
Wilkinson ($r = 2$)	1.9464	2.5472	2.9611
Wilkinson ($r = 3$)		1.8972	2.5389
Wilkinson ($r = 4$)			1.8447

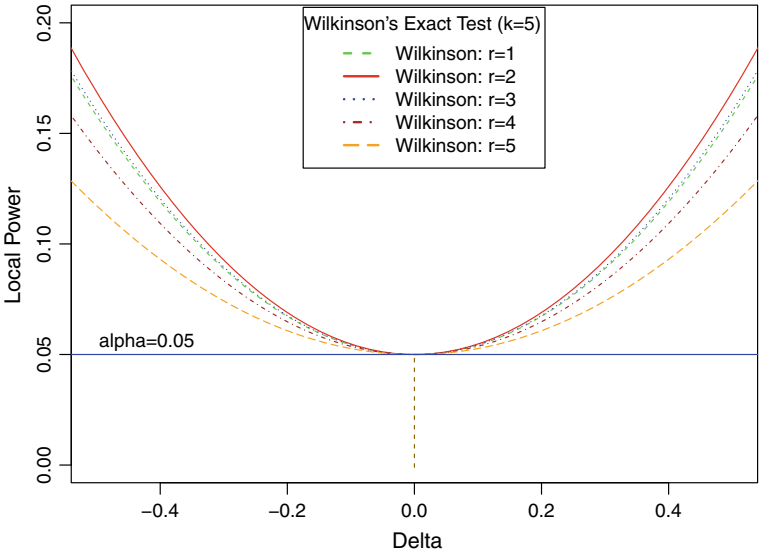

Fig. 2 Comparison of local powers of Wilkinson's exact test for $n = 15$, $k = 5$ and $\Psi = 1$

Table 6 Comparison of Modified t and Modified F local powers and Monte Carlo simulated powers for different values of n, Δ^2, $\sigma_i^2 \in \{1.0, 1.5, 2.0, 0.5, 0.3\}$ and $k = 5$

n	Δ^2	Local Power ($\alpha = 5\%$)		
		Modified t	Modified F	MC simulated
15	0.002	0.0583	0.0585	0.0563
	0.004	0.0666	0.0669	0.0628
	0.006	0.0749	0.0754	0.0708
	0.008	0.0832	0.0838	0.0833
	0.010	0.0915	0.0923	0.0956
25	0.002	0.0642	0.0647	0.0623
	0.004	0.0785	0.0794	0.0774
	0.006	0.0927	0.0941	0.0938
	0.008	0.1069	0.1088	0.1133
	0.010	0.1212	0.1235	0.1339
40	0.002	0.0730	0.0742	0.0723
	0.004	0.0961	0.0984	0.1005
	0.006	0.1191	0.1226	0.1310
	0.008	0.1422	0.1468	0.1653
	0.010	0.1652	0.1710	0.2041

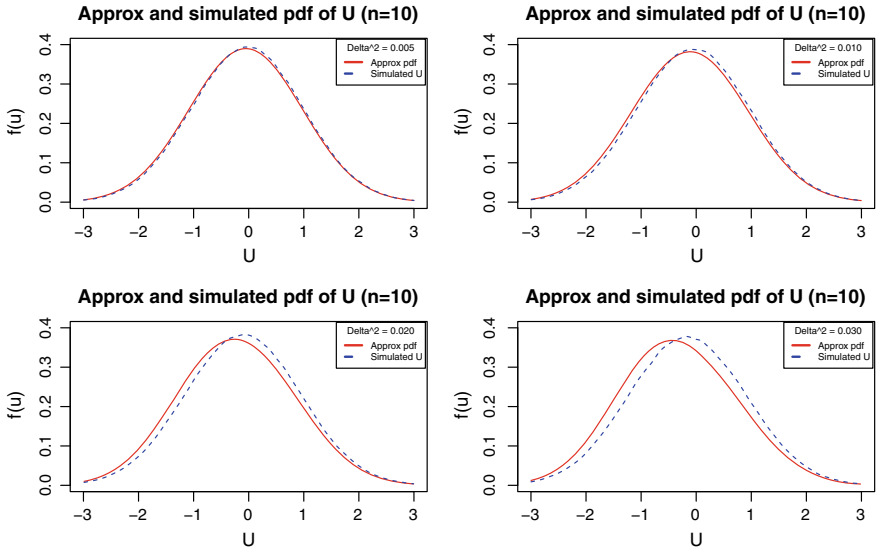

Fig. 3 Approximate pdf of U and simulated pdf of U for different values of $\Delta^2 \in \{0.005, 0.010, 0.020, 0.030\}$

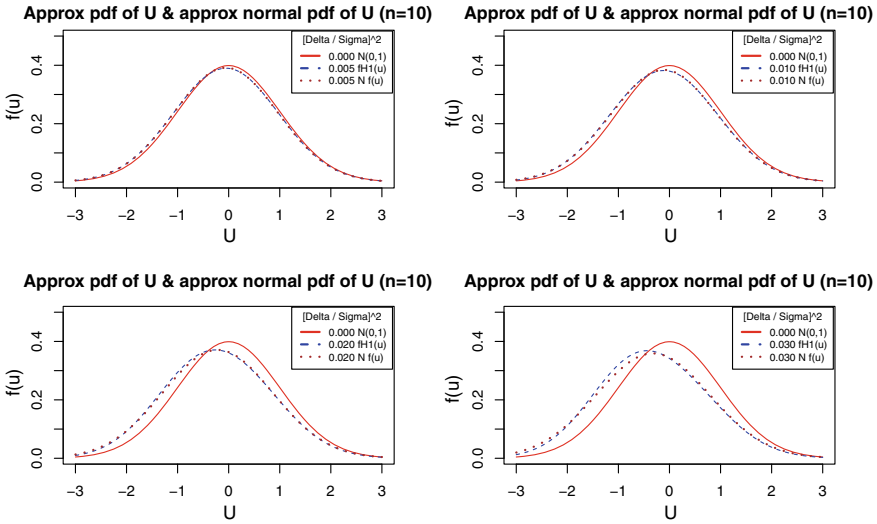

Fig. 4 Approximate pdf of U and approximate normal pdf of U for different values of $[\Delta/\sigma]^2$

5 Conclusion

Based on our computations of local powers of the available exact tests, we have noted that a uniform comparison of them, irrespective of the values of the unknown variances, can be readily made in case of equal sample size, and it turns out that both modified F and modified t tests perform the best. Inverse normal-based exact test also performs reasonably well in the case of equal sample size with the added advantage that its cutoff point can be readily obtained without any simulation. Some limited computations of local powers in case of unequal sample sizes also reveal the superiority of these two modified tests compared to the other exact tests.

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Appendix 1: Proofs of Local Powers of Six Exact Tests

We begin by stating a result related to the distribution of a P-value under the alternative hypothesis $H_0 : \mu = \mu_1$, which will be crucial for providing the main results on local power of all tests based on the P-values. We denote $F_\nu(\cdot)$ to represent the cdf of a central t-distribution with ν degrees of freedom.

Lemma 1

$$Pr\{P > c|H_1\} \approx (1-c) + \frac{n\Delta^2}{2\sigma^2}\xi_\nu(c). \tag{7}$$

Proof

$$\begin{aligned}
Pr\{P > c|H_1\} &= Pr\left\{Pr\left[|t_\nu| > |\frac{\sqrt{n}(\bar{X}-\mu_0)}{S}|\right] > c|H_1\right\} \\
&= Pr\left\{1 - \left[F_\nu\left(|\frac{\sqrt{n}(\bar{X}-\mu_0)}{S}|\right) - F_\nu\left(-|\frac{\sqrt{n}(\bar{X}-\mu_0}{S}|\right)\right] > c|H_1\right\} \\
&= Pr\left\{\left[F_\nu\left(|\frac{\sqrt{n}(\bar{X}-\mu_0)}{S}|\right) - F_\nu\left(-|\frac{\sqrt{n}(\bar{X}-\mu_0}{S}|\right)\right] < 1-c|H_1\right\} \\
&= Pr\left\{|\frac{\sqrt{n}(\bar{X}-\mu_0)}{S}| < t_\nu(\frac{c}{2})|H_1\right\} \\
&= Pr\left\{-t_\nu(\frac{c}{2}) < \frac{\sqrt{n}(\bar{X}-\mu_0)}{S} < t_\nu(\frac{c}{2})|H_1\right\} \\
&= Pr\left\{-t_\nu(\frac{c}{2}) < t_\nu(\delta) < t_\nu(\frac{c}{2})|H_1\right\} \\
&= \int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} f(x|\nu,\delta)\,dx \qquad \left[f(x|\nu,\delta) \sim \text{non-central} \quad t_\nu\left(\delta = \frac{\sqrt{n}}{\sigma}\Delta\right)\right] \\
&\approx \int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} \left\{f(x|\nu,0) + \delta\left(\frac{\partial f}{\partial\delta}\right)\Big|_{\delta=0} + \frac{\delta^2}{2}\left(\frac{\partial^2 f}{\partial\delta^2}\right)\Big|_{\delta=0}\right\}dx \\
&\approx (1-c) + \frac{n}{2\sigma^2}\Delta^2 \int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} \left\{\frac{\partial^2 f(x|\nu,\delta)}{\partial\delta^2}\Big|_{\delta=0}\right\}dx \\
&\approx (1-c) + \frac{n\Delta^2}{2\sigma^2}\xi_\nu(c)
\end{aligned}$$

where $\xi_\nu(c) = \int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} \left\{\frac{\partial^2 f(x|\nu,\delta)}{\partial\delta^2}\Big|_{\delta=0}\right\}dx = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}} \int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} \left(\frac{x^2-1}{[\frac{x^2}{\nu}+1]^{\frac{\nu+3}{2}}}\right)dx$. It turns out that $\xi_\nu(c) < 0$. □

I. Local Power of Tippett's Test [L P(T)]

Recall that Tippett's test rejects the null hypothesis if $P_{(1)} < \left[1-(1-\alpha)^{\frac{1}{k}}\right] = a_\alpha$. This leads to

$$\text{Power} = 1 - \prod_{i=1}^{k} Pr\{P_i > a_\alpha|H_1\}.$$

Applying Lemma 1, the local power of Tippett's test is calculated as follows:

$$\begin{aligned}
\text{Local power} &\approx 1 - \prod_{i=1}^{k}\left[(1-a_\alpha) + \frac{\Delta^2}{2}\left(\frac{n_i}{\sigma_i^2}\xi_{\nu_i T}(a_\alpha)\right)\right] \\
&\approx 1 - \prod_{i=1}^{k}\left[(1-\alpha)^{\frac{1}{k}} + \frac{\Delta^2}{2}\left(\frac{n_i}{\sigma_i^2}\xi_{\nu_i T}(a_\alpha)\right)\right] \\
&\approx 1 - \left[(1-\alpha) + (1-\alpha)^{\frac{k-1}{k}}\frac{\Delta^2}{2}\left(\sum_{i=1}^{k}\frac{n_i}{\sigma_i^2}\xi_{\nu_i T}(a_\alpha)\right)\right] \\
&\approx \alpha + (1-\alpha)^{\frac{k-1}{k}}\frac{\Delta^2}{2}\left(\sum_{i=1}^{k}\frac{n_i}{\sigma_i^2}|\xi_{\nu_i T}(a_\alpha)|\right).
\end{aligned}$$

For the special case $n_1 = \cdots = n_k = n$; $\nu_1 = \cdots = \nu_k = \nu = n-1$ and $\xi_{\nu_1 T}(a_\alpha) = \cdots = \xi_{\nu_k T}(a_\alpha) = \xi_{\nu T}(a_\alpha)$, the local power of Tippett's test reduces to

$$\begin{aligned}
\text{LP(T)} &\approx \alpha + (1-\alpha)^{\frac{k-1}{k}}\frac{n\Delta^2}{2}|\xi_{\nu T}(a_\alpha)|\left(\sum_{i=1}^{k}\frac{1}{\sigma_i^2}\right) \\
&= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]\left[(1-\alpha)^{\frac{k-1}{k}}\right]|\xi_{\nu T}(a_\alpha)| \qquad \text{where } \Psi = \sum_{i=1}^{k}\frac{1}{\sigma_i^2}.
\end{aligned}$$

II. Local Power of Wilkinson's Test $[LP(W_r)]$

Using r^{th} smallest p-value $P_{(r)}$ as a test statistic, the null hypothesis will be rejected if $P_{(r)} < d_{r,\alpha}$, where $P_{(r)} \sim Beta[r, k-r+1]$ under H_0 and $d_{r,\alpha}$ satisfies $\alpha = Pr\{P_{(r)} < d_{r,\alpha}|H_0\} = \int_0^{d_{r,\alpha}} \frac{u^{r-1}(1-u)^{k-r}}{B[r,k-r+1]}du$. This leads to

$$\begin{aligned}
\text{Power} &= Pr[P_{(r)} < d_{r,\alpha}|H_1] \\
&= \sum_{l=r}^{k} Pr\{P_{i_1}, \ldots, P_{i_l} < d_{r,\alpha} < P_{i_{l+1}}, \ldots, P_{i_k}|H_1\}
\end{aligned}$$

where $(i_1, \cdots, i_l, i_{l+1}, \cdots, i_k)$ is a permutation of $(1, \cdots, k)$. Applying Lemma 1, we get

$$
\begin{aligned}
&Pr\{P_{i_1}, \ldots, P_{i_l} < d_{r,\alpha} < P_{i_{l+1}}, \ldots, P_{i_k} | H_1\} \\
&\quad \approx \left\{ \prod_{j=1}^{l} \left(d_{r,\alpha} - \frac{n_{i_j}\Delta^2}{2\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right) \right\} \left\{ \prod_{j=l+1}^{k} \left(1 - d_{r,\alpha} + \frac{n_{i_j}\Delta^2}{2\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right) \right\} \\
&\quad \approx \left\{ d_{r,\alpha}^{l} - d_{r,\alpha}^{l-1} \frac{\Delta^2}{2} \left(\sum_{j=1}^{l} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right) \right\} \times \\
&\qquad \left\{ (1 - d_{r,\alpha})^{k-l} + (1 - d_{r,\alpha})^{k-l-1} \frac{\Delta^2}{2} \left(\sum_{j=l+1}^{k} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right) \right\} \\
&\quad \approx d_{r,\alpha}^{l} (1 - d_{r,\alpha})^{k-l} + \frac{\Delta^2}{2} \left\{ d_{r,\alpha}^{l} (1 - d_{r,\alpha})^{k-l-1} \left(\sum_{j=l+1}^{k} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right) \right. \\
&\qquad \left. - d_{r,\alpha}^{l-1} (1 - d_{r,\alpha})^{k-l} \left(\sum_{j=1}^{l} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(a_{d_{r,\alpha}}) \right) \right\}.
\end{aligned}
$$

Permuting $(i_1, \ldots, i_k)$ over $(1, \ldots, k)$, we get for any fixed l $(r \le l \le k)$,

$$
\begin{aligned}
\text{1st term} &= \binom{k}{l} d_{r,\alpha}^{l} (1 - d_{r,\alpha})^{k-l} \\
\text{2nd term} &= \frac{\Delta^2}{2} d_{r,\alpha}^{l} (1 - d_{r,\alpha})^{k-l-1} \left\{ \binom{k-1}{k-l-1} \left(\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} \xi_{iW}(d_{r,\alpha}) \right) \right\} \\
\text{3rd term} &= -\frac{\Delta^2}{2} d_{r,\alpha}^{l-1} (1 - d_{r,\alpha})^{k-l} \left\{ \binom{k-1}{l-1} \left(\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} \xi_{iW}(d_{r,\alpha}) \right) \right\}.
\end{aligned}
$$

The second term above follows upon noting that when $\left[\sum_{j=l+1}^{k} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right]$ is permuted over $(i_{l+1} < \cdots < i_k) \subset (1, \ldots, k)$, each term $\frac{n_i}{\sigma_i^2} \xi_{iW}(d_{r,\alpha})$ appears exactly $\binom{k-1}{k-l-1}$ times, for each $i = 1, \cdots, k$. The 3rd term, likewise, follows upon noting that when $\left[\sum_{j=1}^{l} \frac{n_{i_j}}{\sigma_{i_j}^2} \xi_{i_j W}(d_{r,\alpha}) \right]$ is permuted over $(i_1 < \cdots < i_l) \subset (1, \ldots, k)$, each term $\frac{n_i}{\sigma_i^2} \xi_{iW}(d_{r,\alpha})$ appears exactly $\binom{k-1}{l-1}$ times, for each $i = 1, \cdots, k$.

Adding the above three terms and simplifying, we get

$$
LP(W_r) \approx \alpha + \binom{k-1}{r-1} d_{r;\alpha}^{r-1} (1 - d_{r;\alpha})^{k-r} \frac{\Delta^2}{2} \left[\sum_{i=1}^{k} \frac{n_i}{\sigma_i^2} |\xi_{iW}(d_{r,\alpha})| \right].
$$

For the special case $n_1 = \cdots = n_k = n; \nu_1 = \cdots = \nu_k = \nu = n - 1$ and $\xi_{\nu_1 W}(d_{r;\alpha}) = \cdots = \xi_{\nu_k W}(d_{r;\alpha}) = \xi_{\nu W}(d_{r;\alpha})$, the local power of Wilkinson's test reduces to

$$LP(W_r) \approx \alpha + \binom{k-1}{r-1} d_{r;\alpha}^{r-1}(1-d_{r;\alpha})^{k-r}\frac{n\Delta^2}{2}|\xi_{iW}(d_{r,\alpha})|\left(\sum_{i=1}^{k}\frac{1}{\sigma_i^2}\right)$$

$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]\binom{k-1}{r-1}|\xi_{\nu W}(d_{r;\alpha})|d_{r;\alpha}^{r-1}(1-d_{r;\alpha})^{k-r} \quad \text{where} \quad \Psi = \sum_{i=1}^{k}\frac{1}{\sigma_i^2}.$$

III. Local Power of Inverse Normal Test [*LP*(*INN*)]

Under this test, the null hypothesis will be rejected if $\frac{1}{\sqrt{k}}\sum_{i=1}^{k} U_i < -z_\alpha$, where $U_i = \Phi^{-1}(P_i)$, Φ^{-1} is the inverse cdf and z_α is the upper α level critical value of a standard normal distribution. This leads to

$$\text{Power} = Pr\left\{\frac{1}{\sqrt{k}}\sum_{i=1}^{k} U_i < -z_\alpha | H_1\right\}.$$

First, let us determine the pdf of U under H_1, $f_{H_1}(u)$, via its cdf $F_{H_1}(u) = Pr\{U \le u|H_1\}$.

$$\begin{aligned}
Pr\{U \le u|H_1\} &= Pr\{\Phi(U) \le \Phi(u)|H_1\} \\
&= Pr\{P \le \Phi(u)|H_1\} && \left[U = \Phi^{-1}(P) \implies P = \Phi(U)\right] \\
&= 1 - Pr\{P > \Phi(u)|H_1\} \\
&\approx 1 - \left[[1-\Phi(u)] + \frac{n\Delta^2}{2\sigma^2}\left[\xi_\nu(c)\right]_{c=\Phi(u)}\right] && \left[\text{upon applying Lemma 1}\right] \\
&\approx \Phi(u) - \frac{n\Delta^2}{2\sigma^2}\left[\xi_\nu(c)\right]_{c=\Phi(u)}.
\end{aligned}$$

This implies

$$\begin{aligned}
f_{H_1}(u) &\approx \frac{d}{du}\left[\Phi(u) - \frac{n\Delta^2}{2\sigma^2}\left[\xi_\nu(c)\right]_{c=\Phi(u)}\right] \\
&\approx \phi(u)\left[1 - \frac{n\Delta^2}{2\sigma^2}\left(\frac{d}{dc}\left[\xi_\nu(c)\right]_{c=\Phi(u)}\right)\right] \\
&\approx \frac{\phi(u)\left[1 + \frac{n\nu\Delta^2}{2\sigma^2}Q_\nu(u)\right]}{1 + \frac{n\nu\Delta^2}{2\sigma^2}\int_{-\infty}^{\infty}\phi(u)Q_\nu(u)du}, \quad Q_\nu(u) = \left[\frac{x^2-1}{x^2+\nu}\right]_{x=t_\nu(\frac{c}{2}),\ c=\Phi(u)}.
\end{aligned}$$

Here we have used the fact that $\frac{d}{du}[\xi_\nu(c)] = \frac{d}{dc}[\xi_\nu(c)]\frac{dc}{du}$, $\frac{d}{dc}[\xi_\nu(c)] = -\nu Q_\nu(\cdot)$ given below in Eq. (10), upon simplification, and $\frac{dc}{du} = \phi(u)$. The denominator in the last expression is a normalizing constant.

$$\begin{aligned}
\frac{d}{dc}\xi_\nu(c) &= \frac{d}{dc}\Big[\int_{-t_\nu(\frac{c}{2})}^{t_\nu(\frac{c}{2})} f^*(x)dx\Big] \qquad \Big[f^*(x) = \frac{\partial^2 f(x|\nu,\delta)}{\partial\delta^2}\Big|_{\delta=0} = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}}\Big(\frac{x^2-1}{[\frac{x^2}{\nu}+1]^{\frac{\nu+3}{2}}}\Big)\Big] \\
&= \frac{d}{dc}\big[F^*\big(t_\nu(c/2)\big) - F^*\big(-t_\nu(c/2)\big)\big] \\
&= f^*\big(t_\nu(c/2)\big)\big[\frac{d}{dc}t_\nu(c/2)\big] + f^*\big(-t_\nu(c/2)\big)\big[\frac{d}{dc}t_\nu(c/2)\big] \\
&= \frac{d}{dc}t_\nu(c/2)\big[f^*\big(t_\nu(c/2)\big) + f^*\big(-t_\nu(c/2)\big)\big] \qquad f^*(x) \text{ is a symmetric distribution} \\
&= 2f^*\big(t_\nu(c/2)\big)\big[\frac{d}{dc}t_\nu(c/2)\big]. \qquad (8)
\end{aligned}$$

Further $\big[\frac{d}{dc}t_\nu(c/2)\big]$ can be expressed in terms of $f\big(t_\nu(c/2)\big)$ as follows.

$$\begin{aligned}
\frac{c}{2} &= Pr\big[t_\nu \geq t_\nu(c/2)\big] \\
&= \int_{t_\nu(c/2)}^{\infty} f_\nu(x)dx = 1 - F\big(t_\nu(c/2)\big) \qquad \Big[f_\nu(x) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi}\,\Gamma(\frac{\nu}{2})}\Big(1+\frac{x^2}{\nu}\Big)^{-\frac{\nu+1}{2}}\Big] \\
\frac{d}{dc}\big[\frac{c}{2}\big] &= \frac{d}{dc}\big[1 - F\big(t_\nu(c/2)\big)\big] \\
&= -f\big(t_\nu(c/2)\big)\big[\frac{d}{dc}t_\nu(c/2)\big] \\
\Longrightarrow \frac{d}{dc}t_\nu(c/2) &= \frac{-1}{2f\big(t_\nu(c/2)\big)}. \qquad (9)
\end{aligned}$$

Replacing Eq. (9) in (8) results in:

$$\begin{aligned}
\frac{d}{dc}\xi_\nu(c) &= 2f^*\big(t_\nu(c/2)\big)\Big[\frac{-1}{2f\big(t_\nu(c/2)\big)}\Big] = -\frac{f^*\big(t_\nu(c/2)\big)}{f\big(t_\nu(c/2)\big)} \\
&= -\nu\Big[\frac{x^2-1}{x^2+\nu}\Big]_{x=t_\nu(\frac{c}{2}),\ c=\Phi(u)}. \qquad (10)
\end{aligned}$$

Let us define A_ν, B_ν and C_ν as $A_\nu = \int_{-\infty}^{\infty} u\phi(u)Q_\nu(u)du$, $B_\nu = \int_{-\infty}^{\infty} u^2\phi(u)Q_\nu(u)du$ and $C_\nu = \int_{-\infty}^{\infty} \phi(u)Q_\nu(u)du$. Using these three quantities, we now approximate the distribution of U as

$$U \sim N[E(U), Var(U)] \quad \text{where} \quad E(U) = \int_{-\infty}^{\infty} u f_{H_1}(u)du \approx \frac{n\nu\Delta^2}{2\sigma^2}A_\nu \quad \text{and}$$

$$Var(U) = \int_{-\infty}^{\infty} u^2 f_{H_1}(u)du \approx 1 + \frac{n\nu\Delta^2}{2\sigma^2}[B_\nu - C_\nu].$$

This leads to

$$\frac{1}{\sqrt{k}}\sum_{i=1}^{k} U_i \sim N\left[\frac{1}{\sqrt{k}}\sum_{i=1}^{k} E(U_i), \frac{1}{k}\sum_{i=1}^{k} Var(U_i)\right]$$
$$\sim N\left[\frac{\Delta^2}{\sqrt{k}}\delta_1, 1+\frac{\Delta^2}{k}\delta_2\right]$$
$$\text{where } \delta_1 = \sum_{i=1}^{k}\frac{n_i\nu_i}{2\sigma_i^2}A_{\nu_i} \quad \text{and} \quad \delta_2 = \sum_{i=1}^{k}\frac{n_i\nu_i}{2\sigma_i^2}[B_{\nu_i} - C_{\nu_i}].$$

Using the above result, the local power of inverse normal test is obtained by approximating its $Power = Pr\left\{\frac{1}{\sqrt{k}}\sum_{i=1}^{k} U_i < -z_\alpha | H_1\right\}$ as

$$\text{Local power (INN)} \approx \Phi\left[\frac{-z_\alpha - \frac{\Delta^2}{\sqrt{k}}\delta_1}{\sqrt{1+\frac{\Delta^2}{k}\delta_2}}\right]$$
$$\approx \Phi\left[-z_\alpha - \frac{\Delta^2}{\sqrt{k}}\delta_1 + \frac{z_\alpha}{2}\frac{\Delta^2}{k}\delta_2\right]$$
$$\approx \Phi\left[-z_\alpha + \frac{\Delta^2}{\sqrt{k}}\left(\frac{z_\alpha}{2\sqrt{k}}\delta_2 - \delta_1\right)\right]$$
$$\approx \Phi(-z_\alpha) + \frac{\Delta^2}{\sqrt{k}}\phi(z_\alpha)\left[\frac{z_\alpha}{2\sqrt{k}}\delta_2 - \delta_1\right]$$
$$\approx \alpha + \frac{\Delta^2}{\sqrt{k}}\phi(z_\alpha)\left[\frac{z_\alpha}{2\sqrt{k}}\delta_2 - \delta_1\right].$$

Substituting back the expressions for δ_1 and δ_2 results in

$$LP(INN) \approx \alpha + \frac{\Delta^2}{2\sqrt{k}}\phi(z_\alpha)\sum_{i=1}^{k}\frac{n_i\nu_i}{\sigma_i^2}\left[\frac{z_\alpha[B_{\nu_i} - C_{\nu_i}]}{2\sqrt{k}} - A_{\nu_i}\right].$$

For the special case $n_1 = \cdots = n_k = n$ and $\nu_1 = \cdots = \nu_k = \nu = n-1$, the local power of *Inverse Normal test* reduces to

$$LP(INN) \approx \alpha + \frac{n\nu\Delta^2}{2\sqrt{k}}\phi(z_\alpha)\left(\sum_{i=1}^{k}\frac{1}{\sigma_i^2}\right)\left[\frac{z_\alpha[B_\nu - C_\nu]}{2\sqrt{k}} - A_\nu\right]$$
$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]\frac{\nu}{\sqrt{k}}\phi(z_\alpha)\left[\frac{z_\alpha[B_\nu - C_\nu]}{2\sqrt{k}} - A_\nu\right] \quad \text{where } \Psi = \sum_{i=1}^{k}\frac{1}{\sigma_i^2}.$$

IV. Local Power of Fisher's Test [LP(F)]

According to Fisher's exact test, the null hypothesis will be rejected if $\sum_{i=1}^{k} U_i > \chi^2_{2k;\alpha}$, where $U_i = -2\ln(P_i)$, and $\chi^2_{2k;\alpha}$ is the upper α level critical value of a χ^2-distribution with $2k$ degrees of freedom. This leads to

$$\text{Power} = Pr\left\{\sum_{i=1}^{k} U_i > \chi^2_{2k;\alpha} | H_1\right\}.$$

In a similar way to the inverse normal test in Appendix III, first let us determine the pdf of U under H_1, $g_{H_1}(u)$, via its cdf $G_{H_1}(u) = Pr\{U \le u|H_1\}$.

$$\begin{aligned} Pr\{U \le u|H_1\} &= Pr\{-2\ln(P) \le u|H_1\} \\ &= Pr\{\ln(P) > -u/2|H_1\} \\ &= Pr\{P > \exp(-u/2)|H_1\} \\ &\approx [1 - \exp(-u/2)] + \frac{n\Delta^2}{2\sigma^2}\big[\xi_\nu(c)\big]_{c=\exp(-u/2)} \quad \big[\text{upon applying Lemma 1}\big]. \end{aligned}$$

This implies

$$\begin{aligned} g_{H_1}(u) &\approx \frac{d}{du}\left[1 - \exp(-u/2) + \frac{n\Delta^2}{2\sigma^2}\big[\xi_\nu(c)\big]_{c=\exp(-u/2)}\right] \\ &\approx \frac{1}{2}\exp(-u/2) + \Big[\frac{n\Delta^2}{2\sigma^2}\Big]\frac{d}{du}\big[\xi_\nu(c)\big]_{c=\exp(-u/2)} \\ &\approx \frac{1}{2}\exp(-u/2) - \frac{1}{2}\exp(-u/2)\Big[\frac{n\Delta^2}{2\sigma^2}\Big]\frac{d}{dc}\big[\xi_\nu(c)\big]_{c=\exp(-u/2)} \\ &\approx \frac{\frac{1}{2}\exp(-u/2)\big[1 + \frac{n\nu\Delta^2}{2\sigma^2}\Psi_\nu(u)\big]}{1 + \frac{n\nu\Delta^2}{2\sigma^2}\big[\int_0^\infty \frac{1}{2}\exp(-u/2)\Psi_\nu(u)du\big]}, \quad \Psi_\nu(u) = \left[\frac{x^2-1}{x^2+\nu}\right]_{x=t_\nu(\frac{c}{2}),\ c=\exp(-u/2)}. \end{aligned}$$

Here we have used the fact that $\frac{d}{du}[\xi_\nu(c)] = \frac{d}{dc}[\xi_\nu(c)]\frac{dc}{du}$, $\frac{d}{dc}[\xi_\nu(c)] = -\nu\Psi_\nu(\cdot)$ given in Eq. (10), upon simplification, and $\frac{dc}{du} = -\frac{1}{2}\exp(-u/2)$. The denominator in the last expression is a normalizing constant.

Define $D_0 = \int_0^\infty \frac{1}{\Gamma(k)}\exp(-u)u^{k-1}\ln(u)du$ and $D_\nu = \int_0^\infty \frac{1}{2}\exp(-u/2)(u-2)\Psi_\nu(u)du$. Using these quantities, we can now approximate the distribution of U as

$$U \sim Gamma[\beta = 2, \gamma_\nu] \quad \text{where} \quad \gamma_\nu = \big[1 + \frac{n\nu\Delta^2}{4\sigma^2}D_\nu\big].$$

Here Gamma$[\beta, \gamma_\nu]$ stands for a Gamma random variable with scale parameter β and shape parameter γ_ν with the pdf $f(x) = [e^{-x/\beta}x^{\gamma_\nu - 1}]/[\beta^{\gamma_\nu}\Gamma(\gamma_\nu)]$. By the additive property of independent $Gamma[\beta = 2, \gamma_{\nu_1}], \cdots, Gamma[\beta = 2, \gamma_{\nu_k}]$ corresponding to $U_1, \cdots, U_k$, we readily get the approximate distribution of $(U_1 + \cdots + U_k)$ as

$$\sum_{i=1}^{k} U_i \sim Gamma\big[\beta = 2, k + \Delta^2 A\big] \quad \text{where} \quad A = \frac{1}{4}\sum_{i=1}^{k}\frac{n_i\nu_i}{\sigma_i^2}D_{\nu_i}.$$

The local power of Fisher's test under H_1 is then obtained as follows:

$$\text{Local power (F)} \approx \int_{\chi^2_{2k;\alpha}}^{\infty} \frac{\exp(-t/2)t^{k+A\Delta^2-1}}{2^{k+A\Delta^2}\Gamma(k+A\Delta^2)}dt \qquad \left[\text{since } \sum_{i=1}^{k} U_i \sim Gamma\left[\beta = 2, k+\Delta^2 A\right]\right]$$
$$= Q(\Delta^2).$$

We now expand $Q(\Delta^2)$ around $\Delta^2 = 0$ to get

$$\text{Local power (F)} \approx \alpha + \Delta^2 \int_{\chi^2_{2k;\alpha}}^{\infty} \frac{\exp(-t/2)t^{k-1}}{2^k}\left[\frac{\partial}{\partial\Delta^2}\left(\frac{(t/2)^{A\Delta^2}}{\Gamma(k+A\Delta^2)}\right)_{\Delta^2=0}\right]dt$$
$$\approx \alpha + \Delta^2 \int_{\chi^2_{2k;\alpha}}^{\infty} \frac{\exp(-t/2)t^{k-1}}{2^k}\left[\frac{A\ln(t/2)}{\Gamma(k)} - \frac{A\int_0^{\infty}\exp(-u)u^{k-1}\ln(u)du}{\Gamma^2(k)}\right]dt$$
$$\approx \alpha + \Delta^2 A \int_{\chi^2_{2k;\alpha}}^{\infty} \frac{\exp(-t/2)t^{k-1}}{2^k\Gamma(k)}\left[\ln(t/2) - \frac{\int_0^{\infty}\exp(-u)u^{k-1}\ln(u)du}{\Gamma(k)}\right]dt$$
$$\approx \alpha + \Delta^2 A\left[E\left\{\left\{\ln(T/2)\right\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right].$$

Substituting back the expressions for A results in

$$LP(F) \approx \alpha + \frac{\Delta^2}{2}\left[\sum_{i=1}^{k}\frac{n_i\nu_i}{2\sigma_i^2}D_{\nu_i}\right]\left[E\left\{\left\{\ln(T/2)\right\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right].$$

For the special case $n_1 = \cdots = n_k = n$ and $\nu_1 = \cdots = \nu_k = \nu = n-1$, the local power of *Fisher's* test reduces to

$$LP(F) \approx \alpha + \frac{n\Delta^2}{2}\nu D_{\nu}\left[\sum_{i=1}^{k}\frac{1}{2\sigma_i^2}\right]\left[E\left\{\left\{\ln(T/2)\right\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right]$$
$$= \alpha + \left[\frac{n\Delta^2}{2}\Psi\right]\frac{\nu D_{\nu}}{2}\left[E\left\{\left\{\ln(T/2)\right\}I_{\{T\geq\chi^2_{2k;\alpha}\}}\right\}_{T\sim\chi^2_{2k}} - \alpha D_0\right] \qquad \text{where } \Psi = \sum_{i=1}^{k}\frac{1}{\sigma_i^2}.$$

V. Local Power of a Modified t Test $[LP(T_1)]$

Using this exact test based on a modified t, the null hypothesis $H_0 : \mu = \mu_0$ will be rejected if $T_1 > d_{1\alpha}$, where $T_1 = \sum_{i=1}^{k} w_{1i}|t_i|$, $w_{1i} \propto [Var(|t_i|)]^{-1}$, $Var(|t_i|) = [\nu_i(\nu_i-2)^{-1}] - \left([\Gamma(\frac{\nu_i-1}{2})\sqrt{\nu_i}][\Gamma(\frac{\nu_i}{2})\sqrt{\pi}]^{-1}\right)^2$, and $Pr\{T_1 > d_{1\alpha}|H_0\} = \alpha$. In applications $d_{1\alpha}$ is computed by simulation. This leads to

$$\text{Power of } T_1 = Pr\left\{\sum_{i=1}^{k} w_{1i}|t_i| > d_{1\alpha}|H_1\right\}$$
$$= \int\cdots\int_{\sum_{i=1}^{k} w_{1i}|t_i| > d_{1\alpha}} \prod_{i=1}^{k}\left[f_{\nu_i,\delta_i}(t_i)\right]\mathrm{d}t_i \qquad \left[\delta_i = \frac{\sqrt{n_i}\Delta}{\sigma_i}\right]$$

$$\approx \int\cdots\int_{\sum_{i=1}^{k} w_{1i}|t_i|>d_{1\alpha}} \prod_{i=1}^{k}\left[f_{\nu_i}(t_i)+\delta_i\frac{\partial f_{\nu_i,\delta_i}(t_i)}{\partial\delta_i}\Big|_{\delta_i=0}+\frac{\delta_i^2}{2}\frac{\partial^2 f_{\nu_i,\delta_i}(t_i)}{\partial\delta_i^2}\Big|_{\delta_i=0}\right]\mathrm{d}t_i$$

$$\approx \alpha+\sum_{j=1}^{k}\frac{\delta_j^2}{2}\left[\int\cdots\int_{\sum_{i=1}^{k} w_{1i}|t_i|>d_{1\alpha}}\left\{\prod_{i=1}^{k} f_{\nu_i}(t_i)\right\}\left\{\frac{\frac{\partial^2 f_{\nu_j,\delta_j}(t_j)}{\partial\delta^2}\big|_{\delta=0}}{f_{\nu_j}(t_j)}\right\}\right]\prod_{i=1}^{k}\mathrm{d}t_i$$

$$\approx \alpha+\sum_{j=1}^{k}\frac{\delta_j^2}{2}\left[E_{H_0}\left[\left\{\frac{\frac{\partial^2 f_{\nu_j,\delta_j}(t_j)}{\partial\delta_j^2}\big|_{\delta_j=0}}{f_{\nu_j}(t_j)}\right\}I_{\{\sum_{i=1}^{k} w_{1i}|t_i|>d_{1\alpha}\}}\right]\right]$$

$$\approx \alpha+\sum_{j=1}^{k}\frac{\delta_j^2}{2}\left[E_{H_0}\left[\left\{\frac{(t_j^2-1)\nu_j}{t_j^2+\nu_j}\right\}I_{\{\sum_{i=1}^{k} w_{1i}|t_i|>d_{1\alpha}\}}|H_0\right]\right]$$

$$\approx \alpha+\frac{\Delta^2}{2}\left(\sum_{j=1}^{k}\frac{n_j}{\sigma_j^2}E_{H_0}\left[\left\{\frac{(t_j^2-1)\nu_j}{t_j^2+\nu_j}\right\}I_{\{\sum_{i=1}^{k} w_{1i}|t_i|>d_1\alpha\}}\right]\right)\quad\text{using}\quad\left[\delta_j=\frac{\sqrt{n_j}\Delta}{\sigma_j}\right].$$

$E_{H_0}[\cdot]$ above is computed by simulation. It is easy to verify from Sect. 3 that the product terms $\left\{\frac{\partial f_{\nu_i,\delta_i}(t_i)}{\partial\delta_i}\big|_{\delta_i=0}\right\}\times\left\{\frac{\partial f_{\nu_j,\delta_j}(t_j)}{\partial\delta_j}\big|_{\delta_j=0}\right\}$ involve (t_it_j), apart from t_i^2 and t_j^2, whose integral over $\{\sum_{i=1}^{k} w_{1i}|t_i|>d_{1\alpha}\}$ under H_0 is zero.

For the special case $n_1=\cdots=n_k=n$ and $\nu_1=\cdots=\nu_k=\nu=n-1$ which implies $w_{11}=\cdots=w_{1k}=1$, the local power of this exact test based on modified t reduces to

$$LP(T_1)\approx\alpha+\frac{n\Delta^2}{2}\left(\sum_{j=1}^{k}\frac{1}{\sigma_j^2}\right)E_{H_0}\left[\left\{\frac{(t_1^2-1)\nu}{t_1^2+\nu}\right\}I_{\{\sum_{i=1}^{k}|t_i|>d_{1\alpha}\}}\right]$$

$$=\alpha+\left[\frac{n\Delta^2}{2}\Psi\right]E_{H_0}\left[\left\{\frac{(t_1^2-1)\nu}{t_1^2+\nu}\right\}I_{\{\sum_{i=1}^{k}|t_i|>d_{1\alpha}\}}\right]\qquad\text{where}\quad\Psi=\sum_{j=1}^{k}\frac{1}{\sigma_j^2}.$$

VI. Local Power of a Modified F Test $[LP(T_2)]$

According to this exact test based on a modified F, the null hypothesis $H_0:\mu=\mu_0$ will be rejected if $T_2>d_{2\alpha}$, where $T_2=\sum_{i=1}^{k} w_{2i}F_i$, $F_i\sim F(1,\nu_i)$, $w_{2i}\propto[Var(F_i)]^{-1}=[2\nu_i^2(\nu_i-1)]^{-1}[(\nu_i-2)^2(\nu_i-4)]$, and $Pr\{T_2>d_{2\alpha}|H_0\}=\alpha$. In applications $d_{2\alpha}$ is computed by simulation. This leads to

$$\text{Power of } T_2=Pr\left\{\sum_{i=1}^{k} w_{2i}F_i>d_{2\alpha}|H_1\right\}$$

$$=\int\cdots\int_{\sum_{i=1}^{k} w_{2i}F_i>d_{2\alpha}}\prod_{i=1}^{k}[f_{\nu_i,\lambda_i}(F_i)]\mathrm{d}F_i\quad\left[f_{\nu,\lambda}(F)\sim\text{non-central }F_{1,\nu}\left(\lambda=\frac{n\Delta^2}{\sigma^2}\right)\right].$$

Note that $f_{\nu,\lambda}(F)$ and its local expansion around $\lambda = 0$ are give by

$$
\begin{aligned}
f_{\nu,\lambda}(F) &= \exp(-\frac{\lambda}{2}) \sum_{j=0}^{\infty} \frac{(\frac{\lambda}{2})^j}{j!} \left[\frac{(\frac{\nu_1}{\nu_2})^{\frac{\nu_1+2j}{2}} \Gamma(\frac{\nu_1+\nu_2+2j}{2})}{\Gamma(\frac{\nu_1+2j}{2})\Gamma(\frac{\nu_2}{2})} \right] \left[\frac{F^{\frac{\nu_1+2j}{2}-1}}{\left(1+F\frac{\nu_1}{nu_2}\right)^{\frac{\nu_1+\nu_2+2j}{2}}} \right] \\
&\approx f_\nu(F)\left(1-\frac{\lambda}{2}\right) + \left[\frac{(\frac{\lambda}{2})(\frac{\nu_1}{\nu_2})^{\frac{\nu_1+2}{2}} \Gamma(\frac{\nu_1+\nu_2+2}{2})}{\Gamma(\frac{\nu_1+2}{2})\Gamma(\frac{\nu_2}{2})} \right] \left[\frac{F^{\nu_1}}{\left(1+F\frac{\nu_1}{\nu_2}\right)^{\frac{\nu_1+\nu_2+2}{2}}} \right] \\
&= f_\nu(F) + \frac{\lambda}{2}\left[f_\nu^*(F) - f_\nu(F)\right], \quad \text{where} \quad f_\nu^*(F) = \left(\frac{1}{\nu}\right)^{\frac{3}{2}} \left[\frac{F}{(1+\frac{F}{\nu})^{\frac{\nu+3}{2}} B[\frac{3}{2}, \frac{\nu}{2}]} \right].
\end{aligned}
$$

Using the above first-order expansion of $f_{\nu,\lambda}(F)$ leads to the following local power of T_2.

$$
\begin{aligned}
LP(T_2) &\approx \int\cdots\int_{\sum_{i=1}^k w_{2i} F_i > d_{2\alpha}} \left[\prod_{i=1}^k f_{\nu_i}(F_i) + \sum_{j=1}^k \frac{\lambda_j}{2} \left(f_{\nu_j}^*(F_j) - f_{\nu_j}(F_j) \right) \left\{ \prod_{i\neq j} \left[f_{\nu_i}(F_i) \right] \right\} \right] \prod_{i=1}^k \mathrm{d}F_i \\
&\approx \alpha + \left(\sum_{j=1}^k \frac{\lambda_j}{2} E_{H_0} \left[\left\{ \frac{f_{\nu_j}^*(F_j) - f_{\nu_j}(F_j)}{f_{\nu_j}(F_j)} \right\} I_{\{\sum_{i=1}^k w_{2i} F_i > d_{2\alpha}\}} \right] \right) \\
&\quad E_{H_0}[\cdot] \text{ stands for expectation w.r.t } F_1, \ldots, F_k \text{ under } H_0[F_i \sim F(1, \nu_i)]. \\
&\approx \alpha + \left(\sum_{j=1}^k \frac{\lambda_j}{2} E_{H_0} \left[\left\{ \frac{F_j - 1}{\frac{F_j}{\nu_j} + 1} \right\} I_{\{\sum_{i=1}^k w_{2i} F_i > d_{2\alpha}\}} \right] \right) \\
&\approx \alpha + \frac{\Delta^2}{2} \left(\sum_{j=1}^k \frac{n_j}{\sigma_j^2} E_{H_0} \left[\left\{ \frac{[F_j - 1]\nu_j}{F_j + \nu_j} \right\} I_{\{\sum_{i=1}^k w_{2i} F_i > d_{2\alpha}\}} \right] \right) \text{ using } \left[\lambda_j = \frac{n_j \Delta^2}{\sigma_j^2} \right]. \\
&\quad E_{H_0}[\cdot] \text{ is obtained by simulation.}
\end{aligned}
$$

For the special case $n_1 = \cdots = n_k = n$ and $\nu_1 = \cdots = \nu_k = \nu = n - 1$ which implies $w_{21} = \cdots = w_{2k} = 1$, the local power of this exact test based on modified F reduces to

$$
\begin{aligned}
LP(T_2) &\approx \alpha + \frac{n\Delta^2}{2} \left(\sum_{j=1}^k \frac{1}{\sigma_j^2} \right) E_{H_0} \left[\left\{ \frac{[F_1 - 1]\nu}{F_1 + \nu} \right\} I_{\{\sum_{i=1}^k F_i > d_{2\alpha}\}} \right] \\
&= \alpha + \left[\frac{n\Delta^2}{2} \Psi \right] E_{H_0} \left[\left\{ \frac{[F_1 - 1]\nu}{F_1 + \nu} \right\} I_{\{\sum_{i=1}^k F_i > d_{2\alpha}\}} \right] \qquad \text{where} \quad \Psi = \sum_{j=1}^k \frac{1}{\sigma_j^2}.
\end{aligned}
$$

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Quantile Function: Overview of Collaboration with Professor C. R. Rao

G. Jogesh Babu

Abstract The author's collaboration with Professor C. Radhakrishna Rao covers several topics. Some of these results will be presented in this note. In particular, the study of joint asymptotic distribution of the marginal sample quantiles and its use in developing tests of significance for population medians will be discussed. The estimation of the density quantile function at a point, which is needed in evaluating the asymptotic dispersion matrix of vector of sample quantiles, will also be described.

Keywords Asymptotic distribution of marginal sample quantiles · Tests of significance · Median · Estimation of density quantile function · Bahadur's representation of sample quantiles · Pooled estimator

1 Introduction

My collaboration with professor C. R. Rao covers several research projects (Babu et al. 1999, 2000; Babu and Rao 1988, 1990, 1992, 1993, 2003, 2004; Babu et al. 1992; Rao et al. 1991; Lee et al. 2012) including estimation of quantiles, and their applications. The results of Babu and Rao on quantiles developed in Babu and Rao (1988, 1990) make use of Bahadur's representation (Bahadur 1966) of sample quantiles. Bahadur's representation provides an elegant way to study large sample properties of sample quantiles. It also helps in density estimation. In this note, I shall briefly review the results of two of the research projects that I have collaborated with professor Rao. The first one is on nonparametric treatment of joint asymptotic distribution of marginal sample quantiles based on samples from a multivariate population. The second one is on consistent and efficient estimation for the density at a quantile point, where the rates of convergence depend on the smoothness properties

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of the density. Unlike classical density estimation, these estimators do not require knowledge of the actual values of the derivatives of the density. Rate of convergence depends only on the smoothness of the density (number of derivatives).

2 Bahadur's Representation

To describe Bahadur's representation we start with a definition.

Definition For any probability distribution function F on the real-line, the quantile function F^{-1} is defined as

$$F^{-1}(u) = \inf\{x : F(x) \geq u\}, \quad \text{for } 0 < u < 1.$$

For $0 < p < 1$, the p-th sample quantile of $U_1, \ldots, U_n$ is defined as $U_{([np])}$ or $F_n^{-1}(p)$, where $[\,y]$ is the largest integer not exceeding y, and F_n is the empirical distribution function:

$$F_n(x) = \frac{1}{n}\#\{1 \leq i \leq n : U_i \leq x\}.$$

In particular, the sample median $m_n = F_n^{-1}(1/2)$.

Bahadur (1966) developed an elegant way to express a sample quantile in terms of the empirical distribution and the density at a population quantile, with a negligible reminder. Bahadur's representation is presented as Theorem 1 below.

Theorem 1 *Let $U_1, \ldots, U_n$ be i.i.d.r.v.s with common distribution function F. Suppose $F'(F^{-1}(p))$ exists and non-zero at p-th population quantile $F^{-1}(p)$, and*

$$R_n = F_n^{-1}(p) - F^{-1}(p) + \frac{F_n(F^{-1}(p)) - p}{F'(F^{-1}(p))}.$$

Then $\sqrt{n}R_n \to_p 0$ as $n \to \infty$.

A simple proof by Ghosh (1971) establishes this weaker version, which is sufficient for most of the convergence in distribution results. This representation is used to get the joint asymptotic distribution of multiple sample quantiles.

In fact, Bahadur establishes a stronger result,

$$\limsup_{n\to\infty} (n^{3/4}/\log n)|R_n| < \infty \quad a.e.$$

when the second derivative of F exists and is bounded in a neighborhood of $F^{-1}(p)$.

3 Joint Asymptotic Distribution of Marginal Quantiles

In this section, the joint asymptotic distributions of the marginal sample quantiles, and quantile functions based on samples from a k-variate population are described. Of particular interest is the joint asymptotic distribution of marginal sample medians. Based on this, tests of significance for population medians were developed by Babu and Rao (1988). Methods of estimating unknown nuisance parameters are briefly discussed below. The approach is completely nonparametric.

Let $\boldsymbol{T} = (Y_1, \ldots, Y_k)$ be a random vector. Let F_i denotes the marginal distribution of Y_i. Suppose $\boldsymbol{T}_1, \ldots, \boldsymbol{T}_n$ are n independent copies of $\boldsymbol{T}$. Let F_n and $F_{i;n}$ denote the empirical distribution of $\boldsymbol{T}_1, \ldots, \boldsymbol{T}_n$ and their i-th coordinates $Y_{i;1}, \ldots, Y_{i;n}$. For $0 < q_i < 1$, the q_i-th sample quantile $F_{i;n}^{-1}(q_i)$ of the i-th coordinate is a good estimator of the population marginal quantile $F_i^{-1}(q_i)$. Define a diagonal matrix

$$A = diag\left((1/F_1'(F_1^{-1}(q_1)), \ldots, 1/F_k'(F_k^{-1}(q_k))\right), \tag{1}$$

and let

$$\tau_{ij}(t, s) = P\left(Y_i \le F_i^{-1}(t),\ Y_j \le F_j^{-1}(s)\right) - ts. \tag{2}$$

The following theorem on joint asymptotic distribution of marginal sample quantiles $(F_{1;n}^{-1}(q_1), \ldots, F_{k;n}^{-1}(q_k))$ was established by Babu and Rao (1988).

Theorem 2 *Suppose F_i is continuously twice differentiable in a neighborhood of $F_i^{-1}(q_i)$ and $F_i'(F_i^{-1}(q_i)) > 0, i = 1, \ldots, k$. Then the asymptotic distribution of*

$$V_n(q_1, \ldots, q_k) = \sqrt{n}\left(F_{1;n}^{-1}(q_1) - F_1^{-1}(q_1), \ldots, F_{k;n}^{-1}(q_k) - F_k^{-1}(q_k)\right) \tag{3}$$

is a k-variate normal with mean vector zero, and variance-covariance matrix

$$\Sigma = A\mathcal{T}A, \tag{4}$$

where $\mathcal{T}$ is a $k \times k$ matrix with ij-th entry $\tau_{ij}(q_i, q_j)$.

Remark The variance-covariance matrix Σ in the theorem above is not completely known. So in practice, the unknown entries $P(Y_i \le F_i^{-1}(q_i),\ Y_j \le F_j^{-1}(q_j))$ and $F_i'(F_i^{-1}(q_i))$ need to be estimated. By Theorem 2.2 of Babu and Rao (1988), as $n \to \infty$,

$$\frac{1}{n}\#\left\{1 \le k \le n : Y_{i;k} \le F_{i;n}^{-1}(q_i),\ Y_{j;k} \le F_{j;n}^{-1}(q_j)\right\} \to P\left(Y_i \le F_i^{-1}(q_i),\ Y_j \le F_j^{-1}(q_j)\right),$$

with probability 1. Several methods for estimation of density function at a given population quantile exist in the literature. A consistent estimator for the reciprocal of the density at a quantile point was developed in Babu (1986). More details on density quantile estimation are given in Sect. 4. Unlike the classical density estimators, these

density quantile estimators do not require knowledge of the actual values of the derivatives of the density.

The infinite dimensional weak limits of the entire marginal quantile process were also developed by Babu and Rao (1988) under the following *Assumptions* for $j = 1, \ldots, k$:

(i) the marginal distribution F_j of Y_j is twice differentiable on (a_j, b_j), where

$$-\infty \le a_j = \sup\{x : F_j(x) = 0\}, \quad \inf\{x : F_j(x) = 1\} = b_j \le \infty;$$

(ii) $f_j = F_j' \ne 0$ on (a_j, b_j);

(iii) $\max_j \sup_{a_j < x < b_j} F_j(x)(1 - F_j(x))|f_j'(x)|/f_j^2(x) < \infty$;

(iv) f_j is non-decreasing (non-increasing) on an interval to the right of a_j (to the left of b_j).

Theorem 3 *Under assumptions (i) - (iv) on F_j, the process Z_n converges weakly to a Gaussian process $\boldsymbol{W} = (W_1, \ldots, W_k)$, where*

$$\begin{aligned} Z_n(q_1, \ldots, q_k) =& \sqrt{n}\big(F_1'(F_1^{-1}(q_1))(F_{1;n}^{-1}(q_1) - F_1^{-1}(q_1), \\ & \ldots, F_k'(F_k^{-1}(q_k))(F_{k;n}^{-1}(q_k) - F_k^{-1}(q_k))\big) \\ =& V_n(q_1, \ldots, q_k)A^{-1}, \end{aligned} \tag{5}$$

W_j is a Brownian bridge for each j, and the covariance function is given by

$$E(W_i(t)W_j(s)) = \tau_{ij}(t, s). \tag{6}$$

3.1 Tests of Significance for the Vector Medians

Using Theorem 2, tests of significance for the population medians based on the vector of marginal sample medians were developed by Babu and Rao (1988). These results are similar to the classical tests for means in multivariate case. To describe the test, let $\Theta_1, \ldots, \Theta_r$ be k-variate populations. To test that they all have the same vector of marginal medians, let n_i samples be drawn from the i-th population Θ_i; $i = 1, \ldots, r$. Let $\hat{\boldsymbol{m}}_i$ denote the vector of marginal medians based on the sample from Θ_i, and Σ_i denote the corresponding estimate of Σ. See Eq. (4) and the Remark following Theorem 2.

To test the hypothesis that all the marginal population median vectors are identical ($\hat{\boldsymbol{m}}_1 = \cdots = \hat{\boldsymbol{m}}_r$), use the statistic

$$\chi^2 = \text{trace}\left[\sum_{i=1}^{r} n_i \Sigma_i^{-1} \hat{\boldsymbol{m}}_i \hat{\boldsymbol{m}}_i' - \left(\sum_{i=1}^{r} n_i \Sigma_i^{-1}\right) \hat{\boldsymbol{m}} \hat{\boldsymbol{m}}'\right],$$

where

$$\hat{\boldsymbol{m}} = \left(\sum_{i=1}^{r} n_i \Sigma_i^{-1}\right)^{-1} \sum_{i=1}^{r} n_i \Sigma_i^{-1} \hat{\boldsymbol{m}}_i.$$

This statistic has approximately chi-square distribution with $k(r-1)$ degrees of freedom, provided the sample sizes $n_1, \ldots, n_r$ are large.

4 Estimation of Density Quantile Function

As seen in Sect. 3, the density at a quantile appears as a nuisance parameter for the inference on quantiles. Similarly, inference based on least absolute deviation (L_1) norm also involves such nuisance parameters. These unknown nuisance parameters may be substituted by their estimates in the analysis. We now focus on consistent estimators for the reciprocal of the density at a quantile point in the univariate case. Note that the reciprocal of the density at a quantile is the derivative of the quantile function. Building on an estimator proposed in Babu (1986), the rates of convergence for the estimator of reciprocal of the density at a quantile point were developed by Babu and Rao (1990). The rates of convergence depend on the smoothness properties of the density only.

Let U be a random variable with a differentiable distribution function F. Suppose the quantile density function $F'(F^{-1}(p)) > 0$ for a fixed $0 < p < 1$, and assume that F is twice continuously differentiable in a neighborhood of $F^{-1}(p)$.

We now concentrate on efficient estimation of $\alpha = (1/F'(F^{-1}(p))) = (F^{-1})'(p)$, based on $i.i.d.$ random variables $U_1, \ldots, U_n$, with finite second moment and a common distribution function F.

For $0 < \delta < \frac{1}{2}$, and an integer $n \geq 3$, let

$$\begin{aligned} D_n(\delta; h) &= n^{\delta} \int_0^{\min\{\log n, (1-p)n^{\delta}\}} \left(F_n^{-1}(p + un^{-\delta}) - F_n^{-1}(p)\right) h(u) e^{-u}\, du \\ H_n(\delta; h) &= n^{\delta} \int_0^{\min\{\log n, (1-p)n^{\delta}\}} \left(F^{-1}(p + un^{-\delta}) - F^{-1}(p)\right) h(u) e^{-u}\, du, \end{aligned} \tag{7}$$

where F_n is the empirical distribution function of the sample, and h is a polynomial such that

$$\int_0^{\infty} uh(u)e^{-u}\, du = \int_0^{\infty} h(u)e^{-u}\, du = 1. \tag{8}$$

For example, the polynomials $h_1(y) = 1,\ h_2(y) = 2y - \frac{1}{2}y^2,\ h_3(y) = -2 + 8y - \frac{7}{2}y^2 + \frac{1}{3}y^3$ and $h_4(y) = -5 + 20y - \frac{25}{2}y^2 + \frac{7}{3}y^3 - \frac{1}{8}y^4$ satisfy Eq. (8). The choice of polynomial h depends on the assumed number of derivatives of the density only. The following result is established in Babu and Rao (1990).

Theorem 4 *As* $n \to \infty$,

$$n^{(1-\delta)/2}\alpha^{-1}(D_n(\delta; h) - H_n(\delta; h)) \xrightarrow{\mathcal{D}} \sigma\, Z,$$

where Z *has standard normal distribution and*

$$\sigma^2 = \int_0^\infty \int_0^\infty \min(u, v)h(u)h(v)\, du\, dv.$$

The rates of convergence in Theorem 4 is dependent on finding a polynomial h_m (for $m \geq 2$) of degree not exceeding m and satisfying the integral equation

$$\int_0^\infty y^j h_m(y)e^{-y}dy = \begin{cases} 1 & \text{for} \quad j = 0, 1, \\ 0 & \text{for} \quad j = 2, \ldots, m. \end{cases} \tag{9}$$

Such a distinctive polynomial is constructed in Babu (1986). The construction is surprisingly simple and uses a positive definite matrix B with $(m + 1)$ columns and its ij-th entry is $(i + j)!, i, j = 0, \ldots, m$. As $\int_0^\infty y^j e^{-y}dy = j!$. The required function h_m is defined as

$$h_m(y) = \sum_{j=0}^{m} u_j y^j,$$

where $(u_0, \ldots, u_m) = (1, 1, 0, \ldots, 0)B^{-1}$, and

$$u_j = \frac{(-1)^{j+1}}{j!}\left(m\binom{m+1}{j+1} - \binom{m+2}{j+2}\right),\ j = 0, 1, \ldots, m.$$

Until this point δ is arbitrary. From a computational point of view, $D_n(\delta; h_m)$ is a good estimator if F is m times continuously differentiable in a neighborhood of $F^{-1}(p)$ and $\delta = 1/(2m - 1)$. In this case, by (9),

$$\begin{aligned} H_n(\delta; h_m) =& \alpha + o\left(\int_0^{\log n} n^{-(m-1)\delta}u^m |h_m(u)|\, du\right) \\ =& \alpha + o\left(n^{(1-\delta)/2}\right), \end{aligned} \tag{10}$$

and

$$bias = E\left(D_n(\delta; h_m)\right) - \alpha = o\left(\left(E\left(D_n(\delta; h_m) - \alpha\right)^2\right)^{1/2}\right).$$

Thus, it follows from Theorem 4 and Eq. (10), that

$$n^{(m-1)/(2m-1)}\alpha^{-1}(D_n(\delta; h_m) - \alpha) \xrightarrow{\mathcal{D}} \sigma\, Z, \tag{11}$$

where Z and σ are as in Theorem 4.

4.1 Location Family

Using the above results, Babu and Rao proposed two estimators based on several samples from a location family in Babu and Rao (1990). The samples are drawn from a family with unknown and different location parameters. Such results are needed in estimating the asymptotic dispersion matrix of several sample quantiles as they involve density at population quantiles.

Theorem 4 was extended to a case when the i.i.d. random variable $Y_{i1}, \ldots, Y_{in_i}$ are drawn from a location family G^i, $i = 1, \ldots, r$. Here F is a continuous distribution function that links these distributions as $G^i(x) = F(x - \beta_i)$ for all x, where location parameter m_i is the p-th quantile of G^i. Thus Y_{ij} are from the same population except for differences in location; that is

$$Y_{i1} - \beta_i, \ldots, Y_{in_i} - \beta_i \tag{12}$$

are i.i.d. random variables with the common distribution F. We assume, as before that F is m times continuously differentiable in a neighborhood of $F^{-1}(p)$. Let $N = n_1 + \cdots + n_r$. It is natural to assume none of the sample sizes are negligible compared to the others. That is, we assume $Na \le n_i \le Nb$ for some positive constants a, b.

Two estimators of $\alpha = 1/F'(F^{-1}(p)) > 0$ based on (i) pooled, and (ii) location adjusted combined sample are considered in Babu and Rao (1990).

4.1.1 Pooled Estimator

Pooled estimator $d_N^* = \sum_{i=1}^r \gamma_i D_{n_i}(1/(2m-1); h_m)$ is a linear combination of individual estimators, where $\gamma_i > 0$, $\sum_{i=1}^r \gamma_i = 1$ and D_n is defined in (7). The estimates D_{n_i} are independent of location parameters β_i as D_{n_i} depends only on the differences of order statistics. In this case Theorem 2 of Babu and Rao (1990) shows that

$$\left(\sum_{i=1}^r \gamma_i^2 n_i^{2(m-1)/(2m-1)}\right)^{1/2} \alpha^{-1}(d_N^* - \alpha) \xrightarrow{\mathcal{D}} \sigma\, Z,$$

and the mean square error σ_{N1}^2 of $\alpha^{-1}d_N^*$ satisfies

$$\sigma_{N1}^2 \sim \left(\sum_{i=1}^r \gamma_i^2 n_i^{-2(m-1)/(2m-1)}\right)\sigma^2. \tag{13}$$

This leads to the optimal choice for γ_i as

$$\gamma_i = n_i^{2(m-1)/(2m-1)} \left(\sum_{j=1}^{r} n_j^{2(m-1)/(2m-1)} \right)^{-1}.$$

4.1.2 Location Adjusted Combined Sample Estimator

The second method involves adjusting the observations in each sample for location and constructing the estimate based on the resultant combined sample of size N. More precisely, obtain the empirical distribution

$$F_N^*(x) = \sum_{i=1}^{r} \frac{n_i}{N} G_n^i(x + \beta_{iN} - \beta_i)$$

of the combined adjusted sample,

$$Y_{i1} - \beta_{iN}, \ldots, Y_{in_i} - \beta_{iN}, \ i = 1, \ldots, r,$$

where β_{iN} is the p-th sample quantile of the i-th sample and G_n^i is the empirical distribution function based on the sample in Eq. (12). We now consider the combined adjusted estimator

$$d_N^c = N^{1/(2m-1)} \int_0^{\log N} \left(F_N^{*-1}(p + uN^{-1/(2m-1)}) - F_N^{*-1}(p) \right) h(u) e^{-u} \, du.$$

Theorem 3 of Babu and Rao (1990) establishes

$$N^{(m-1)/(2m-1)} \alpha^{-1} (d_N^c - \alpha) \xrightarrow{\mathcal{D}} \sigma \, Z, \ as \ N \to \infty,$$

and the mean square error σ_{N2}^2 of $\alpha^{-1} d_N^c$ satisfies

$$\sigma_{N2}^2 \sim N^{-2(m-1)/(2m-1)} \sigma^2. \tag{14}$$

From Eqs. (13) and (14), it follows that $\sigma_{N1}^2 / \sigma_{N2}^2 \sim \nu < 1$. Thus pooled estimator seems to be better than location adjusted combined sample estimator.

5 Concluding Remarks

A brief description of some of the results of my collaboration with Professor C. R. Rao is given above. The main focus of this article is on the large sample theory for a vector of marginal sample quantiles, and estimation of density at a quantile point.

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Distribution Theory

Some Bivariate and Multivariate Models Involving Independent Gamma Distributed Components

Barry C. Arnold

Abstract Several multivariate models involving independent gamma distributed components (three of which are new) are described. The flexible bivariate beta(2) model introduced by Arnold and Ng (2011) provides the template for the other models. It involved ratios of sums of independent gamma variables. The other models involve differences, sums, products, and minima rather than ratios.

Keywords Beta(2) distribution · Asymmetric Laplace distribution · Gamma difference · Gamma product · Copulas

1 Introduction

Arnold and Ng (2011) introduced a bivariate second kind beta or beta(2) distribution involving 8 independent random variables with gamma distributions (subsequently such random variables will be referred to as gamma distributed variables or, more simply, as gamma variables). Recall that a random variable X has a second kind beta distribution with parameters δ_1 and δ_2 if its density is of the form

$$f_X(x) = \frac{x^{\delta_1 - 1} I(x > 0)}{B(\delta_1, \delta_2)(1 + x)^{\delta_1 + \delta_2}}, \tag{1}$$

where $\delta_1 > 0$ and $\delta_2 > 0$. In this formula $B(\delta_1, \delta_2)$ denotes the classical Beta function and indicator function notation is used so that $I(P(x))$ is equal to 1 if the proposition $P(x)$ is true and is equal 0 otherwise. A convenient stochastic representation of such beta(2) variables is available. If X has density (1) then it has the same distribution as the ratio of two independent gamma distributed random variables. Specifically we

For C. R. Rao on his 100th Birthday.

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have

$$X \stackrel{d}{=} \frac{U_1}{U_2}, \tag{2}$$

where U_1 and U_2 are independent gamma variables with $U_i \sim \Gamma(\delta_i, 1)$ for $i = 1, 2$. The flexible Arnold–Ng model subsumed and extended several previously available bivariate beta(2) models. The construction of this bivariate model relies on two well-known facts. (1) A sum of independent gamma variables with a common scale parameter has again a gamma distribution. (2) Ratios of independent gamma variables with a common scale parameter have beta distributions of the second kind. A convenient source for discussion of the history, properties, and applications of the gamma distribution is Chap. 17 of Johnson et al. (1994).

Arnold and Ng (2011) sought to identify the most general bivariate distribution whose marginals are ratios of sums of independent gamma variables. The most general model turns out to involve 8 independent gamma component variables. For this model, we begin with $U_1, U_2, ..., U_8$ a set of 8 independent variables with $U_j \sim \Gamma(\delta_j, 1)$, $j = 1, 2, ..., 8$. We then define the two-dimensional random vector (X, Y) by

$$\begin{aligned} X &= \frac{U_1 + U_5 + U_7}{U_3 + U_6 + U_8}, \\ Y &= \frac{U_2 + U_6 + U_7}{U_4 + U_5 + U_8}. \end{aligned} \tag{3}$$

This clearly defines an 8-parameter family of bivariate distributions with beta(2) marginal distributions. If (X, Y) is defined as in (3) then we write: $(X, Y) \sim BB(2)(\underline{\delta})$, to be read as (X, Y) has a bivariate second kind beta distribution with parameter vector $\underline{\delta}$.

Some explanation regarding the placement of the U_j's in (3) and why there are no more than 8 of them, will perhaps be helpful. There are four locations where a particular U_j may be placed. (1) In the numerator of X. (2) In the denominator of X. (3) In the numerator of Y and (4) In the denominator of Y. The variables U_1, U_2, U_3, and U_4 appear only once and each one of them appears in only one of the four possible locations. A variable U_j cannot appear in both the numerator and denominator of X, nor of Y, since otherwise the independence of numerators and denominators, required for beta(2) marginals, would be destroyed. U_5 appears in the numerator of X and in the denominator of Y. U_6 appears in the denominator of X and the numerator of Y. U_7 appears in both numerators, while U_8 appears in both denominators. No U_j can appear in 3 or in 4 of the possible locations, since that would destroy the required independence of at least one numerator and its corresponding denominator. If an additional independent gamma variable is introduced in one or two permissible locations in (3) then it can be combined with one of the existing 8 U_j's and no enrichment of the model will result. Thus, for example, if U_9 is added to both numerators, then $U_7 + U_9$ will continue to play the role of U_7 with an adjusted

shape parameter $\delta_7 + \delta_9$. In this fashion it becomes apparent that the most general bivariate model involving ratios of sums of independent gamma variables will involve 8 such random variables. This number of independent component variables will be subsequently observed in the general models to be introduced in Sects. 3, 4 and 5.

We adopt the convention that a random variable with a $\Gamma(\delta, 1)$ distribution with $\delta = 0$ will be defined to be a random variable that is degenerate at 0, By setting some of the δ_j's in the Arnold–Ng model (3) equal to zero, simplified sub-models (some of which have been discussed in the literature, e.g., Olkin and Liu 2003) will be obtained. Note that after setting certain δ_j's equal to zero, we must retain $\delta_1 + \delta_5 + \delta_7 > 0$, $\delta_3 + \delta_6 + \delta_8 > 0$, $\delta_2 + \delta_6 + \delta_7 > 0$, and $\delta_4 + \delta_5 + \delta_8 > 0$, in order to continue to have beta(2) marginal distributions.

The bivariate beta(2) model is clearly closed under reciprocation, since the univariate beta(2) distribution has this property. Thus if (X, Y) has a BB(2) distribution then so do each of the related random vectors $(X, 1/Y)$, $(1/X, Y)$, and $(1/X, 1/Y)$.

In the case of the bivariate beta(2) model, we dealt with ratios of sums of gamma variables. In subsequent sections of this paper we will consider replacing ratios with products, sums, and differences and we will also consider two other 8 parameter constructions which are closely related.

2 Concerning Flexible Copulas

If X has a beta(2) distribution then $V = X/(1 + X)$ has a beta distribution of the first kind, i.e., the usual beta distribution. Consequently, if $(X, Y) \sim BB(2)(\underline{\delta})$ then $(V, W) = (X/[1 + X]), Y/[1 + Y])$ has a bivariate distribution with beta(1) marginals. Specifically, $V \sim B(\delta_1 + \delta_5 + \delta_7, \delta_3 + \delta_6 + \delta_8)$ and $W \sim B(\delta_2 + \delta_6 + \delta_7, \delta_4 + \delta_5 + \delta_8)$. If we impose the constraints, $\delta_1 + \delta_5 + \delta_7 = 1$, $\delta_3 + \delta_6 + \delta_8 = 1$, $\delta_2 + \delta_6 + \delta_7 = 1$, and $\delta_4 + \delta_5 + \delta_8 = 1$, then (V, W) will have $Uniform(0, 1)$ marginal distributions. That is to say, (V, W) has a joint distribution function that is a copula. We thus have available a 4 parameter family of copulas, Most copula families have only one or perhaps two parameters. Arvanitis (2018) provides detailed discussion of this flexible 4 parameter family of copulas.

3 A Bivariate Gamma-Product Model

If W_1 and W_2 are independent gamma distributed random variables with $W_j \sim \Gamma(\delta_j, 1)$ $j = 1, 2$, then the product $Z = W_1 W_2$ has what is known as a gamma-product distribution with parameters δ_1 and δ_2. Note that this model is not identifiable, since interchanging the roles of δ_1 and δ_2 will not change the distribution. Identifiability will be assured if we impose the constraint that $\delta_1 \leq \delta_2$. If a random variable Z has a gamma-product distribution then we write $Z \sim GP(\delta_1, \delta_2)$, and we may verify that the density of Z is given by

$$f_Z(z) = \frac{2}{\Gamma(\delta_1)\Gamma(\delta_2)} z^{[\delta_1+\delta_2]-1} K_{\delta_1-\delta_2}(2\sqrt{z}) I(z > 0), \tag{4}$$

where $K_u(v)$ is a modified Bessel function of the third kind (see Johnson et al. 1994).

Although this is not the most simple density, it must be remarked that simulation of realizations from this distribution is readily accomplished.

Discussion of products of independent gamma variables as special cases of products of generalized gamma variables may be found in Mathai (1972). Muhammed et al. (2019) discuss the role of such distributions in certain stochastic volatility models.

With this definition at hand, we turn to the problem of developing flexible bivariate models with gamma-product marginal distributions. When the word flexible is used here, it is used to reflect the fact that model has the capacity to exhibit a wide spectrum of dependence relations between the coordinate variables. When the word tractable is used to describe a model, it typically refers to the fact that some distributional features of the distribution are readily derived and that, at the very least, simulation of realizations from the distribution are easily accomplished. The models discussed in this paper are generally both flexible and tractable.

To the end of developing a bivariate gamma-product distribution, we begin as in Sect. 1, with 8 independent gamma variables $U_1, U_2, ..., U_8$ with $U_j \sim \Gamma(\delta_j, 1)$, $j = 1, 2, ..., 8$. We then define (X, Y) by

$$\begin{aligned} X &= (U_1 + U_5 + U_7)(U_3 + U_6 + U_8), \\ Y &= (U_2 + U_6 + U_7)(U_4 + U_5 + U_8), \end{aligned} \tag{5}$$

analogous to (3). If (X, Y) is as defined by (5) then we write $(X, Y) \sim BGP(\underline{\delta})$, to be read as a bivariate gamma-product distribution. Clearly (X, Y) has gamma-product marginals. Since $W_1 W_2 = W_2 W_1$, the BGP model is not identifiable. Identifiability can be assured by imposing the constraint that $\delta_7 \leq \delta_8$. If we consider sub-models obtained by setting some of the δ_j's equal to zero, it may be necessary to impose a different constraint to ensure identifiability.

The means and variances for the BGP model are readily calculated recalling that the U_j's are independent gamma variables. Thus

$$E(X) = (\delta_1 + \delta_5 + \delta_7)(\delta_3 + \delta_6 + \delta_8), \tag{6}$$

$$E(Y) = (\delta_2 + \delta_6 + \delta_7)(\delta_4 + \delta_5 + \delta_8), \tag{7}$$

$$var(X) = E(X)[1 + \delta_1 + \delta_5 + \delta_7 + \delta_3 + \delta_6 + \delta_8], \tag{8}$$

$$var(Y) = E(Y)[1 + \delta_2 + \delta_6 + \delta_7 + \delta_4 + \delta_5 + \delta_8], \tag{9}$$

Expressions for the covariance of X and Y and their correlation, though elementary, are quite complicated and will not be included here.

Simplified sub-models obtained by setting certain of the δ_j's equal to zero, or by imposing linear constraints on them, will in some cases allow for simple expressions for the covariance, and may be preferable as models for some data sets.

4 A Bivariate Gamma-Difference Model

If W_1 and W_2 are independent gamma distributed random variables with $W_j \sim \Gamma(\delta_j, 1)$ $j = 1, 2$, then the difference $Z = W_1 - W_2$ has what is known as a gamma-difference distribution with parameters δ_1 and δ_2, and we write $Z \sim GD(\delta_1, \delta_2)$, A recent paper by Klar (2015) provides details, possible applications and historical perspective on this model. Many early appearances of the model dealt with the symmetric case in which $\delta_1 = \delta_2$.

If $Z \sim GD(\delta_1, \delta_2)$ it follows that its moment generating function is of the form

$$M_Z(t) = (1-t)^{-\delta_1}(1+t)^{-\delta_2}, \quad |t| < 1. \tag{10}$$

The moments of Z could be obtained from this moment generating function, but they may more easily be obtained by expanding $(W_1 - W_2)^k$, where k is a positive integer, and using available expressions for gamma moments. The mean, variance ad skewness of Z are thus, respectively:

$$\delta_1 - \delta_2 \qquad \delta_1 + \delta_2 \qquad \frac{2(\delta_1 - \delta_2)}{(\delta_1 + \delta_2)^{3/2}}. \tag{11}$$

The distribution of Z is asymmetric unless $\delta_1 = \delta_2$. Klar (2015) provides the following expression for the density of Z.

$$f_Z(z) = \begin{cases} [\Gamma(\delta_1)\Gamma(\delta_2)]^{-1} e^z \int_z^\infty x^{\delta_1 - 1}(x-z)^{\delta_2 - 1} e^{-2x} dx, & z > 0, \\ [\Gamma(\delta_1)\Gamma(\delta_2)]^{-1} e^{-z} \int_{-z}^\infty x^{\delta_1 - 1}(x+z)^{\delta_2 - 1} e^{-2x} dx, & z < 0. \end{cases} \tag{12}$$

He points out that the integrals in (12) can be evaluated in terms of Whittaker-W functions, although he cautions that there may be some problems for certain choices of δ_1 and δ_2. Of course, if δ_1 and δ_2 are positive integers, successive integration by parts can be used to evaluate the integrals.

The representation $Z = X_1 - X_2$ not only allows for ready computation of the moments of Z, but also permits straightforward simulation of realizations from its distribution. Klar (2015), observing the simplicity of the expression for the characteristic function of Z, suggests a parameter estimation strategy using the empirical characteristic function. Variations of the method of moments could also be used to estimate (δ_1, δ_2).

Simple bivariate versions of the GD distribution can be developed using the "variables in common" methodology. For it, we can begin with 3 independent gamma variables U_1, U_2, and U_3 with $U_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, 3$. Then define $X = U_1 - U_3$ and $Y = U_2 - U_3$.

Instead, in order to develop a more flexible bivariate model, we can behave in a manner analogous to that used in the earlier sections of this paper. We begin, as usual, with 8 independent gamma variables $U_1, U_2, ..., U_8$ with $U_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, ..., 8$. We then define (X, Y) by

$$\begin{aligned} X &= (U_1 + U_5 + U_7) - (U_3 + U_6 + U_8), \\ Y &= (U_2 + U_6 + U_7) - (U_4 + U_5 + U_8), \end{aligned} \tag{13}$$

analogous to (3). If (X, Y) is as defined by (13) then we write $(X, Y) \sim BGD(\underline{\delta})$, to be read as a bivariate gamma-difference distribution. Clearly (X, Y) has gamma-difference marginals. The BGD distribution is identifiable. Observe that each U_j plays a different role in the construction. Moreover, the BGD model represents the most general model in which both X and Y are linear combinations of independent gamma variables with all coefficients equal to 1 or -1. Of course sub-models of (13), in which certain δ_j's are set equal to 0 with the usual convention that the corresponding U_j's are equal to 0 with probability 1, may frequently be found adequate to model particular data sets. For example, the three-parameter "variables in common" model described in the previous paragraph is identifiable as a special case obtained by setting 5 of the parameters equal to 0. It exhibits a limited range of correlation values (only non-negative ones). Alternatively, it is sometimes appropriate to impose linear constraints on the δ_j's to arrive at a model with a parameter space of reduced dimension. An example, in which linear constraints are imposed is provided by one of the bivariate asymmetric Laplace model to be described in the next section.

Moments of the BGD distribution are generally not difficult to evaluate, since they are functions of available gamma moments. For example, we have

$$E(X) = \delta_1 + \delta_5 + \delta_7 - \delta_3 - \delta_6 - \delta_8, \tag{14}$$

$$E(Y) = \delta_2 + \delta_6 + \delta_7 - \delta_4 - \delta_5 - \delta_8, \tag{15}$$

$$var(X) = \delta_1 + \delta_5 + \delta_7 + \delta_3 + \delta_6 + \delta_8, \tag{16}$$

$$var(Y) = \delta_2 + \delta_6 + \delta_7 + \delta_4 + \delta_5 + \delta_8, \tag{17}$$

and

$$cov(X, Y) = -\delta_5 - \delta_6 + \delta_7 + \delta_8. \tag{18}$$

In this bivariate model, a simple expression is at hand for the covariance, in contrast to the situation in the other bivariate models that have been discussed. It is clearly possible to have a full range of correlations in the BGD model. Zero correlation can occur even though X and Y are dependent. It only requires that $-\delta_5 - \delta_6 + \delta_7 + \delta_8 = 0$. Independence will be the case if $\delta_5 = \delta_6 = \delta_7 = \delta_8 = 0$.

5 Bivariate Asymmetric Laplace Distributions

A special case of the gamma-difference distribution when $\delta_1 = \delta_2 = 1$ is more tractable than the general model. For in that case, we are dealing with a difference of two independent standard exponential random variables. It is of course well-known that such a difference has a Laplace distribution. Not so well known, but not much more difficult to deal with, is the case in which the exponential variables have different intensity parameters, denoted by λ_1 and λ_2. Thus we begin with two independent random variables W_1 and W_2 with $W_j \sim exp(\lambda_j), \quad j = 1, 2.$

As in the general gamma-difference case (but this time not having unit scale parameters), we define $Z = W_1 - W_2$. The moment generating function of Z is then of the form

$$M_Z(t) = \left(1 - \frac{t}{\lambda_1}\right)^{-1} \left(1 + \frac{t}{\lambda_2}\right)^{-1}, \quad |t| < \widetilde{\lambda} = min\{\lambda_1, \lambda_2\}. \tag{19}$$

Expanding this expression via partial fractions, we obtain

$$M_Z(t) = \frac{\lambda_2}{\lambda_1 + \lambda_2} \left(1 - \frac{t}{\lambda_1}\right)^{-1} + \frac{\lambda_1}{\lambda_1 + \lambda_2} \left(1 + \frac{t}{\lambda_2}\right)^{-1}, \quad |t| < \widetilde{\lambda} \tag{20}$$

This can be recognized as a mixture of two moment generating functions, one corresponding to an exponential random variable and the other to a random variable that is the negative of an exponential variable. From this observation we obtain the following expression for the density of Z:

$$f_Z(z) = \begin{cases} \frac{\lambda_1 \lambda_2}{\lambda_1 + \lambda_2} e^{-\lambda_1 z}, & z > 0, \\ \\ \frac{\lambda_1 \lambda_2}{\lambda_1 + \lambda_2} e^{\lambda_2 z}, & z < 0, \end{cases} \tag{21}$$

The random variable Z, in this case is said to have an asymmetric Laplace distribution with parameters λ_1 and λ_2. To indicate this, we write $Z \sim AL(\lambda_1, \lambda_2)$. Note that, if $\lambda_1 = \lambda_2$ this reduces to become the usual (symmetric) Laplace distribution. Moments of the asymmetric Laplace distribution are easily obtained, making use of the representation $Z = W_1 - W_2$, thus:

$$E(Z) = \lambda_1^{-1} - \lambda_2^{-1}, \tag{22}$$

$$var(Z) = \lambda_1^{-2} + \lambda_2^{-2}. \tag{23}$$

Some discussion of the asymmetric Laplace distribution may be found in Kozubowski and Podgórski (2000), using different notation.

Two different bivariate asymmetric Laplace distributions will be described in this section. Before introducing them, we will review two features of the exponential distribution that will be used in the discussion. First we note that if we have three inde-

pendent gamma variables U_1, U_2, and U_3 with $U_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, 3$ then, if $\delta_1 + \delta_2 + \delta_3 = 1$ then the random variable $\lambda^{-1}(U_1 + U_2 + U_3) \sim exp(\lambda)$. Next note that if V_1, V_2, and V_3 are independent exponential variables with $V_j \sim exp(\lambda_j), \ j = 1, 2, 3$, then $V = min\{V_1, V_2, V_3\} \sim exp(\lambda)$ where $\lambda = \lambda_1 + \lambda_2 + \lambda_3$.

5.1 *Bivariate Asymmetric Laplace Distribution of the First Kind (BAL(I))*

The first bivariate asymmetric Laplace model was introduced by Arvanitis (2018) and we refer the reader to that source for detailed discussion of the model. Construction of the model begins with the components used in Sect. 4 in developing the bivariate gamma-difference model. Thus we begin with 8 independent gamma variables $U_1, U_2, ..., U_8$ with $U_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, ..., 8$. We then define (X, Y) by

$$\begin{aligned} X &= \lambda_{11}^{-1}(U_1 + U_5 + U_7) - \lambda_{12}^{-1}(U_3 + U_6 + U_8), \\ Y &= \lambda_{21}^{-1}(U_2 + U_6 + U_7) - \lambda_{22}^{-1}(U_4 + U_5 + U_8), \end{aligned} \tag{24}$$

where it is assumed that the constraints, $\delta_1 + \delta_5 + \delta_7 = 1$, $\delta_3 + \delta_6 + \delta_8 = 1$, $\delta_2 + \delta_6 + \delta_7 = 1$, and $\delta_4 + \delta_5 + \delta_8 = 1$, have been imposed. This model will be called the bivariate asymmetric Laplace model of the first kind and if (X, Y) is as defined in (24) we will write $(X, Y) \sim BAL(1)(\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}, \underline{\delta})$, Since there were four constraints on the δ_j's, this is an 8 parameter model. The marginal distributions depend only on the four λ parameters, thus:

$$X \sim AL(\lambda_{11}, \lambda_{12}), \quad Y \sim AL(\lambda_{21}, \lambda_{22}). \tag{25}$$

Moments are obtainable from the representation (24):

$$E(X) = \lambda_{11}^{-1} - \lambda_{12}^{-1}, \tag{26}$$

$$E(Y) = \lambda_{21}^{-1} - \lambda_{22}^{-1}, \tag{27}$$

$$var(X) = \lambda_{11}^{-2} + \lambda_{12}^{-2}, \tag{28}$$

$$var(Y) = \lambda_{21}^{-2} + \lambda_{22}^{-2}, \tag{29}$$

and

$$cov(X, Y) = -\lambda_{11}^{-1}\lambda_{22}^{-1}\delta_5^2 - \lambda_{12}^{-1}\lambda_{21}^{-1}\delta_6^2 + \lambda_{11}^{-1}\lambda_{21}^{-1}\delta_7^2 + \lambda_{12}^{-1}\lambda_{22}^{-1}\delta_8^2. \tag{30}$$

It is evident from (30), that a full range of correlations are available in this model. A submodel with non-negative correlations can be identified by setting $\delta_5 = \delta_6 = 0$.

5.2 Bivariate Asymmetric Laplace Distribution of the Second Kind ($BAL(II)$)

The second bivariate asymmetric Laplace model that we will consider will utilize the closure under minimization property of the exponential distribution. For it we again begin, as is becoming customary in this paper, with 8 independent random variables, $V_1, V_2, ..., V_8$ but this time we assume that they are exponentially distributed, thus $V_j \sim exp(\lambda_j), \quad j = 1, 2, ..., 8$. We then define

$$\begin{aligned} X &= min\{V_1, V_5, V_7\} - min\{V_3, V_6, V_8\}, \\ Y &= min\{V_2, V_6, V_7\} - min\{V_4, V_5, V_8\}, \end{aligned} \tag{31}$$

using a construction somewhat parallel to that used in the construction of models earlier described in this paper. If (X, Y) has the structure shown in (31) then we will write $(X, Y) \sim BAL(II)(\underline{\lambda})$ and say that it has a bivariate asymmetric Laplace distribution of the second kind with parameter vector $\underline{\lambda}$. Note that both the first kind and the second kind bivariate asymmetric Laplace distributions have an 8 dimensional parameter space. The marginal distributions of the BAL(II) distribution are of the asymmetric Laplace form, Thus:

$$X \sim AL(\lambda_1 + \lambda_5 + \lambda_7, \lambda_3 + \lambda_6 + \lambda_8), \tag{32}$$

$$Y \sim AL(\lambda_2 + \lambda_6 + \lambda_7, \lambda_4 + \lambda_5 + \lambda_8). \tag{33}$$

The moments of the BAL(II) distribution are thus given by

$$E(X) = [\lambda_1 + \lambda_5 + \lambda_7]^{-1} - [\lambda_3 + \lambda_6 + \lambda_8]^{-1}, \tag{34}$$

$$E(Y) = [\lambda_2 + \lambda_6 + \lambda_7]^{-1} - [\lambda_4 + \lambda_5 + \lambda_8]^{-1}, \tag{35}$$

$$var(X) = [\lambda_1 + \lambda_5 + \lambda_7]^{-2} + [\lambda_3 + \lambda_6 + \lambda_8]^{-2}, \tag{36}$$

$$var(Y) = [\lambda_2 + \lambda_6 + \lambda_7]^{-2} + [\lambda_4 + \lambda_5 + \lambda_8]^{-2}, \tag{37}$$

and

$$\begin{aligned} cov(X, Y) &= \xi(\lambda_1 + \lambda_5, \lambda_2 + \lambda_6, \lambda_7) - \xi(\lambda_1 + \lambda_7, \lambda_4 + \lambda_8, \lambda_5) \\ &\quad -\xi(\lambda_3 + \lambda_8, \lambda_2 + \lambda_7, \lambda_6) + \xi(\lambda_3 + \lambda_6, \lambda_4 + \lambda_5, \lambda_8), \end{aligned} \tag{38}$$

in which we use the notation $\xi(\tau_1, \tau_2, \tau_3)$ to denote

$$cov(min\{W_1, W_3\}, min\{W_2, W_3\})$$

where the W_i's are independent with $W_i \sim exp(\tau_i), \quad i = 1, 2, 3$. The value of $\xi(\tau_1, \tau_2, \tau_3)$ is most easily approximated by simulation. In fact, one could just evaluate $cov(X, Y)$ directly by simulation using the definition (31).

If we adopt a convention that a random variable that has an exponential distribution with parameter $\lambda = 0$ is equal to $+\infty$ with probability 1, then we can consider various sub-models of (31) obtained by setting certain of the λ_j's equal to 0. For many data fitting applications such simplified models may be adequate. Of course the expressions for the moments of such sub-models will be less complicated than they would be for the full model.

6 The Case in Which Addition Is Used Instead of Subtraction, Multiplication, Division, and Minimization

Parallel to the construction in (13) in which differences of sums of independent gamma variables are considered, it is natural to ask "What happens if we replace differences by sums?"

In such a case we would begin, once more, with 8 independent gamma variables $U_1, U_2, ..., U_8$ with $U_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, ..., 8$. We then define (X, Y) by

$$\begin{aligned} X &= (U_1 + U_5 + U_7) + (U_3 + U_6 + U_8), \\ Y &= (U_2 + U_6 + U_7) + (U_4 + U_5 + U_8), \end{aligned} \tag{39}$$

However, if we define

$$\begin{aligned} W_1 &= U_1 + U_3, \\ W_2 &= U_2 + U_4, \\ W_3 &= U_5 + U_6 + U_7 + U_8, \end{aligned}$$

then the W_j's are independent gamma random variables, and the model (39) is equivalent to

$$\begin{aligned} X &= W_1 + W_3, \\ Y &= W_2 + W_3, \end{aligned} \tag{40}$$

where the W_j's are independent with $W_j \sim \Gamma(\delta_j, 1), \quad j = 1, 2, 3$. This then is just a well-known bivariate gamma distribution known as Cheriyan's distribution (which was later reinvented by several other researchers, so in re-inventing it, we have good company!). For this model (40) we have

$$E(X) = \delta_1 + \delta_3, \tag{41}$$
$$E(Y) = \delta_2 + \delta_3, \tag{42}$$
$$var(X) = \delta_1 + \delta_3, \tag{43}$$
$$var(Y) = \delta_2 + \delta_3, \tag{44}$$

and

$$cov(X, Y) = \delta_3. \tag{45}$$

Only non-negative correlations are encountered in this model.

In the Sect. 8, we will briefly consider multivariate versions of the bivariate models introduced in Sects. 3–5. We will see that, unless we set many of the parameters in the corresponding multivariate models equal to zero, the dimension of the parameter space, which in the bivariate case was 8 (often already considered by some to be excessively large), will become much larger in higher dimensional models. In the k dimensional model there will turn out to be $3^k - 1$ parameters. In contrast it is not difficult to construct k-dimensional versions of the Cheriyan model that involve a more reasonable number of parameters. We can illustrate this in the 3-dimensional case. Begin with 7 independent gamma variables, $W_j \sim \Gamma(\delta_j, 1) \quad j = 1, 2, ..., 7$. Then define:

$$\begin{aligned} X &= W_1 + W_4 + W_5 + W_7, \\ Y &= W_2 + W_4 + W_6 + W_7, \\ Z &= W_3 + W_5 + W_6 + W_7. \end{aligned} \tag{46}$$

The number of parameters in this model is $\binom{3}{1} + \binom{3}{2} + \binom{3}{3} = 2^3 - 1 = 7$. The k-dimensional version of this model will have $\sum_{j=1}^{k} \binom{k}{j} = 2^k - 1$ parameters, a considerably smaller number than $3^k - 1$. Note also that the computation of means, variances, and covariances for the multivariate Cheriyan models is not difficult. A negative feature of these distributions is that all correlations in the model are non-negative.

It is not easy to identify papers dealing with the use of Cheriyan's model to analyze real-world data. However, multivariate versions of it have been utilized. Prekopa and Szantai (1978) used a 6-dimensional Cheriyan model in an analysis of streamflow data.

7 Possible Extensions Involving Dependent Component Variables

The flexible models discussed thus far all share the feature that the basic building blocks consisted of 8 independent variables, having gamma distributions or exponential distributions. A referee suggests that it may be worthwhile investigating similar

models in which 8 dependent gamma variables replace the independent ones. In the case of the models in Sects. 2, 3, 4, and 5.1, one might endow the vector $\underline{U}$ with a multivariate gamma distribution of the kind introduced by Mathai and Moschopoulos (1992) or that introduced by Furman (2008). Instead, one might assume a multivariate Tweedie distribution for $\underline{U}$ (Furman and Landsman 2010). In the case of the model in Sect. 5.2, instead of having independent exponential components, one could consider that $\underline{U}$ obeys a multivariate exponential model as introduced in Marshall and Olkin (1967).

8 On Multivariate Versions of the Models in Sects. 3–5

k-dimensional versions of the Arnold–Ng beta(2) distribution were mentioned in Arnold and Ghosh (2014), in a context of copula models. We will describe the approach with reference to the bivariate gamma-difference distribution. The reader will readily recognize how to develop analogous k-variate models involving gamma products, and asymmetric Laplace distributions. After describing the three dimensional case, it will be evident how to deal with higher dimensions. A three dimensional gamma-difference distribution will be one whose structure is of a form which involves 26 U_j's. This is the appropriate number of gamma distributed components since a trivariate model (X, Y, Z) expressed as differences of two independent sums of independent gamma variables (with unit scale parameter), will involve 6 places where a particular U can appear, three places in the first sums and three places in the subtracted second sums. But a particular U cannot appear in both the first sum and the subtracted second sum of any of the three variables X, Y, and Z, There will be 6 U's which appear in just one of the 6 possible places. These will be denoted by $U_1, U_2, ..., U_6$. There will be 12 U's that appear in exactly two of the 6 possible positions, denoted by $U_7, U_8, ..., U_{18}$. Finally there are 8 U's that appear in 3 places, namely, $U_{19}, U_{20}, ..., U_{26}$. No U can appear in more than 3 places without violating the requirement that first sums must be independent of their corresponding subtracted second sums.

Thus, there are a total of 26 parameters in the model where $U_j,\ j = 1, 2, ..., 26$ are independent variables with $U_j \sim \Gamma(\delta_j, 1)$ for each j. The model can then be expressed in the following form.

$$\begin{aligned} X = &(U_1 + U_7 + U_8 + U_9 + U_{10} + U_{19} + U_{20} + U_{21} + U_{22}) \\ &-(U_4 + U_{11} + U_{12} + U_{13} + U_{14} + U_{23} + U_{24} + U_{25} + U_{26}), \end{aligned} \tag{47}$$

$$\begin{aligned} Y = &(U_2 + U_7 + U_{11} + U_{15} + U_{16} + U_{19} + U_{20} + U_{23} + U_{24}) \\ &-(U_5 + U_9 + U_{13} + U_{17} + U_{18} + U_{21} + U_{22} + U_{25} + U_{26}), \end{aligned} \tag{48}$$

and

$$Z = (U_3 + U_8 + U_{12} + U_{15} + U_{17} + U_{19} + U_{21} + U_{23} + U_{25}) \\ -(U_6 + U_{10} + U_{14} + U_{16} + U_{18} + U_{20} + U_{22} + U_{24} + U_{26}). \tag{49}$$

The pattern for the dimensions of the parameter spaces of the multivariate models should now be clear. The univariate model involves 2 U's, i.e., $3^1 - 1$. The bivariate model involves 8 U's, i.e., $3^2 - 1$. The trivariate case involves 26 U's, i.e., $3^3 - 1$, and, in general, the k-dimensional model involves $3^k - 1$ U's.

Use of the fully parameterized k-dimensional model would not usually be recommended, if ever. Instead simplified sub-models, obtained by setting many of the δ's equal to zero, can be expected to be adequate for many data sets.

9 Discussion

Inference questions concerning the models described in Sects. 3, 4 and 5, will be the subjects of separate reports. The present paper has provided an introduction to a broad spectrum of bivariate models and sub-models which can potentially be useful additions to the modeler's tool kit. These new flexible models can be expected to find application in cases in which the simpler well-known models prove to be inadequate to adapt to particular data sets.

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An Absolute Continuous Bivariate Inverse Generalized Exponential Distribution: Properties, Inference and Extensions

Debasis Kundu

Abstract The aim of this paper is to introduce an absolutely continuous bivariate inverse generalized exponential (BIGE) distribution. The proposed distribution has been obtained by removing the singular component from the BIGE distribution similarly as the Block and Basu absolute continuous bivariate exponential distribution. This distribution has four parameters, and due to this, the joint probability density function can take variety of shapes. This distribution can be used quite effectively if there are no ties in the bivariate data set and particularly if the marginals are from a heavy tailed distribution. We have developed different properties of this distribution and provided classical inference of the unknown parameters. The maximum likelihood (ML) estimators cannot be obtained in closed form and one needs to solve a four-dimensional optimization problem to compute the ML estimators in this case. To avoid that, we propose to use the expectation maximization (EM) algorithm to compute the ML estimators of the unknown parameters. The analysis of one data set has been performed to see the effectiveness of the proposed algorithm and extended the results to the multivariate case also. Finally, we conclude the paper with several open problems for future research.

Keywords Generalized exponential distribution · Maximum likelihood estimators · Absolutely continuous distribution · Expectaion maximization algorithm · Fisher information matrix · Competing risks

1 Introduction

Two-parameter generalized exponential (GE) has received a considerable amount of attention in the last two decades. It has been introduced by Gupta and Kundu (1999) as a special case of the three-parameter exponentiated Weibull distribution originally proposed by Mudholkar and Srivastava (1993). It can also be obtained as a special

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case of the three-parameter generalized Gompertz–Verhulst family of distributions introduced by Ahuja and Nash (1967); see also Verhulst (1945) in this respect.

The two-parameter GE distribution has the following cumulative distribution function (CDF), probability density function (PDF) and hazard function (HF) for $x > 0$, $\alpha > 0$, $\lambda > 0$:

$$F_{GE}(x; \alpha, \lambda) = (1 - e^{-\lambda x})^{\alpha} \tag{1}$$

$$f_{GE}(x; \alpha, \lambda) = \alpha\lambda e^{-\lambda x}(1 - e^{-\lambda x})^{\alpha-1}, \tag{2}$$

$$h_{GE}(x; \alpha, \lambda) = \frac{\alpha\lambda e^{-\lambda x}(1 - e^{-\lambda x})^{\alpha-1}}{1 - (1 - e^{-\lambda x})^{\alpha}}. \tag{3}$$

Here, α is the shape parameter and λ is the scale parameter. The PDF (2) of a GE distribution can be either a decreasing or a unimodal function depending on the values of α. If $\alpha \leq 1$, the PDF is a decreasing function, otherwise it becomes a unimodal function. When $\alpha = 1$, it coincides with the one-parameter exponential distribution. The hazard function of a GE distribution (3) can be increasing ($\alpha > 1$), decreasing ($\alpha < 1$) or constant ($\alpha = 1$). It is observed by Gupta and Kundu (1999) that the GE distribution behaves very similarly as the two-parameter gamma distribution. But because of the explicit expression of the CDF, it can be used very effectively for the censored data. Due to this reason, an extensive amount of work has been done in establishing different properties and also developing various inferential procedures of the unknown parameters of this model. A book length treatment can be found in Al-Hussaini and Ahsanullah (2015), see also the review articles by Gupta and Kundu (2007), Nadarajah (2011) and the references cited therein.

Although the GE distribution is a very flexible distribution, it cannot have a non-monotone hazard function or heavy tailed property. Due to this reason, Oguntunde and Adejumo (2015) introduced the inverted GE distribution (IGE) similar to the inverted Weibull distribution; see, for example, Murthy et al. (2004). The IGE distribution has the following survival function (SF), PDF and HF for $x > 0$, $\alpha > 0$ and $\lambda > 0$:

$$S_{IGE}(x; \alpha, \lambda) = (1 - e^{-\frac{\lambda}{x}})^{\alpha} \tag{4}$$

$$f_{IGE}(x; \alpha, \lambda) = \frac{\alpha\lambda}{x^2} e^{-\frac{\lambda}{x}}(1 - e^{-\frac{\lambda}{x}})^{\alpha-1} \tag{5}$$

$$h_{IGE}(x; \alpha, \lambda) = \frac{\alpha\lambda}{x^2(e^{-\frac{\lambda}{x}} - 1)}. \tag{6}$$

The PDF and the HF of an IGE distribution are always unimodal for all values of $\alpha > 0$ and $\lambda > 0$. When $\lambda = 1$, the mode of an IGE is at $1/2$ if $\alpha = 1$, for $\alpha > 1$, the mode is less than $1/2$ and for $\alpha \leq 1$, the mode is greater than $1/2$. Moreover, depending on the values of α, it becomes a heavy tailed distribution. If $\alpha \leq 1$, the mean does not exist. If $1 < \alpha \leq 2$, the mean exists, but the variance does not exist. For $\alpha > 2$, the variance exists. From now on, an absolutely continuous random variable with PDF (5) will be denoted by IGE(α, λ).

Recently, Alqallaf and Kundu (2020) introduced a bivariate IGE distribution similar to the Marshall–Olkin bivariate exponential (MOBE) distribution or bivariate generalied exponential distribution, see, for example, Marshall and Olkin (1967) and Kundu and Gupta (2009).

Definition 1 Suppose U_1 follows ($\sim$) IGE(α_1, λ), $U_2 \sim$ IGE(α_2, λ) and $U_0 \sim$ IGE(α_0, λ), and they are independently distributed. If $X = \min\{U_1, U_0\}$ and $Y = \min\{U_2, U_0\}$, then the distribution of (X, Y) is said to have a bivariate IGE (BIGE) distribution with parameters α_1, α_2, α_0 and λ.

We denote this by BIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$). It may be mentioned that this BIGE distribution has the same interpretation as the shock model similar to the MOBE model. Here the shock appears following an IGE distribution, which can be heavy tailed.

The BIGE introduced by Alqallaf and Kundu (2020) has a singular component along $X = Y$, i.e. $P(X = Y) > 0$, similar to the MOBE distribution. Therefore, if there are no ties in the data, it may not be reasonable to use BIGE distribution in this case. It may be recalled that since MOBE has a singular component, it is not used when there are no ties in the data. Due to this reason, Block and Basu (1974) introduced an absolutely continuous bivariate exponential distribution, from now on, we call it as the Block and Basu bivariate exponential (BBBE) distribution, by removing the singular component from the MOBE distribution. Although the MOBE is a singular distribution, the BBBE distribution enjoys all the properties of an absolutely continuous distribution. It can be used quite effectively to analyze a bivariate data set when there are no ties in the data.

The main aim of this paper is to introduce absolutely continuous BIGE (ABIGE) by removing the singular component of a BIGE distribution. Clearly, ABIGE is an absolutely continuous distribution with four parameters. We study different properties of the ABIGE distribution and its marginals. Due to presence of the four parameters, the joint PDF of an ABIGE can take variety of shapes. Moreover, the marginals of an ABIGE can be heavy tailed also. Hence, the ABIGE model can be used quite effectively for a bivariate data set when there are no ties. The ML estimators of the unknown parameters of a ABIGE cannot be obtained in explicit forms. They have to be obtained by solving four non-linear equations simultaneously. Therefore, some numerical algorithms like Newton–Raphson or Gauss–Newton method may be used to solve these non-linear equations. Hence, very accurate initial values are needed to start the iterative process, otherwise it may not converge or it may converge to some local optimum. To avoid that, we have proposed an EM algorithm to compute the ML estimators. The proposed EM algorithm requires solving only one-dimensional optimization problem at each 'E'-step of the EM algorithm. Hence, the implementation of the proposed EM algorithm is quite simple in practice. The analysis of one data set has been performed to see the performances of the proposed EM algorithm and the effectiveness of the model. Finally, we have introduced the absolute continuous multivariate IGE (AMIGE) and showed how the EM algorithm can be developed for the multivariate model also. We have indicated several open problems for further research.

The rest of the paper is organized as follows. In Sect. 2, we have defined the ABIGE model and discuss its different properties. The inference procedure has been developed in Sect. 3. In Sect. 4, we provide the analysis of one bivariate data set. In Sect. 5, we have discussed AMIGE distribution, and finally we conclude the paper and provide several open problems for future work, in Sect. 6.

2 Model Description and Properties

2.1 Model Description

We have already introduced BIGE in Sect. 1. If $(X, Y) \sim \text{BIGE}(\alpha_1, \alpha_2, \alpha_0, \lambda)$, then the joint SF of X and Y for $x > 0$ and $y > 0$ becomes

$$S_{X,Y}(x, y) = P(X > x, Y > y) = \begin{cases} (1 - e^{-\frac{\lambda}{x}})^{\alpha_1}(1 - e^{-\frac{\lambda}{y}})^{\alpha_2+\alpha_0} & \text{if } 0 < x < y < \infty \\ (1 - e^{-\frac{\lambda}{x}})^{\alpha_1+\alpha_0}(1 - e^{-\frac{\lambda}{y}})^{\alpha_2} & \text{if } 0 < y < x < \infty \\ (1 - e^{-\frac{\lambda}{x}})^{\alpha_1+\alpha_2+\alpha_0} & \text{if } 0 < x = y < \infty. \end{cases}$$

The joint SF of X and Y has the following unique decomposition:

$$S_{X,Y}(x, y) = \frac{\alpha_1 + \alpha_2}{\alpha_1 + \alpha_2 + \alpha_0} S_{ac}(x, y) + \frac{\alpha_0}{\alpha_1 + \alpha_2 + \alpha_0} S_{si}(x, y)$$

Here,

$$S_{si}(x, y) = \begin{cases} (1 - e^{-\frac{\lambda}{x}})^{\alpha_1+\alpha_2+\alpha_0} & \text{if } x = y, \\ 0 & \text{if } x \neq y, \end{cases}$$

and

$$S_{ac}(x, y) = \frac{\alpha_1 + \alpha_2 + \alpha_0}{\alpha_1 + \alpha_2}(1 - e^{-\frac{\lambda}{x}})^{\alpha_1}(1 - e^{-\frac{\lambda}{y}})^{\alpha_2}(1 - e^{-\frac{\lambda}{z}})^{\alpha_0} - \frac{\alpha_0}{\alpha_1 + \alpha_2}(1 - e^{-\frac{\lambda}{x}})^{\alpha_1+\alpha_2+\alpha_0},$$

here $z = \max\{x, y\}$. Note that here $S_{ac}(x, y)$ is the absolute continuous part and $S_{si}(x, y)$ is the singular part.

From the joint SF, the joint PDF of X and Y can be obtained as follows:

$$f_{X,Y}(x, y) = \frac{\alpha_1 + \alpha_2}{\alpha_1 + \alpha_2 + \alpha_0} f_{ac}(x, y) + \frac{\alpha_0}{\alpha_1 + \alpha_2 + \alpha_0} f_{si}(u), \tag{7}$$

where

$$f_{ac}(x,y)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}\times\begin{cases} f_{IGE}(x;\alpha_1,\lambda)f_{IGE}(y;\alpha_2+\alpha_0,\lambda) \text{ if } 0<x<y<\infty \\ f_{IGE}(x;\alpha_1+\alpha_0,\lambda)f_{IGE}(y;\alpha_2,\lambda) \text{ if } 0<y<x<\infty, \end{cases}$$

and for $x=y=u$,

$$f_{si}(u)=f_{IGE}(u;\alpha_1+\alpha_2+\alpha_0,\lambda).$$

It should be mentioned that when we write the joint PDF of X and Y as in (7), it is understood that $f_{ac}(x,y)$ is a PDF with respect to two-dimensional Lebesgue measure and $f_{si}(u)$ is a PDF with respect to one-dimensional Lebesgue measure; see, for example, Bemis et al. (1972).

Now we define ABIGE by removing the singular component from the BIGE, similar to the construction of BBBE from MOBE distribution, as follows:

Definition 2 If the joint PDF of the random variables U and V is

$$f_{U,V}(u,v)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}\times\begin{cases} f_{IGE}(u;\alpha_1,\lambda)f_{IGE}(v;\alpha_2+\alpha_0,\lambda) \text{ if } 0<u<v<\infty \\ f_{IGE}(u;\alpha_1+\alpha_0,\lambda)f_{IGE}(v;\alpha_2,\lambda) \text{ if } 0<v<u<\infty, \end{cases}$$

then (U,V) is said to have ABIGE distribution with parameters α_1, α_2, α_0, λ and it will be denoted by ABIGE$(\alpha_1,\alpha_2,\alpha_0,\lambda)$.

The joint survival function of (U,V) becomes

$$S_{U,V}(u,v)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}(1-e^{-\frac{\lambda}{u}})^{\alpha_1}(1-e^{-\frac{\lambda}{v}})^{\alpha_2}(1-e^{-\frac{\lambda}{w}})^{\alpha_0}-\frac{\alpha_0}{\alpha_1+\alpha_2}(1-e^{-\frac{\lambda}{u}})^{\alpha_1+\alpha_2+\alpha_0},$$

here $w=\max\{u,v\}$. The marginal survival functions of U and V become:

$$S_U(u)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}\left(1-e^{-\frac{\lambda}{u}}\right)^{\alpha_1+\alpha_0}-\frac{\alpha_0}{\alpha_1+\alpha_2}\left(1-e^{-\frac{\lambda}{u}}\right)^{\alpha_1+\alpha_2+\alpha_0}$$
$$S_V(v)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}\left(1-e^{-\frac{\lambda}{v}}\right)^{\alpha_2+\alpha_0}-\frac{\alpha_0}{\alpha_1+\alpha_2}\left(1-e^{-\frac{\lambda}{v}}\right)^{\alpha_1+\alpha_2+\alpha_0},$$

respectively. The marginal PDFs of U and V become

$$f_U(u)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}f_{IGE}(u;\alpha_1+\alpha_0,\lambda)-\frac{\alpha_0}{\alpha_1+\alpha_2}f_{IGE}(u;\alpha_1+\alpha_2+\alpha_0,\lambda)$$
$$f_V(v)=\frac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}f_{IGE}(v;\alpha_2+\alpha_0,\lambda)-\frac{\alpha_0}{\alpha_1+\alpha_2}f_{IGE}(v;\alpha_1+\alpha_2+\alpha_0,\lambda),$$

respectively. It may be observed that the relation between the BIGE and ABIGE is the following:

$$(U,V)=(X,Y)|\{X\neq Y\}. \tag{8}$$

The above relation (8) can be used quite effectively to generate ABIGE distribution. The following algorithm can be used to generate $(U, V) \sim \text{ABIGE}(\alpha_1, \alpha_2, \alpha_0, \lambda)$ as follows:

Algorithm

Step 1: Generate $U_1 \sim \text{IGE}(\alpha_1, \lambda)$, $U_2 \sim \text{IGE}(\alpha_2, \lambda)$ and $U_0 \sim \text{IGE}(\alpha_0, \lambda)$.
Step 2: If $U_0 < \min\{U_1, U_2\}$, go to Step 1.
Step 3: $U = \min\{U_1, U_0\}$ and $V = \min\{U_2, U_0\}$.

2.2 Properties

The following result provides the shape of the joint PDF of ABIGE.

Theorem 1 *Let $(U, V) \sim ABIGE(\alpha_1, \alpha_2, \alpha_0, \lambda)$. We use the following notations. $S_0 = \{(u, v); 0 < u = v < \infty\}$, $S_1 = \{(u, v); 0 < u < v < \infty\}$, $S_2 = \{(u, v); 0 < v < u < \infty\}$.*
(a) If $\alpha_1 = \alpha_2 = \alpha$, then $f_{U,V}(u, v)$ is continuous on $S_0 \cup S_1 \cup S_2 = \mathbb{R}^2$, $f_{U,V}(u, v)$ is unimodal and the mode is at $(x_0, x_0) \in S_0$, where x_0 is the unique solution of the non-linear equation

$$2(e^{\frac{1}{x}} - 1)(1 - 2x) = (2\alpha + \alpha_0 - 2). \tag{9}$$

(b) If $\alpha_2 + \alpha_0 < 1 < \alpha_1$, then $f_{U,V}(u, v)$ is continuous on $S_1 \cup S_2$, $f_{U,V}(u, v)$ is unimodal and the mode is at $(x_1, x_2) \in S_1$, where x_1 and x_2 are unique solutions of the non-linear equations

$$(e^{\frac{1}{x}} - 1)(1 - 2x) = (\alpha_1 - 1) \tag{10}$$
$$(e^{\frac{1}{x}} - 1)(1 - 2x) = (\alpha_2 + \alpha_0 - 1). \tag{11}$$

(c) If $\alpha_1 + \alpha_0 < 1 < \alpha_2$, then $f_{U,V}(u, v)$ is continuous on $S_1 \cup S_2$, $f_{U,V}(u, v)$ is unimodal and the mode is at $(x_1, x_2) \in S_2$, where x_1 and x_2 are unique solutions of the non-linear equations

$$(e^{\frac{1}{x}} - 1)(1 - 2x) = (\alpha_2 - 1) \tag{12}$$
$$(e^{\frac{1}{x}} - 1)(1 - 2x) = (\alpha_1 + \alpha_0 - 1). \tag{13}$$

Proof See Appendix 1.

In Figs. 1, 2, 3 and 4, we have provided the surface plots of the of the joint PDF of ABIGE$(\alpha_1, \alpha_2, \alpha_0, \lambda)$ for different values of α_1, α_2 and α_0 keeping $\lambda = 1$. It is observed that for all values of α_1, α_2 and α_0, the joint PDF is an unimodal function. □

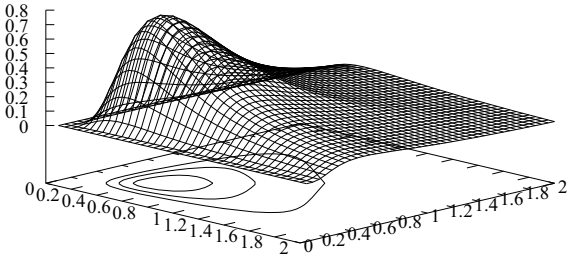

Fig. 1 Bivariate surface plots of BIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$) distribution for $(\alpha_1, \alpha_2, \alpha_0, \lambda) =$ (1.0, 1.0, 1.0, 1.0)

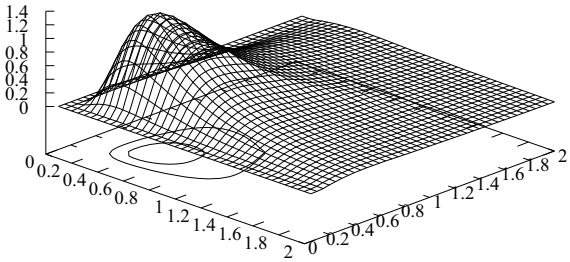

Fig. 2 Bivariate surface plots of BIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$) distribution for $(\alpha_1, \alpha_2, \alpha_0, \lambda) =$ (1.0, 1.0, 2.0, 1.0)

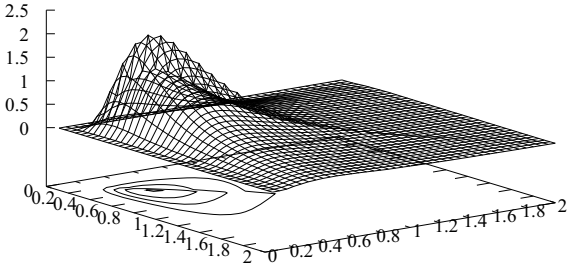

Fig. 3 Bivariate surface plots of BIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$) distribution for $(\alpha_1, \alpha_2, \alpha_0, \lambda) =$ (1.0, 2.0, 1.0, 1.0)

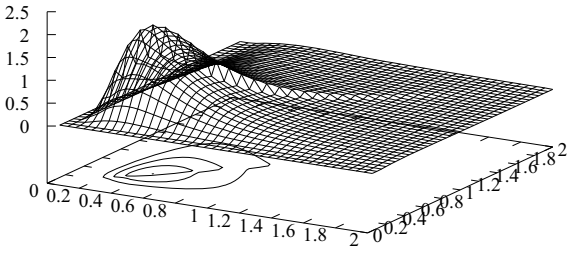

Fig. 4 Bivariate surface plots of BIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$) distribution for $(\alpha_1, \alpha_2, \alpha_0, \lambda) =$ (2.0, 1.0, 2.0, 1.0)

3 Inference

In this section, we derive the ML estimators of the unknown parameters of a ABIGE($\alpha_1, \alpha_2, \alpha_0, \lambda$) based on a random sample of size n and it is as follows:

$$Data = \{(u_1, v_1), \ldots, (u_n, v_n)\}. \tag{14}$$

We use the following notations $I_1 = \{i : u_i < v_i\}$, $I_2 = \{i : u_i > v_i\}$ and $\boldsymbol{\Theta} = (\alpha_1, \alpha_2, \alpha_0, \lambda)^\top$. Moreover, $n_1 = |I_1|$ = number of elements in I_1 and similarly, $n_2 = |I_2|$. Based on the sample (14), the log-likelihood function can be written as

$$\begin{aligned} l(\boldsymbol{\Theta}|Data) &= n\ln(\alpha_1+\alpha_2+\alpha_0) - n\ln(\alpha_1+\alpha_2) + \\ &\quad \sum_{i\in I_1} \ln f_{IGE}(u_i;\alpha_1,\lambda) + \sum_{i\in I_1} \ln f_{IGE}(v_i;\alpha_2+\alpha_0,\lambda) + \\ &\quad \sum_{i\in I_2} \ln f_{IGE}(u_i;\alpha_1+\alpha_0,\lambda) + \sum_{i\in I_2} \ln f_{IGE}(v_i;\alpha_2,\lambda) \\ &= C + n\ln(\alpha_1+\alpha_2+\alpha_0) - n\ln(\alpha_1+\alpha_2) - A\lambda + 2n\ln\lambda + \\ &\quad n_1(\ln\alpha_1 + \ln(\alpha_2+\alpha_0)) + n_2(\ln(\alpha_1+\alpha_0)+\ln\alpha_2) + \\ &\quad (\alpha_1-1)\sum_{i\in I_1}\ln(1-e^{-\frac{\lambda}{u_i}}) + (\alpha_2+\alpha_0-1)\sum_{i\in I_1}\ln(1-e^{-\frac{\lambda}{v_i}}) + \\ &\quad (\alpha_1+\alpha_0-1)\sum_{i\in I_2}\ln(1-e^{-\frac{\lambda}{u_i}}) + (\alpha_2-1)\sum_{i\in I_2}\ln(1-e^{-\frac{\lambda}{v_i}}). \end{aligned} \tag{15}$$

Here C is a constant does not depend on the parameters and $A = \sum_{i=1}^{n}(u_i^{-1} + v_i^{-1})$. The ML estimate of $\boldsymbol{\Theta}$ can be obtained by maximizing (15) with respect to the unknown parameters. It is immediate that it cannot be obtained in explicit form. It has to be obtained by solving a four-dimensional optimization problem. Therefore, one needs to use some iterative algorithms like Newton–Raphson or Gauss–Newton method to compute the ML estimates. Any iterative algorithm needs very good initial guesses, which may not be a trivial issue in four dimension. Moreover, it may converge to a local maximum rather than the global maximum.

To avoid that we treat this problem as a missing value problem, and we will show that if we have the complete data set, then the ML estimates of $\boldsymbol{\Theta}$ can be obtained by solving only one non-linear equation. Hence, we propose to use a very simple EM algorithm, where at each 'E'-step, the corresponding 'M'-step can be performed by solving only one non-linear equation, and that is the main motivation of the proposed EM algorithm.

Suppose instead of observing only (U, V), we also observe the indicator vector (Δ_1, Δ_2) associate with the corresponding U_1, U_2, U_0 defined before as follows:
Case 1: $(U < V) : \Delta_1 = 1$ and

$$\Delta_2 = \begin{cases} 2 \text{ if } V = U_2 \\ 3 \text{ if } V = U_0. \end{cases}$$

Case 2: $(V < U) : \Delta_2 = 2$ and

$$\Delta_1 = \begin{cases} 1 \text{ if } U = U_1 \\ 3 \text{ if } U = U_0. \end{cases}$$

Now we will provide the log-likelihood contribution of a typical data point $(u, v, \delta_1, \delta_2)$ for different cases.
Case 1: $u < v$, $\delta_1 = 1$ and $\delta_2 = 2$. The log-likelihood contribution becomes

$$\ln f_{IGE}(u; \alpha_1, \lambda) + \ln f_{IGE}(v; \alpha_2, \lambda) + \ln S_{IGE}(v; \alpha_0, \lambda).$$

Case 2: $u < v$, $\delta_1 = 1$ and $\delta_2 = 3$. The log-likelihood contribution becomes

$$\ln f_{IGE}(u; \alpha_1, \lambda) + \ln f_{IGE}(v; \alpha_0, \lambda) + \ln S_{IGE}(v; \alpha_2, \lambda).$$

Case 3: $v < u$, $\delta_1 = 1$ and $\delta_2 = 2$. The log-likelihood contribution becomes

$$\ln f_{IGE}(u; \alpha_1, \lambda) + \ln f_{IGE}(v; \alpha_2, \lambda) + \ln S_{IGE}(u; \alpha_0, \lambda).$$

Case 4: $u < v$, $\delta_1 = 3$ and $\delta_2 = 2$. The log-likelihood contribution becomes

$$\ln f_{IGE}(u; \alpha_0, \lambda) + \ln f_{IGE}(v; \alpha_2, \lambda) + \ln S_{IGE}(u; \alpha_1, \lambda).$$

In this case, it can be easily shown that for the complete data set, namely, $\{(u_i, v_i, \delta_{1i}, \delta_{2i}); i = 1, \ldots, n\}$, the ML estimates of α_1, α_2 and α_0 can be obtained in explicit forms if λ is known. Hence, the ML estimate of λ can be obtained by maximizing the profile log-likelihood function in one dimension only. The following Table 1 will be useful for further development of the EM algorithm.

Now following the idea of Dinse (1982), see also Kundu (2004) in this respect, for each incomplete data (u, v), we form 'pseudo observations' by fractioning (u, v) to two partially complete 'pseudo observation' of the form $\{(u, v, w_1), (u, v, 1 - w_1)\}$ and $\{(u, v, w_2), (u, v, 1 - w_2)\}$ depending on whether $u > v$ or $u < v$, respectively. Here, w_1 is the conditional probability that $U_1 < U_0$ given that $V < U$. Similarly, w_2 is the conditional probability that $U_2 < U_0$, given that $U < V$. From Table 1

$$w_1 = \frac{\alpha_1}{\alpha_1 + \alpha_0} \quad \text{and} \quad w_2 = \frac{\alpha_2}{\alpha_2 + \alpha_0}.$$

Now let us denote by $\Theta^{(k)} = (\alpha_1^{(k)}, \alpha_2^{(k)}, \alpha_0^{(k)}, \lambda^{(k)})^\top$ as the estimates of the parameters at the k-th stage of the EM algorithm. Similarly, let us denote $w_1^{(k)}$ and $w_2^{(k)}$ as the estimates of w_1 and w_2, respectively, at the k-th stage. At the k-th stage the 'pseudo-log-likelihood' function can be written as follows:

Table 1 Possible configuration of U_1, U_2, U_0 and the associated probabilities

Set	Relation between U and V	Possible configuration of U_0, U_1, U_2	Observed variable	Conditional probability	(Δ_1, Δ_2)
I_1	$U < V$	$U_1 < U_2 < U_0$	$U = U_1, V = U_2$	$\frac{\alpha_2}{(\alpha_2+\alpha_0)}$	(1, 2)
		$U_1 < U_0 < U_2$	$U = U_1, V = U_0$	$\frac{\alpha_0}{(\alpha_2+\alpha_0)}$	(1, 3)
I_2	$V < U$	$U_2 < U_1 < U_0$	$U = U_1, V = U_2$	$\frac{\alpha_1}{(\alpha_1+\alpha_0)}$	(1, 2)
		$U_2 < U_0 < U_1$	$U = U_0, V = U_2$	$\frac{\alpha_0}{(\alpha_1+\alpha_0)}$	(3, 2)

$$
\begin{aligned}
l(\boldsymbol{\Theta}|\boldsymbol{\Theta}^{(k)}) = {} & w_2^{(k)} \sum_{i\in I_1} (\ln f_{IGE}(u_i;\alpha_1,\lambda) + \ln f_{IGE}(v_i;\alpha_2,\lambda) + \ln S_{IGE}(v_i;\alpha_0,\lambda)) + \\
& (1-w_2^{(k)}) \sum_{i\in I_1} (\ln f_{IGE}(u_i;\alpha_1,\lambda) + \ln f_{IGE}(v_i;\alpha_0,\lambda) + \ln S_{IGE}(v_i;\alpha_2,\lambda)) + \\
& w_1^{(k)} \sum_{i\in I_2} (\ln f_{IGE}(u_i;\alpha_1,\lambda) + \ln f_{IGE}(v_i;\alpha_2,\lambda) + \ln S_{IGE}(u_i;\alpha_0,\lambda)) + \\
& (1-w_1^{(k)}) \sum_{i\in I_2} (\ln f_{IGE}(u_i;\alpha_0,\lambda) + \ln f_{IGE}(v_i;\alpha_2,\lambda) + \ln S_{IGE}(u_i;\alpha_1,\lambda)) \\
= {} & \sum_{i\in I_1} \ln f_{IGE}(u_i;\alpha_1,\lambda) + \sum_{i\in I_2} \ln f_{IGE}(v_i;\alpha_2,\lambda) + \\
& \sum_{i\in I_2} \left\{ w_1^{(k)} \ln f_{IGE}(u_i;\alpha_1,\lambda) + (1-w_1^{(k)}) \ln S_{IGE}(u_i;\alpha_1,\lambda) \right\} + \\
& \sum_{i\in I_1} \left\{ w_2^{(k)} \ln f_{IGE}(v_i;\alpha_2,\lambda) + (1-w_2^{(k)}) \ln S_{IGE}(v_i;\alpha_2,\lambda) \right\} + \\
& w_2^{(k)} \sum_{i\in I_1} \ln S_{IGE}(v_i;\alpha_0,\lambda) + (1-w_2^{(k)}) \sum_{i\in I_1} \ln f_{IGE}(v_i;\alpha_0,\lambda) + \\
& w_1^{(k)} \sum_{i\in I_2} \ln S_{IGE}(u_i;\alpha_0,\lambda) + (1-w_1^{(k)}) \sum_{i\in I_2} \ln f_{IGE}(u_i;\alpha_0,\lambda). \qquad (16)
\end{aligned}
$$

Therefore, $\boldsymbol{\Theta}^{(k+1)}$ can be obtained from $\boldsymbol{\Theta}^{(k)}$ by maximizing (16) with respect to $\boldsymbol{\Theta}$. For a fixed λ

$$
\alpha_1^{(k+1)}(\lambda) = -\frac{n_1 + w_1^{(k)} n_2}{\sum_{i\in I} \ln(1 - e^{-\frac{\lambda}{u_i}})}
$$

$$
\alpha_2^{(k+1)}(\lambda) = -\frac{n_2 + w_2^{(k)} n_1}{\sum_{i\in I} \ln(1 - e^{-\frac{\lambda}{v_i}})}
$$

$$\alpha_0^{(k+1)}(\lambda) = -\frac{n_1(1-w_2^{(k)}) + n_2(1-w_1^{(k)})}{\sum_{i\in I_1}\ln(1-e^{-\frac{\lambda}{v_i}}) + \sum_{i\in I_2}\ln(1-e^{-\frac{\lambda}{u_i}})},$$

maximize (16). Hence, $\lambda^{(k+1)}$ which maximizes (16) can be obtained by maximizing the profile log-likelihood function, i.e. $\lambda^{(k+1)} = \text{argmax}\ g(\lambda)$, where

$$g(\lambda) = 2(n_1+n_2)\ln\lambda + (n_1+w_1^{(k)}n_2)\ln\alpha_1^{(k+1)}(\lambda) + (n_2+w_2^{(k)}n_1)\ln\alpha_2^{(k+1)}(\lambda) + (n_1(1-w_2^{(k)}) + n_2(1-w_1^{(k)}))\ln\alpha_0^{(k+1)}(\lambda) - \lambda\left(\sum_{i\in I_1\cup I_2}\frac{1}{u_i}+\frac{1}{v_i}\right) - \sum_{i\in I_1\cup I_2}\left(\ln(1-e^{-\frac{\lambda}{u_i}}) + \ln(1-e^{-\frac{\lambda}{v_i}})\right).$$

Therefore,

$$\alpha_1^{(k+1)} = \alpha_1^{(k+1)}(\lambda^{(k+1)}), \quad \alpha_2^{(k+1)} = \alpha_2^{(k+1)}(\lambda^{(k+1)}), \quad \alpha_0^{(k+1)} = \alpha_0^{(k+1)}(\lambda^{(k+1)}).$$

Once the ML estimates of α_1, α_2, α_3 and λ are obtained the associated confidence intervals can be obtained from the observed Fisher information matrix as suggested by Louis (1982). In Appendix 2, we have provided the observed Fisher information matrix.

4 Data Analysis

In this section, we provide the analysis of a real data set to show how the proposed EM algorithm can be implemented in practice. This data set is obtained from Johnson and Wichern (1999) and it represents the cholesterol level of 23 adults at two different times. It is presented below for easy reference: (317, 275), (186, 190), (377, 368), (229, 282), (276, 306), (272, 250), (219, 236), (260, 264), (284, 241), (365, 294), (298, 341), (274, 262), (232, 244), (367, 358), (253, 247), (230, 245), (190, 212), (290, 291), (337, 383), (283, 277), (325, 288), (266,253), (338, 307).

Before progressing further, we have subtracted 165 and divided by 10 for each data point, mainly for computational purposes. It is not going to affect the inference procedure. One natural question arises whether ABIGE can be used to analyze this data set or not. First of all, there are no ties in the data set. We have fitted the IGE to the minimum of the two cholesterol levels, and the ML estimates of the shape and scale parameters are 4.7691 and 17.5489, respectively. The Kolmogorov-Smirnov distance between the fitted and empirical distribution is 0.1451 and the associated p value is 0.7178. Therefore, it is clear that IGE distribution fits the minimum quite well. Hence, we have fitted ABIGE distribution to the above bivariate data set.

We have used the EM algorithm to compute the ML estimates of the unknown parameters. The following initial values have been used: $\alpha_1 = \alpha_2 = \alpha_0 = 1$ and $\lambda =$

17.0. We have started the EM algorithm with these initial values and the EM algorithm stops when the relative difference between the two consecutive log-likelihood values is less than 10^{-6}. The iteration stops after 20 steps. The ML estimates and the associated 95% confidence intervals based on the observed Fisher information matrix are provided below

$$\widehat{\alpha}_1 = 3.2683(\mp 0.9876), \quad \widehat{\alpha}_2 = 3.5433(\mp 1.0145), \quad \widehat{\alpha}_0 = 2.4060(\mp 0.7655)$$

$$\widehat{\lambda} = 19.6523(\mp 4.1276).$$

We have tried the above EM algorithm with different initial guesses, it converges to the same point, although the number of iterations are different. Another natural question is whether the EM algorithm converges to the global maximum or not. To verify that, we have tried to find the maximum of the log-likelihood function using the grid search method. We have taken the range of α_0, α_1 and α_2 as $(0, 5)$ and the range of λ as $(0, 30)$ with grid size 0.0001 for each parameter. It gives the maximum at the same point although it took more than three hours to execute, whereas in the same machine the EM algorithm converges in few seconds.

5 Absolute Continuous Multivariate IGE Distribution

In this section, we define absolute continuous multivariate IGE (AMIGE) distribution along the same way as the multivariate Block and Basu absolutely continuous exponential distribution, see for example Pradhan and Kundu (2016). The basic idea is the same. First, we define the multivariate IGE distribution as follows:

Definition 3 Suppose $U_0, \ldots, U_p$ are independent IGE distributions, and $U_i \sim \text{IGE}(\alpha_i, \lambda)$, for $i = 0, \ldots, p$. Now, define $X_j = \min\{U_j, U_0\}$, for $j = 1, \ldots, p$. Then, $(X_1, \ldots, X_p)^\top$ is called the MIGE distribution with parameters $\alpha_0, \ldots, \alpha_p, \lambda$ and it is denoted by $\text{MIGE}(\alpha_1, \ldots, \alpha_p, \alpha_0, \lambda)$.

Now, an AMIGE distribution can be constructed from a MIGE distribution by removing the singular components. We give the formal definition of a AMIGE distribution.

Definition 4 A random vector $(Y_1, \ldots, Y_p)^\top$ is said to have a p-variate AMIGE distribution with parameters $\alpha_0, \alpha_1, \ldots, \alpha_p$ and λ, if the joint PDF of $(Y_1, \ldots, Y_p)^\top$ is of the form

$$f_{Y_1,\ldots,Y_p}(y_1, \ldots, y_p) = c f_{IGE}(y_{i_1}; \alpha_{i_1}, \lambda) \times \ldots \times f_{IGE}(y_{i_{p-1}}; \alpha_{i_{p-1}}, \lambda) \times f_{IGE}(y_{i_p}; \alpha_{i_p} + \alpha_0, \lambda), \tag{17}$$

here c is the normalizing constant and $\{i_1, \ldots, i_p\}$ is a permutation of $\{1, \ldots, p\}$, where $y_{i_1} < \ldots < y_{i_p}$. From now on, it will be denoted by $\text{AMIGE}(\alpha_1, \ldots, \alpha_p, \alpha_0, \lambda)$.

The normalizing constant c is such that

$$\int_{\mathbb{R}^p} f_{Y_1,\ldots,Y_p}(y_1,\ldots,y_p)dy_1\ldots dy_p = 1.$$

It can be seen (see Appendix 3) from the simple multiple integration that

$$c^{-1} = \sum_{\mathcal{P}} \frac{\alpha_{i_1}}{\alpha_{i_1}+\ldots+\alpha_{i_p}+\alpha_0} \times \ldots \times \frac{\alpha_{i_{p-1}}}{\alpha_{i_{p-1}}+\alpha_{i_p}+\alpha_0}. \tag{18}$$

Here, $\mathcal{P}$ denotes the set of all permutations of $\{1,\ldots,p\}$. Note that when $p=2$, $c = \dfrac{\alpha_1+\alpha_2+\alpha_0}{\alpha_1+\alpha_2}$. The relation between a MIGE and AMIGE can be described as follows:

$$(Y_1,\ldots,Y_p)^\top = (X_1,\ldots,X_p)^\top | \{X_{i_1} \neq X_{i_j}, 1 \le i_1, i_j \le p\}. \tag{19}$$

The above relation (19) can be easily used to generate random samples from a AMIGE distribution. We have the following results.

Theorem 2 *Let* $(Y_1,\ldots,Y_p)^\top \sim AMIGE(\alpha_1,\ldots,\alpha_p,\alpha_0,\lambda)$.
(a) If $q < p$, *then* $(Y_1,\ldots,Y_q)^\top \sim AMIGE(\alpha_1,\ldots,\alpha_q,\alpha_0,\lambda)$.
(b) If $\alpha_1 = \ldots = \alpha_p = 1$, *then* $f_{Y_1,\ldots,Y_p}(y_1,\ldots,y_p)$ *is continuous on* $\mathbb{R}^p$, $f_{Y_1,\ldots,Y_p}(y_1,\ldots,y_p)$ *is unimodal and the mode is at* $(x_0,\ldots,x_0)$, *where* x_0 *is the unique solution of the non-linear equation*

$$n(e^{\frac{1}{x}}-1)(1-2x) = n(\alpha-1)+\alpha_0.$$

(c) $Z = \min\{Y_1,\ldots,Y_p\} \sim IGE(\alpha_1+\ldots+\alpha_p+\alpha_0,\lambda)$.
(d) $P(Y_i < Y_j) = \dfrac{\alpha_i}{\alpha_i+\alpha_j}$.
(e) $Y_i|\{Y_i < Y_j\} \sim IGE(\alpha_i+\alpha_j+\alpha_0,\lambda)$.

Proof See Appendix 4.

Now we consider the estimation of the unknown parameters based on a random sample from a AMIGE distribution. For notational simplicity, we illustrate the procedure for $p=3$, although the result can be easily obtained for a general p also. It is assumed that we have a random sample of size n from AMIGE$(\alpha_1,\alpha_2,\alpha_3,\alpha_0,\lambda)$ as follows:

$$Data = \{(y_{1i}, y_{2i}, y_{3i}); i = 1,\ldots,n\}. \tag{20}$$

In this case also, we use the same notations as before, i.e. $\boldsymbol{\Theta} = (\alpha_1,\alpha_2,\alpha_3,\alpha_0,\lambda)^\top$. It is clear that the MLE of $\boldsymbol{\Theta}$ cannot be obtained in explicit forms, and we use the EM algorithm as before. We use the following notations $I_{jkm} = \{i : y_{ji} < y_{ki} < y_{mi}\}$, here $\{jkm\}$ belongs to the class of all permutations of $\{1,2,3\}$. Moreover,

$$w_1 = \frac{\alpha_1}{\alpha_1 + \alpha_0}, \quad w_2 = \frac{\alpha_2}{\alpha_2 + \alpha_0}, \quad w_3 = \frac{\alpha_3}{\alpha_3 + \alpha_0}.$$

Let us denote $n_1 = |I_{123}| + |I_{213}| + |I_{312}| + |I_{132}|$, $n_2 = |I_{123}| + |I_{213}| + |I_{321}| + |I_{231}|$, $n_3 = |I_{312}| + |I_{321}| + |I_{231}| + |I_{132}|$. The 'pseudo-log-likelihood' function at the k-th stage of the EM algorithm can be written as follows:

$$\begin{aligned}
l(\boldsymbol{\Theta}|\boldsymbol{\Theta}_k) = & \sum_{i \in I_{123} \cup I_{132} \cup I_{213} \cup I_{312}} \ln f_{IGE}(y_{1i}; \alpha_1, \lambda) + \\
& \sum_{i \in I_{231} \cup I_{321}} \left\{ w_1^{(k)} \ln f_{IGE}(y_{1i}; \alpha_1, \lambda) + (1 - w_1^{(k)}) \ln S_{IGE}(y_{1i}; \alpha_1, \lambda) \right\} + \\
& \sum_{i \in I_{123} \cup I_{213} \cup I_{321} \cup I_{231}} \ln f_{IGE}(y_{2i}; \alpha_2, \lambda) + \\
& \sum_{i \in I_{132} \cup I_{312}} \left\{ w_2^{(k)} \ln f_{IGE}(y_{2i}; \alpha_2, \lambda) + (1 - w_2^{(k)}) \ln S_{IGE}(y_{2i}; \alpha_2, \lambda) \right\} + \\
& \sum_{i \in I_{312} \cup I_{132} \cup I_{321} \cup I_{231}} \ln f_{IGE}(y_{3i}; \alpha_3, \lambda) + \\
& \sum_{i \in I_{123} \cup I_{213}} \left\{ w_3^{(k)} \ln f_{IGE}(y_{3i}; \alpha_3, \lambda) + (1 - w_3^{(k)}) \ln S_{IGE}(y_{3i}; \alpha_3, \lambda) \right\} + \\
& \sum_{i \in I_{231} \cup I_{321}} \left\{ w_1^{(k)} \ln S_{IGE}(y_{1i}; \alpha_0, \lambda) + (1 - w_1^{(k)}) \ln f_{IGE}(y_{1i}; \alpha_0, \lambda) \right\} + \\
& \sum_{i \in I_{132} \cup I_{312}} \left\{ w_2^{(k)} \ln S_{IGE}(y_{2i}; \alpha_0, \lambda) + (1 - w_2^{(k)}) \ln f_{IGE}(y_{2i}; \alpha_0, \lambda) \right\} + \\
& \sum_{i \in I_{123} \cup I_{213}} \left\{ w_3^{(k)} \ln S_{IGE}(y_{3i}; \alpha_0, \lambda) + (1 - w_3^{(k)}) \ln f_{IGE}(y_{3i}; \alpha_0, \lambda) \right\} \quad (21)
\end{aligned}$$

It is clear that for a given λ

$$\begin{aligned}
\widehat{\alpha}_1^{(k+1)}(\lambda) &= \frac{n_1 + w_1^{(k)}(n - n_1)}{\sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{1i}}})}, \\
\widehat{\alpha}_2^{(k+1)}(\lambda) &= \frac{n_2 + w_2^{(k)}(n - n_2)}{\sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{2i}}})}, \\
\widehat{\alpha}_3^{(k+1)}(\lambda) &= \frac{n_3 + w_3^{(k)}(n - n_3)}{\sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{3i}}})}, \\
\widehat{\alpha}_0^{(k+1)}(\lambda) &= \frac{(n - n_1)(1 - w_1^{(k)}) + (n - n_2)(1 - w_2^{(k)}) + (n - n_3)(1 - w_3^{(k)})}{\sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{1i}}}) + \sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{2i}}}) + \sum_{i \in I} \ln(1 - e^{-\frac{\lambda}{y_{3i}}})},
\end{aligned}$$

maximize (21). Moreover, $\lambda^{(k+1)}$ can be obtained by maximizing the profile 'pseudo-log-likelihood' function of λ. Hence, 'M'-step can be performed by solving only one one-dimensional optimization problem. □

6 Conclusions and Some Open Problems

In this paper, we have introduced a new absolutely continuous bivariate distribution by removing the singular component of the singular bivariate inverse generalized exponential distribution. The marginals of the present bivariate distribution can be heavy tailed and have non-monotone hazard function. Due to the presence of four parameters, the proposed distribution is very flexible. We have developed an EM algorithm which can be used very conveniently to compute the ML estimators of the unknown parameters. The method has been extended to the multivariate case also.

As it has been mentioned before that the GE distribution can be obtained as a special case of the generalized Gompertz–Verhulst (GGV) distribution as introduced by Ahuja and Nash (1967). The CDF of a GGV distribution with parameters $p > 0$, $\sigma > 0$ and $\theta > 0$ takes the following form:

$$F_{GGV}(x;\theta,\sigma,p) = \begin{cases} 0 & \text{if } x \le \sigma \ln p \\ \left(1 - pe^{-\frac{x}{\sigma}}\right)^{\theta} & \text{if } x > \sigma \ln p. \end{cases} \tag{22}$$

Therefore, if we reparameterize as $\lambda = \sigma^{-1}$ and $\mu = \sigma \ln p$, then (22) can be written as

$$F_{GGV}(x;\theta,\lambda,\mu) = \begin{cases} 0 & \text{if } x \le \mu \\ \left(1 - e^{-\lambda(x-\mu)}\right)^{\theta} & \text{if } x > \mu. \end{cases} \tag{23}$$

Hence, the GGV distribution is the same as the three-parameter (location shift) GE distribution. Three-parameter IGE can be analogously defined from the three-parameter GE distribution. Similarly, five-parameter ABIGE can be defined with one location, one scale and three shape parameters and all the properties also remain the same. If the common location parameter is known, then the proposed EM algorithm can be used to compute the MLEs of the unknown parameters. All the results can be easily generalized to the multivariate case also. But if the location parameter is unknown, then it is no more a regular family and MLEs may not exist always. It will be interesting to develop a proper inference procedure in this case. More work is needed in this direction.

Recently, Feizjavadian and Hashemi (2015), Cai et al. (2017) and Shen and Xu (2018) developed dependent competing risks model based Marshall–Olkin bivariate Weibull distribution. The main assumption in developing the model based on Marshall–Olkin bivariate Weibull distribution is that, an experimental unit can fail at a particular time due to two competing causes simultaneously. But it may not be true in many cases. It seems this distribution can be used to develop dependent compet-

ing risks data when there are no ties on the cause of failure. The detailed inference procedure needs to be developed. The work is in progress, it will be reported later.

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Appendix 1: Proof of Theorem 1

Proof (a) It is clear that $f_{U,V}(u, v)$ is continuous in $S_1 \cup S_2$. Since $f_{U,V}(x, x) = \lim_{u,v\to x} f_{U,V}(u, v)$, it follows that $f_{U,V}(u, v)$ is continuous in $S_0 \cup S_1 \cup S_2$. Since for all $0 < u, v < \infty$,

$$f_{U,V}(0, 0) = f_{U,V}(\infty, \infty) = f_{U,V}(u, 0) = f_{U,V}(u, \infty) = f_{U,V}(0, v) = f_{U,V}(\infty, v) = 0,$$

that $f_{U,V}(u, v)$ has a local maximum. It can be easily checked by taking derivatives of $\ln f_{U,V}(u, v)$ that $f_{U,V}(u, v)$ does not have any critical point in the region $S_1 \cup S_2$, hence $f_{U,V}(u, v)$ does not have any critical point in the region $S_1 \cup S_2$, hence it does not have any local maximum in $S_1 \cup S_2$. Therefore, in this case, the local maximum will be at S_0. By taking derivative with respect to x of $\ln f_{U,V}(x, x)$ and equating it to zero, we can get one needs to solve the Eq. (9). It can be easily seen that the left-hand side of (9) is a decreasing function of x, and it decreases from ∞ to -4. Hence, it has a unique solution.
(b) Note that since $\alpha_1 > 1$ and $\alpha_2 + \alpha_0 < 1$, it can be easily seen by taking partial derivatives of $\ln f_{U,V}(u, v)$ that $f_{U,V}(u, v)$ has a critical point at (x_1, x_2), where x_1 and x_2 are solutions of the non-linear Eqs. (10) and (11), respectively. Clearly, $x_1 < 1/2$, since $\alpha_1 > 1$ and $x_2 < 1/2$, since $\alpha_2 + \alpha_0 < 1$. Hence, $(x_1, x_2) \in S_1$. Uniqueness follows using the same argument as in (a). It can be easily checked that $f_{U,V}(u, v)$ does not have a critical point in S_2.
(c) Follows similarly as in (b). □

Appendix 2: Observed Fisher Information Matrix

Using the same notation as Louis (1982), the observed Fisher information matrix can be written as

$$\boldsymbol{F}_{obs} = \boldsymbol{B} - \boldsymbol{S}\boldsymbol{S}^{\top},$$

here $\boldsymbol{B}$ is the negative of the second derivative of the log-likelihood function and $\boldsymbol{S}$ is the derivative vector. We provide the elements of the matrix $\boldsymbol{B}$ and the vector $\boldsymbol{S}$. We will use the following notation for brevity.

$$a_{11} = \sum_{i \in I_1} \frac{1}{u_i^2 (1 - e^{-\frac{\widehat{\lambda}}{u_i}})^2}, \quad a_{12} = \sum_{i \in I_2} \frac{1}{u_i^2 (1 - e^{-\frac{\widehat{\lambda}}{u_i}})^2},$$

$$a_{22} = \sum_{i \in I_2} \frac{1}{v_i^2 (1 - e^{-\frac{\widehat{\lambda}}{v_i}})^2}, \quad a_{21} = \sum_{i \in I_1} \frac{1}{v_i^2 (1 - e^{-\frac{\widehat{\lambda}}{v_i}})^2}$$

$$b_{11} = \sum_{i \in I_1} \frac{1}{u_i (1 - e^{-\frac{\widehat{\lambda}}{u_i}})}, \quad b_{12} = \sum_{i \in I_2} \frac{1}{u_i (1 - e^{-\frac{\widehat{\lambda}}{u_i}})},$$

$$b_{22} = \sum_{i \in I_2} \frac{1}{v_i (1 - e^{-\frac{\widehat{\lambda}}{v_i}})}, \quad b_{21} = \sum_{i \in I_1} \frac{1}{v_i (1 - e^{-\frac{\widehat{\lambda}}{v_i}})}$$

$$c_{11} = \sum_{i \in I_1} \frac{1}{u_i}, \quad c_{12} = \sum_{i \in I_2} \frac{1}{u_i}, c_{22} = \sum_{i \in I_2} \frac{1}{v_i}, \quad c_{21} = \sum_{i \in I_1} \frac{1}{v_i},$$

$$d_{11} = \sum_{i \in I_1} \ln(1 - e^{-\frac{\lambda}{u_i}}), d_{12} = \sum_{i \in I_2} \ln(1 - e^{-\frac{\lambda}{u_i}})$$

$$d_{22} = \sum_{i \in I_2} \ln(1 - e^{-\frac{\lambda}{v_i}}), d_{21} = \sum_{i \in I_1} \ln(1 - e^{-\frac{\lambda}{v_i}}).$$

If the (i, j)-th element of the matrix $\boldsymbol{B}$ is $B(i, j)$, then $B(i, j) = B(j, i)$, for $1 \leq i, j \leq 4$, and for $1 \leq i \leq j \leq 4$,

$$B(1,1) = \frac{n_1 + n_2 w_2}{\widehat{\alpha}_1^2}, \quad B(2,2) = \frac{n_2 + n_1 w_1}{\widehat{\alpha}_2^2}, \quad B(3,3) = \frac{n_1(1 - w_1) + n_2(1 - w_2)}{\widehat{\alpha}_0^2},$$

$$B(4,4) = \frac{2}{\widehat{\lambda}^2} + a_{11}[\widehat{\alpha}_1 - 1] + a_{22}[\widehat{\alpha}_2 - 1] + a_{12}[\widehat{\alpha}_1 + \widehat{\alpha}_0 - 1] + a_{21}[\widehat{\alpha}_2 + \widehat{\alpha}_0 - 1]$$

$$B(1,4) = -\frac{1}{\widehat{\lambda}^2} - (c_{11} + b_{11}), B(2,4) = -\frac{1}{\widehat{\lambda}^2} - (c_{22} + b_{22}), B(3,4) = b_{12} + b_{21},$$

$$B(1,3) = B(2,3) = B(1,2) = 0.$$

If $\boldsymbol{S} = (S(1), S(2), S(3), S(4))^\top$, then

$$S(1) = \frac{n_1 + w_2 n_2}{\widehat{\alpha}_1} + (d_{11} + d_{12}), S(2) = \frac{n_2 + w_1 n_1}{\widehat{\alpha}_2} + (d_{22} + d_{21}), S(3) = d_{12} + d_{21},$$

$$S(4) = \widehat{\lambda}(c_{11}+c_{12}+c_{21}+c_{22}) - \frac{2n}{\widehat{\lambda}} - \widehat{\alpha}_1(b_{11}+b_{12}) + \widehat{\alpha}_2(b_{22}+b_{21}) + \widehat{\alpha}_0(b_{21}+b_{12}) + (b_{11}+b_{12}+b_{21}+b_{22}).$$

Appendix 3: Normalizing Constant *c*

In this section, we show that the normalizing constant c satisfies (18). We will show the result for $p = 3$, the general result easily follows from there. If $(Y_1, Y_2, Y_3)^\top$ follows a AMIGE with parameters α_0, α_1, α_2, α_3 and λ, then for $\boldsymbol{Y} = (Y_1, Y_2, Y_3)$ and $\boldsymbol{y} = (y_1, y_2, y_3)$

$$f_{\boldsymbol{Y}}(\boldsymbol{y}) = c \begin{cases} f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_2;\alpha_2,\lambda) f_{IGE}(y_3;\alpha_0+\alpha_3,\lambda) \text{ if } y_1 < y_2 < y_3 \\ f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_3;\alpha_3,\lambda) f_{IGE}(y_2;\alpha_0+\alpha_2,\lambda) \text{ if } y_1 < y_3 < y_2 \\ f_{IGE}(y_2;\alpha_2,\lambda) f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_3;\alpha_0+\alpha_3,\lambda) \text{ if } y_2 < y_1 < y_3 \\ f_{IGE}(y_2;\alpha_2,\lambda) f_{IGE}(y_3;\alpha_3,\lambda) f_{IGE}(y_1;\alpha_0+\alpha_1,\lambda) \text{ if } y_2 < y_3 < y_1 \\ f_{IGE}(y_3;\alpha_3,\lambda) f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_2;\alpha_0+\alpha_2,\lambda) \text{ if } y_3 < y_1 < y_2 \\ f_{IGE}(y_3;\alpha_3,\lambda) f_{IGE}(y_2;\alpha_2,\lambda) f_{IGE}(y_1;\alpha_0+\alpha_1,\lambda) \text{ if } y_3 < y_2 < y_1. \end{cases}$$

Now, note that

$$\int_0^\infty \int_{y_1}^\infty \int_{y_2}^\infty f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_2;\alpha_2,\lambda) f_{IGE}(y_3;\alpha_0+\alpha_3,\lambda) dy_3 dy_2 dy_1 =$$
$$\int_0^\infty \int_{y_1}^\infty f_{IGE}(y_1;\alpha_1,\lambda) f_{IGE}(y_2;\alpha_2,\lambda) S_{IGE}(y_2;\alpha_0+\alpha_3,\lambda) dy_3 dy_2 =$$
$$\frac{\alpha_2}{\alpha_2+\alpha_3+\alpha_0} \int_0^\infty \int_{y_1}^\infty f_{IGE}(y_1;\alpha_1,\lambda) S_{IGE}(y_1;\alpha_2+\alpha_3+\alpha_0,\lambda) =$$
$$\frac{\alpha_1}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_2}{\alpha_2+\alpha_3+\alpha_0}.$$

Similarly, the other integrations also can be obtained. Hence

$$c^{-1} = \frac{\alpha_1}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_2}{\alpha_2+\alpha_3+\alpha_0} + \frac{\alpha_1}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_3}{\alpha_2+\alpha_3+\alpha_0} +$$
$$\frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_1}{\alpha_1+\alpha_3+\alpha_0} + \frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_3}{\alpha_1+\alpha_3+\alpha_0} +$$
$$\frac{\alpha_3}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_1}{\alpha_1+\alpha_2+\alpha_0} + \frac{\alpha_3}{\alpha_1+\alpha_2+\alpha_3+\alpha_0} \times \frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_0}.$$

Appendix 4: Proof of Theorem 2

Proof (a) Follows from the definition.
(b) Proof follows along the same way as the proof of Part (a) of Theorem 2.1.
(c)

$$\begin{aligned} P(Z > z) &= P(U_1 > z, \ldots, U_p > z, U_0 > z) \\ &= S_{IGE}(z; \alpha_1, \lambda) \times \ldots \times S_{IGE}(z; \alpha_p, \lambda) S_{IGE}(z; \alpha_0, \lambda) \\ &= S_{IGE}(z; \alpha_1 + \ldots + \alpha_p + \alpha_0, \lambda). \end{aligned}$$

(d) Observe that $(Y_i, Y_j) \sim \text{ABIGE}(\alpha_i, \alpha_j, \lambda)$. Hence,

$$\begin{aligned} P(Y_i < Y_j) &= \frac{\alpha_i + \alpha_j + \alpha_0}{\alpha_i + \alpha_j} \int_0^\infty \int_u^\infty f_{IGE}(u; \alpha_i, \lambda) f_{IGE}(v; \alpha_j + \alpha_0, \lambda) dv du \\ &= \frac{\alpha_i + \alpha_j + \alpha_0}{\alpha_i + \alpha_j} \int_0^\infty f_{IGE}(u; \alpha_i, \lambda) S_{IGE}(u; \alpha_j + \alpha_0, \lambda) du \\ &= \frac{\alpha_i}{\alpha_i + \alpha_j}. \end{aligned}$$

(e) Observe that $(Y_i, Y_j) \sim \text{ABIGE}(\alpha_i, \alpha_j, \lambda)$. Hence,

$$\begin{aligned} P(Y_i > a | Y_i < Y_j) &= \frac{P(a < Y_i < Y_j)}{P(Y_i < Y_j)} \\ &= \frac{\alpha_i + \alpha_j + \alpha_0}{\alpha_i} \int_a^\infty \int_u^\infty f_{IGE}(u; \alpha_i, \lambda) f_{IGE}(v, \alpha_j + \alpha_0, \lambda) dv du \\ &= \frac{\alpha_i + \alpha_j + \alpha_0}{\alpha_i} \int_a^\infty f_{IGE}(u; \alpha_i, \lambda) S_{IGE}(u, \alpha_j + \alpha_0, \lambda) du \\ &= S_{IGE}(a; \alpha_i + \alpha_j + \alpha_0, \lambda). \end{aligned}$$

□

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Multivariate Analysis

The Likelihood Ratio Test of Equality of Mean Vectors with a Doubly Exchangeable Covariance Matrix

Carlos A. Coelho and Jolanta Pielaszkiewicz

Abstract The authors derive the LRT statistic for the test of equality of mean vectors when the covariance matrix has what is called a double exchangeable structure. A second expression for this statistic, based on determinants of Wishart matrices with a block-diagonal parameter matrix, allowed for the expression of the distribution of this statistic as that of a product of independent Beta random variables. Moreover, the split of the LRT statistic into three independent components, induced by this second representation, will then allow for the expression of the exact distribution of the LRT statistic in a very manageable finite closed form for most cases and the obtention of very sharp near-exact distributions for the other cases. Numerical studies show that, as expected, due to the way they are built, these near-exact distributions are indeed asymptotic not only for increasing sample sizes but also for increasing values of all other parameters in the distribution, besides lying very close to the exact distribution even for extremely small samples.

Keywords Asymptoticity for all parameters · Exact distribution · Near-exact distributions · Product of Betas · Quadratic space · Small samples

1 Introduction

Let us suppose we have a multivariate random vector $\underline{X}$ which is split into m subvectors $\underline{X}_i$ $(i = 1, \ldots, m)$, all of the same length vr, each of which is, in turn, split into v subvectors $\underline{X}_{ij}$ $(j = 1, \ldots, v)$, each of them of length r, that is, we have

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$$\underline{X} = \big[\underbrace{\underline{X}_{11}, \underline{X}_{12}, \ldots, \underline{X}_{1v}}_{\underline{X}_1}, \underbrace{\underline{X}_{21}, \underline{X}_{22}, \ldots, \underline{X}_{2v}}_{\underline{X}_2}, \ldots, \underbrace{\underline{X}_{m1}, \underline{X}_{m2}, \ldots, \underline{X}_{mv}}_{\underline{X}_m}\big]'$$

where each $\underline{X}_{ij}$ $(i = 1, \ldots, m;\ j = 1, \ldots, v)$ is of dimension r.

The $\underline{X}_i$ may correspond for example to different times of measurement $(i = 1, \ldots, m)$, with the $\underline{X}_{ij}$ $(j = 1, \ldots, v)$, for a given i, corresponding to the set of r variables measured at different v locations at that given time i.

Then it may make sense to assume a covariance structure where we have, for $i = 1, \ldots, m$,

$$Var(\underline{X}_i) = I_v \otimes U + (I_v - J_v) \otimes V = \begin{bmatrix} U & V & \ldots & V \\ V & U & \ldots & V \\ \vdots & \vdots & \ddots & \vdots \\ V & V & \ldots & U \end{bmatrix}$$

and for $i \neq i'$ $(i, i' \in \{1, \ldots, m\})$

$$Cov(\underline{X}_i, \underline{X}_{i'}) = J_v \otimes M = \begin{bmatrix} M & M & \ldots & M \\ M & M & \ldots & M \\ \vdots & \vdots & \ddots & \vdots \\ M & M & \ldots & M \end{bmatrix}$$

where I_p represents an identity matrix of order p and J_p a matrix of 1's of dimensions $p \times p$, so that for any $i = 1, \ldots, m$ and $j = 1, \ldots, v$

$$Var(\underline{X}_{ij}) = U$$

and for $j \neq j'$ $(j, j' \in \{1, \ldots, v\})$ and $i \neq i'$ $(i, i' \in \{1, \ldots, m\})$

$$Cov(\underline{X}_{ij}, \underline{X}_{ij'}) = V \quad \text{and} \quad Cov(\underline{X}_{ij}, \underline{X}_{i'j'}) = Cov(\underline{X}_{ij}, \underline{X}_{i'j}) = M\,.$$

In this case the covariance matrix for our random vector $\underline{X}$ will have what we call a double exchangeable structure, with

$$\Sigma = I_{vm} \otimes U + \{I_m \otimes (J_v - I_v)\} \otimes V + \{J_{vm} - (I_m \otimes J_v)\} \otimes M\,, \qquad (1)$$

for any positive-definite $r \times r$ matrices U and symmetric $r \times r$ matrices V and M, such that $U - V$, $U - V + v(V - M)$ and $U - V + v(V - M) + vmM$ are positive-definite.

An account of the properties of this covariance structure was given by several authors and its applicability in spatial/time analyses established (Roy and Fonseca 2012; Pavlenko and Roy 2017; Coelho and Roy 2020). It also has as particular cases several covariance structures of interest as for example the well-known compound-

symmetric structure, for $r = 1$ and $m = 1$ or $v = 1$, the block-compound-symmetric structure, for $m = 1$ or $v = 1$, and the double complete symmetry (Coelho and Singull 2020) for $r = 1$.

For example for $m = 4$ and $v = 3$, Σ would have the following structure

$$\Sigma = \begin{bmatrix} U & V & V & M & M & M & M & M & M & M & M & M \\ V & U & V & M & M & M & M & M & M & M & M & M \\ V & V & U & M & M & M & M & M & M & M & M & M \\ M & M & M & U & V & V & M & M & M & M & M & M \\ M & M & M & V & U & V & M & M & M & M & M & M \\ M & M & M & V & V & U & M & M & M & M & M & M \\ M & M & M & M & M & M & U & V & V & M & M & M \\ M & M & M & M & M & M & V & U & V & M & M & M \\ M & M & M & M & M & M & V & V & U & M & M & M \\ M & M & M & M & M & M & M & M & M & U & V & V \\ M & M & M & M & M & M & M & M & M & V & U & V \\ M & M & M & M & M & M & M & M & M & V & V & U \end{bmatrix}.$$

Let us suppose that we have q independent replicates of $\underline{X}$, which we will denote by $\underline{X}^{(k)}$, for $k = 1, \ldots, q$, with

$$E\left(\underline{X}^{(k)}\right) = \underline{\mu}^{(k)} \quad \text{and} \quad Var(\underline{X}^{(k)}) = \Sigma\,,$$

where Σ has the above double exchangeable structure, and let us suppose that we are then interested in testing the null hypothesis

$$H_0 : \underline{\mu}^{(1)} = \cdots = \underline{\mu}^{(q)}\,, \tag{2}$$

based on q independent samples, one from each $\underline{X}^{(k)}$, accounting for the structure of Σ in (1).

In the next section we obtain the LRT statistic for this test, deriving the MLE's for Σ, under the null and the alternative hypotheses, using a strategy based on the fact that both Σ and Σ^{-1} have a similar structure. Then in Sect. 3 we first rewrite the expression for this LRT statistic, expressing it in terms of determinants of diagonal blocks of Wishart matrices with a block-diagonal parameter matrix. This will enable us to obtain the distribution of the LRT statistic in terms of the distribution of a product of independent Beta r.v.'s. This form of the distribution will in turn enable us to obtain the exact distribution of this LRT statistic in a closed finite and very manageable form for all cases where q is odd or r is even and also to develop very sharp near-exact distributions for all other cases. Finally in Sect. 4 conclusions are drawn and a discussion is undertaken upon the methods and techniques used.

2 The LRT Statistic

Let $\underline{X}^{(k)} \sim N_{vmr}(\underline{\mu}^{(k)}, \Sigma)$ $(k = 1, \ldots, q)$, where Σ has the double exchangeable structure in (1) and let us suppose that we are interested in testing the null hypothesis in (2).

Let

$$A = \sum_{k=1}^{q} (n_k - 1) S_k \quad \text{and} \quad B = \sum_{k=1}^{q} n_k (\overline{\underline{X}}^{(k)} - \overline{\underline{X}})(\overline{\underline{X}}^{(k)} - \overline{\underline{X}})' \tag{3}$$

where n_k is the size of the sample from $\underline{X}^{(k)}$ and S_k and $\overline{\underline{X}}^{(k)}$ are respectively the sample covariance matrix and mean vector of the k-th sample and where

$$\overline{\underline{X}} = \frac{1}{n} \sum_{k=1}^{q} n_k \overline{\underline{X}}^{(k)} ,$$

for $n = \sum_{k=1}^{q} n_k$. Then, see for example Kshirsagar (1972, Sect. 9.1), the $(2/n)$-th power of the LRT statistic to test H_0 in (2), without accounting for the structure in Σ, is

$$\Lambda = \frac{|A|}{|A + B|} ,$$

where A and $A + B$ are the unstructured MLEs of Σ, respectively under the alternative and under the null hypotheses.

So, the question now is: which will be the ($(2/n)$-th power of the) LRT statistic to test H_0 in (2), accounting for the structure of Σ in (1)?

It is not too hard to show that the answer is: it is a statistic of the form

$$\Lambda = \frac{|A^*|}{|A^* + B^*|} , \tag{4}$$

where A^* and $A^* + B^*$ will be the MLEs of Σ, respectively under the alternative and under the null hypotheses, both of them accounting for the double exchangeable structure of Σ.

So, the next question is: how will we be able to obtain A^* and B^*?

We may note that, not only the space of doubly exchangeable covariance matrices is itself a quadratic space (Seely 1971), as well as if we let Γ_p denote an orthogonal Helmert matrix whose first row is proportional to a vector of 1's, and consider the orthogonal matrix

$$\Gamma = \Gamma_m \otimes \Gamma_v \otimes I_r , \tag{5}$$

then we have, for Σ in (1) (Roy and Fonseca 2012),

$$\Gamma \Sigma \Gamma' = \Psi ,$$

with

$$\Psi = bdiag(\Psi_1, \underbrace{\Psi_3, \ldots, \Psi_3}_{v-1}, \underbrace{\Psi_2, \underbrace{\Psi_3, \ldots, \Psi_3}_{v-1}, \ldots, \Psi_2, \underbrace{\Psi_3, \ldots, \Psi_3}_{v-1}}_{m-1}), \tag{6}$$

where $bdiag$ denotes a block-diagonal matrix and where Ψ_1, Ψ_2 and Ψ_3 are all $r \times r$ positive-definite matrices, with

$$\begin{aligned} \Psi_1 &= U + (v-1)V + v(m-1)M \\ \Psi_2 &= U + (v-1)V - vM \\ \Psi_3 &= U - V\,. \end{aligned} \tag{7}$$

But then, since we will have

$$\Psi^{-1} = bdiag(\Psi_1^{-1}, \underbrace{\Psi_3^{-1}, \ldots, \Psi_3^{-1}}_{v-1}, \underbrace{\Psi_2^{-1}, \underbrace{\Psi_3^{-1}, \ldots, \Psi_3^{-1}}_{v-1}, \ldots, \Psi_2^{-1}, \underbrace{\Psi_3^{-1}, \ldots, \Psi_3^{-1}}_{v-1}}_{m-1}),$$

we may write

$$\Sigma^{-1} = \Gamma \Psi^{-1} \Gamma'\,,$$

which shows that both Σ and Σ^{-1} have the double exchangeable structure, what allows us to use the results in Szatrowski (1978, 1980) and Seely (1971) in order to obtain the MLEs of Σ under H_0, as well as under the alternative hypothesis, built from the MLEs of the corresponding blocks of dimensions $r \times r$, which will then be obtained by averaging the corresponding blocks of the unstructured MLE.

This way, under the alternative hypothesis $H_1 : \exists_{k,k' \in \{1,\ldots,q\}} : \underline{\mu}^{(k)} \neq \underline{\mu}^{(k')}$, the MLE of Σ is

$$A^* = I_{vm} \otimes \widehat{U}_{|H_1} + [I_m \otimes (J_v - I_v)] \otimes \widehat{V}_{|H_1} + [J_{vm} - (I_m \otimes J_v)] \otimes \widehat{M}_{|H_1}\,, \tag{8}$$

where

$$\widehat{U}_{|H_1} = \frac{1}{mv} \sum_{j=1}^{mv} A_{jj}\,, \tag{9}$$

$$\widehat{V}_{|H_1} = \frac{1}{v(v-1)m} \sum_{j=0}^{m-1} \sum_{k=1}^{v-1} \sum_{\ell=1}^{v-k} A_{jv+k,jv+k+\ell} + A'_{jv+k,jv+k+\ell}\,, \tag{10}$$

and

$$\widehat{M}_{|H_1} = \frac{1}{v^2 m(m-1)} \sum_{j=0}^{m-2} \sum_{k=1}^{v} \sum_{\ell=0}^{vm-(j+1)v-1} A_{jv+k,(j+1)v+1+\ell} + A'_{jv+k,(j+1)v+1+\ell}\,, \quad (11)$$

with A_{jk} representing the $r \times r$ block of A starting at row $r(j-1)+1$ and column $r(k-1)+1$.

Under the null hypothesis in (2) the MLE of Σ is

$$A^* + B^* = I_{vm} \otimes \widehat{U}_{|H_0} + [I_m \otimes (J_v - I_v)] \otimes \widehat{V}_{|H_0} + [J_{vm} - (I_m \otimes J_v)] \otimes \widehat{M}_{|H_0}\,,$$

where

$$\widehat{U}_{|H_0} = \frac{1}{mv} \sum_{j=1}^{mv} A_{jj} + B_{jj}\,,$$

$$\widehat{V}_{|H_0} = \frac{1}{v(v-1)m} \sum_{j=0}^{m-1} \sum_{k=1}^{v-1} \sum_{\ell=1}^{v-k} \big(A_{jv+k,jv+k+\ell} + A'_{jv+k,jv+k+\ell} + B_{jv+k,jv+k+\ell} + B'_{jv+k,jv+k+\ell}\big)$$

and

$$\widehat{M}_{|H_0} = \frac{1}{v^2 m(m-1)} \sum_{j=0}^{m-2} \sum_{k=1}^{v} \sum_{\ell=0}^{vm-(j+1)v-1} \big(A_{jv+k,(j+1)v+1+\ell} + A'_{jv+k,(j+1)v+1+\ell} + B_{jv+k,(j+1)v+1+\ell} + B'_{jv+k,(j+1)v+1+\ell}\big),$$

where A_{jk} and B_{jk} represent respectively the $r \times r$ blocks of A and B starting at row $r(j-1)+1$ and column $r(k-1)+1$.

Then, for a sample of size $n = \sum_{k=1}^{q} n_k$, the $(2/n)$-th power of the LRT statistic to test H_0 in (2) is the statistic Λ in (4).

However, although that expression may be used to obtain the computed value of the statistic, it is much useful in helping us derive the distribution of Λ. In order to do this the best way is to take the approach in the next section.

3 The Distribution of the l.r.t. Statistic

The results on the distribution of the statistic Λ in (4), which will be used to obtain its distribution in a finite closed form for most cases and near-exact approximations for the remaining cases, are summarized in the following Theorem, whose Corollary shows that the results in Coelho (2017) are indeed a particular case of the present results.

Theorem 1 *The distribution of Λ in (4) is the same as that of*

$$\left\{\prod_{j=1}^{r} Y_j\right\} \times \left\{\prod_{j=1}^{r} \left(Y_j^*\right)^{m-1}\right\} \times \left\{\prod_{j=1}^{r} \left(Y_j^{**}\right)^{(v-1)m}\right\}, \tag{12}$$

where, for $j = 1, \ldots, r$, and for $n > q + r - 1$,

$$\begin{aligned} Y_j &\sim Beta\left(\frac{n-q+1-j}{2}, \frac{q-1}{2}\right) \\ Y_j^* &\sim Beta\left(\frac{(m-1)(n-q)}{2} + \frac{1-j}{2}, \frac{(m-1)(q-1)}{2}\right) \\ Y_j^{**} &\sim Beta\left(\frac{(v-1)m(n-q)}{2} + \frac{1-j}{2}, \frac{(v-1)m(q-1)}{2}\right) \end{aligned} \tag{13}$$

form three sets of independent r.v.'s, also all independent among themselves.

Proof Let us consider the matrices

$$A^{**} = \Gamma A \Gamma' \quad \text{and} \quad B^{**} = \Gamma B \Gamma', \tag{14}$$

for Γ in (5). Then, we should remark that, given the fact that the matrices A and B in (3) are independent, with

$$A \sim W_{vmr}(n-q, \Sigma) \quad \text{and} \quad B \sim W_{vmr}(q-1, \Sigma),$$

then, A^{**} and B^{**} will be two independent matrices, with

$$A^{**} \sim W_{vmr}(n-q, \Psi) \quad \text{and} \quad B^{**} \sim W_{vmr}(q-1, \Psi), \tag{15}$$

for Ψ in (6).

Then, it is possible to show that (see Appendix 1)

$$\begin{aligned} |A^*| = |\underbrace{A_1^{**}}_{A_1^{***}}| \left(\left|\frac{1}{m-1} \underbrace{\sum_{j=1}^{m-1} A_{jv+1}^{**}}_{A_2^{***}}\right|\right)^{m-1} \\ \times \left(\left|\frac{1}{(v-1)m} \underbrace{\sum_{j=1}^{m} \sum_{k=1}^{v-1} A_{(j-1)v+1+k}^{**}}_{A_3^{***}}\right|\right)^{(v-1)m}, \end{aligned} \tag{16}$$

and

$$|A^* + B^*| = |\underbrace{A_1^{**} + B_1^{**}}_{A_1^{***}+B_1^{***}}| \left(\left| \frac{1}{m-1} \underbrace{\sum_{j=1}^{m-1} A_{jv+1}^{**} + B_{jv+1}^{**}}_{A_2^{***}+B_2^{***}} \right| \right)^{m-1}$$
$$\times \left(\left| \frac{1}{(v-1)m} \underbrace{\sum_{j=1}^{m} \sum_{k=1}^{v-1} A_{(j-1)v+1+k}^{**} + B_{(j-1)v+1+k}^{**}}_{A_3^{***}+B_3^{***}} \right| \right)^{(v-1)m}, \tag{17}$$

where A_j^{**} and B_j^{**} represent the j-th diagonal block of dimensions $r \times r$ respectively of A^{**} and B^{**}.

But then, from (4), (16) and (17) we may write

$$\Lambda = \underbrace{\frac{|A_1^{***}|}{|A_1^{***} + B_1^{***}|}}_{\Lambda_1} \underbrace{\left(\frac{|A_2^{***}|}{|A_2^{***} + B_2^{***}|} \right)^{m-1}}_{\Lambda_2} \underbrace{\left(\frac{|A_3^{***}|}{|A_3^{***} + B_3^{***}|} \right)^{(v-1)m}}_{\Lambda_3} \tag{18}$$

where, under H_0 in (2), given the distributions of A^{**} and B^{**} in (15) and the fact that Ψ is a block-diagonal matrix, A_1^{***}, A_2^{***}, A_3^{***}, B_1^{***}, B_2^{***} and B_3^{***} are all independent, with

$$A_1^{***} \sim W_r(n-q, \Psi_1)$$
$$A_2^{***} \sim W_r\big((m-1)(n-q), \Psi_2\big)$$
$$A_3^{***} \sim W_r\big((r-1)m(n-q), \Psi_3\big)$$

and

$$B_1^{***} \sim W_r(q-1, \Psi_1)$$
$$B_2^{***} \sim W_r\big((m-1)(q-1), \Psi_2\big)$$
$$B_3^{***} \sim W_r\big((r-1)m(q-1), \Psi_3\big)$$

for Ψ_1, Ψ_2 and Ψ_3 in (6), so that, under H_0 in (2), we have (Coelho and Arnold 2019, Chap. 5, App. A)

$$\Lambda_1 \overset{\text{st}}{\sim} \prod_{j=1}^{r} Y_j\,, \quad \Lambda_2 \overset{\text{st}}{\sim} \prod_{j=1}^{r} \big(Y_j^*\big)^{m-1} \quad \text{and} \quad \Lambda_3 \overset{\text{st}}{\sim} \prod_{j=1}^{r} \big(Y_j^{**}\big)^{(v-1)m}\,,$$

where, for $j = 1, \ldots, r$, and for $n > q + r - 1$, the r.v.'s Y_j, Y_j^* and Y_j^{**} form three sets of independent r.v.'s, which, given the independence of Λ_1, Λ_2 and Λ_3, consequence of the block-diagonal structure of the matrix Ψ, are also independent among themselves, with the distributions in (13). □

For $r = 1$ and $v = 1$ or for $r = 1$ and $m = 1$, the matrix Σ is a compound-symmetric matrix, and as such, for these values of the parameters it is possible to

establish the following Corollary, which shows that the results in Coelho (2017) are a particular case of the results in the present paper.

Corollary 1 *For $r = 1$, $v = 1$ and $m = p$, or for $r = 1$, $m = 1$ and $v = p$, we may write, from (16)–(18), the statistic Λ as*

$$\Lambda = \frac{a_{11}^{***}}{c_{11}^{***}} \frac{(a^{***})^{p-1}}{(c^{***})^{p-1}}$$

for

$$c_{11}^{***} = a_{11}^{***} + b_{11}^{***} \quad \text{and} \quad c^{***} = a^{***} + b^{***},$$

where a_{11}^{***} and b_{11}^{***} stand for the only diagonal element in A_1^{***} and B_1^{***} respectively, which are now 1×1 matrices, and where a^{***} and b^{***} represent respectively either the sum or the average of the A_j^{**} and the B_j^{**} for $j = 2, \ldots, p$.

Furthermore, for $r = 1$, $v = 1$ and $m = p$ we have, from (12) and (13), the distribution of Λ as that of

$$Y_1 \left(Y_1^*\right)^{p-1},$$

where

$$Y_1 \sim Beta\left(\frac{n-q}{2}, \frac{q-1}{2}\right) \quad \text{and} \quad Y_1^* \sim Beta\left(\frac{(p-1)(n-q)}{2}, \frac{(p-1)(q-1)}{2}\right),$$

are two independent r.v.'s, and for $r = 1$, $m = 1$ and $v = p$, as that of

$$Y_1 \left(Y_1^{**}\right)^{p-1},$$

where Y_1^{**} has exactly the same distribution as that of Y_1^* above, being also independent of Y_1.

These results establish those in Coelho (2017) as a particular case of the present ones.

In addressing the distribution of the l.r.t. statistic in (18) we will have to consider four different scenarios, split into two main scenarios, the second of which, itself split into three sub-scenarios.

The two main scenarios to consider are:

(i) the case of odd q or even r, where we will be able to obtain the exact distribution of Λ in a closed manageable form,

(ii) the case of even q and odd r, where we will have to approximate the distribution of Λ using near-exact distributions, which will be shown to lay very close to the exact distribution, and where we will have to consider three sub-scenarios:

(ii.a) where m and v are odd, in which case we may still obtain the distribution of Λ_1 and Λ_2 in a closed finite manageable form,

(ii.b) where m is odd and v is even, in which case we may obtain only the distribution of Λ_2 in a closed finite manageable form, and

(ii.c) where m is even, in which case only the distribution of Λ_3 may be obtained in a closed finite manageable form.

This enchaining of scenarios is addressed in the following subsections.

3.1 The Case of Odd q and Even r

When either q is odd or r is even we are actually able to obtain the exact distribution of Λ in a closed finite and very manageable form.

This is so because in this case we may use Theorem 3.2 in Coelho and Arnold (2019) to obtain, for odd q or even r the exact distribution of Λ_1, Λ_2 and Λ_3 in a closed finite and very manageable form, which moreover, given the independence of the three statistics, will then open the way for obtaining the exact distribution of Λ in a closed finite and very manageable form.

We have thus the following Theorem, which gives the exact distribution of Λ for odd q or even r in a closed finite and very manageable form.

Theorem 2 *For odd q or even r the exact distribution of Λ is an EGIG distribution (Arnold et al. 2013) of depth at most $3r + vm(q-1) - 6$, with rate parameters*

$$\lambda_{jk} = \frac{n-1}{2} - \frac{j+1}{2c_k}, \quad j = 1, \ldots, r + c_k(q-1) - 2;\ k = 1, \ldots, 3, \tag{19}$$

for

$$c_1 = 1, \quad c_2 = m - 1 \quad \text{and} \quad c_3 = (v-1)m, \tag{20}$$

and shape parameters

$$r_{jk} = \begin{cases} h_{jk} & j = 1, 2 \\ h_{jk} + r_{j-2,k} & j = 3, \ldots, r + c_k(q-1) - 2 \end{cases} \tag{21}$$

where

$$\begin{aligned} h_{jk} &= (\#\ \textit{of elements in}\ \{r, c_k(q-1)\} \geq j) - 1 \\ &= \begin{cases} 1 & j = 1, \ldots, \min(r, c_k(q-1)) \\ 0 & j = 1 + \min(r, c_k(q-1)), \ldots, \max(r, c_k(q-1)) \\ -1 & j = 1 + \max(r, c_k(q-1)), \ldots, r + c_k(q-1) - 2, \end{cases} \end{aligned} \tag{22}$$

with p.d.f. and c.d.f. respectively given by

$$f_\Lambda(z) = f^{EGIG}\left(z \,\middle|\, \overset{\approx}{\{r_{jk}\}}, \overset{\approx}{\widetilde{\{\lambda_{jk}\}}}; \widetilde{\#\{\lambda_{jk}\}}\right) \tag{23}$$

and

$$F_{\Lambda}(z) = F^{EGIG}\left(z \,\middle|\, \underset{\approx}{\{r_{jk}\}}, \widetilde{\{\lambda_{jk}\}}; \#\widetilde{\{\lambda_{jk}\}}\right), \tag{24}$$

for $0 < z < 1$, *and where* f^{EGIG} *and* F^{EGIG} *denote respectively the p.d.f. and the c.d.f. of the EGIG distribution, with the full notation being explained in Appendix 2, and with* $\widetilde{\{\lambda_{jk}\}}$ *denoting the set of unique* λ_{jk} *in (19) (given the fact that for different* k *some of the* λ_{jk} *may be equal) and with* $\underset{\approx}{\{r_{jk}\}}$ *denoting the set of corresponding shape parameters, where the original shape parameters* r_{jk} *that correspond to equal* $\lambda'_{jk}s$ *are added together (this has to be done because the definition of the EGIG p.d.f. and c.d.f. requests a set of unique rate parameters). The depth of this distribution, which is the number of different Gamma distributions involved and the product of whose exponentials form the EGIG distribution, is then equal to* $\#\widetilde{\{\lambda_{jk}\}}$ *or* $\#\ \underset{\approx}{\{r_{jk}\}}$, *where* # *denotes the cardinality of the set.*

Proof Let $W_k = -\log \Lambda_k$, for $k = 1, \ldots, 3$. Then, for even r, the distribution of Λ_k and W_k $(k = 1, \ldots, 3)$ are given, for c_k in (20), by Theorem 3.2 in Coelho and Arnold (2019) for

$$m^* = 1\,,\ \ k_1 = 2\,,\ \ n_1 = r/2\,,\ \ m_1 = c_k(q-1)\ \text{ and }\ a_1 = \frac{c_k(n-q)}{2} + \frac{1}{2}\,,$$

or, for odd q, for

$$m^* = 1\,,\ \ k_1 = 2\,,\ \ n_1 = c_k(q-1)/2\,,\ \ m_1 = r\ \text{ and }\ a_1 = \frac{c_k(n-1)-r}{2} + \frac{1}{2}\,, \tag{25}$$

yielding, in either case,

$$W_k \overset{\mathrm{d}}{\equiv} \sum_{j=1}^{r+c_k(q-1)-2} Z_{jk} \quad \text{or} \quad \Lambda_k \overset{\mathrm{d}}{\equiv} \prod_{j=1}^{r+c_k(q-1)-2} e^{-Z_{jk}} \tag{26}$$

where "$\overset{\mathrm{d}}{\equiv}$" stands for "is equivalent in distribution to" and

$$Z_{jk} \sim \Gamma(r_{jk}, \lambda_{jk})\,, \quad j = 1, \ldots, r + c_k(q-1) - 2 \tag{27}$$

are a set of independent r.v.'s, with r_{jk} given by (21)–(22) and

$$\lambda_{jk} = \frac{n-q}{2} + \frac{j-r}{2c_k}\,,\ \ j = 1, \ldots, r + c_k(q-1) - 2; k = 1, \ldots, 3\,,$$

thus yielding for W_k a GIG distribution (Coelho 1998) and for Λ_k an EGIG distribution (Arnold et al. 2013) of depth $r + mv(q-1) - 2$ (where $mv = c_1 + c_2 + c_3$),

with rate parameters λ_{jk} and shape parameters r_{jk} $(j = 1, \ldots, r + c_k(q-1) - 2; k = 1, 2, 3)$.

Given the fact that the shape parameters r_{jk} are symmetric for $j = 1, \ldots, r + c_k(q-1) - 2$, for any $k = 1, \ldots, 3$, we may reverse the index j in the expression for λ_{jk}, writing these parameters as in (19). This will render simpler expressions and a simpler approach later in Sect. 3.2.

The exact characteristic function (c.f.) of W_k $(k = 1, \ldots, 3)$ is thus,

$$\Phi_{W_k}(t) = \prod_{j=1}^{r+c_k(q-1)-2} \lambda_{jk}^{r_{jk}} \left(\lambda_{jk} - \mathrm{i}t\right)^{-r_{jk}} , \tag{28}$$

for r_{jk} given by (21)–(22), λ_{jk} given by (19) and c_k given by (20), and therefore, given the independence of Λ_1, Λ_2 and Λ_3, and as such also that of W_1, W_2 and W_3, the exact c.f. of $W = -\log \Lambda = W_1 + W_2 + W_3$ is

$$\Phi_W(t) = \Phi_{W_1}(t)\, \Phi_{W_2}(t)\, \Phi_{W_3}(t)$$

and the exact distribution of W is, therefore, a GIG distribution of depth at most $3r + (c_1 + c_2 + c_3)(q-1) - 6$ with rate parameters λ_{jk} and shape parameters r_{jk} $(k = 1, \ldots, 3; j = 1, \ldots, r + c_k(q-1) - 2)$ and that of Λ an EGIG distribution of the same depth and with the same rate and shape parameters. We say that the depth of this GIG distribution, that is, the number of different rate parameters it has, is at most $3r + (c_1 + c_2 + c_3)(q-1) - 6$, since for some combinations of values of the parameters m, q, v and r, some of the rate parameters λ_{jk} may be equal for different k's. In this case the depth of the GIG and of the EGIG distributions will be smaller than $3r + (c_1 + c_2 + c_3)(q-1) - 6$ since we will have to "collapse", or more precisely, to add together the Gamma r.v.'s with the same rate parameters into a single Gamma r.v. with that same rate parameter and a shape parameter that is the sum of the shape parameters for the original Gamma r.v.'s with that same rate parameter. We could arrange for a rather intricate play of indexes to index all these different rate parameters and also to indicate which would collapse for different possible relations among the parameters m, q, v and r, but since we will anyway need a software to compute the values of the p.d.f. and the c.d.f. of Λ or W, this "selection" of the different rate parameters may then be easily done by this software using a function similar to the function `Tally` in Mathematica®.

Using the notation in Appendix 2 for the GIG p.d.f. and c.d.f., and using for the sets of rate and shape parameters the notation used and explained in the statement of the Theorem, we will write, for $w > 0$, the exact p.d.f. of W as

$$f_W(w) = f^{GIG}\left(w \,\middle|\, \widetilde{\widetilde{\{r_{jk}\}}}, \widetilde{\{\lambda_{jk}\}}; \#\widetilde{\{\lambda_{jk}\}}\right)$$

and its c.d.f. as

$$F_W(w) = F^{GIG}\left(w \,\middle|\, \overset{\approx}{\{r_{jk}\}}, \overset{\approx}{\{\widetilde{\lambda}_{jk}\}}; \#\{\widetilde{\lambda}_{jk}\}\right),$$

The corresponding exact p.d.f. and c.d.f. of $\Lambda = e^{-W}$ are then easily obtained by simple transformation, and may be expressed in terms of the p.d.f. and c.d.f. of the EGIG distribution, as in (23) and (24). □

The following Corollary shows that the exact distribution in Theorem 2 fully matches the exact distribution obtained for odd q in Coelho (2017) for the case when Σ is a compound-symmetric matrix, that is, when $r = 1$ and either $v = 1$ or $m = 1$. Although in face of Corollary 1 such result would be fully expected, it may be not immediately discernible from the result in Theorem 2, besides the fact that there is a small typo in expression (13) in Coelho (2017) which matters to correct.

Corollary 2 *For $r = 1$, $v = 1$ and $m = p$, or for $r = 1$, $m = 1$ and $v = p$, and odd q, the exact distribution of Λ is an EGIG distribution of depth $(q-1)(p-1)/2$, with rate parameters*

$$\lambda_j = \frac{n-q}{2} + \frac{j-1}{p-1}, \quad j = 1, \ldots, (q-1)(p-1)/2 \tag{29}$$

and shape parameters

$$r_j = \begin{cases} 1\,, \; j = 1, \ldots, (q-1)(p-1)/2 \\ \quad j \neq (\ell-1)(p-1)+1 \; \textit{for} \; \ell = 1, \ldots, (q-1)/2 \\ 2\,, \; j = (\ell-1)(p-1)+1 \; \textit{for} \; \ell = 1, \ldots, (q-1)/2 \end{cases} \tag{30}$$

with p.d.f. and c.d.f.

$$f_\Lambda(z) = f^{EGIG}\left(z \,\middle|\, \{r_j\}_{j=1:g}, \left\{\frac{n-q}{2} - \frac{j-1}{p-1}\right\}_{j=1:g}; g\right) \tag{31}$$

and

$$F_\Lambda(z) = F^{EGIG}\left(z \,\middle|\, \{r_j\}_{j=1:g}, \left\{\frac{n-q}{2} - \frac{j-1}{p-1}\right\}_{j=1:g}; g\right) \tag{32}$$

for $g = (q-1)(p-1)/2$ and r_j given by (30).

Proof Being a direct Corollary of Theorem 2, no formal proof is indeed necessary. All one has to do is to set $r = 1$, $v = 1$ and $m = p$ in Theorem 2, and notice that in this case we have, from (20),

$$c_1 = 1\,, \quad c_2 = p-1 \quad \text{and} \quad c_3 = 0\,,$$

so that we have, from (19),

$$\lambda_{j1} = \frac{n-q}{2} + \frac{j-1}{2}, \quad j = 1, \ldots, q-2$$

and

$$\lambda_{j2} = \frac{n-q}{2} + \frac{j-1}{2(p-1)}, \quad j = 1, \ldots, (p-1)(q-1)-1,$$

while the λ_{j3} vanish. Furthermore, from (22) we have

$$h_{j1} = \begin{cases} 1, & j = 1 \\ 0, & j = 2, \ldots, q-2 \end{cases}$$

so that, from (21) we obtain

$$r_{j1} = \begin{cases} 1, \text{for odd } j, \text{ i.e. } j = 1, \ldots, q-2, \text{ step } 2 \\ 0, \text{for even } j, \text{ i.e. } j = 2, \ldots, q-3, \text{ step } 2 \end{cases}$$

and

$$h_{j2} = \begin{cases} 1, & j = 1 \\ 0, & j = 2, \ldots, (p-1)(q-1)-1 \end{cases}$$

which gives

$$r_{j2} = \begin{cases} 1, \text{for odd } j, \text{ i.e. } j = 1, \ldots, (p-1)(q-1)-1, \text{ step } 2 \\ 0, \text{for even } j, \text{ i.e. } j = 2, \ldots, (p-1)(q-1)-2, \text{ step } 2. \end{cases}$$

We may thus write the c.f. of W_1 as

$$\Phi_{W_1}(t) = \prod_{j=1}^{q-2} \lambda_{j1}^{r_{j1}} \left(\lambda_{j1} - \mathrm{i}t\right)^{-r_{j1}} = \prod_{j=0}^{\frac{q-1}{2}} \left(\frac{n-q}{2} + j\right)^{1} \left(\frac{n-q}{2} + j - \mathrm{i}t\right)^{-1} \tag{33}$$

and the c.f. of W_2 as

$$\begin{aligned} \Phi_{W_2}(t) &= \prod_{j=1}^{(p-1)(q-1)-2} \lambda_{j2}^{r_{j2}} \left(\lambda_{j2} - \mathrm{i}t\right)^{-r_{j2}} \\ &= \prod_{j=1}^{(p-1)(q-1)/2} \left(\frac{n-q}{2} + \frac{j-1}{p-1}\right)^{1} \left(\frac{n-q}{2} + \frac{j-1}{p-1} - \mathrm{i}t\right)^{-1}, \end{aligned}$$

while Λ_3 and W_3 vanish. This gives for W a c.f. which is

$$\Phi_W(t) = \Phi_{W_1}(t)\,\Phi_{W_2}(t) = \prod_{j=1}^{(p-1)(q-1)/2} \lambda_j^{r_j}\,(\lambda_j - \mathrm{i}t)^{-r_j} \tag{34}$$

for λ_j in (29) and r_j in (30), which is exactly the c.f. on page 24 of Coelho (2017), thus confirming that result as a particular case of the result in Theorem 2. In this reference there is a small typo on the second row of expression (13), where a j appears where there should be an ℓ.

For $r = 1$, $m = 1$ and $v = p$, in Theorem 2,we have

$$c_1 = 1\,, \quad c_2 = 0 \quad \text{and} \quad c_3 = p - 1$$

so that we will have again the c.f. of W_1 given by (33) and W_3 with a similar distribution to that of W_2 for the case $r = 1$, $v = 1$ and $m = p$, while Λ_2 and W_2 vanish, this way giving again the c.f. of W as that in (34), confirming, also for this case, the result in Coelho (2017) as a particular case of the result in Theorem 2. □

3.2 The Case of Even q and Odd r

When q is even and r is odd there are indeed a number of sub-cases to consider. That is what we do in the next subsections. On our study of these cases we will need to obtain the c.f.'s of W_1, W_2, and W_3, for situations where the distributions of these statistics will not have a closed finite form representation, in a form suitable for the development of near-exact approximations.

In order to fulfill this aim we may use the results in Appendix A2 of Marques et al. (2011) concerning the statistic Λ_2 in that paper.

Using these results, we may write the c.f. of W_1, when r is odd and q is even, the c.f. of W_2 when r is odd, q is even and m is also even or the c.f. of W_3 when r is odd, q is even, m is odd and v is even, as

$$\Phi_{W_k}(t) = \underbrace{\left\{ \prod_{j=1}^{r+c_k(q-1)-2} \lambda_{jk}^{r_{jk}} \left(\lambda_{jk} - \mathrm{i}t\right)^{-r_{jk}} \right\}}_{\Phi_{W_{k,1}}(t)} \times \underbrace{\frac{\Gamma\left(\frac{c_k(n-1)}{2}\right)\Gamma\left(\frac{c_k(n-1)-1}{2} - c_k\mathrm{i}t\right)}{\Gamma\left(\frac{c_k(n-1)-1}{2}\right)\Gamma\left(\frac{c_k(n-1)}{2} - c_k\mathrm{i}t\right)}}_{\Phi_{W_{k,2}}(t)} \tag{35}$$

now with

$$r_{jk} = \begin{cases} h_{jk} + (-1)^j\,, & j = 1, 2 \\ h_{jk} + r_{j-2,k}\,, & j = 3, \ldots, r + c_k(q-1) - 2 \end{cases} \tag{36}$$

for h_{jk} still given by (22), and thus yielding $r_{1k} = 0$ and $r_{2k} = 2$ ($k = 1, \ldots, 3$), and λ_{jk} and c_k, respectively, given by (19) and (20).

In all other cases the c.f.'s of W_1, W_2, and W_3 will be given by (28), with λ_{jk} and r_{jk} respectively given by (19) and (21)–(22).

3.2.1 The Case of Even q, Odd r, Odd m, and Odd v

We should note that in this case we still have the exact distribution of Λ_2 and Λ_3, and as such also that of W_2 and W_3, given by Theorem 3.2 in Coelho and Arnold (2019), for $m^* = 1$ and k_1, n_1, m_1, and a_1 given by (25).

Then we have the following Theorem, which gives near-exact distributions for Λ when q is even, r is odd and m and v are also both odd.

Theorem 3 *For even q and odd r, m and v, near-exact distributions for Λ will have p.d.f.'s and c.d.f.'s respectively of the form*

$$f_\Lambda(z) = \sum_{\ell=0}^{v} \pi_\ell\, f^{GNIG}\Big(-\log z \,\Big|\, \overset{\approx}{\{r_{jk}\}}, \overset{\approx}{\frac{1}{2}+2\ell}; \widetilde{\{\lambda_{jk}\}}, \frac{n-2}{2} - \frac{1}{4}; \#\widetilde{\{\lambda_{jk}\}}+1\Big)\,\frac{1}{z} \tag{37}$$

and

$$F_\Lambda(z) = \sum_{\ell=0}^{v} \pi_\ell \left(1 - F^{GNIG}\Big(-\log z \,\Big|\, \overset{\approx}{\{r_{jk}\}}, \overset{\approx}{\frac{1}{2}+2\ell}; \widetilde{\{\lambda_{jk}\}}, \frac{n-2}{2} - \frac{1}{4}; \#\widetilde{\{\lambda_{jk}\}}+1\Big)\right), \tag{38}$$

for $0 < z < 1$, where f^{GNIG} and F^{GNIG} stand respectively for the p.d.f. and c.d.f. of the GNIG distribution (Coelho 2004), using the notation in Appendix 2, and where λ_{jk} are given by (19) and r_{jk} are given by (36) and (22) for $k = 1$ and by (21)–(22) for $k = 2, 3$, and where the notations $\widetilde{\{\lambda_{jk}\}}$ and $\overset{\approx}{\{r_{jk}\}}$ are the same as the ones used in Theorem 2.

Proof Given the remark right before the statement of this Theorem, on the distributions of W_2 and W_3, in order to build a near-exact distribution for Λ we will use, for even q, odd r, and odd m and v, the c.f. of W_1 given by (35) and those of W_2 and W_3 given by (28) and write

$$\Phi_W(t) = \underbrace{\Phi_{W_1,1}(t)\,\Phi_{W_2}(t)\,\Phi_{W_3}(t)}_{\Phi_1(t)}\,\underbrace{\Phi_{W_1,2}(t)}_{\Phi_2(t)}, \tag{39}$$

where we will keep untouched $\Phi_1(t)$ and will approximate asymptotically $\Phi_2(t)$, in such a way that the c.f. that will work as its asymptotic replacement may then be "joined" back together with $\Phi_1(t)$ to produce the c.f. of a manageable distribution. Since $\Phi_2(t)$ is the c.f. of a single $Logbeta\left(\frac{n-2}{2}, \frac{1}{2}\right)$ r.v., we will use the approach in Sect. 3.3 in Coelho and Alberto (2021) and we will replace $\Phi_2(t)$ in (39) by

$$\widetilde{\Phi}_2(t) = \sum_{\ell=0}^{\nu} \pi_k \left(\frac{n-2}{2} - \frac{1}{4}\right)^{\frac{1}{2}+2\ell} \left(\frac{n-2}{2} - \frac{1}{4} - \mathrm{i}t\right)^{-\left(\frac{1}{2}+2\ell\right)} \tag{40}$$

which is the c.f. of a finite mixture with $\nu+1$ components which are Gamma distributions, all with the same rate parameter $\frac{n-2}{2} - \frac{1}{4}$ and shape parameters $\frac{1}{2} + 2\ell$ ($\ell = 0, \ldots, \nu$), whose weights π_ℓ for $\ell = 0, \ldots, \nu - 1$ will be obtained through the numerical solution of the linear system of ν equations

$$\left.\frac{\partial^\ell}{\partial t^\ell} \Phi_2(t)\right|_{t=0} = \left.\frac{\partial^\ell}{\partial t^\ell} \widetilde{\Phi}_2(t)\right|_{t=0}, \quad \ell = 1, \ldots, \nu\,,$$

with $\pi_\nu = 1 - \sum_{\ell=0}^{\nu-1} \pi_\ell$.

This approach will lead to near-exact distributions that match the first ν exact moments of $W = -\log \Lambda$ and yields for this r.v. the near-exact c.f.

$$\widetilde{\Phi}_W(t) = \Phi_1(t)\, \widetilde{\Phi}_2(t) = \sum_{\ell=0}^{\nu} \pi_k\, \Phi_1(t) \left(\frac{n-2}{2} - \frac{1}{4}\right)^{\frac{1}{2}+2\ell} \left(\frac{n-2}{2} - \frac{1}{4} - \mathrm{i}t\right)^{-\left(\frac{1}{2}+2\ell\right)}$$

with $\Phi_1(t)$ given by (39) and $\widetilde{\Phi}_2(t)$ by (40), which gives as near-exact distributions for W a mixture of $\nu+1$ GNIG (Generalized Near-Integer Gamma) distributions (Coelho 2004) with integer shape parameters r_{jk} ($k = 1, \ldots, 3$; $j = 1, \ldots, r + c_k(q-1) - 2$), given by (21) and (22) for $k = 3$ and by (36) and (22) for $k = 1$, and non-integer shape parameter $\frac{1}{2} + 2\ell$ ($\ell = 0, \ldots, \nu$) and corresponding rate parameters λ_{jk} ($k = 1, \ldots, 3$; $j = 1, \ldots, r + c_k(q-1) - 2$), given by (19), and $\frac{n-2}{2} - \frac{1}{4}$.

This yields near-exact distributions for W with p.d.f.'s given by

$$f_W(w) = \sum_{\ell=0}^{\nu} \pi_\ell\, f^{GNIG}\left(w \,\middle|\, \overset{\approx}{\{r_{jk}\}}, \frac{1}{2} + 2\ell; \widetilde{\{\lambda_{jk}\}}, \frac{n-2}{2} - \frac{1}{4}; \#\widetilde{\{\lambda_{jk}\}} + 1\right)$$

and c.d.f.'s given by

$$F_W(w) = \sum_{\ell=0}^{\nu} \pi_\ell\, F^{GNIG}\left(w \,\middle|\, \overset{\approx}{\{r_{jk}\}}, \frac{1}{2} + 2\ell; \widetilde{\{\lambda_{jk}\}}, \frac{n-2}{2} - \frac{1}{4}; \#\widetilde{\{\lambda_{jk}\}} + 1\right)$$

for $w > 0$, and where we use for the GNIG p.d.f. and c.d.f. the notation in Appendix 2.

The corresponding near-exact distributions for Λ may then be easily obtained through the transformation $\Lambda = e^{-W}$ and these have p.d.f.'s and c.d.f.'s given by (37) and (38). □

These near-exact distributions will be asymptotic not only for increasing sample sizes but also for increasing values of all other parameters in the distribution of Λ and W, that is, for r, q, m, and v, as it is shown by the values in Tables 1 and 2, where are displayed values of the measure

$$\Delta = \int_{-\infty}^{+\infty} \left| \frac{\Phi_W(t) - \widetilde{\Phi}_W(t)}{t} \right| dt \,. \tag{41}$$

This measure gives a very sharp upper-bound on the absolute value of the difference between the exact and the near-exact c.d.f.'s of W or Λ, with

$$\Delta \geq \max_{w>0} \left| F_W(w) - \widetilde{F}_W(w) \right| = \max_{0<z<1} \left| F_\Lambda(z) - \widetilde{F}_\Lambda(z) \right| ,$$

where $F_W(\cdot)$ and $\widetilde{F}_W(\cdot)$ represent, respectively, the exact and the near-exact c.d.f.'s of W, and $F_\Lambda(\cdot)$ and $\widetilde{F}_\Lambda(\cdot)$ represent, respectively, the exact and near-exact c.d.f.'s of Λ.

As we may see from the values of the measure Δ in Tables 1 and 2, the near-exact distributions exhibit very low values of Δ, showing their great closeness to the exact distribution, even for extremely small sample sizes, as it is the case of the sample sizes of $n = q + r$, which are the smallest possible ones, and even for the smaller values of v, the number of exact moments of W matched by the near-exact distributions. The values in these Tables also show the asymptotic behavior of these near-exact distributions for increasing values of all other parameters, q, r, m and v, with a more marked asymptotic trend for larger values of v, that is, with a more accentuated decrease in the values of Δ for the near-exact distributions that match more of the exact moments of W.

Although it is possible to obtain different forms of analytical upper bounds on $\max_{\{w>0\}} |F_W(w) - \widetilde{F}_W(w)|$ or $\max_{\{0<z<1\}} |F_\Lambda(z) - \widetilde{F}_\Lambda(z)|$, the ones obtained so far are not sharp enough. Given the fact that the measure Δ in (41) gives a really sharp upper-bound on these quantities, the analysis of the values of this measure in Tables 1 and 2, for different values of the parameters in the distribution, gives a much better idea of the asymptotic characteristics of the near-exact distributions obtained and their closeness to the exact distribution.

For $r = 1$, $m = 1$ and $v = p$, the near-exact distributions in Theorem 3 may be used as near-exact distributions for the statistic studied in Coelho (2017), for even q and odd p, exhibiting some advantages, in terms of closeness to the exact distribution, over the near-exact distributions developed in Sect. 5.2 of that reference.

Table 1 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r, odd m, and odd v, for increasing values of q and r and sample sizes of $r + q + \{0, 100, 200, 500\}$

n	r	q	m	v	ν (number of exact moments matched)			
					2	4	6	10
7	3	4	5	7	5.58×10^{-9}	6.28×10^{-12}	3.25×10^{-14}	9.35×10^{-18}
107					9.83×10^{-17}	1.79×10^{-24}	3.03×10^{-31}	5.52×10^{-43}
207					1.76×10^{-18}	2.20×10^{-27}	2.55×10^{-35}	2.23×10^{-49}
507					7.81×10^{-21}	2.64×10^{-31}	8.31×10^{-41}	5.35×10^{-58}
13	9	4	5	7	9.98×10^{-12}	3.20×10^{-16}	7.32×10^{-20}	1.03×10^{-25}
113					1.37×10^{-17}	6.87×10^{-26}	3.26×10^{-33}	4.97×10^{-46}
213					2.88×10^{-19}	1.11×10^{-28}	4.03×10^{-37}	3.66×10^{-52}
513					1.42×10^{-21}	1.58×10^{-32}	1.68×10^{-42}	1.29×10^{-60}
23	19	4	5	7	5.11×10^{-14}	6.12×10^{-20}	6.52×10^{-25}	3.67×10^{-33}
123					2.63×10^{-18}	4.45×10^{-27}	7.15×10^{-35}	1.27×10^{-48}
223					7.10×10^{-20}	1.08×10^{-29}	1.57×10^{-38}	2.29×10^{-54}
523					4.13×10^{-22}	2.04×10^{-33}	9.57×10^{-44}	1.48×10^{-62}
29	19	10	5	7	1.81×10^{-15}	2.32×10^{-22}	2.71×10^{-28}	2.04×10^{-38}
129					3.53×10^{-19}	1.57×10^{-28}	6.65×10^{-37}	8.32×10^{-52}
229					1.12×10^{-20}	4.99×10^{-31}	2.13×10^{-40}	2.72×10^{-57}
529					7.32×10^{-23}	1.14×10^{-34}	1.71×10^{-45}	2.68×10^{-65}
39	19	20	5	7	5.93×10^{-17}	7.93×10^{-25}	9.87×10^{-32}	9.41×10^{-44}
139					6.51×10^{-20}	9.38×10^{-30}	1.29×10^{-38}	1.71×10^{-54}
239					2.64×10^{-21}	4.50×10^{-32}	7.35×10^{-42}	1.38×10^{-59}
539					2.07×10^{-23}	1.40×10^{-35}	9.02×10^{-47}	2.65×10^{-67}

Table 2 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r, odd m, and odd v, for increasing values of m and v and sample sizes of $r + q + \{0, 100, 200, 500\}$

n	r	q	m	v	ν (number of exact moments matched)			
					2	4	6	10
39	19	20	5	7	5.93×10^{-17}	7.93×10^{-25}	9.87×10^{-32}	9.41×10^{-44}
139					6.51×10^{-20}	9.38×10^{-30}	1.29×10^{-38}	1.71×10^{-54}
239					2.64×10^{-21}	4.50×10^{-32}	7.35×10^{-42}	1.38×10^{-59}
539					2.07×10^{-23}	1.40×10^{-35}	9.02×10^{-47}	2.65×10^{-67}
39	19	20	15	7	1.45×10^{-17}	7.50×10^{-26}	3.59×10^{-33}	4.99×10^{-46}
139					1.27×10^{-20}	6.17×10^{-31}	2.86×10^{-40}	4.31×10^{-57}
239					5.13×10^{-22}	2.93×10^{-33}	1.61×10^{-43}	3.40×10^{-62}
539					4.01×10^{-24}	9.02×10^{-37}	1.95×10^{-48}	6.43×10^{-70}
39	19	20	25	7	7.11×10^{-18}	2.29×10^{-26}	6.79×10^{-34}	3.62×10^{-47}
139					5.93×10^{-21}	1.73×10^{-31}	4.82×10^{-41}	2.63×10^{-58}
239					2.39×10^{-22}	8.19×10^{-34}	2.70×10^{-44}	2.06×10^{-63}
539					1.86×10^{-24}	2.52×10^{-37}	3.27×10^{-49}	3.89×10^{-71}
39	19	20	25	17	1.98×10^{-18}	2.70×10^{-27}	3.41×10^{-35}	3.28×10^{-49}
139					1.57×10^{-21}	1.89×10^{-32}	2.17×10^{-42}	2.02×10^{-60}
239					6.32×10^{-23}	8.94×10^{-35}	1.21×10^{-45}	1.57×10^{-65}
539					4.93×10^{-25}	2.74×10^{-38}	1.47×10^{-50}	2.96×10^{-73}
39	19	20	25	27	1.00×10^{-18}	8.69×10^{-28}	6.97×10^{-36}	2.70×10^{-50}
139					7.85×10^{-22}	5.95×10^{-33}	4.31×10^{-43}	1.59×10^{-61}
239					3.16×10^{-23}	2.81×10^{-35}	2.40×10^{-46}	1.24×10^{-66}
539					2.46×10^{-25}	8.63×10^{-39}	2.90×10^{-51}	2.33×10^{-74}

3.2.2 The Case of Even q, Odd r, Odd m and Even v

In this case we still have the exact distribution of Λ_2 and W_2 given by Theorem 3.2 in Coelho and Arnold (2019), for $m^* = 1$ and k_1, n_1, m_1 and a_1 given by (25), while for W_1 and W_3 we will have to take their c.f.'s given by (35), with c_k given by (20) for $k = 1$ and $k = 3$.

We then have the following Theorem, which gives near-exact distributions for Λ when q is even, r and m are odd and v is even.

Theorem 4 *For even q and odd r and m and even v, near-exact distributions for Λ will have p.d.f.'s and c.d.f.'s respectively of the form*

$$f_\Lambda(z) = \sum_{\ell=0}^{v} \pi_\ell \, f^{EGIG}\left(z \,\middle|\, \overset{\approx}{\{r_{jk}\}}, 1+\ell; \widetilde{\{\lambda_{jk}\}}, \lambda; \#\widetilde{\{\lambda_{jk}\}}+1\right) \tag{42}$$

and

$$F_\Lambda(z) = \sum_{\ell=0}^{v} \pi_\ell \, F^{EGIG}\left(z \,\middle|\, \overset{\approx}{\{r_{jk}\}}, 1+\ell; \widetilde{\{\lambda_{jk}\}}, \lambda; \#\widetilde{\{\lambda_{jk}\}}+1\right), \tag{43}$$

for $0 < z < 1$, where f^{EGIG} and F^{EGIG} stand, respectively, for the p.d.f. and c.d.f. of the EGIG distribution, using the notation in Appendix 2, and where λ_{jk} are given by (19) and r_{jk} are given by (36) and (22) for $k = 1, 3$ and by (21)–(22) for $k = 2$, and λ is obtained from the numerical solution of the system of equations (46), and where the notations $\widetilde{\{\lambda_{jk}\}}$ and $\overset{\approx}{\{r_{jk}\}}$ are the same as the ones used in Theorem 2.

Proof Given the remark at the beginning of the present subsection, in order to build near-exact distributions for Λ and $W = -\log \Lambda$, for the case of even q, odd r and m and even v, we will take $\Phi_{W_2}(t)$ given by (28) and $\Phi_{W_1}(t)$ and $\Phi_{W_3}(t)$ given by (35), and write

$$\Phi_W(t) = \underbrace{\Phi_{W_1,1}(t)\, \Phi_{W_2}(t)\, \Phi_{W_3,1}(t)}_{\Phi_1(t)} \, \underbrace{\Phi_{W_1,2}(t)\, \Phi_{W_3,2}(t)}_{\Phi_2(t)}, \tag{44}$$

where, as we did in the previous subsection, we will keep $\Phi_1(t)$ unchanged and will approximate asymptotically $\Phi_2(t)$. We may note that in this case $\Phi_2(t)$ is the c.f. of the sum of two independent Logbeta r.v.'s, one with parameters $\frac{n-2}{2}$ and $\frac{1}{2}$ and the other with parameters $\frac{(v-1)m(n-1)-1}{2}$ and $\frac{1}{2}$, this last one multiplied by $(v-1)m$. As such, we will replace $\Phi_2(t)$ by

$$\widetilde{\Phi}_2(t) = \sum_{\ell=0}^{v} \pi_\ell \, \lambda^{1+\ell} (\lambda - \mathrm{i}t)^{-(1+\ell)}, \tag{45}$$

where the parameter λ is obtained as the rate parameter in a mixture of two Gamma distributions.

This approximation is based on a somewhat heuristic approach, which was already used in similar situations where it proved to be extremely effective (Coelho et al. 2010, 2015; Coelho and Marques 2013; Coelho and Roy 2020) and which is based on the fact that from the results in Sect. 5 of Tricomi and Erdélyi (1951) we may asymptotically approximate a $Logbeta(a, b)$ distribution by a mixture of $\Gamma(b + k, a)$ $(k = 0, 1, \dots)$ distributions. The parameter λ in (45) is itself obtained through the numerical solution of the system of four equations

$$\left.\frac{\partial^\ell}{\partial t^\ell}\,\Phi_2(t)\right|_{t=0} = \left.\frac{\partial^\ell}{\partial t^\ell}\,\Phi^*(t)\right|_{t=0}, \quad \ell = 1, \dots, 4\,, \tag{46}$$

where

$$\Phi^*(t) = \theta\,\lambda^{s_1}(\lambda - \mathrm{i}t)^{-s_1} + (1-\theta)\lambda^{s_2}(\lambda - \mathrm{i}t)^{-s_2}$$

is the c.f. of a mixture of two Gamma distributions, both with the same rate parameter λ. The weights π_ℓ $(\ell = 0, \dots, \nu)$ are obtained in a similar manner to the one used in Sect. 3.2.1, where now $\widetilde{\Phi}_2(t)$ is given by (45) and where the 1 in $1 + \ell$ comes exactly from the sum of the second parameters of the Logbeta r.v.'s in $\Phi_2(t)$.

This way we obtain, for $\Phi_1(t)$ in (44), as near-exact c.f. for W

$$\widetilde{\Phi}_W(t) = \Phi_1(t)\,\widetilde{\Phi}_2(t) = \sum_{\ell=0}^{\nu} \pi_\ell\,\Phi_1(t)\,\lambda^{1+\ell}(\lambda - \mathrm{i}t)^{-(1+\ell)} \tag{47}$$

which is the c.f. of a mixture of GIG distributions with integer shape parameters r_{jk} $(k = 1, \dots, 3;\ j = 1, \dots, r + c_k(q-1) - 2)$, given by (21) and (22) for $k = 2$ and by (36) and (22) for $k = 2, 3$, and $1 + \ell$ $(\ell = 0, \dots, \nu)$ and rate parameters λ_{jk}, given by (19), and λ.

The corresponding near-exact p.d.f.'s and c.d.f.'s for W are given by (using the notation in Appendix 2)

$$f_W(w) = \sum_{\ell=0}^{\nu} \pi_\ell\, f^{GIG}\left(w \,\middle|\, \widetilde{\{r_{jk}\}}, 1+\ell; \widetilde{\{\lambda_{jk}\}}, \lambda; \#\widetilde{\{\lambda_{jk}\}} + 1\right)$$

and c.d.f.'s given by

$$F_W(w) = \sum_{\ell=0}^{\nu} \pi_\ell\, F^{GIG}\left(w \,\middle|\, \widetilde{\{r_{jk}\}}, 1+\ell; \widetilde{\{\lambda_{jk}\}}, \lambda; \#\widetilde{\{\lambda_{jk}\}} + 1\right)$$

for $w > 0$.

The corresponding near-exact distributions for Λ, may then, once again, be easily obtained through the transformation $\Lambda = e^{-W}$ and will have p.d.f.'s and c.d.f.'s given by (42) and (43), respectively. □

Given the fact that these near-exact distributions are based on the approximation of the distribution of a sum of two independent Logbeta r.v.'s and not on the approximation of the distribution of a single Logbeta r.v., as it happened in the previous subsection, they will yield larger values of the measure Δ in (41) than those near-exact distributions, anyway still showing very low values of this measure, mainly when four or more of the exact moments of W are matched by these distributions, thus showing also for this case an extreme closeness to the exact distribution. Values of the measure Δ for these near-exact distributions are shown in Tables 3 and 4.

From these values we can see that once again these near-exact distributions display a very good performance even for extremely small sample sizes and an asymptotic behavior not only for increasing sample sizes but also for increasing values of all the other parameters in the distributions of Λ and W, once again with this asymptotic character being more accentuated for larger values of ν, the number exact moments of W matched by these near-exact distributions.

For $r = 1$, $m = 1$ and $v = p$, the near-exact distributions in Theorem 4 may be used as near-exact distributions for the statistic studied in Coelho (2017), yielding equivalent near-exact distributions to the ones obtained in Sect. 5.1 of that reference.

3.2.3 The Case of Even q, Odd r and Even m

In this case we have the exact distribution of Λ_3 and W_3 given by Theorem 3.2 in Coelho and Arnold (2019), for $m^* = 1$ and k_1, n_1, m_1, and a_1 given by (25), while for W_1 and W_2 we will have to take their c.f.'s given by (35), with c_k given by (20) for $k = 1$ and $k = 2$. Hence we have the following Theorem.

Theorem 5 *For even q, odd r and even m we have near-exact distributions for Λ with p.d.f.'s and c.d.f.'s similar to the ones in (42) and (43), now with r_{jk} given by (21) for $k = 3$ and by (36) for $k = 1, 2$.*

Proof For even q, odd r and even m, in order to build near-exact distributions for Λ and $W = -\log \Lambda$ we will follow an approach in all similar to the one taken in the previous subsection, taking into account the remark at the beginning of this subsection and thus taking $\Phi_{W_3}(t)$ given by (28) and $\Phi_{W_1}(t)$ and $\Phi_{W_2}(t)$ given by (35) and writing

$$\Phi_W(t) = \underbrace{\Phi_{W_1,1}(t)\,\Phi_{W_2,1}(t)\,\Phi_{W_3}(t)}_{\Phi_1(t)}\ \underbrace{\Phi_{W_1,2}(t)\,\Phi_{W_2,2}(t)}_{\Phi_2(t)}\,, \tag{48}$$

Table 3 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r, odd m, and even v, for increasing values of q and r and sample sizes of $r + q + \{0, 100, 200, 500\}$

n	r	q	m	v	v (number of exact moments matched)			
					2	4	6	10
7	3	4	5	8	2.63×10^{-8}	9.29×10^{-13}	1.24×10^{-15}	2.49×10^{-21}
107					1.24×10^{-11}	5.32×10^{-19}	6.49×10^{-23}	4.87×10^{-32}
207					1.70×10^{-12}	5.96×10^{-21}	5.94×10^{-25}	3.04×10^{-35}
507					1.15×10^{-13}	3.10×10^{-23}	1.07×10^{-27}	1.44×10^{-39}
13	9	4	5	8	8.85×10^{-10}	5.43×10^{-15}	1.44×10^{-18}	2.58×10^{-25}
113					2.01×10^{-12}	2.41×10^{-20}	9.55×10^{-25}	6.70×10^{-35}
213					3.00×10^{-13}	3.13×10^{-22}	1.06×10^{-26}	5.66×10^{-38}
513					2.14×10^{-14}	1.93×10^{-24}	2.16×10^{-29}	3.26×10^{-42}
23	19	4	5	8	4.17×10^{-11}	2.39×10^{-17}	1.61×10^{-21}	2.71×10^{-30}
123					5.03×10^{-13}	2.12×10^{-21}	3.76×10^{-26}	4.20×10^{-37}
223					8.48×10^{-14}	3.39×10^{-23}	5.59×10^{-28}	5.60×10^{-40}
523					6.58×10^{-15}	2.81×10^{-25}	1.38×10^{-30}	4.39×10^{-44}
29	19	10	5	8	3.30×10^{-12}	2.74×10^{-19}	3.93×10^{-24}	3.68×10^{-34}
129					7.80×10^{-14}	8.84×10^{-23}	4.85×10^{-28}	4.54×10^{-40}
229					1.45×10^{-14}	1.65×10^{-24}	9.07×10^{-30}	8.65×10^{-43}
529					1.20×10^{-15}	1.69×10^{-26}	2.64×10^{-32}	8.75×10^{-47}
39	19	20	5	8	2.95×10^{-13}	3.61×10^{-21}	1.32×10^{-26}	6.54×10^{-38}
139					1.81×10^{-14}	6.88×10^{-24}	1.60×10^{-29}	2.13×10^{-42}
239					3.89×10^{-15}	1.63×10^{-25}	4.22×10^{-31}	6.97×10^{-45}
539					3.61×10^{-16}	2.36×10^{-27}	1.59×10^{-33}	1.06×10^{-48}

Table 4 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r, odd m and even v, for increasing values of m and v and sample sizes of $r+q+\{0, 100, 200, 500\}$

n	r	q	m	v	v (number of exact moments matched)			
					2	4	6	10
39	19	20	5	8	2.95×10^{-13}	3.61×10^{-21}	1.32×10^{-26}	6.54×10^{-38}
139					1.81×10^{-14}	6.88×10^{-24}	1.60×10^{-29}	2.13×10^{-42}
239					3.89×10^{-15}	1.63×10^{-25}	4.22×10^{-31}	6.97×10^{-45}
539					3.61×10^{-16}	2.36×10^{-27}	1.59×10^{-33}	1.06×10^{-48}
39	19	20	15	8	7.13×10^{-14}	1.68×10^{-22}	4.51×10^{-28}	3.22×10^{-40}
139					3.60×10^{-15}	7.41×10^{-25}	3.46×10^{-31}	5.17×10^{-45}
239					7.68×10^{-16}	8.14×10^{-26}	9.01×10^{-33}	1.65×10^{-47}
539					7.10×10^{-17}	1.91×10^{-27}	3.35×10^{-35}	2.45×10^{-51}
39	19	20	25	8	3.49×10^{-14}	4.09×10^{-23}	8.41×10^{-29}	2.29×10^{-41}
139					1.68×10^{-15}	2.76×10^{-25}	5.81×10^{-32}	3.13×10^{-46}
239					3.59×10^{-16}	2.80×10^{-26}	1.51×10^{-33}	9.93×10^{-49}
539					3.31×10^{-17}	6.33×10^{-28}	5.60×10^{-36}	1.47×10^{-52}
39	19	20	25	18	1.08×10^{-14}	4.53×10^{-24}	5.40×10^{-30}	3.08×10^{-43}
139					5.01×10^{-16}	4.45×10^{-26}	3.41×10^{-33}	3.63×10^{-48}
239					1.07×10^{-16}	4.31×10^{-27}	8.82×10^{-35}	1.15×10^{-50}
539					9.86×10^{-18}	9.51×10^{-29}	3.27×10^{-37}	1.69×10^{-54}
39	19	20	25	28	5.64×10^{-15}	1.42×10^{-24}	1.18×10^{-30}	2.83×10^{-44}
139					2.58×10^{-16}	1.54×10^{-26}	7.26×10^{-34}	3.20×10^{-49}
239					5.51×10^{-17}	1.48×10^{-27}	1.88×10^{-35}	1.01×10^{-51}
539					5.09×10^{-18}	3.25×10^{-29}	6.96×10^{-38}	1.48×10^{-55}

where, as we did in the previous subsections, we will once again keep $\Phi_1(t)$ unchanged and will approximate asymptotically $\Phi_2(t)$. As we said, we will take an approach in all similar to the one taken in the previous subsection. In the present case $\Phi_2(t)$ is the c.f. of the sum of two independent Logbeta r.v.'s, one with parameters $\frac{n-2}{2}$ and $\frac{1}{2}$ and the other with parameters $\frac{(m-1)(n-1)-1}{2}$ and $\frac{1}{2}$, this last one multiplied by $(m-1)$.

So, following the same approach as we did in the previous subsection, we will replace $\Phi_2(t)$ by $\widetilde{\Phi}_2(t)$, with a similar structure to the one in (45) and with λ obtained in a similar manner to the one described in Sect. 3.2.2, and where the 1 in $1+\ell$ comes once again from the sum of the second parameters of the Logbeta r.v.'s in $\Phi_2(t)$.

The weights π_ℓ $(\ell = 0, \ldots, \nu)$ are obtained in a similar manner to the one used in Sects. 3.2.1 and 3.2.2, and in this way we obtain, for $\Phi_1(t)$ in (48), as near-exact c.f. for W a c.f. with a similar expression to the one in (47), which is, as in the previous subsection, the c.f. of a mixture of GIG distributions with integer shape parameters r_{jk} $(k = 1, \ldots, 3;\ j = 1, \ldots, r + c_k(q-1) - 2)$, but now given by (21) and (22) for $k = 3$ and by (36) and (22) for $k = 1, 2$, and $1 + \ell$ $(\ell = 0, \ldots, \nu)$, and rate parameters λ_{jk}, given by (19), and λ, which now, although being computed in a somewhat similar manner, will have different values than the ones obtained in the previous subsection.

The corresponding near-exact p.d.f.'s and c.d.f.'s for W and Λ will have similar expressions to the ones in the previous subsection, now with the differences in the parameters pointed out above. □

In Tables 5 and 6 we may analyze the values of the measure Δ in (41) for these near-exact distributions. We may how generally they have quite similar values to the ones in Tables 3 and 4 for the near-exact distributions in the previous subsection, which was indeed expected, given the similitude in structure and building approach between the near-exact distributions obtained in the present subsection and the ones obtained in the previous subsection. Once again, these near-exact distributions show their asymptotic character not only for increasing sample sizes but also for increasing values of all other parameters, that is, for increasing values of the overall number of variables involved in the test, at the same time that they keep showing very good performances even for very small sample sizes.

For $r = 1$, $v = 1$ and $m = p$, the near-exact distributions in Theorem 5 will yield for the statistic studied in Coelho (2017), similar near-exact distributions to the ones obtained for this statistic from the results in Theorem 4, and thus also similar to the ones developed in Sect. 5.1 of that reference, for even q and even p.

Table 5 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r and even m, for increasing values of q and r and sample sizes of $r + q + \{0, 100, 200, 500\}$

n	r	q	m	v	ν (number of exact moments matched)			
					2	4	6	10
7	3	4	6	8	2.03×10^{-8}	1.09×10^{-12}	2.32×10^{-15}	1.02×10^{-20}
107					7.57×10^{-12}	4.51×10^{-18}	3.82×10^{-23}	2.00×10^{-32}
207					1.03×10^{-12}	1.59×10^{-19}	3.59×10^{-25}	1.33×10^{-35}
507					6.96×10^{-14}	1.75×10^{-21}	6.54×10^{-28}	6.63×10^{-40}
13	9	4	6	8	6.47×10^{-10}	7.60×10^{-15}	5.35×10^{-19}	1.74×10^{-25}
113					1.23×10^{-12}	2.20×10^{-19}	5.63×10^{-25}	2.73×10^{-35}
213					1.82×10^{-13}	8.90×10^{-21}	6.39×10^{-27}	2.46×10^{-38}
513					1.29×10^{-14}	1.07×10^{-22}	1.32×10^{-29}	1.48×10^{-42}
23	19	4	6	8	2.95×10^{-11}	4.97×10^{-17}	9.33×10^{-22}	4.47×10^{-32}
123					3.08×10^{-13}	2.18×10^{-20}	2.23×10^{-26}	1.74×10^{-37}
223					5.15×10^{-14}	1.09×10^{-21}	3.37×10^{-28}	2.44×10^{-40}
523					3.98×10^{-15}	1.50×10^{-23}	8.45×10^{-31}	1.99×10^{-44}
29	19	10	6	8	2.25×10^{-12}	6.58×10^{-19}	2.31×10^{-24}	9.77×10^{-35}
129					4.77×10^{-14}	9.75×10^{-22}	2.88×10^{-28}	1.88×10^{-40}
229					8.79×10^{-15}	5.71×10^{-23}	5.47×10^{-30}	3.77×10^{-43}
529					7.27×10^{-16}	8.84×10^{-25}	1.61×10^{-32}	3.97×10^{-47}
39	19	20	6	8	1.95×10^{-13}	1.10×10^{-20}	7.92×10^{-27}	2.34×10^{-38}
139					1.11×10^{-14}	8.51×10^{-23}	9.50×10^{-30}	8.89×10^{-43}
239					2.36×10^{-15}	6.38×10^{-24}	2.54×10^{-31}	3.04×10^{-45}
539					2.18×10^{-16}	1.19×10^{-25}	9.67×10^{-34}	4.79×10^{-49}

Table 6 Values of Δ for near-exact distributions of Λ or W for the case of even q, odd r and even m, for increasing values of m and v and sample sizes of $r + q + \{0, 100, 200, 500\}$

n	r	q	m	v	v (number of exact moments matched)			
					2	4	6	10
39	19	20	6	8	1.95×10^{-13}	1.10×10^{-20}	7.92×10^{-27}	2.34×10^{-38}
139					1.11×10^{-14}	8.51×10^{-23}	9.50×10^{-30}	8.89×10^{-43}
239					2.36×10^{-15}	6.38×10^{-24}	2.54×10^{-31}	3.04×10^{-45}
539					2.18×10^{-16}	1.19×10^{-25}	9.67×10^{-34}	4.79×10^{-49}
39	19	20	16	8	6.23×10^{-14}	5.43×10^{-22}	3.72×10^{-28}	2.25×10^{-40}
139					3.08×10^{-15}	2.29×10^{-24}	2.89×10^{-31}	3.88×10^{-45}
239					6.56×10^{-16}	1.56×10^{-25}	7.57×10^{-33}	1.26×10^{-47}
539					6.05×10^{-17}	2.67×10^{-27}	2.83×10^{-35}	1.90×10^{-51}
39	19	20	26	8	3.21×10^{-14}	1.16×10^{-22}	7.46×10^{-29}	1.84×10^{-41}
139					1.53×10^{-15}	2.90×10^{-25}	5.21×10^{-32}	2.63×10^{-46}
239					3.27×10^{-16}	1.62×10^{-26}	1.36×10^{-33}	8.45×10^{-49}
539					3.01×10^{-17}	2.19×10^{-28}	5.04×10^{-36}	1.26×10^{-52}
39	19	20	26	18	9.91×10^{-15}	1.63×10^{-23}	4.78×10^{-30}	2.45×10^{-43}
139					4.55×10^{-16}	3.83×10^{-26}	3.06×10^{-33}	3.07×10^{-48}
239					9.69×10^{-17}	2.14×10^{-27}	7.95×10^{-35}	9.81×10^{-51}
539					8.94×10^{-18}	2.89×10^{-29}	2.96×10^{-37}	1.46×10^{-54}
39	19	20	26	28	5.17×10^{-15}	5.51×10^{-24}	1.05×10^{-30}	2.25×10^{-44}
139					2.35×10^{-16}	1.27×10^{-26}	6.53×10^{-34}	2.71×10^{-49}
239					4.99×10^{-17}	7.09×10^{-28}	1.70×10^{-35}	8.65×10^{-52}
539					4.61×10^{-18}	9.58×10^{-30}	6.30×10^{-38}	1.29×10^{-55}

4 Conclusions and Discussion

The problem addressed seemed to pose a couple of interesting challenges. The first of these challenges was the question of the approach that had to be followed in order to be able to express the distribution of the LRT statistic in the form of that of a product of independent Beta distributed r.v.'s. Then, there was the question of the possible existence of several scenarios to be considered, in terms of different combinations of values of the five parameters in the distribution of the LRT statistic, and if for any of them it would be possible to obtain the distribution of the LRT in a closed finite and manageable form and yet if for the other cases, using the so-called near-exact distributions, it would be possible to build approximations that would be asymptotic for all five parameters involved in the distribution of Λ, while performing very well even for small samples.

The way around that was taken in trying to express the distribution of Λ in terms of that of a product of independent Beta r.v.'s, not taking an approach directly based on the expression for Λ in (4) but rather using a different approach by rewriting the determinants that appear in the numerator and denominator in that expression in terms of the diagonal blocks of another matrix which has a Wishart distribution with a block-diagonal parameter matrix, proved itself very effective. Indeed somewhat similar approaches had already proven effective in somewhat similar situations, but in our case the proof of the relation in (16) or (17) was quite a challenge.

Then, once the distribution of Λ was obtained in the form of that of a product of independent Beta distributed r.v.'s, Theorem 3.2 in Coelho and Arnold (2019) proved itself extremely useful in being able to very quickly and quite easily obtain the exact distribution of Λ_1, Λ_2 and Λ_3 and as such also of Λ in a closed finite and manageable form for the cases where q is odd or r is even.

It remained then the problem of building near-exact distributions for the remaining cases. A detailed check of these cases showed that there were indeed three sub-cases to be taken into account and which should be considered individually since this would allow for a more dedicated approach to each sub-case. This allowed us to see that in each of these three sub-cases there was always one or two of the partial statistics Λ_1, Λ_2 or Λ_3, for which we could obtain the exact distribution in a closed finite form, while for the other or others it was possible to obtain a decomposition of the c.f. of its or their logarithm which might lead to very sharp near-exact distributions. Typically these distributions, when properly built, are supposed to be asymptotic for increasing values of all the parameters involved in the exact distribution, but anyway this was a challenge for a distribution that has five parameters, four of which related with the number of variables in the analysis. Indeed, the approach followed proved effective in obtaining near-exact distributions that not only perform very well for very small samples, but which besides that are asymptotic not only for increasing sample sizes but also for increasing values of all other parameters, which are related with the overall number of variables involved in the testing procedure.

Given the ease of computation for the form of the exact distribution for the cases where q is odd or r is even, which are indeed the majority of the cases, and given the quite easy computability of the near-exact distributions obtained, the authors feel that the results in the present work may not only be useful for practical applications but also they may encourage the pursual of the obtention of similar results for situations that at first may seem very complicated or very challenging to approach, while the techniques used showed to be quite effective in addressing the problem and as such seem to be possible to be applied in a wide range of situations.

The results in Sect. 11 of Chap. 8 of Anderson (2003), namely the one in Theorem 8.11.3, together with the properties of the double exchangeable covariance matrix, namely the one that makes it part of a quadratic space, allow us to foresee that the present test statistic should have the same null distribution for elliptically contoured and left-spherical distributions.

Taking into account the particular cases of the double exchangeable covariance structure enumerated in the Introduction, for $r = 1$ and $m = 1$ or $v = 1$ we have the test of equality of mean vectors with compound-symmetric matrices, and for just $m = 1$ or $v = 1$, the test of equality of mean vectors for block compound-symmetric covariance matrices, while for $r = 1$ we have the same test for double complete symmetric covariance matrices.

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Appendix A: Proof of Expression (16)

For ease of exposition let us split the proof of (16) into the proof of three consecutive results. First let us prove the following result.

Result 1: The MLE of Σ under H_1, which is A^* into (8), may be equivalently written as

$$A^* = P_{vm} \otimes \widehat{\Psi}_{1|H_1} + Q_{vm} \otimes \widehat{\Psi}_{2|H_1} + R_{vm} \otimes \widehat{\Psi}_{3|H_1}, \tag{A.1}$$

where, from (7),

$$\begin{aligned} \widehat{\Psi}_{1|H_1} &= \widehat{U}_{|H_1} + (v-1)\widehat{V}_{|H_1} + v(m-1)\widehat{M}_{|H_1} \\ \widehat{\Psi}_{2|H_1} &= \widehat{U}_{|H_1} + (v-1)\widehat{V}_{H_1} - v\widehat{M}_{|H_1} \\ \widehat{\Psi}_{3|H_1} &= \widehat{U}_{|H_1} - \widehat{V}_{|H_1}\,, \end{aligned} \tag{A.2}$$

and

$$
\begin{aligned}
P_{vm} &= \frac{1}{mv} J_{vm} \\
Q_{vm} &= \frac{1}{v}(I_m \otimes J_v) - P_{vm} \\
R_{vm} &= I_{vm} - Q_{vm} - P_{vm}\,.
\end{aligned}
\tag{A.3}
$$

Proof The proof is easier if we start from (A.1) and try to end with (8), by using (A.2) and (A.3) to write

$$
\begin{aligned}
&P_{vm} \otimes \widehat{\Psi}_{1|H_1} + Q_{vm} \otimes \widehat{\Psi}_{2|H_1} + R_{vm} \otimes \widehat{\Psi}_{3|H_1} \\
&\quad = \frac{1}{mv} J_{vm} \otimes \left(\widehat{U}_{|H_1} + (v-1)\widehat{V}_{|H_1} + v(m-1)\widehat{M}_{|H_1}\right) \\
&\quad + \left(\frac{1}{v}(I_m \otimes J_v) - \frac{1}{mv} J_{vm}\right) \otimes \left(\widehat{U}_{|H_1} + (v-1)\widehat{V}_{|H_1} - v\widehat{M}_{|H_1}\right) \\
&\quad + \left(I_{vm} - \tfrac{1}{v}(I_m \otimes J_v) + P_{vm} - P_{vm}\right) \otimes (\widehat{U}_{|H_1} - \widehat{V}_{|H_1}) \\
&= \left(\frac{1}{mv} J_{vm} + \frac{1}{v}(I_m \otimes J_v) - \frac{1}{mv} J_{vm} + I_{vm} - \frac{1}{v}(I_m \otimes J_v)\right) \otimes \widehat{U}_{|H_1} \\
&\quad + \left(\frac{v-1}{mv} J_{vm} + \frac{v-1}{v}(I_m \otimes J_v) - \frac{v-1}{mv} J_{vm} - I_{vm} + \frac{1}{v}(I_m \otimes J_v)\right) \otimes \widehat{V}_{|H_1} \\
&\quad + \left(\frac{m-1}{m} J_{vm} - (I_m \otimes J_v) + \frac{1}{m} J_{vm}\right) \otimes \widehat{M}_{|H_1} \\
&= I_{vm} \otimes \widehat{U}_{|H_1} + (I_m \otimes (J_v - I_v)) \otimes \widehat{V}_{|H_1} + (J_{vm} - (I_m \otimes J_m)) \otimes \widehat{M}_{|H_1}
\end{aligned}
$$

which is (8). □

We now prove that P_{vm}, Q_{vm} and R_{vm} in (A.3) are indeed mutually orthogonal projectors.

Result 2: P_{vm}, Q_{vm} and R_{vm} in (A.3) are mutually orthogonal projectors with $\text{rank}(P_{vm}) = 1$, $\text{rank}(Q_{vm}) = m - 1$, $\text{rank}(R_{vm}) = m(v-1)$.

Proof P_{vm}, Q_{vm} and R_{vm} in (A.3) are idempotent, since

$$
\begin{aligned}
P_{vm} P_{vm} &= \frac{1}{mv} J_{vm} \frac{1}{mv} J_{vm} = \frac{1}{(mv)^2} mv J_{vm} = \frac{1}{mv} J_{vm} = P_{vm}, \\
Q_{vm} Q_{vm} &= \left(\frac{1}{v}(I_m \otimes J_v) - P_{vm}\right)\left(\frac{1}{v}(I_m \otimes J_v) - P_{vm}\right) \\
&= \frac{1}{v^2}(I_m \otimes J_v)(I_m \otimes J_v) - \frac{1}{v}(I_m \otimes J_v) P_{vm} - \frac{1}{v} P_{vm}(I_m \otimes J_v) + P_{vm} \\
&= \frac{1}{v}(I_m \otimes J_v) - \frac{2}{vm} J_{vm} + \frac{1}{vm} J_{vm} = \frac{1}{v}(I_m \otimes J_v) - P_{vm} = Q_{vm},
\end{aligned}
$$

$$\begin{aligned} R_{vm}R_{vm} &= (I_{vm} - Q_{vm} - P_{vm})(I_{vm} - Q_{vm} - P_{vm}) = I_{vm} - Q_{vm} - P_{vm} \\ &\quad -Q_{vm} + Q_{vm}Q_{vm} + Q_{vm}P_{vm} - P_{vm} + P_{vm}Q_{vm} + P_{vm}P_{vm} \\ &= I_{vm} - Q_{vm} - P_{vm} - Q_{vm} + Q_{vm} - P_{vm} + P_{vm} \\ &= I_{vm} - Q_{vm} - P_{vm} = R_{vm}, \end{aligned}$$

and they are mutually orthogonal since

$$\begin{aligned} P_{vm}Q_{vm} &= P_{vm}\left(\tfrac{1}{v}(I_m \otimes J_v) - P_{vm}\right) = \tfrac{1}{v}P_{vm}(I_m \otimes J_v) - P_{vm} \\ &= \frac{1}{vm}J_{vm}\left(\frac{1}{v}(I_m \otimes J_v) - I_{vm}\right) = 0_{vm}, \\ R_{vm}P_{vm} &= (I_{vm} - Q_{vm} - P_{vm})P_{vm} = P_{vm} - P_{vm} = 0_{vm}, \\ R_{vm}Q_{vm} &= (I_{vm} - Q_{vm} - P_{vm})Q_{vm} = Q_{vm} - Q_{vm} = 0_{vm}. \end{aligned}$$

Since P_{vm}, Q_{vm} and R_{vm} are idempotent, we have

$$\begin{aligned} &\operatorname{rank}(P_{vm}) = \operatorname{tr}(P_{vm}) = \frac{1}{vm}\operatorname{tr}(I_{vm}) = 1 \\ &\operatorname{rank}(Q_{vm}) = \operatorname{tr}(Q_{vm}) = \frac{1}{v}\operatorname{tr}(I_m \otimes J_v) - \operatorname{tr}(P_{vm}) = \frac{mv}{v} - 1 = m - 1 \\ &\operatorname{rank}(R_{vm}) = \operatorname{tr}(R_{vm}) = \operatorname{tr}(I_{vm}) - \operatorname{tr}(Q_{vm}) - \operatorname{tr}(P_{vm}) = vm - m = (v-1)m. \end{aligned}$$

□

Setting together the previous two results with the next one, we will finally be able to prove (16).

Result 3: For the matrix A^{**} in (14), we may write

$$\begin{aligned} \widehat{\Psi}_{1|H_1} &= A_1^{**}, \\ \widehat{\Psi}_{2|H_1} &= \frac{1}{m-1}\sum_{j=1}^{m-1} A_{jv+1}^{**}, \\ \widehat{\Psi}_{3|H_1} &= \frac{1}{m(v-1)}\sum_{j=1}^{m}\sum_{k=1}^{v-1} A_{(j-1)v+k+1}^{**}. \end{aligned}$$

Proof Let $\mathrm{BTr}_r(A)$ denote the sum of all $r\times r$ diagonal blocks of A. Then, for $U_{|H_1}$, $V_{|H_1}$ and $W_{|H_1}$ in (9)–(11) we may write

$$\begin{aligned}
\widehat{U}_{|H_1} &= \frac{1}{mv}\mathrm{BTr}_r(A),\\
\widehat{V}_{|H_1} &= \frac{1}{mv(v-1)}\left(\mathrm{BTr}_r((I_m\otimes J_v\otimes I_r)A)-\mathrm{BTr}_r(A)\right),\\
\widehat{M}_{|H_1} &= \frac{1}{mv^2(m-1)}\left(\mathrm{BTr}_r((J_{vm}\otimes I_r)A)-\mathrm{BTr}_r((I_m\otimes J_v\otimes I_r)A)\right).
\end{aligned}$$

Then, since from (14) we may write

$$A=\Gamma' A^{**}\Gamma\,, \tag{A.4}$$

from (A.2), and from the definition of the matrix Γ in (5), we have

$$\begin{aligned}
\widehat{\Psi}_{1|H_1} &= \widehat{U}_{|H_1}+(v-1)\widehat{V}_{|H_1}+v(m-1)\widehat{M}_{|H_1}\\
&= \frac{1}{mv}\mathrm{BTr}_r(A)+\frac{1}{mv}\left(\mathrm{BTr}_r((I_m\otimes J_v\otimes I_r)A)-\mathrm{BTr}_r(A)\right)\\
&\quad+\frac{1}{mv}\left(\mathrm{BTr}_r((J_{vm}\otimes I_r)A)-\mathrm{BTr}_r((I_m\otimes J_v\otimes I_r)A)\right)\\
&= \frac{1}{mv}\mathrm{BTr}_r((J_{vm}\otimes I_r)A)=\mathrm{BTr}_r((P_{vm}\otimes I_r)A)\\
&= \mathrm{BTr}_r((P_{vm}\otimes I_r)\Gamma' A^{**}\Gamma)=\mathrm{BTr}_r(\Gamma(P_{vm}\otimes I_r)\Gamma' A^{**})\\
&= \mathrm{BTr}_r((\underbrace{((\Gamma_m\otimes\Gamma_v)P_{vm}(\Gamma_m\otimes\Gamma_v)')}_{=diag(\underbrace{1,0,\ldots,0}_{vm})}\otimes I_r)A^{**})=A_1^{**}\,,
\end{aligned}$$

where A_1^{**} represents the first diagonal block of A^{**} of dimensions $r\times r$, since, given the definition of a Helmert matrix, $\Gamma_m\otimes\Gamma_v$ is a $vm\times vm$ matrix whose first row is equal to $\frac{1}{\sqrt{vm}}\underline{1}'_{vm}$, where $\underline{1}_{vm}$ denotes a vector of 1's of dimension vm, and as such $(\Gamma_m\otimes\Gamma_v)P_{vm}$ is a $vm\times vm$ matrix whose first row is equal to $\frac{1}{\sqrt{vm}}\underline{1}'_{vm}$ and all other rows are null, so that

$$(\Gamma_m\otimes\Gamma_v)P_{vm}(\Gamma_m\otimes\Gamma_v)'=diag(\underbrace{1,0,\ldots,0}_{vm})\,, \tag{A.5}$$

what implies

$$((\Gamma_m\otimes\Gamma_v)P_{vm}(\Gamma_m\otimes\Gamma_v)')\otimes I_r=bdiag(I_r,0_{v(m-1)\times v(m-1)})\,.$$

Using (A.4), and once again the definition of the matrix Γ in (5), we also have

$$\begin{aligned}
\widehat{\Psi}_{2|H_1} &= \widehat{U}_{|H_1} + (v-1)\widehat{V}_{|H_1} - v\widehat{M}_{|H_1} \\
&= \frac{1}{mv}\mathrm{BTr}_r(A) + \frac{1}{mv}\left(\mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A) - \mathrm{BTr}_r(A)\right) \\
&\quad - \frac{1}{mv(m-1)}\left(\mathrm{BTr}_r((J_{vm} \otimes I_r)A) - \mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A)\right) \\
&= \frac{1}{mv}\left(1 + \frac{1}{m-1}\right)\mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A) \\
&\quad - \frac{1}{mv(m-1)}\mathrm{BTr}_r((J_{vm} \otimes I_r)A) \\
&= \frac{1}{m-1}\mathrm{BTr}_r\left(\left(\left(\frac{1}{v}(I_m \otimes J_v) - \frac{1}{mv}J_{vm}\right) \otimes I_r\right)A\right) \\
&= \frac{1}{m-1}\mathrm{BTr}_r\left((Q_{vm} \otimes I_r)\,A\right) = \frac{1}{m-1}\mathrm{BTr}_r((Q_{vm} \otimes I_r)\Gamma' A^{**}\Gamma) \\
&= \frac{1}{m-1}\mathrm{BTr}_r(\Gamma(Q_{vm} \otimes I_r)\Gamma' A^{**}) \\
&= \frac{1}{m-1}\mathrm{BTr}_r((((\Gamma_m \otimes \Gamma_v)Q_{vm}(\Gamma_m \otimes \Gamma_v)) \otimes I_r)A^{**}) \\
&= \frac{1}{m-1}\sum_{j=1}^{m-1} A^{**}_{jv+1}\,,
\end{aligned}$$

where A^{**}_j represents the j-th diagonal block of A^{**} of dimensions $r \times r$, since

$$(\Gamma_m \otimes \Gamma_v)Q_{vm}(\Gamma_m \otimes \Gamma_v)' = diag(\underbrace{0,\ldots,0}_{v},\underbrace{\underbrace{1,0,\ldots,0}_{v},\ldots,\underbrace{1,0,\ldots,0}_{v}}_{m-1 \text{ times}}) \quad \text{(A.6)}$$

and as such,

$$\begin{aligned}
&((\Gamma_m \otimes \Gamma_v)Q_{vm}(\Gamma_m \otimes \Gamma_v)') \otimes I_r \\
&\qquad = bdiag(I_{vr\times vr}, \underbrace{\underbrace{I_r, 0_{(v-1)r\times(v-1)r}}_{},\ldots,\underbrace{I_r, 0_{(v-1)r\times(v-1)r}}_{}}_{m-1})\,.
\end{aligned}$$

This is so because, given the definition of a Helmert matrix, for a $v \times v$ Helmert matrix Γ_v, we have that $\Gamma_v J_v$ is a matrix whose first row is equal to $\frac{1}{\sqrt{v}}\underline{1}_v'$, and as such we have

$$\Gamma_v J_v \Gamma_v' = diag(\underbrace{v, 0, \ldots, 0}_{v}),$$

so that we have

$$\begin{aligned}
&\frac{1}{v}\left(I_m \otimes \Gamma_v J_v \Gamma_v'\right) \\
&\quad = bdiag(\underbrace{diag(\underbrace{1, 0, \ldots, 0}_{v}), diag(\underbrace{1, 0, \ldots, 0}_{v}), \ldots, diag(\underbrace{1, 0, \ldots, 0}_{v})}_{m}) \\
&\quad = diag(\underbrace{\underbrace{1, 0, \ldots, 0}_{v}, \underbrace{1, 0, \ldots, 0}_{v}, \ldots, \underbrace{1, 0, \ldots, 0}_{v}}_{m})
\end{aligned}$$

and as such we may write, using the relation in (A.5),

$$\begin{aligned}
&(\Gamma_m \otimes \Gamma_v) Q_{vm} (\Gamma_m \otimes \Gamma_v)' \\
&\quad = (\Gamma_m \otimes \Gamma_v)\left(\frac{1}{v}(I_m \otimes J_v) - p_{vm}\right)(\Gamma_m \otimes \Gamma_v)' \\
&\quad = \left(\frac{1}{v}(\Gamma_m \otimes \Gamma_v J_v) - (\Gamma_m \otimes \Gamma_v) P_{vm}\right)(\Gamma_m \otimes \Gamma_v)' \\
&\quad = \frac{1}{v}(\Gamma_m \otimes \Gamma_v J_v)(\Gamma_m \otimes \Gamma_v)' - (\Gamma_m \otimes \Gamma_v) P_{vm} (\Gamma_m \otimes \Gamma_v)' \\
&\quad = \frac{1}{v}(\Gamma_m \Gamma_m' \otimes \Gamma_v J_v \Gamma_v') - (\Gamma_m \otimes \Gamma_v) P_{vm} (\Gamma_m \otimes \Gamma_v)' \\
&\quad = \frac{1}{v}(I_m \otimes \Gamma_v J_v \Gamma_v')) - diag(\underbrace{1, 0, \ldots, 0}_{vm}) \\
&\quad = diag(\underbrace{\underbrace{1, 0, \ldots, 0}_{v}, \underbrace{1, 0, \ldots, 0}_{v}, \ldots, \underbrace{1, 0, \ldots, 0}_{v}}_{m}) - diag(\underbrace{1, 0, \ldots, 0}_{vm}) \\
&\quad = diag(\underbrace{0, \ldots, 0}_{v}, \underbrace{\underbrace{1, 0, \ldots, 0}_{v}, \ldots, \underbrace{1, 0, \ldots, 0}_{v}}_{m-1 \text{ times}}).
\end{aligned}$$

And finally, using once again (A.4), and the definition of R_{vm} in (A.3), we have

$$
\begin{aligned}
\widehat{\Psi}_{3|H_1} &= \widehat{U}_{|H_1} - \widehat{V}_{|H_1} \\
&= \frac{1}{mv}\mathrm{BTr}_r(A) - \frac{1}{mv(v-1)}\left(\mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A) - \mathrm{BTr}_r(A)\right) \\
&= \frac{1}{mv}\left(1 + \frac{1}{v-1}\right)\mathrm{BTr}_r(A) - \frac{1}{mv(v-1)}\mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A) \\
&= \frac{1}{m(v-1)}\left(\mathrm{BTr}_r(A) - \frac{1}{v}\mathrm{BTr}_r((I_m \otimes J_v \otimes I_r)A)\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r\left((I_{mvr} - \frac{1}{v}(I_m \otimes J_v \otimes I_r))A\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r\left(((I_{mv} - \frac{1}{v}(I_m \otimes J_v)) \otimes I_r)A\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r\left((R_{vm} \otimes I_r)A\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r\left((R_{vm} \otimes I_r)\Gamma' A^{**}\Gamma\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r\left(\Gamma(R_{vm} \otimes I_r)\Gamma' A^{**}\right) \\
&= \frac{1}{m(v-1)}\mathrm{BTr}_r((((\Gamma_m \otimes \Gamma_v)R_{vm}(\Gamma_m \otimes \Gamma_v)') \otimes I_r)A^{**}) \\
&= \frac{1}{m(v-1)}\sum_{j=1}^{m}\sum_{k=1}^{v-1} A^{**}_{(j-1)v+k+1}\,,
\end{aligned}
$$

where, once again, A^{**}_j represents the j-th diagonal block of A^{**} of dimensions $r \times r$.

This is so given that from the definition of R_{vm} in (A.3) and from (A.5) and (A.6) it is clear that we have

$$
\begin{aligned}
&(\Gamma_m \otimes \Gamma_v)R_{vm}(\Gamma_m \otimes \Gamma_v)' \\
&\quad = (\Gamma_m \otimes \Gamma_v)(\Gamma_m \otimes \Gamma_v)' - (\Gamma_m \otimes \Gamma_v)Q_{vm}(\Gamma_m \otimes \Gamma_v)' \\
&\qquad\qquad\qquad\qquad -(\Gamma_m \otimes \Gamma_v)P_{vm}(\Gamma_m \otimes \Gamma_v)' \\
&\quad = I_{vm} - diag(\underbrace{0,\ldots,0}_{v},\underbrace{\underbrace{1,0,\ldots,0}_{v},\ldots,\underbrace{1,0,\ldots,0}_{v}}_{m-1 \text{ times}}) - diag(\underbrace{1,0,\ldots,0}_{vm}) \\
&\quad = diag(0,\underbrace{\underbrace{1,\ldots,1}_{v-1},0,\underbrace{1,\ldots,1}_{v-1},\ldots,0,\underbrace{1,\ldots,1}_{v-1}}_{m \text{ times}})\,,
\end{aligned}
$$

so that

$$((\Gamma_m \otimes \Gamma_v) R_{vm} (\Gamma_m \otimes \Gamma_v)') \otimes I_r$$
$$= bdiag(\underbrace{0_{r\times r}, I_{(v-1)r}, 0_{r\times r}, I_{(v-1)r}, \ldots, 0_{r\times r}, I_{(v-1)r}}_{m \text{ times}}).$$

□

Finally, expression (16) holds since from Result 1 and the mutual orthogonality of P_{vm}, Q_{vm} and R_{vm} proven in Result 2 and yet the rank results therein, we may write

$$|A^*| = |\widehat{\Psi}_{1|H_1}|\,|\widehat{\Psi}_{2|H_1}|^{m-1}\,|\widehat{\Psi}_{3|H_1}|^{m(v-1)},$$

which given the expressions obtained in Result 3 for $\widehat{\Psi}_{1|H_1}$, $\widehat{\Psi}_{2|H_1}$ and $\widehat{\Psi}_{3|H_1}$ yields (16).

Expression (17) would be proven in a completely similar way.

Appendix B: The GIG, EGIG and GNIG distributions

In this appendix we define the GIG (Generalized Integer Gamma), EGIG (Exponentiated Generalized Integer Gamma) and GNIG (Generalized Near-Integer Gamma) distributions and establish the notation used concerning their p.d.f.'s and c.d.f.'s.

We say that the r.v. (random variable) X has a Gamma distribution with shape parameter r (> 0) and rate parameter λ (> 0), and we will denote this fact by $X \sim \Gamma(r, \lambda)$, if the p.d.f. of X is

$$f_X(x) = \frac{\lambda^r}{\Gamma(r)}\, e^{-\lambda x}\, x^{r-1} \quad (x > 0)\,.$$

Let $X_j \sim \Gamma(r_j, \lambda_j)$ $(j = 1, \ldots, p)$ be a set of p independent r.v.'s and consider the r.v.

$$W = \sum_{j=1}^{p} X_j\,.$$

In case all the $r_j \in \mathbb{N}$, the distribution of W is what we call a GIG distribution (Coelho 1998). If all the λ_j are different, W has a GIG distribution of depth p, with shape parameters r_j and rate parameters λ_j, with p.d.f.

$$f_W(w) = f^{GIG}\Big(w \,\Big|\, \{r_j\}_{j=1:p};\, \{\lambda_j\}_{j=1:p};\, p\Big) = K \sum_{j=1}^{p} P_j(w)\, e^{-\lambda_j w}\,,$$

and c.d.f.

$$F_W(w) = F^{GIG}\Big(w \,\Big|\, \{r_j\}_{j=1:p};\, \{\lambda_j\}_{j=1:p};\, p\Big) = 1 - K \sum_{j=1}^{p} P_j^*(w)\, e^{-\lambda_j w}\,,$$

for $w > 0$, where

$$K = \prod_{j=1}^{p} \lambda_j^{r_j}\,, \qquad P_j(w) = \sum_{k=1}^{r_j} c_{j,k}\, w^{k-1} \tag{B.1}$$

and

$$P_j^*(w) = \sum_{k=1}^{r_j} c_{j,k}(k-1)! \sum_{i=0}^{k-1} \frac{w^i}{i!\,\lambda_j^{k-i}}\,, \tag{B.2}$$

with

$$c_{j,r_j} = \frac{1}{(r_j-1)!} \prod_{\substack{i=1 \\ i\neq j}}^{p} (\lambda_i - \lambda_j)^{-r_i}\,, \quad j = 1, \ldots, p\,, \tag{B.3}$$

and, for $k = 1, \ldots, r_j - 1$ and $j = 1, \ldots, p$,

$$c_{j,r_j-k} = \frac{1}{k} \sum_{i=1}^{k} \frac{(r_j - k + i - 1)!}{(r_j - k - 1)!}\, R(i, j, p)\, c_{j,r_j-(k-i)}\,, \tag{B.4}$$

where

$$R(i, j, p) = \sum_{\substack{k=1 \\ k\neq j}}^{p} r_k (\lambda_j - \lambda_k)^{-i} \quad (i = 1, \ldots, r_j - 1)\,. \tag{B.5}$$

In case some of the λ_j assume the same value as other λ_j's, the distribution of W still is a GIG distribution, but in this case with a reduced depth. In this more general case, let $\widetilde{\{\lambda_\ell\}}_{\ell=1:g(\leq p)}$ be the set of different λ_j's and let $\overset{\approx}{\{r_\ell\}}_{\ell=1:g(\leq p)}$ be the set of the corresponding shape parameters, with r_ℓ ($\ell = 1, \ldots, g$) being the sum of all r_j ($j \in \{1, \ldots, p\}$) which correspond to the λ_j assuming the value λ_ℓ. In this case W will have a GIG distribution of depth g, with shape parameters r_ℓ and rate parameters λ_ℓ ($\ell = 1, \ldots, g$).

The r.v. $Z = e^{-W}$ has then what Arnold et al. (2013) call an Exponentiated Generalized Integer Gamma (EGIG) distribution of depth g, with p.d.f.

$$
\begin{aligned}
f_Z(z) &= f^{EGIG}\left(z \mid \overset{\approx}{\{r_\ell\}}_{\ell=1:g}; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}; g\right) \\
&= f^{GIG}\left(-\log z \mid \overset{\approx}{\{r_\ell\}}_{j=1:g}; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}; g\right)\frac{1}{z} \qquad \text{(B.6)} \\
&= K^* \sum_{\ell=1}^{g} P_\ell(-\log z)\, z^{\lambda_\ell - 1} \qquad (0 < z < 1)
\end{aligned}
$$

and c.d.f.

$$
\begin{aligned}
F_Z(z) &= F^{EGIG}\left(z \mid \overset{\approx}{\{r_\ell\}}_{\ell=1:g}; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}; g\right) \\
&= 1 - F^{GIG}\left(-\log z \mid \overset{\approx}{\{r_\ell\}}_{\ell=1:g}; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}; g\right) \qquad \text{(B.7)} \\
&= K^* \sum_{\ell=1}^{g} P_\ell^*(-\log z)\, z^{\lambda_\ell} \qquad (0 < z < 1)\,,
\end{aligned}
$$

for

$$
K^* = \prod_{\ell=1}^{g} \lambda_\ell^{r_\ell} \qquad \text{(B.8)}
$$

and $P_\ell(\cdot)$ and $P_\ell^*(\cdot)$ given by (B.1) and (B.2), with j replaced by ℓ.

Then let W be a r.v. with a GIG distribution of depth g, with rate parameters $\widetilde{\{\lambda_\ell\}}_{\ell=1:g}$ and shape parameters $\overset{\approx}{\{r_\ell\}}_{\ell=1:g}$ $(\in \mathbb{N})$ and let $W^* \sim \Gamma(r, \lambda)$, with $r \in \mathbb{R}^+ \backslash \mathbb{N}$. Let further W and W^* be two independent r.v.'s. Then the r.v.

$$
Y = W + W^*
$$

has a Generalized Near-Integer Gamma (GNIG) distribution (Coelho 2004) of depth $g+1$, with rate parameters $\widetilde{\{\lambda_\ell\}}_{\ell=1:g}$ and λ and corresponding shape parameters $\overset{\approx}{\{r_\ell\}}_{\ell=1:g}$ $(\in \mathbb{N})$ and r, with p.d.f.

$$
\begin{aligned}
f_Y(y) &= f^{GNIG}\left(y \mid \overset{\approx}{\{r_\ell\}}_{\ell=1:g}, r; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}, \lambda; g+1\right) \\
&= K^* \lambda^r \sum_{\ell=1}^{g} e^{-\lambda_\ell y} \sum_{k=1}^{r_\ell} \left\{ c_{\ell,k} \frac{\Gamma(k)}{\Gamma(k+r)} y^{k+r-1}\, {}_1F_1\left(r, k+r, -(\lambda - \lambda_\ell) y\right) \right\}
\end{aligned}
$$

and c.d.f.

$$
\begin{aligned}
F_Y(y) &= F^{GNIG}\Big(y \mid \overset{\approx}{\{r_\ell\}}_{\ell=1:g}, r; \widetilde{\{\lambda_\ell\}}_{\ell=1:g}, \lambda; g+1\Big) \\
&= \frac{\lambda^r\, y^r}{\Gamma(r+1)}\, {}_1F_1\big(r, r+1, -\lambda y\big) \\
&\quad - K^{**} \sum_{\ell=1}^{g} e^{-\lambda_\ell y} \sum_{k=1}^{r_\ell} c^*_{\ell,k} \sum_{i=0}^{k-1} \left\{ \frac{y^{r+i}\, \lambda_\ell^i}{\Gamma(r^*+i)}\, {}_1F_1\big(r, r^*+i, -(\lambda-\lambda_\ell)y\big) \right\}
\end{aligned}
$$

where $z > 0$, $K^{**} = K^* \lambda^r$, for K^* in (B.8), $r^* = r + 1$, and

$$
c^*_{\ell,k} = \frac{c_{\ell,k}}{\lambda_\ell^k}\, \Gamma(k)
$$

for $c_{\ell,k}$ given by (B.3)–(B.5) with j replaced by ℓ, and

$$
{}_1F_1(a, b, y) = \sum_{i=0}^{\infty} \frac{\Gamma(a+i)}{\Gamma(b+i)} \frac{\Gamma(b)}{\Gamma(a)} \frac{z^i}{i!}
$$

is the Kummer confluent hypergeometric function.

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Bilinear Regression with Rank Restrictions on the Mean and Dispersion Matrix

Dietrich von Rosen

Abstract A bilinear regression model with rank restrictions imposed on the mean-parameter matrix and the dispersion matrix is studied. Maximum likelihood-inspired estimates are derived. The approach generalizes classical reduced rank regression analysis and principal component analysis. It is illustrabed via a simulation study and a real example that even for small dimensions, the method works similarly to reduced rank regression analysis whereas the approach in this article also can be used when the dimension is large.

Keywords Bilinear regression model · Latent processes · Rank restriction on the dispersion · Rank restriction on the mean

1 Introduction

The rapid development of technology enables the use of various types of sensors together with advanced computer facilities in modern empirical studies which often results in data with quite complex structures. Well-established models do not exist in this case since one only has a vague idea of what should be included in a model adequately describing the data. For example, a huge number of chemical soil characteristics can be observed which, however, are all governed by a few latent processes, or brain activity can be measured via EEG signals from a large number of electrodes which are placed on the scalp though there are a few latent processes which direct the signals. At the end of this section, another example is presented in some detail.

Our philosophy is that latent processes should be looked upon as non-observable processes on which we do not want to put a distribution. The concept of latent variables appears in the literature in different contexts. Sometimes, latent variables are motivating mixed linear models. Other examples where latent variables are men-

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tioned are finite mixtures of regression models and the terms latent class models and latent factor models are also often used. In this article, we relate latent variables to rank restrictions on parameter matrices which according to data analysis seems to be a rewarding strategy.

Statistical modeling under a normality assumption often means joint modeling of the mean and dispersion. The available literature comprises results on using latent variables to model the mean (reduced rank regression, cointegration; e.g. see Anderson 1951; Johansen 1991; Reinsel and Velu 1998) or to model the dispersion (principal component analysis, among other methods; e.g. see Jolliffe 2002). To our knowledge there are, however, no results concerning jointly modeling multiprocesses, i.e. the case when simultaneously some latent processes are affecting the mean whereas other latent processes steer the dispersion.

In this article, the focus is on the bilinear regression model (BRM) which is often called the growth curve model or generalized multivariate analysis model (GMANOVA). The model was introduced by Potthoff and Roy (1964) although other authors had earlier considered similar models. For general references about the model, e.g. see Woolson and Leeper (1980), von Rosen (1991), Kshirsagar and Smith (1995) and von Rosen (2018).

As has been mentioned above, the inference in this article is based on the fact that latent processes can be described through rank restrictions on parameters. For references to results and applications of rank restrictions on the mean, including the mean structure of the BRM, we refer the readers to the book by Reinsel and Velu (1998), Albert and Kshirsagar (1993), Reinsel and Velu (2003) or to a recent work by von Rosen and von Rosen (2017). Today, high-dimensional statistical analysis is rapidly developing. A pure high-dimensional perspective on rank restrictions on the mean is presented in an interesting article by Kargin (2015) and Chen and Huang (2012) combined reduced rank regression with a variable selection method. Further, there exists extensive literature on linear models when the dispersion matrix is proportional to a known positive semi-definite matrix (the Gauss-Markov model), e.g. see Rao (1973a, 1979), Nordström (1985) and Baksalary et al. (1992). However, when the dispersion matrix is unknown, only a few references exist (see Wong and Cheng 2001 and Srivastava and von Rosen 2002).

The aim of this work is to find estimates of the mean and dispersion parameters under simultaneous rank restrictions on the matrix of regression coefficients and the dispersion matrix.

Grizzle and Allen (1969) published a data set which later was analyzed by Albert and Kshirsagar (1993) who used a reduced rank restriction on the mean parameter in order to discriminate groups of independent observations which is linked to canonical correlation analysis (see Tso 1981; Johansen 1988). The data set consists of 36 dogs randomly assigned to four groups. For each dog, measurements of potassium were obtained at seven equally spaced time points, and then a reduced rank growth curve model was applied. As Grizzle and Allen (1969), the authors used a cubic regression model and tested what rank on the mean parameters would be natural to assume. Albert and Kshirsagar (1993) suggested the rank to be one. Moreover, Albert and Kshirsagar (1993) aimed to reduce the dimensionality in data via rank restrictions on

the mean (similar to canonical correlation analysis) whereas in this article we also employ ideas from principal component analysis and additionally reduce the data via rank restrictions on the dispersion matrix.

The following notation will be used. Bold upper cases denote matrices: $\mathcal{C}(\boldsymbol{A})$ is the column vector space generated by the columns of $\boldsymbol{A}$, and $\mathcal{C}(\boldsymbol{A})^{\perp}$ denotes its orthogonal complement; $\boldsymbol{A}^{o}$ denotes any matrix of full rank which generates $\mathcal{C}(\boldsymbol{A})^{\perp}$. The orthogonal projector on $\mathcal{C}(\boldsymbol{A})$ is denoted by $\boldsymbol{P}_{A}$ and equals $\boldsymbol{P}_{A} = \boldsymbol{A}(\boldsymbol{A}'\boldsymbol{A})^{-}\boldsymbol{A}'$, where "$-$" denotes an arbitrary generalized inverse (g-inverse). Moreover, we will often write $(\boldsymbol{Q})()'$ instead of $(\boldsymbol{Q})(\boldsymbol{Q})'$, where $\boldsymbol{Q}$ represents any matrix expression. Additionally, necessary notation will be introduced in the following sections.

2 The Model

Consider the BRM with normally distributed error which without loss of generality can be written as

$$\boldsymbol{X} = \boldsymbol{ABC} + \boldsymbol{E}, \tag{1}$$

where $\boldsymbol{X}$: $p \times n$ consists of independent response vectors, $\boldsymbol{A}$: $p \times q$ is a known within-individuals design matrix, $\boldsymbol{C}$: $k \times n$ is a known between-individuals design matrix, $\boldsymbol{E} \sim N_{p,n}(\boldsymbol{0}, \boldsymbol{\Sigma}, \boldsymbol{I}_n)$, i.e. $\boldsymbol{E}$ is a matrix normally distributed (see Ohlson et al. 2013), the mean matrix $\boldsymbol{B}$: $q \times k$ and the dispersion matrix $\boldsymbol{\Sigma}$: $p \times p$ are unknown parameter matrices. A distinguishing characteristic of the BRM studied here are the following reduced-rank restrictions on the model parameters

$$r(\boldsymbol{B}) = f < \min(q, k), \tag{2}$$

$$r(\boldsymbol{\Sigma}) = r < p, r \geq f, \tag{3}$$

where both f and r are supposed to be known. Thus, $\boldsymbol{\Sigma}$ is positive semi-definite instead of being positive definite, which is a usual assumption. As mentioned in the introduction, the main aim of this article is to estimate the parameters $\boldsymbol{B}$ and $\boldsymbol{\Sigma}$ in (1) when the rank restrictions (2) and (3) hold so that the model can be used for prediction. Note that in the majority of published articles, $\boldsymbol{B}$ is interpretable or one wants to find interpretable scores such as in Albert and Kshirsagar (1993) which can be difficult in practice. However, it is possible that $\boldsymbol{B}$ constitutes an object with rank restrictions corresponding to latent processes where we really do not know the implications of these processes. The latent process can not only have a clear interpretation of the "between-individuals" structure of the model but can also be interpretable in terms of the "within-individuals" structure. In both cases (precise or vague interpretation of $\boldsymbol{B}$), the mathematics will be the same when deriving estimators, i.e. the only thing which matters is the interpretation of the estimators. In this article, we focus on statistical inference rather than interpreting the results which can depend on the data and purpose of the empirical study.

3 Preliminaries

We will present three lemmas which are used to derive the estimates in model (1). The first lemma is essentially a restatement of Theorem 1.5.3 in Srivastava and Khatri (1979).

Lemma 1 *For any $\boldsymbol{\Theta}$: $q \times k$, with rank restrictions, say $r(\boldsymbol{\Theta}) = f$, there exist $\boldsymbol{\Theta}_1$: $q \times f$, $\boldsymbol{\Theta}_2$: $f \times k$, $r(\boldsymbol{\Theta}_i) = f$, $i = 1, 2$, such that $\boldsymbol{\Theta} = \boldsymbol{\Theta}_1\boldsymbol{\Theta}_2$.*

Note that $\boldsymbol{\Theta}_1$ and $\boldsymbol{\Theta}_2$ together can include more unknown elements than $\boldsymbol{\Theta}$. In this case, the estimation strategy is to consider a larger parameter space than the original one, i.e. some type of imbedding takes place. On the other hand, if $r(\boldsymbol{\Theta}) = f$ there exist $k - f$ linear combinations of $\boldsymbol{\Theta}$ which equal $\mathbf{0}$, say $\boldsymbol{L}\boldsymbol{\Theta} = \mathbf{0}$, where $\boldsymbol{L}$ is of size $(q - f) \times q$, or $\boldsymbol{L}\boldsymbol{\Theta}' = \mathbf{0}$, where $\boldsymbol{L}$ is of size $(k - f) \times k$. Both conditions imply, since $\boldsymbol{L}$ is unknown, that $\boldsymbol{\Theta} = \boldsymbol{\Theta}_1\boldsymbol{\Theta}_2$, and thus the factorization of $\boldsymbol{\Theta}$ is a natural approach to apply. However, what type of restrictions exist can be important for the interpretation of the analysis. The next lemma is also well known.

Lemma 2 (spectral decomposition) *Let $\boldsymbol{\Sigma}$: $p \times p$ be positive semi-definite of rank $r(\boldsymbol{\Sigma}) = r$. Then there exists a semi-orthogonal matrix $\boldsymbol{\Gamma}$, i.e. $\boldsymbol{\Gamma}'\boldsymbol{\Gamma} = \boldsymbol{I}_r$ and a diagonal matrix $\boldsymbol{\Delta}$: $r \times r$ with positive diagonal elements, such that $\boldsymbol{\Sigma} = \boldsymbol{\Gamma}\boldsymbol{\Delta}\boldsymbol{\Gamma}'$.*

It is well known that $\mathcal{C}(\boldsymbol{S}) \subseteq \mathcal{C}(\boldsymbol{\Sigma})$, when $\boldsymbol{S} \sim \boldsymbol{W}_p(\boldsymbol{\Sigma}, n)$, i.e. Wishart distributed. Furthermore, if $n \geq r(\boldsymbol{\Sigma})$, then $\mathcal{C}(\boldsymbol{S}) = \mathcal{C}(\boldsymbol{\Sigma})$ holds with probability 1 (e.g. see Srivastava and von Rosen 2002, Lemma 3.1). In this article, $\boldsymbol{S} = \boldsymbol{X}(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{X}' \sim W_p(\boldsymbol{\Sigma}, n - r(\boldsymbol{C}))$. Let $\boldsymbol{S} = \boldsymbol{H}\boldsymbol{D}\boldsymbol{H}'$ where $\boldsymbol{H}$ consists of eigenvectors of $\boldsymbol{S}$, and $\boldsymbol{D}$ is a diagonal matrix with eigenvalues of $\boldsymbol{S}$ on its diagonal. If we have observations $\boldsymbol{X}_o$, i.e. realizations of $\boldsymbol{X}$, we can calculate $\boldsymbol{H}_o$ which is the observed $\boldsymbol{H}$, where however eigenvectors corresponding to the $p - r$ smallest eigenvalues of $\boldsymbol{X}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{X}_o'$ have been removed, and $\boldsymbol{D}_o$ is the diagonal matrix consisting of the observed eigenvalues of $\boldsymbol{X}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{X}_o'$, where the $p - r$ smallest eigenvalues have been removed. Then

$$\boldsymbol{S}_o = \boldsymbol{H}_o\boldsymbol{D}_o\boldsymbol{H}_o' \tag{4}$$

does not represent the observed $\boldsymbol{S}$ but a quantity corresponding to $\boldsymbol{S}$, where the $p - r$ smallest eigenvalues have been put to 0. The way of defining $\boldsymbol{S}_o$ is fundamental for the results of this article.

Furthermore, throughout the paper we make the following two crucial assumptions.

Assumption 1 For the model in (1), it is assumed that $\mathcal{C}(\boldsymbol{X}_o) \subseteq \mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{\Sigma})$.

Assumption 2 For the model in (1), if $n \geq r + r(\boldsymbol{C})$, it is assumed that $\mathcal{C}(\boldsymbol{S}_o) = \mathcal{C}(\boldsymbol{\Sigma})$.

Removing the $p - r$ smallest eigenvalues in (4) is not obvious. However, Assumption 2, i.e. $\mathcal{C}(\boldsymbol{S}_o) = \mathcal{C}(\boldsymbol{\Sigma})$, is motivated by $\mathcal{C}(\boldsymbol{S}) = \mathcal{C}(\boldsymbol{\Sigma})$ which as noted before holds with probability 1. Therefore, under Assumption 2,

$$\mathcal{C}(\boldsymbol{H}_o) = \mathcal{C}(\boldsymbol{S}_o) = \mathcal{C}(\boldsymbol{\Sigma}) = \mathcal{C}(\boldsymbol{\Gamma}). \tag{5}$$

It is worth noting that the equality $\mathcal{C}(\boldsymbol{H}_o) = \mathcal{C}(\boldsymbol{\Gamma})$. Instead of Assumption 1, we can use $\mathcal{C}(\boldsymbol{X}_o) \subseteq \mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{S})$, and using Assumption 2, $\mathcal{C}(\boldsymbol{S})$ can be replaced by $\mathcal{C}(\boldsymbol{S}_o)$. In reality, it means that before analyzing data, $\boldsymbol{X}_o$ has to be preprocessed, i.e. $\boldsymbol{X}_o$ should be projected on $\mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{S}_o)$, and then Assumption 1 holds. In the Gauss-Markov literature, Assumption 1 is a so called consistency assumption.

Lemma 3 *Let $\boldsymbol{\Gamma}$ and $\boldsymbol{H}_o$, defined in Lemma 2 and (4), respectively, be the matrices of eigenvectors corresponding to $\boldsymbol{\Sigma}$ and $\boldsymbol{S}_o$, respectively, and suppose $n \geq r + r(\boldsymbol{C})$. Then, for some orthogonal matrix $\boldsymbol{Q}$, under Assumption 2,*

$$\boldsymbol{\Gamma} = \boldsymbol{H}_o \boldsymbol{Q}.$$

Proof The proof follows from (5) and a few calculations: $\boldsymbol{I}_r = \boldsymbol{\Gamma}'\boldsymbol{\Gamma} = \boldsymbol{Q}'\boldsymbol{H}_o'\boldsymbol{H}_o\boldsymbol{Q} = \boldsymbol{Q}'\boldsymbol{Q}$. □

Corollary 1 *Let $\boldsymbol{\Gamma}$ and $\boldsymbol{S}_o$ be defined as in Lemma 3; $\boldsymbol{X}_o$ is the realization of $\boldsymbol{X}$ in (1) where also $\boldsymbol{C}$ is given. Then, under Assumption 2,*

$$\boldsymbol{\Gamma}'\boldsymbol{X}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{X}_o'\boldsymbol{\Gamma} - \boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma} = \boldsymbol{0}.$$

Proof According to Lemma (3), $\boldsymbol{\Gamma} = \boldsymbol{H}_o\boldsymbol{Q}$ and thus

$$\boldsymbol{Q}'\boldsymbol{H}_o'(\boldsymbol{X}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{X}_o' - \boldsymbol{S}_o)\boldsymbol{H}_o\boldsymbol{Q} = \boldsymbol{0}.$$

□

Corollary 2 *Let $\boldsymbol{\Gamma}$ and $\boldsymbol{S}_o$ be defined as in Lemma 3. Then*

$$\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}' = \boldsymbol{S}_o^+,$$

where "+" denotes the Moore-Penrose generalized inverse (e.g. see Rao 1973b; p. 26).

Proof Since $\boldsymbol{\Gamma} = \boldsymbol{H}_o\boldsymbol{Q}$ for some orthogonal $\boldsymbol{Q}$, the Moore-Penrose generalized inverse is established by verification of its four defining conditions. □

The next lemma can be found, for example, in Rao (1973b; pp. 64–65), and it follows from the Poincaré separation theorem concerning eigenvalues.

Lemma 4 *Let $\boldsymbol{F}$: $p \times q$ satisfy $\boldsymbol{F}'\boldsymbol{F} = \boldsymbol{I}_q$, and let $\boldsymbol{U}$: $p \times p$ be positive definite. Then*

$$|\boldsymbol{F}'\boldsymbol{U}\boldsymbol{F}| \geq \prod_{i=1}^{q} \lambda_i,$$

where $\lambda_q \geq \lambda_{q-1} \geq \cdots \geq \lambda_1$ *are the* q *smallest eigenvalues of* $\boldsymbol{U}$.

Equality holds in Lemma 4 if $\boldsymbol{F}$ comprises the eigenvectors corresponding to the q smallest eigenvalues of $\boldsymbol{U}$ which follows, for example, from Lemma 2.

4 Estimation

In this section, the goal is to estimate $\boldsymbol{B}$ and $\boldsymbol{\Sigma}$ in (1) under the constraints in (2) and (3). The following decomposition of the whole space,

$$\mathcal{C}(\boldsymbol{\Sigma}) \boxplus \mathcal{C}(\boldsymbol{\Sigma})^{\perp} \cap \mathcal{C}(\boldsymbol{A} : \boldsymbol{\Sigma}) \boxplus \mathcal{C}(\boldsymbol{A} : \boldsymbol{\Sigma})^{\perp},$$

where $\boxplus$ denotes the "orthogonal sum" of linear spaces, yields a one-one transformation of the original model presented in (1):

$$\begin{pmatrix} \boldsymbol{\Gamma}' \\ \boldsymbol{A}'(\boldsymbol{I} - \boldsymbol{\Gamma}\boldsymbol{\Gamma}') \\ (\boldsymbol{A} : \boldsymbol{\Sigma})^{o'} \end{pmatrix} \boldsymbol{X},$$

where it has been utilized that $\mathcal{C}((\boldsymbol{I} - \boldsymbol{\Gamma}\boldsymbol{\Gamma}')\boldsymbol{A}) = \mathcal{C}(\boldsymbol{\Sigma})^{\perp} \cap \mathcal{C}(\boldsymbol{A} : \boldsymbol{\Sigma})$ (e.g. see Kollo and von Rosen 2005; Theorem 1.2.16). Thus, we obtain three relations which are fundamental for obtaining the estimates of the parameters:

$$\boldsymbol{\Gamma}'\boldsymbol{X} = \boldsymbol{\Gamma}'\boldsymbol{A}\boldsymbol{B}\boldsymbol{C} + \boldsymbol{\Delta}^{1/2}\widetilde{\boldsymbol{E}}, \qquad \widetilde{\boldsymbol{E}} \sim N_{r,n}(\boldsymbol{0}, \boldsymbol{I}_r, \boldsymbol{I}_n), \tag{6}$$

$$\boldsymbol{A}'(\boldsymbol{I} - \boldsymbol{\Gamma}\boldsymbol{\Gamma}')\boldsymbol{X} = \boldsymbol{A}'(\boldsymbol{I} - \boldsymbol{\Gamma}\boldsymbol{\Gamma}')\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}, \tag{7}$$

$$(\boldsymbol{A} : \boldsymbol{\Sigma})^{o'}\boldsymbol{X} = \boldsymbol{0}. \tag{8}$$

Note that "=" in (6) stands for equality in distribution whereas "=" in (7) and (8) means equality with probability 1. To perform likelihood inference, we should replace $\boldsymbol{X}$ by $\boldsymbol{X}_o$ in these equations. In (6), the density is a function of $\boldsymbol{X}_o$. Because of Assumption 1, (8) is trivially satisfied when $\boldsymbol{X}$ is replaced by $\boldsymbol{X}_o$, and will not be considered anymore. We call (6) to be the random part of the original model and (7) to be the deterministic part. Next, (7) will be exploited. From Lemma 3, it follows that we should study

$$\boldsymbol{A}'(\boldsymbol{I} - \boldsymbol{H}_o\boldsymbol{H}_o')\boldsymbol{X}_o = \boldsymbol{A}'(\boldsymbol{I} - \boldsymbol{H}_o\boldsymbol{H}_o')\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}$$

which is identical to

$$\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o = \boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}. \tag{9}$$

Thus, data put restrictions on $\boldsymbol{B}$ which is unusual and not obvious on how to handle. One strategy is to ignore them, but here we will think that utilizing the restrictions will improve our estimators. Assumption 1 implies that

$$\mathcal{C}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o) \subseteq \mathcal{C}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A}'). \tag{10}$$

Moreover, it will be further assumed that

$$\mathcal{C}(\boldsymbol{X}_o'\boldsymbol{H}_o^o) \subseteq \mathcal{C}(\boldsymbol{C}') \tag{11}$$

and therefore instead of $\boldsymbol{X}_o'\boldsymbol{H}_o^o$ its orthogonal projection on $\mathcal{C}(\boldsymbol{C}')$,

$$\boldsymbol{P}_{C'}\boldsymbol{X}_o'\boldsymbol{H}_o^{o'},$$

will be used when estimating the parameters. The projection could also have taken place in a preprocessing step of $\boldsymbol{X}_o$. Note that $\mathcal{C}(\boldsymbol{X}'\boldsymbol{H}_o^o) \subseteq \mathcal{C}(\boldsymbol{C}')$ holds with probability 1. Hence, we replace (9) by

$$\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{P}_{C'} = \boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}, \tag{12}$$

and we have now a consistent system of linear equations. A general solution to (12) is given by (see Kollo and von Rosen 2005; Theorem 1.3.4)

$$\begin{aligned}\boldsymbol{B} = {} & (\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^- + (\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Theta}_1 \\ & + \boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A}\boldsymbol{\Theta}_2\boldsymbol{C}^{o'},\end{aligned} \tag{13}$$

where $\boldsymbol{\Theta}_1$: $(q - r(\boldsymbol{A}'\boldsymbol{H}_o^o)) \times k$, and $\boldsymbol{\Theta}_2$: $q \times (k - r(\boldsymbol{C}))$, are new parameters.

However, $\boldsymbol{H}_o^{o'}\boldsymbol{A}$ has to be considered in some detail. The first observation is that if $\boldsymbol{H}_o^{o'}\boldsymbol{A} = \boldsymbol{0}$ or $\boldsymbol{H}_o'\boldsymbol{A} = \boldsymbol{0}$, which in principle never will hold mathematically, we cannot use the model in (1), with rank restrictions given by (2) and (3), and thus it will be assumed that $\boldsymbol{H}_o^{o'}\boldsymbol{A} = \boldsymbol{0}$ or $\boldsymbol{H}_o'\boldsymbol{A} = \boldsymbol{0}$ will not occur, which was implicitly assumed in the above discussion. In the following subsections, two cases will be studied:

(a) $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma}) = \{\boldsymbol{0}\}$, $q \leq p - r$, which implies $r(\boldsymbol{H}_o^{o'}\boldsymbol{A}) = q$;
(b) $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma}) \neq \{\boldsymbol{0}\}$.

In (b) there exists a special case, $r(\boldsymbol{H}_o^{o'}\boldsymbol{A}) = p - r < q$, which, however, will not be considered because the treatment of the model under this condition follows the case discussed in the forthcoming Sect. 4.2. The only difference is that if $r(\boldsymbol{H}_o^{o'}\boldsymbol{A}) = p - r$ holds, Assumption 1 is not needed, since in this case $\mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{\Sigma})$ spans the whole space and $\boldsymbol{X}_o$ belongs always to this space.

4.1 Estimation Under the Condition $\mathcal{C}(A) \cap \mathcal{C}(\Sigma) = \{0\}$

If $q \leq p - r, \mathcal{C}(A) \cap \mathcal{C}(\Sigma) = \{0\}$ yields $r(H_o^{o'} A) = q$, we get from (13) the relation

$$B = (A' H_o^o H_o^{o'} A)^{-1} A' H_o^o H_o^{o'} X_o C' (CC')^- + A' H_o^o H_o^{o'} A \Theta_2 C^{o'}, \tag{14}$$

because now $(A' H_o^o)^o = 0$. However, the estimation of Θ_2 which only can be performed via (6) is impossible, because the term involving Θ_2 will disappear when inserting B, given by (14), into (6). Thus, we can only estimate Σ but not B.

Theorem 1 *Let the model be defined in (1) with rank restrictions given by (2) and (3). Assume that* $\mathcal{C}(A) \cap \mathcal{C}(\Sigma) = \{0\}$, $H_o^{o'} A \neq 0$, $H_o' A \neq 0$, $\mathcal{C}(X_o) \subseteq \mathcal{C}(A) + \mathcal{C}(\Sigma)$ *and* $\mathcal{C}(X_o' H_o) \subseteq \mathcal{C}(C')$. *Put*

$$Y_o = (I - A(A' H_o^o H_o^{o'} A)^+ A' H_o^o H_o^{o'}) X_o.$$

Then

$$n\widehat{\Sigma} = \widehat{\Gamma}_o \widehat{\Delta}_o \widehat{\Gamma}_o',$$

where the estimate $n\widehat{\Delta}_o$ *equals the diagonal matrix with the* r *largest eigenvalues of* $Y_o Y_o'$ *on the diagonal, and* $\widehat{\Gamma}_o$ *comprises the eigenvectors of* $Y_o Y_o'$ *corresponding to these eigenvalues.*

Proof The proof follows from the proof of Theorem 2. □

4.2 Estimation Under the Condition $\mathcal{C}(A) \cap \mathcal{C}(\Sigma) \neq \{0\}$

According to (2), there exists the rank restriction $r(B) = f$ and it will be assumed that $f - r(H_o^{o'} X_o) < \min((q - r(H_o^{o'} X_o)), k)$. To estimate parameters, the idea is to insert an appropriate chosen B in (6), for example, based on (13). It seems reasonable to consider, instead of (13), the following solution:

$$B = (A' H_o^o H_o^{o'} A)^+ A' H_o^o H_o^{o'} X_o C' (CC')^- + (A' H_o^o)^o \Theta_1, \tag{15}$$

because when inserting this B into (6) Θ_2 disappears, and when choosing B according to (15) the effect of the rank restrictions will be "maximal". Thus, the challenge is to put appropriate rank restrictions on Θ_1 so that $r(B) = f$ holds. It is noted that

$$\begin{aligned} &r((A' H_o^o H_o^{o'} A)^+ A' H_o^o H_o^{o'} X_o C' (CC')^- : (A' H_o^o)^o \Theta_1) \\ &\quad = r((A' H_o^o H_o^{o'} A)^+ A' H_o^o H_o^{o'} X_o C' (CC')^-) + r((A' H_o^o)^o \Theta_1), \end{aligned}$$

since $(\boldsymbol{A}'\boldsymbol{H}_o^o)^{o'}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+ = \boldsymbol{0}$ because $\mathcal{C}((\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+) = \mathcal{C}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})$ (see Harville 1997; Theorem 20.5.1). It can be remarked that it is essential that the Moore-Penrose generalized inverse has been chosen. Hence, from (15)

$$\begin{aligned} f &= r((\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^-) + r((\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Theta}_1) \\ &= r(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^-) + r((\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Theta}_1) \\ &= r(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{C}') + r(\boldsymbol{\Theta}_1), \end{aligned}$$

where it has been utilized that $r((\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Theta}_1)=r(\boldsymbol{\Theta}_1 : \boldsymbol{A}'\boldsymbol{H}_o^o) - r(\boldsymbol{A}'\boldsymbol{H}_o^o)=r(\boldsymbol{\Theta}_1)$, with an underlying assumption that the spaces generated by $\boldsymbol{A}'\boldsymbol{H}_o^o$ and $\boldsymbol{\Theta}_1$, respectively, are disjoint. The relations in (10) and (11) show that

$$f = r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o) + r(\boldsymbol{\Theta}_1)$$

and therefore $\boldsymbol{\Theta}_1$ can be factored as $\boldsymbol{\Theta}_1 = \boldsymbol{\Psi}_1\boldsymbol{\Psi}_2$, with

$$\begin{aligned} &\boldsymbol{\Psi}_1 : (q - r(\boldsymbol{H}_o^{o'}\boldsymbol{A})) \times (f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o)), \\ &\boldsymbol{\Psi}_2 : (f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o)) \times k. \end{aligned}$$

Here, it is seen why the condition $f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o) < \min((q - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o)), k)$ is needed. Inserting the expression for $\boldsymbol{\Theta}_1$ into (13) yields an appropriate parametrization of $\boldsymbol{B}$ which then is inserted in (6). Thus, the model in (1) becomes

$$\boldsymbol{\Gamma}'\boldsymbol{X} = \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o + \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C} + \boldsymbol{\Delta}^{1/2}\widetilde{\boldsymbol{E}}, \quad (16)$$

where $\widetilde{\boldsymbol{E}} \sim N_{r,n}(\boldsymbol{0}, \boldsymbol{I}_r, \boldsymbol{I}_n)$. Via this model, the parameters $\boldsymbol{B}$, $\boldsymbol{\Psi}_1$, $\boldsymbol{\Psi}_2$, $\boldsymbol{\Delta}$, $\boldsymbol{\Gamma}$ and $\boldsymbol{\Sigma}$, or sometimes linear combinations of them, e.g. $\boldsymbol{L}'\boldsymbol{B}$ or $\boldsymbol{L}'\boldsymbol{\Psi}_1$, for some $\boldsymbol{L}$, will be discussed.

Let

$$\boldsymbol{Y}_o = (\boldsymbol{I} - \boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'})\boldsymbol{X}_o, \quad (17)$$

$$\boldsymbol{Y} = \boldsymbol{X} - \boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o. \quad (18)$$

The model in (16) can be rewritten as

$$\boldsymbol{\Gamma}'\boldsymbol{Y} = \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C} + \boldsymbol{\Delta}^{1/2}\widetilde{\boldsymbol{E}}.$$

The likelihood for $\boldsymbol{\Gamma}'\boldsymbol{Y}$ equals

$$\begin{aligned} &L(\boldsymbol{\Psi}_1, \boldsymbol{\Psi}_2, \boldsymbol{\Gamma}, \boldsymbol{\Delta}) \\ &\quad = c|\boldsymbol{\Delta}|^{-n/2}\exp\{-\tfrac{1}{2}\mathrm{tr}\{\boldsymbol{\Delta}^{-1}(\boldsymbol{\Gamma}'\boldsymbol{Y}_o - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'\}\} \\ &\quad \le c|\tfrac{1}{n}\{(\boldsymbol{\Gamma}'\boldsymbol{Y}_o - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'\}_d|^{-\frac{n}{2}}\exp\{-\tfrac{1}{2}rn\}, \end{aligned} \quad (19)$$

where $c = (2\pi)^{-\frac{1}{2}rn}$ and $\{\boldsymbol{W}\}_d$ is the diagonal matrix with non-zero elements equal to elements on the main diagonal of $\boldsymbol{W}$. The proof of the inequality can be obtained from the proof of Theorem 1.10.4 in Srivastava and Khatri (1978). Equality in (19) holds if and only if

$$n\boldsymbol{\Delta} = \{(\boldsymbol{\Gamma}'\boldsymbol{Y}_o - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'\}_d. \tag{20}$$

Moreover, from (19) it follows that we shall study the following determinant:

$$\begin{aligned}&|\{(\boldsymbol{\Gamma}'\boldsymbol{Y}_o - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'\}_d| \\ &\quad \geq |(\boldsymbol{\Gamma}'\boldsymbol{Y}_o - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'|\end{aligned} \tag{21}$$

and equality holds if $\boldsymbol{\Gamma}$ comprises the eigenvectors corresponding to the r smallest eigenvalues of $(\boldsymbol{Y}_o - \boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'$. Thus, $\boldsymbol{\Gamma}$ can be estimated if $\boldsymbol{\Psi}_1$ and $\boldsymbol{\Psi}_2$ can be estimated.

Now the goal is to minimize the determinant on the right-hand side of (21). Let $\boldsymbol{S}_o$ be defined as in (4), where $\boldsymbol{H}_o$ consists of the r eigenvectors corresponding to the r largest eigenvalues of $\boldsymbol{Y}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{Y}_o'$ which are placed in the diagonal matrix $\boldsymbol{D}_o$. Hence, the right-hand side of (21) equals (see Corollary 1)

$$\begin{aligned}&|(\boldsymbol{\Gamma}'(\boldsymbol{Y}_o(\boldsymbol{I} - \boldsymbol{P}_{C'})\boldsymbol{Y}_o' - \boldsymbol{S}_o)\boldsymbol{\Gamma} + \boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma} \\ &\qquad +(\boldsymbol{\Gamma}'\boldsymbol{Y}_o\boldsymbol{P}_{C'} - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'| \\ &\quad = |\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma} + (\boldsymbol{\Gamma}'\boldsymbol{Y}_o\boldsymbol{P}_{C'} - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})()'| \\ &\quad = |\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma}||\boldsymbol{I} + (\boldsymbol{\Gamma}'\boldsymbol{Y}_o\boldsymbol{P}_{C'} - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})'(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1} \\ &\qquad \times(\boldsymbol{\Gamma}'\boldsymbol{Y}_o\boldsymbol{P}_{C'} - \boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\boldsymbol{\Psi}_2\boldsymbol{C})|.\end{aligned} \tag{22}$$

Let

$$\boldsymbol{T} = \boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1, \tag{23}$$

which is of size $p \times (f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o))$. In order to estimate $\boldsymbol{\Psi}_2$ as a function of $\boldsymbol{\Psi}_1$, we are going to apply the same technique used to find maximum likelihood estimates in the growth curve model (e.g. see Kollo and von Rosen 2005; pp. 358–361). We can note that Tso (1981) used the same approach as in this article whereas Johansen (1988) estimated first $\boldsymbol{\Psi}_1$ as a function of $\boldsymbol{\Psi}_2$. Below, some calculations are presented showing the estimation approach. An important result is (for a proof, e.g. see Kollo and von Rosen 2005; Theorem 1.2.25)

$$\begin{aligned}(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1} &= (\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}'\boldsymbol{T}(\boldsymbol{T}'\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}'\boldsymbol{T})^-\boldsymbol{T}'\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1} \\ &\quad +(\boldsymbol{\Gamma}'\boldsymbol{T})^o((\boldsymbol{\Gamma}'\boldsymbol{T})^{o'}\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{T})^o)^-(\boldsymbol{\Gamma}'\boldsymbol{T})^{o'}.\end{aligned} \tag{24}$$

Applying this result yields that the right-hand side of (22) is larger or equal to

$$|\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma}||\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{T})^o((\boldsymbol{\Gamma}'\boldsymbol{T})^{o'}\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{T})^o)^-(\boldsymbol{\Gamma}'\boldsymbol{T})^{o'}\boldsymbol{\Gamma}'\boldsymbol{Y}_o\boldsymbol{P}_{C'}| \quad (25)$$

and equality holds if and only if

$$\boldsymbol{T}'\boldsymbol{\Gamma}(\boldsymbol{\Gamma}'\boldsymbol{S}_o\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}'(\boldsymbol{Y}_o\boldsymbol{P}_{C'}-\boldsymbol{T}\boldsymbol{\Psi}_2\boldsymbol{C})=\boldsymbol{0},$$

which is identical to (see Corollary 2)

$$\boldsymbol{T}'\boldsymbol{S}_o^+(\boldsymbol{Y}_o\boldsymbol{P}_{C'}-\boldsymbol{T}\boldsymbol{\Psi}_2\boldsymbol{C})=\boldsymbol{0}.$$

This is a consistent system of linear equations in $\boldsymbol{\Psi}_2$ and all solutions satisfy

$$\boldsymbol{T}\boldsymbol{\Psi}_2\boldsymbol{C}=\boldsymbol{T}(\boldsymbol{T}'\boldsymbol{S}_o^+\boldsymbol{T})^{-1}\boldsymbol{T}'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'}. \quad (26)$$

Note that the solutions are independent of the choice of $\boldsymbol{\Gamma}$ and that the inverse in (26) exists. Moreover, (25) is identical to

$$|\boldsymbol{D}_o^{-1}||\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o(\boldsymbol{H}_o'\boldsymbol{T})^o((\boldsymbol{H}_o'\boldsymbol{T})^{o'}\boldsymbol{D}_o(\boldsymbol{H}_o'\boldsymbol{T})^o)^-(\boldsymbol{H}_o'\boldsymbol{T})^{o'}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}| \quad (27)$$

which also is independent of $\boldsymbol{\Gamma}$. Now an appropriate linear combination of $\boldsymbol{\Psi}_1$ which is included in $\boldsymbol{T}$ will be estimated. Using (24) again, the relation in (27) will be manipulated, i.e. (27) is identical to

$$\begin{aligned}&|\boldsymbol{D}_o^{-1}||\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'}\\&\quad-\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{T}(\boldsymbol{T}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{T})^{-1}\boldsymbol{T}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}|. \quad (28)\end{aligned}$$

Let

$$\boldsymbol{F}=\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{T}(\boldsymbol{T}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{T})^{-1/2}, \quad (29)$$

where the square root is supposed to be symmetric. Then (28) can be written as

$$\begin{aligned}&|\boldsymbol{D}_o^{-1}||\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'}|\\&\quad\times|\boldsymbol{I}-\boldsymbol{F}'\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}(\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'})^{-1}\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1/2}\boldsymbol{F}|\\&=|\boldsymbol{D}_o^{-1}||\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'}|\\&\quad\times|\boldsymbol{F}'(\boldsymbol{I}-\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}(\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'})^{-1}\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1/2})\boldsymbol{F}|. \quad (30)\end{aligned}$$

Since (e.g. see Kollo and von Rosen 2005; Proposition 1.3.5) the following matrix

$$\begin{aligned}&\boldsymbol{I}-\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}(\boldsymbol{I}+\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'})^{-1}\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1/2}\\&\quad=(\boldsymbol{I}+\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1/2})^{-1}\end{aligned}$$

is positive definite and $\boldsymbol{F}$ is of full rank, Lemma 4 can be applied. Thus, a lower bound of (30) is given by

$$|\boldsymbol{D}_o^{-1}||\boldsymbol{I} + \boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{S}_o^{+}\boldsymbol{Y}_o\boldsymbol{P}_{C'}|\prod_{i=1}^{g}\delta_i, \tag{31}$$

where $\delta_1, \ldots, \delta_g$ ($g = f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o)$) are the g smallest eigenvalues of

$$(\boldsymbol{I}_r + \boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}\boldsymbol{Y}_o'\boldsymbol{H}_o\boldsymbol{D}_o^{-1/2})^{-1} \tag{32}$$

which do not depend on any unknown parameters. Therefore, we have to find an estimator of $\boldsymbol{\Psi}_1$ so that the lower bound is attained. Let

$$\widehat{\boldsymbol{F}} = (\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_g),$$

where $\{\boldsymbol{v}_i\}$ are the eigenvectors which correspond to the g eigenvalues $\{\delta_i\}$. If it is possible to solve the following non-linear equation in $\boldsymbol{\Psi}_1$, see Eq. (29),

$$\begin{aligned}\widehat{\boldsymbol{F}} &= \boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{T}\{\boldsymbol{T}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{T}\}^{-1/2} \\ &= \boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\{\boldsymbol{\Psi}_1'(\boldsymbol{A}'\boldsymbol{H}_o^o)^{o'}\boldsymbol{A}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1\}^{-1/2},\end{aligned} \tag{33}$$

there is chance to find an estimator of $\boldsymbol{\Psi}_1$ but it is known from the usual BRM that without any rank condition on $\boldsymbol{A}$ it is not possible to estimate $\boldsymbol{\Psi}_1$. The linear combinations

$$\boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\boldsymbol{\Psi}_1 = \boldsymbol{H}_o'\boldsymbol{T}$$

are, however, estimable and

$$\boldsymbol{H}_o'\boldsymbol{A}\widehat{(\boldsymbol{A}'\boldsymbol{H}_o^o)^o}\boldsymbol{\Psi}_1 = \boldsymbol{D}_o^{1/2}\widehat{\boldsymbol{F}} \tag{34}$$

which is verified by inserting this expression in (33) and using that the eigenvectors $\widehat{\boldsymbol{F}}$ are of unit length, i.e. $\widehat{\boldsymbol{F}}'\widehat{\boldsymbol{F}} = \boldsymbol{I}$. Note that $\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o$ is connected to the fact that we only consider $\boldsymbol{B}$ in (13) to be a function of $\boldsymbol{\Theta}_1$, and $\boldsymbol{H}_o'$ is used because we are now working with the random part of the model in (6). If $\boldsymbol{A} = \boldsymbol{I}$, the parameter $\boldsymbol{\Psi}_1$ is always estimable whereas if $\boldsymbol{\Sigma}$ is positive definite $\boldsymbol{A}\boldsymbol{\Psi}_1$ is always estimable and if additionally $r(\boldsymbol{A}) = q$, $\boldsymbol{\Psi}_1$ is estimable. Moreover, if $r((\boldsymbol{H}_o'\boldsymbol{A}^o)^o) = p - r$ then $\mathcal{C}(\boldsymbol{H}_o) \subseteq \mathcal{C}(\boldsymbol{A})$ and $\boldsymbol{\Psi}_1$ is estimable.

Proposition 1 *Let the model be defined in (1) with rank restrictions given by (2) and (3). If* $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma}) \neq \{\boldsymbol{0}\}$, $\boldsymbol{H}_o^{o'}\boldsymbol{A} \neq \boldsymbol{0}$, $\boldsymbol{H}_o'\boldsymbol{A} \neq \boldsymbol{0}$, $\mathcal{C}(\boldsymbol{X}_o) \subseteq \mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{\Sigma})$, $\mathcal{C}(\boldsymbol{X}_o'\boldsymbol{H}_o) \subseteq \mathcal{C}(\boldsymbol{C}')$ *and*

$$\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C} = \widehat{\boldsymbol{F}}'\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'},$$
$$\boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\widehat{\boldsymbol{\Psi}}_1 = \boldsymbol{D}_o^{1/2}\widehat{\boldsymbol{F}},$$

where $\boldsymbol{D}_o$, $\boldsymbol{Y}_o$ and $\widehat{\boldsymbol{F}}$ are presented in (4), (17) and (33), respectively, then

$$\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C} = \boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{P}_{C'} + \boldsymbol{D}_o^{1/2}\widehat{\boldsymbol{F}}\widehat{\boldsymbol{F}}'\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'}.$$

Motivation: First, we show the relation for $\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C}$. From (26), it follows that

$$\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C} = (\widehat{\boldsymbol{T}}'\boldsymbol{S}_o^+\widehat{\boldsymbol{T}})^{-1}\widehat{\boldsymbol{T}}'\boldsymbol{S}_o^+\boldsymbol{Y}_o\boldsymbol{P}_{C'} = (\widehat{\boldsymbol{T}}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\widehat{\boldsymbol{T}})^{-1}\widehat{\boldsymbol{T}}'\boldsymbol{H}_o\boldsymbol{D}_o^{-1}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{P}_{C'},$$

where according to (23) and (34) $\boldsymbol{H}_o'\widehat{\boldsymbol{T}} = \boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\widehat{\boldsymbol{\Psi}}_1 = \boldsymbol{D}_o^{1/2}\widehat{\boldsymbol{F}}$. A few calculations show that $\widehat{\boldsymbol{T}}'\boldsymbol{S}_o^+\widehat{\boldsymbol{T}} = \widehat{\boldsymbol{F}}'\widehat{\boldsymbol{F}} = \boldsymbol{I}_g$, $g = f - r(\boldsymbol{H}_o^{o'}\boldsymbol{X}_o)$ and $\widehat{\boldsymbol{T}}'\boldsymbol{S}_o^+\boldsymbol{Y}_o = \widehat{\boldsymbol{F}}'\boldsymbol{D}_o^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o$ which establish $\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C}$.

From (13), one can see that

$$\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C} = \boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{P}_{C'} + \boldsymbol{H}_o'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o)^o\widehat{\boldsymbol{\Psi}}_1\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C},$$

and using (34) together with $\widehat{\boldsymbol{\Psi}}_2\boldsymbol{C}$, presented above, implies the expression for $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$.

In Proposition 1, we have estimated $\boldsymbol{ABC}$ within the random part of the model. However, in most realistic situations we can make a stronger statement.

Proposition 2 *Assume that $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma})^\perp = \{0\}$, $r(\boldsymbol{A}) = q$ and $r(\boldsymbol{C}) = k$, and let the matrices be as in Proposition 1. Then $\boldsymbol{B}$ can be estimated using*

$$\widehat{\boldsymbol{B}} = (\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1} + (\boldsymbol{A}'\boldsymbol{H}_o\boldsymbol{H}_o'\boldsymbol{A})^{-1}\boldsymbol{A}'\boldsymbol{H}_o\boldsymbol{D}^{1/2}\widehat{\boldsymbol{F}}\widehat{\boldsymbol{F}}'\boldsymbol{D}^{-1/2}\boldsymbol{H}_o'\boldsymbol{Y}_o\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}.$$

Motivation: By assumption, it follows that $(\boldsymbol{A}'\boldsymbol{H}_o\boldsymbol{H}_o'\boldsymbol{A})^{-1}$ exists and therefore premultiplying $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ by $(\boldsymbol{A}'\boldsymbol{H}_o\boldsymbol{H}_o'\boldsymbol{A})^{-1}\boldsymbol{A}'\boldsymbol{H}_o$ establishes the statement.

The assumption $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma})^\perp = \{0\}$ in Proposition 2 is natural since inference about the mean parameters is connected to the random part of the model in (1).

Proposition 3 *Let the model be defined in (1) with rank restrictions given by (2) and (3). Assume that $\mathcal{C}(\boldsymbol{A}) \cap \mathcal{C}(\boldsymbol{\Sigma}) \neq \{\boldsymbol{0}\}$, $\boldsymbol{H}_o^{o'}\boldsymbol{A} \neq \boldsymbol{0}$, $\boldsymbol{H}_o'\boldsymbol{A} \neq \boldsymbol{0}$, $\mathcal{C}(\boldsymbol{X}_o) \subseteq \mathcal{C}(\boldsymbol{A}) + \mathcal{C}(\boldsymbol{\Sigma})$, $\mathcal{C}(\boldsymbol{X}_o'\boldsymbol{H}_o) \subseteq \mathcal{C}(\boldsymbol{C}')$ and $\boldsymbol{Y}_o$ is given in (17). The estimate $n\widehat{\boldsymbol{\Delta}}_o$ equals the diagonal matrix with the r smallest eigenvalues of $(\boldsymbol{Y}_o - \boldsymbol{H}_o\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C})()'$ on its main diagonal, and $\widehat{\boldsymbol{\Gamma}}_o$ is given by the eigenvectors of $(\boldsymbol{Y}_o - \boldsymbol{H}_o\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C})()'$ corresponding to the r eigenvalues, where $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ is presented in Proposition 1. Then*

$$n\widehat{\boldsymbol{\Sigma}} = \widehat{\boldsymbol{\Gamma}}_o\widehat{\boldsymbol{\Delta}}_o\widehat{\boldsymbol{\Gamma}}_o'.$$

Motivation: The result follows from (19), (20), (21) and the fact that $\boldsymbol{\Gamma}' = \boldsymbol{\Gamma}'(\boldsymbol{H}_o\boldsymbol{H}_o' + \boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}) = \boldsymbol{\Gamma}'\boldsymbol{H}_o\boldsymbol{H}_o'$. □

Theorem 2 *If choosing* $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ *as in Proposition 1 and* $\widehat{\boldsymbol{\Sigma}}$ *as in Proposition 3, the likelihood which corresponds to (6), with restrictions on* $\boldsymbol{B}$ *given by (7), is maximized.*

We end this section by studying $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ when $n \to \infty$. Firstly, it is observed that the "largest" eigenvalues of $\frac{1}{n}\boldsymbol{S}$ converge in probability to the non-zero eigenvalues of $\boldsymbol{\Sigma}$ which for simplicity are supposed to be of multiplicity 1. Moreover, the corresponding eigenvectors of $\frac{1}{n}\boldsymbol{S}$ which correspond to $\boldsymbol{H}_o$ converge to $\boldsymbol{\Gamma}$. We will not be able to say anything about $\boldsymbol{H}^o$ and therefore in our expressions, $\boldsymbol{H}_o^o$ is kept and not replaced by any random variable. To show that the eigenvectors converge, it can be noted that $\boldsymbol{S} = \boldsymbol{Z}\boldsymbol{Z}'$, for $\boldsymbol{Z} \sim N_{p,n-r(\boldsymbol{C})}(\boldsymbol{0}, \boldsymbol{\Sigma}, \boldsymbol{I})$, $r(\boldsymbol{Z}) = r$, and then its density which is defined on a subspace (see Srivastava and Khatri, p. 43) can be used. Based on this density, $\boldsymbol{D}$ and $\boldsymbol{H}$ ($\boldsymbol{D}$ and $\boldsymbol{H}$ correspond to $\boldsymbol{D}_o$ and $\boldsymbol{H}_o$) are maximum likelihood estimators and therefore they are also consistent. Hence, in probability,

$$\boldsymbol{H} \to \boldsymbol{\Gamma}, \qquad \tfrac{1}{n}\boldsymbol{D} \to \boldsymbol{\Delta}.$$

Now we study what happens with the random version of $\boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ (which will be called $\boldsymbol{H}'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$):

$$\begin{aligned}\boldsymbol{H}'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C} = {} & \boldsymbol{H}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{P}_{C'} \\ & + \boldsymbol{D}^{1/2}\widehat{\boldsymbol{F}}\widehat{\boldsymbol{F}}'\boldsymbol{D}^{-1/2}\boldsymbol{H}'\boldsymbol{Y}\boldsymbol{P}_{C'}, \end{aligned} \tag{35}$$

where $\boldsymbol{Y}$ is given by (18) and now $\widehat{\boldsymbol{F}}$ is a random variable. The crucial point is to observe that the random version of (32) converges to $\boldsymbol{I}_r$. This holds since $\sqrt{n}\boldsymbol{D}^{-1/2} \to \boldsymbol{\Delta}^{-1/2}$ and $n^{-1}\boldsymbol{Y}\boldsymbol{P}_{C'}\boldsymbol{Y}' \to \boldsymbol{0}$ in probability, under some mild assumptions on $\boldsymbol{C}$, which are supposed to hold. Therefore, the eigenvalues of (32) converge to 1. Since $\widehat{\boldsymbol{F}}\widehat{\boldsymbol{F}}'$ is an eigenprojector, we will construct our result so that its limit also is an eigenprojector. Thus, $\widehat{\boldsymbol{F}} \to (\boldsymbol{I}_g : \boldsymbol{0})'$, in probability, implying the result

$$\widehat{\boldsymbol{F}}\widehat{\boldsymbol{F}}' \to \begin{pmatrix} \boldsymbol{I}_g & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}, \qquad \widehat{\boldsymbol{F}}'\widehat{\boldsymbol{F}} = \boldsymbol{I}_g,$$

where obviously $\begin{pmatrix} \boldsymbol{I}_g & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}$ is a projector.

Theorem 3 *The expression* $\boldsymbol{H}'\boldsymbol{A}\widehat{\boldsymbol{B}}\boldsymbol{C}$ *in (35) is asymptotically equivalent to*

$$\boldsymbol{\Gamma}'\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{A})^+\boldsymbol{A}'\boldsymbol{H}_o^o\boldsymbol{H}_o^{o'}\boldsymbol{X}_o\boldsymbol{P}_{C'} + \begin{pmatrix} \boldsymbol{I}_g & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}\boldsymbol{\Gamma}'\boldsymbol{Y}\boldsymbol{P}_{C'}$$

which is normally distributed.

A final remark is that if assuming $\boldsymbol{H}_o^o = \boldsymbol{0}$, i.e. $\boldsymbol{\Sigma}$ is positive definite, then the estimates in Propositions 1 and 3 for $\boldsymbol{B}$ and $\boldsymbol{\Sigma}$ under rank restrictions on $\boldsymbol{B}$ are identical to known estimates of the parameters of the growth curve model with rank restrictions on $\boldsymbol{B}$.

5 Illustrations

Example 1 Firstly, we present a small simulation study showing that our estimators make sense. Since $\boldsymbol{B}$ with rank restrictions is difficult to interpret, the focus will be on prediction, i.e. $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1} = \boldsymbol{H}_o'\boldsymbol{A}\widehat{\boldsymbol{B}}$ will be considered, and is obtained from Proposition 1. Note that for small n, there is rather much variation in $\boldsymbol{H}_o$. It is not obvious how to evaluate $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}$, but we have decided to compare $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ with $\boldsymbol{H}_o'\boldsymbol{P}_A\boldsymbol{X}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ which for a fixed $\boldsymbol{H}_o$ is an unbiased estimator of $\boldsymbol{H}_o'\boldsymbol{A}\boldsymbol{B}$, irrespectively if there exist rank restrictions on $\boldsymbol{B}$ or there are no rank restrictions.

Let

$$\boldsymbol{A} = \begin{pmatrix} 1 & 8 & 64 \\ 1 & 10 & 100 \\ 1 & 12 & 144 \\ 1 & 14 & 196 \end{pmatrix}, \quad \boldsymbol{B} = \begin{pmatrix} 17.1 & 37.1 & 34.2 \\ 0.54 & 0.23 & 1.08 \\ -0.003 & 0.0020 & -0.006 \end{pmatrix},$$

$$\boldsymbol{C} = \left(\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \boldsymbol{1}_{10}' : \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \boldsymbol{1}_9' : \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \boldsymbol{1}_8' \right), \quad \boldsymbol{\Sigma}_0 = \begin{pmatrix} 5.1 & 2.4 & 3.6 & 2.5 \\ & 3.9 & 2.7 & 3.1 \\ & & 6.0 & 3.8 \\ & & & 4.6 \end{pmatrix}.$$

This means that we have a growth curve model with polynomial growth of order two and three groups, respectively, consisting of 10, 9 and 8 independent observations. Data were generated from the model $\boldsymbol{X} = \boldsymbol{A}\boldsymbol{B}\boldsymbol{C} + \boldsymbol{E}$, where $\boldsymbol{E} \sim N_{p,27}(\boldsymbol{0}, \boldsymbol{\Sigma}, \boldsymbol{I}_{27})$ and $\boldsymbol{\Sigma} = \boldsymbol{H}\boldsymbol{D}\boldsymbol{H}'$, where $\boldsymbol{D}$ is a diagonal matrix which consists of the three largest eigenvalues of $\boldsymbol{\Sigma}_0$ and $\boldsymbol{H}$ is the matrix of corresponding eigenvectors. Thus $r(\boldsymbol{\Sigma}) = 3$. Note that the third column of $\boldsymbol{B}$ equals two times its first column, meaning that the rank of $\boldsymbol{B}$ equals 2. Then 1000 simulations took place and $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ was compared to $\boldsymbol{H}_o'\boldsymbol{P}_A\boldsymbol{X}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$, where $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ follows from Proposition 1. Since the size of these matrices is 3×3, there are nine elements which are to be compared. The results of the simulation study are presented in Table 1. One conclusion is that there is almost no difference between the two estimators besides that $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ is of rank equal to two and the other estimator is of rank three. Thus, we can conclude that our approach makes sense from a point of view that even in small samples the estimators seem to be appropriate.

Example 2 Now we turn to the real data example utilized by Albert and Kshirsagar (1993) which was mentioned in the introduction. Group averages for potassium values are plotted separately for each group of dogs in Fig. 1.

The $\boldsymbol{A}$ and $\boldsymbol{C}$ matrices equal

Table 1 Let $\boldsymbol{p} = \mathrm{vec}(\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1})$ and p_i be the ith element of $\boldsymbol{p}$. Correspondingly, let $\boldsymbol{q} = \mathrm{vec}(\boldsymbol{H}_o'\boldsymbol{P}_A\boldsymbol{X}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1})$ and let q_i be the ith element of $\boldsymbol{q}$

	p_1	q_1	p_2	q_2	p_3	q_3	p_4	q_4	p_5	q_5
Mean	44.6	44.6	78.5	78.4	89.1	89.2	4.54	4.53	8.08	8.09
Std	1.4	1.4	1.8	1.8	1.9	1.9	3.6	3.7	6.0	6.0
Min	39.7	39.8	70.1	69.9	80.3	80.3	−1.9	−2.4	−1.6	−1.7
Max	39.7	48.2	83.9	84.3	94.7	94.8	19.4	19.0	34.6	34.6
	p_6	q_6	p_7	q_7	p_8	q_8	p_9	q_9		
Mean	9.08	9.08	4.61	4.56	8.68	8.79	9.22	9.14		
Std	7.3	7.4	3.6	3.6	6.2	6.2	7.2	7.2		
Min	−3.7	−4.7	−1.9	−2.5	−1.6	−1.5	−3.8	−3.9		
Max	38.7	38.9	20.3	20.1	35.7	35.8	40.7	40.9		

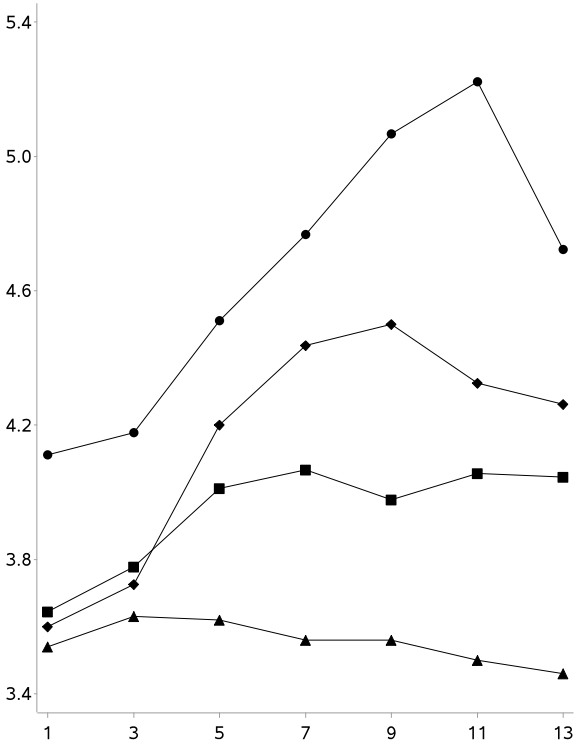

Fig. 1 The dogs' data used in Grizzle and Allen (1969) and Albert and Kshirsagar (1993) are presented. Each line corresponds to one group of dogs where the average values are plotted over time

$$\boldsymbol{A} = \begin{pmatrix} 0.378 & -0.567 & 0.546 & -0.408 \\ 0.378 & -0.378 & 0 & 0.408 \\ 0.378 & -0.189 & -0.327 & 0.40 \\ 0.378 & 0 & -0.436 & 0 \\ 0.378 & 0.189 & -0.327 & -0.408 \\ 0.378 & 0.378 & 0 & -0.408 \\ 0.378 & 0.567 & 0.546 & 0.408 \end{pmatrix}$$

$$\boldsymbol{C} = \left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{1}_9' : \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{1}_{10}' : \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{1}_8' : \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \otimes \mathbf{1}_9' \right).$$

We will assume that $r(\boldsymbol{\Sigma})$ equals 7, 6 or 5. When $r(\boldsymbol{\Sigma}) = 7$, i.e. the dispersion matrix is of full rank, Albert and Kshirsagar (1993) developed a testing strategy to decide about the rank of $\boldsymbol{B}$. We will compare four models by assuming

$$r(\boldsymbol{\Sigma}) = 7, r(\boldsymbol{B}) = 4; r(\boldsymbol{\Sigma}) = 7, r(\boldsymbol{B}) = 1; r(\boldsymbol{\Sigma}) = 6, r(\boldsymbol{B}) = 2 \text{ or } r(\boldsymbol{\Sigma}) = 5, r(\boldsymbol{B}) = 3.$$

The first case is a model without any rank restrictions. In the second alternative, we only have rank restrictions on the mean parameters, which was the case treated by Albert and Kshirsagar (1993), and for the other two cases we have rank restrictions on both the mean parameters and the dispersion matrix. As in the simulation study (Example 1), we will compare it with $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ where the choice of $\boldsymbol{H}_o$ depends on $r(\boldsymbol{\Sigma})$, in particular the length of the column in $\boldsymbol{H}_o$ depends on the rank assumption. Moreover, it is impossible to present all elements in $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ and therefore the focus will be on the first and last rows of $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ of which each consists of four elements. Table 2 shows similar prediction values for the different models. For the last row, i.e. p_{l1}–p_{l4}, some differences appear but it should not be forgotten that different $\boldsymbol{H}_o$ matrices are used in the different models so these minor differences are not unexpected.

Thus, as with the simulation study, we find an agreement between existing methods and our new approach where rank restrictions on the mean are combined with

Table 2 Let $p_{ij} = (\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1})_{ij}$, $i = 1, l$, (l stands for the last row), $j = 1, 2, 3, 4$, where $\boldsymbol{H}_o'\widehat{\boldsymbol{X}}\boldsymbol{C}'(\boldsymbol{C}\boldsymbol{C}')^{-1}$ follows from Proposition 1

	p_{11}	p_{12}	p_{13}	p_{14}	p_{l1}	p_{l2}	p_{l3}	p_{l4}
$r(\boldsymbol{\Sigma}) = 7, r(\boldsymbol{B}) = 4$	12.3	9.2	10.7	10.1	−0.003	0.06	0.07	0.1
$r(\boldsymbol{\Sigma}) = 7, r(\boldsymbol{B}) = 1$	11.7	10.0	10.3	10.3	0.09	0.08	0.08	0.08
$r(\boldsymbol{\Sigma}) = 6, r(\boldsymbol{B}) = 2$	12.4	9.3	10.6	10.0	0.7	0.6	0.7	0.7
$r(\boldsymbol{\Sigma}) = 5, r(\boldsymbol{B}) = 3$	11.9	10.2	10.2	10.0	0.1	0.2	0.3	0.3

rank restrictions on the dispersion. Moreover, if p is large, those existing methods mentioned above cannot be used because the dispersion matrix cannot be estimated and $\boldsymbol{S}$ cannot be inverted which in our approach can take place. Therefore, we believe that it is worth continuing to study the new approach presented in this article.

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Limiting Canonical Distribution of Two Large-Dimensional Random Vectors

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Abstract In multivariate analysis, canonical correlation analysis is a powerful tool to deal with the relationship between two random vectors. In this paper, we establish a functional relation between the sample canonical correlation matrix and a special noncentral Fisher matrix. And under the large-dimensional setting, i.e., the dimensions of the random vectors tend to infinity proportionally to the sample size, we develop a phase transition and a central limit theorem for the sample spiked eigenvalues of the noncentral Fisher matrix. By these results, we further derive the limits and fluctuations of the sample canonical correlation coefficients.

Keywords Canonical correlation analysis · Noncentral fisher matrix · Spiked eigenvalues · Central limit theorem

1 Introduction

Canonical correlation analysis (CCA) is one of the most classical and important tools in multivariate statistics, which has been widely used in various fields to explore the

Dedicated to the great statistician C. R. Rao on his 100th birthday.

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relation between two sets of variables measured on the sample. The basic theory of CCA was initiated by Hotelling (1936). Under the condition that the dimensions of the random vectors are fixed and the sample size tend to infinity, Hsu (1941) presented the limiting distribution of the sample canonical correlations, which can be used to evaluate the population canonical coefficients.

However, rapid development of modern technology necessitates statistical inference on high-dimensional data in many scientific fields, such as image processing, genetic engineering, signal processing, microarray, finance, and economics. A consensus amongst the statisticians is that the classical statistical inferences need to be re-examined when they meet high-dimensional data. So far, there are only a handful of works to the high-dimensional CCA. By extended Fisher's z-transformation, Fujikoshi and Sakurai (2009) concluded the asymptotic distributions of the canonical correlation coefficients and their asymptotic expansions under the condition that one dimension of the two random vectors tends to infinity proportionally to the sample size while the other dimension is fixed. The above results are based on that the population eigenvalues are distinguished with each other. Later, under the same assumptions in Fujikoshi and Sakurai (2009) except the multiplicities the population characteristic roots greater than unity, Fujikoshi (2016) obtained the asymptotic distributions of the canonical correlation coefficients. Gao et al. (2015, 2017) focused on the sparse CCA. The former introduced a method to estimate the leading canonical correlation directions and the latter considered adaptive minimax and computationally tractable estimation of leading sparse canonical coefficient vectors. Han et al. (2018) proposed a unified matrix model and got asymptotic distributions of the maximum eigenvalues of it. In this model, the authors transformed the unified matrix into a canonical correlation matrix by selecting a certain matrix. Johnstone and Onatski (2015) derived the asymptotic properties of the likelihood ratio processes of CCA. Recently, Bao et al. (2019) investigated the asymptotic behavior of the sample canonical correlation coefficients under the assumption that the rank of the population canonical correlation matrix is finite.

In this paper, we will establish a relationship between the sample canonical correlation matrix and a special noncentral spiked Fisher matrix. Actually, the central spiked matrix has been widely investigated since Johnstone (2001) proposed the spiked model with the application for principal component analysis (PCA). Baik and Silverstein (2006) proved the almost sure version of phase transition phenomena about the limits of the sample spiked eigenvalues. Paul (2007) considered the central limit theorem (CLT) for the sample spiked eigenvalues under the Gaussian assumption, and Bai and Yao (2008, 2012) obtained the CLT for the spiked eigenvalues under the moment assumptions. Under more general assumption, Cai et al. (2017) and Jiang and Bai (2018) improved these results under some more general assumption. For two samples case, Wang and Yao (2017) proposed the concept of spiked Fisher matrix and established the phase transition phenomena and CLT for the extreme eigenvalues. Based on Zheng et al. (2017), Jiang et al. (2019) proposed a concept of the general spiked Fisher matrix. Then, Jiang et al. (2019) derived the CLT for the sample spiked eigenvalues of the general spiked Fisher matrix.

It's remarkable that all the results introduced above mainly focused on the central sample covariance matrix or central Fisher matrix. The works devoted to the noncentral sample covariance matrix or noncentral Fisher matrix are relatively limit. Dozier and Silverstein (2007) accomplished the global spectral properties of the information-plus-noise type matrix, which can be viewed as a noncentral sample covariance matrix. Bodnar et al. (2019) derived the CLT for linear spectral statistics of large-dimensional noncentral Fisher matrices under normality assumption.

In this paper, we build a bridge between sample canonical correlation coefficients and the eigenvalues of a special noncentral Fisher matrix. Then via establishing a phase transition and a CLT for the sample spiked eigenvalues of this kind of noncentral Fisher matrix, we derive the limits and fluctuations of the sample canonical correlation coefficients under high-dimensional setting. One of the contributions of this paper is using a different approach from Bao et al. (2019), but obtaining the same results, such as limits and fluctuations of the extreme sample canonical correlation coefficients.

To guarantee the coherence and readability of this paper, we introduce some essential concepts here. For any $n \times n$ matrix $\mathbf{A}_n$ with only real eigenvalues, let F_n be the *empirical spectral distribution* (ESD) function of $\mathbf{A}_n$, that is,

$$F_n(x) = \frac{1}{n} Card\{i; \lambda_i^{\mathbf{A}_n} \leq x\},$$

where $\lambda_i^{\mathbf{A}_n}$ denotes the i-th largest eigenvalue of $\mathbf{A}_n$. If $F^{\mathbf{A}_n}$ has a limiting distribution F, then we call it the *limiting special distribution* (LSD) of sequence $\{\mathbf{A}_n\}$. For any function of bounded variation G on the real line, its *Stieltjes transform* is defined by

$$m(z) = \int \frac{1}{\lambda - z} dG(\lambda), \quad z \in \mathbb{C}^+.$$

The rest of the paper is organized as follows. In Sect. 2, we give some preliminaries and show the relationship between the eigenvalues of the sample canonical correlation matrix and the noncentral Fisher matrix. In Sects. 3 and 4, we present the limits and fluctuations of spiked eigenvalues of the noncentral sample covariance matrix and noncentral Fisher matrix, respectively. In Sect. 5, we derive the limits and fluctuations of the sample canonical correlation matrix. All the technical proofs are presented in Sect. 6.

2 A Functional Relationship

Let $\mathbf{z}_i = (\mathbf{x}_i^T, \mathbf{y}_i^T)^T, i = 1, \ldots, n$, be independent observations from a $(p+q)$-dimensional normal distribution with mean zero and covariance matrix

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{xx} & \mathbf{\Sigma}_{xy} \\ \mathbf{\Sigma}_{yx} & \mathbf{\Sigma}_{yy} \end{pmatrix}, \tag{1}$$

where $\mathbf{x}_i$ and $\mathbf{y}_i$ are p-dimensional and q-dimensional vectors with the population covariance matrices $\mathbf{\Sigma}_{xx}$ and $\mathbf{\Sigma}_{yy}$, respectively. Without loss of generality, we assume that $p \leq q$. Define the corresponding sample covariance matrix of as

$$\boldsymbol{S}_n = \frac{1}{n} \sum_{i=1}^{n} z_i z_i^T \tag{2}$$

which can be formed as

$$\boldsymbol{S}_n = \begin{pmatrix} \boldsymbol{S}_{xx} & \boldsymbol{S}_{xy} \\ \boldsymbol{S}_{yx} & \boldsymbol{S}_{yy} \end{pmatrix} = \frac{1}{n} \begin{pmatrix} \boldsymbol{X}\boldsymbol{X}^T & \boldsymbol{X}\boldsymbol{Y}^T \\ \boldsymbol{Y}\boldsymbol{X}^T & \boldsymbol{Y}\boldsymbol{Y}^T \end{pmatrix} \tag{3}$$

with

$$\boldsymbol{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)_{p \times n}, \quad \boldsymbol{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_n)_{q \times n}, \tag{4}$$

In the sequel, $\mathbf{\Sigma}_{xx}^{-1} \mathbf{\Sigma}_{xy} \mathbf{\Sigma}_{yy}^{-1} \mathbf{\Sigma}_{yx}$ is called as the population canonical correlation matrix and its eigenvalues are denoted as

$$1 > \rho_1^2 \geq \rho_2^2 \geq \cdots \geq \rho_p^2. \tag{5}$$

According to Theorem 12.2.1 of Anderson (2003), the nonnegative square roots $\rho_1, \ldots, \rho_p$ are the population canonical correlation coefficients. Correspondingly, we call $\mathbf{S}_{xx}^{-1} \mathbf{S}_{xy} \mathbf{S}_{yy}^{-1} \mathbf{S}_{yx}$ the sample canonical correlation matrix and its eigenvalues are denoted by

$$\lambda_1^2 \geq \lambda_2^2 \geq \cdots \geq \lambda_p^2. \tag{6}$$

By the singular value decomposition, we have that

$$\mathbf{\Sigma}_{xx}^{-\frac{1}{2}} \mathbf{\Sigma}_{xy} \mathbf{\Sigma}_{yy}^{-\frac{1}{2}} = \mathbf{P}_1 \mathbf{\Lambda} \mathbf{P}_2^T, \tag{7}$$

where

$$\mathbf{\Lambda} = \begin{pmatrix} \mathbf{\Lambda}_{11} & \mathbf{0}_{12} \end{pmatrix},$$

$\mathbf{\Lambda}_{11} = \text{diag}(\rho_1, \rho_2, \ldots, \rho_p)$, $\mathbf{0}_{12}$ is a $p \times (q - p)$ zero matrix, $\mathbf{P}_1$ and $\mathbf{P}_2$ are orthogonal matrix with size $p \times p$ and $q \times q$, respectively. It follows that $\rho_1^2, \rho_2^2, \ldots, \rho_p^2$ are also the eigenvalues of the diagonal matrix $\mathbf{\Lambda}\mathbf{\Lambda}^T$.

Inspired by Johnstone and Nadler (2017) and Jiang et al. (2013), we find $\lambda_i^2/(1 - \lambda_i^2)$ happen to be the eigenvalues of a special noncentral Fisher matrix, the detailed

presentation is postponed in next section. Before that we need some preliminaries. Define the population

$$\tilde{\mathbf{z}} = \begin{pmatrix} \tilde{\mathbf{x}} \\ \tilde{\mathbf{y}} \end{pmatrix} = \begin{pmatrix} \mathbf{P}_1^T & 0 \\ 0 & \mathbf{P}_2^T \end{pmatrix} \begin{pmatrix} \boldsymbol{\Sigma}_{xx}^{-\frac{1}{2}} & 0 \\ 0 & \boldsymbol{\Sigma}_{yy}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}, \tag{8}$$

then

$$\mathrm{Cov}\,(\tilde{\mathbf{z}}) = \begin{pmatrix} \mathbf{I}_p & \boldsymbol{\Lambda} \\ \boldsymbol{\Lambda}^T & \mathbf{I}_q \end{pmatrix}.$$

Let

$$\tilde{\mathbf{x}}_i = \boldsymbol{\Lambda}\tilde{\mathbf{y}}_i + \boldsymbol{\Gamma}\tilde{\mathbf{w}}_i \quad i = 1, \ldots, n, \tag{9}$$

where $\tilde{\mathbf{w}}_i \overset{i.i.d}{\sim} \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ independent of $\tilde{\mathbf{y}}_i$ and $\boldsymbol{\Gamma}$ satisfies

$$\boldsymbol{\Gamma}^2 = \mathbf{I}_p - \boldsymbol{\Lambda}\boldsymbol{\Lambda}^T = \mathbf{I}_p - \boldsymbol{\Lambda}_{11}\boldsymbol{\Lambda}_{11}^T.$$

Let

$$\boldsymbol{\Delta}\boldsymbol{\Delta}^T = \widetilde{\mathbf{Y}}^T(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{-1}\widetilde{\mathbf{Y}}, \quad \boldsymbol{\Theta}\boldsymbol{\Theta}^T = \mathbf{I}_n - \widetilde{\mathbf{Y}}^T(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{-1}\widetilde{\mathbf{Y}}, \tag{10}$$

where

$$\widetilde{\mathbf{X}} = (\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_n)_{p\times n}, \quad \widetilde{\mathbf{Y}} = (\tilde{\mathbf{y}}_1, \ldots, \tilde{\mathbf{y}}_n)_{q\times n}, \quad \widetilde{\mathbf{W}} = (\tilde{\mathbf{w}}_1, \ldots, \tilde{\mathbf{w}}_n)_{p\times n},$$

$\boldsymbol{\Delta}$ and $\boldsymbol{\Theta}$ are $n \times q$ and $n \times (n-q)$ matrices, respectively. Now let $\mathbf{B} = \widetilde{\mathbf{W}}\boldsymbol{\Delta}$, $\mathbf{C} = \widetilde{\mathbf{W}}\boldsymbol{\Theta}$ and

$$\widetilde{S}_1 = \frac{1}{q}(\boldsymbol{\Gamma}^{-1}\boldsymbol{\Lambda}(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2}+\mathbf{B})((\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2}\boldsymbol{\Lambda}^T\boldsymbol{\Gamma}^{-1}+\mathbf{B}^T), \tag{11}$$

$$\widetilde{S}_2 = \frac{1}{n-q}\mathbf{C}\mathbf{C}^T. \tag{12}$$

Apparently, $\mathbf{B}$ and $\mathbf{C}$ are independent random matrices with i.i.d standard normal entries. Because the distributions of $\mathbf{B}$ and $\mathbf{C}$ are independent of $\widetilde{\mathbf{Y}}$, the matrices $\mathbf{B}$ and $\mathbf{C}$ are independent of $\widetilde{\mathbf{Y}}$. According to Dozier and Silverstein (2007), the matrix $\widetilde{S}_1$ defined in (11) can be viewed as an information-plus-noise type matrix conditional on $\widetilde{\mathbf{Y}}$, which also can be reguareded as a noncentral sample covariance matrix. Denote $\widehat{\mathbf{Y}}$ be the first p rows of $\widetilde{\mathbf{Y}}$, $\mathbf{T} = \boldsymbol{\Gamma}^{-1}\boldsymbol{\Lambda}_{11}$ and

$$\boldsymbol{\Xi} := \frac{1}{q}\boldsymbol{\Gamma}^{-1}\boldsymbol{\Lambda}\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T\boldsymbol{\Lambda}^T\boldsymbol{\Gamma}^{-1} = \frac{1}{q}\boldsymbol{\Gamma}^{-1}\boldsymbol{\Lambda}_{11}\widehat{\mathbf{Y}}\widehat{\mathbf{Y}}^T\boldsymbol{\Lambda}_{11}\boldsymbol{\Gamma}^{-1} = \frac{n}{q}\mathbf{T}(n^{-1}\widehat{\mathbf{Y}}\widehat{\mathbf{Y}}^T)\mathbf{T}^T \tag{13}$$

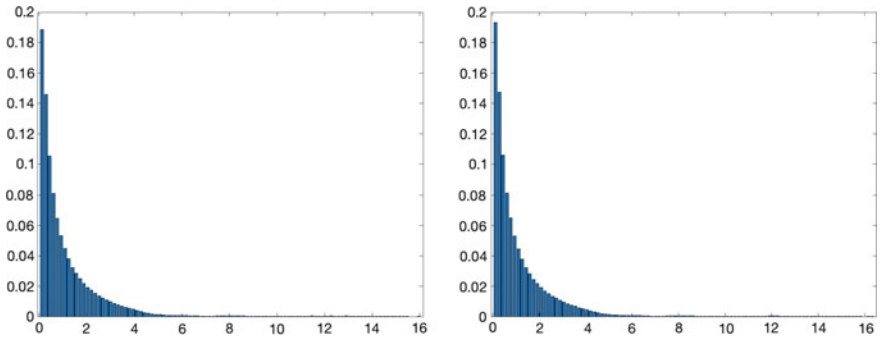

Fig. 1 Comparison of the ESD of $\mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}(\mathbf{I}_p - \mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx})^{-1}$ (the left panel) and $\boldsymbol{F}(\boldsymbol{\Xi})/k_{n,q}$ (the right panel) with $(\rho_1^2, \rho_2^2, \ldots, \rho_5^2, \ldots, \rho_p^2) = (0.8, 0.7, \ldots, 0.4, 0, \ldots, 0)$, $(p, q, n) = (200, 600, 1000)$

be the noncentral parameter matrix, then we have the noncentral Fisher matrix

$$\boldsymbol{F}(\boldsymbol{\Xi}) := \widetilde{\mathbf{S}}_1\widetilde{\mathbf{S}}_2^{-1}. \tag{14}$$

We are now in a position to form the functional relationship between the eigenvalues of sample canonical correlation matrix and that of the noncentral Fisher matrix (14). Before describing the theorem, we make the following assumption throughout the work.

Assumption 1 Assume that $(\mathbf{x}_i^T, \mathbf{y}_i^T)^T$, $i = 1, \ldots, n$, is a sample of i.i.d. observations from a $(p+q)$-dimensional normal distribution with mean zero and covariance matrix $\boldsymbol{\Sigma}$ defined in (1).

Theorem 1 *Suppose that λ_i^2, $i = 1, \ldots, p$, are the ordered eigenvalues of the sample canonical correlation matrix $\mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}$. Then, under Assumption 1, there exists a noncentral Fisher matrix $\boldsymbol{F}(\boldsymbol{\Xi})$, such that $l_i = \frac{(n-q)\lambda_i^2}{q(1-\lambda_i^2)}$, $i = 1, \ldots, p$, where l_i are the ordered eigenvalues of $\boldsymbol{F}(\boldsymbol{\Xi})$.*

To illustrate Theorem 1, we present a numerical result. In this simulation, we compare the ESD between $\mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}(\mathbf{I}_p - \mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx})^{-1}$ and $\boldsymbol{F}(\boldsymbol{\Xi})/k_{n,q}$ with 3000 realizations. According to Fig. 1, we find the ESD of them are almost identical.

Remark 1 In the sequel, we denote $k_{n,q} := n/q - 1$ and the functional relationship between the eigenvalues of $\mathbf{S}_{xx}^{-1}\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}$ and the noncentral Fisher matrix be

$$l_i := g(\lambda_i^2) = k_{n,q} \cdot \frac{\lambda_i^2}{1-\lambda_i^2} \quad i = 1, \ldots, p. \tag{15}$$

Note that the function g is strictly increasing. Hence, the limits and fluctuations of the sample canonical correlation coefficients λ_i can be obtained by that of the eigenvalues of the noncentral Fisher matrix.

3 Fluctuations for the Eigenvalues of $\widetilde{S}_1$

Throughout the paper, we consider the following assumptions about the high-dimensional setting and the spiked structure.

Assumption 2 Assume that as $\min(p, q, n) \to \infty$, $c_{1n} := p/n \to c_1 \in (0, 1)$, $c_{2n} := q/n \to c_2 \in (0, 1)$ and $c_1 + c_2 < 1$.

Assumption 3 Assume that ρ_i^2, $i = 1, \ldots, p$, are the ordered eigenvalues of the diagonal matrix $\mathbf{\Lambda}\mathbf{\Lambda}^T$, satisfying

$$\rho_1^2 = \cdots = \rho_{m_1}^2 > \rho_{m_1+1}^2 = \cdots = \rho_{m_1+m_2}^2 > \cdots > \rho_{\sum_{i=1}^{K-1} m_i+1}^2 = \cdots = \rho_M^2 > 0,$$

and

$$a_k = \rho_{m_{k-1}+1}^2 = \cdots = \rho_{m_{k-1}+m_k}^2, \quad k \in \{1, \ldots, K\},$$

where $M = \sum_{i=1}^K m_i$ is a fixed positive integer with convention $m_0 = 0$. In addition, we assume that there exits $\epsilon > 0$, a constant independent of n, such that $\rho_1^2 < 1 - \epsilon$, $\rho_M^2 > \epsilon$, for any $1 \le i < K$, $\rho_{m_{i+1}}^2 - \rho_{m_i}^2 > \epsilon$, and for all $i > M$, $\rho_i = 0$.

In the following, we discuss the CLT for the sample spiked eigenvalues of $\widetilde{S}_1$ defined in (11), that is

$$\widetilde{S}_1 = (\mathbf{\Xi}_{1/2} + q^{-1/2}\mathbf{B})(\mathbf{\Xi}_{1/2} + q^{-1/2}\mathbf{B})^T, \tag{16}$$

where $\mathbf{\Xi}_{1/2} := q^{-1/2}\mathbf{\Gamma}^{-1}\mathbf{\Lambda}(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2}$. Before that, we first introduce some known results for the spiked eigenvalues of $\mathbf{\Xi}$.

By the definition of $\mathbf{T}$ in (13) and Assumption 3, we denote the eigenvalues of $\frac{n}{q}\mathbf{T}\mathbf{T}^T$ be

$$a_1^{\mathbf{T}} > a_2^{\mathbf{T}} > \cdots > a_K^{\mathbf{T}} > 0, \tag{17}$$

with multiplicity m_k, $k = 1, \ldots, K$, respectively. Thus, we have that $m_1 + \cdots + m_K = M$ and

$$a_k^{\mathbf{T}} = \frac{n}{q} \cdot \frac{\rho_{j_k}^2}{1 - \rho_{j_k}^2}, \quad k = 1, \ldots, K, \tag{18}$$

where $j_k = \sum_{i=0}^{k-1} m_i + 1$.

In addition, we denote the eigenvalues of $\mathbf{\Xi}$ be

$$l_1^{\mathbf{\Xi}} \geq l_2^{\mathbf{\Xi}} \geq \cdots \geq l_M^{\mathbf{\Xi}}. \tag{19}$$

Here one should note that $a_k^{\mathbf{T}}, k = 1, \ldots, K$, are constant but $l_i^{\mathbf{\Xi}}, i = 1, \ldots, M$, are random variables. For the phase transition of the spiked eigenvalues of the noncentral parameter matrix $\mathbf{\Xi}$, by the law of large numbers we have the following lemma.

Lemma 1 *Suppose Assumptions 1–3 hold. For any* $j \in \mathcal{J}_k := \{j_k + 1, \ldots, j_k + m_k\}$, *we have that*

$$\frac{l_j^{\mathbf{\Xi}}}{a_k^{\mathbf{T}}} \xrightarrow{a.s.} 1. \tag{20}$$

In the following, we will present the CLT for the sample spiked eigenvalues, which can be verified from Lindeberg-Feller CLT easily.

Lemma 2 *If Assumptions 1–3 hold, then the* m_k*-dimensional random vector*

$$\boldsymbol{\gamma}_k^{\mathbf{\Xi}} = \sqrt{n}\left\{\frac{l_i^{\mathbf{\Xi}}}{a_k^{\mathbf{T}}} - 1, \quad i \in \mathcal{J}_k\right\}$$

converges weakly to the joint distribution of the m_k *eigenvalues of random matrix*

$$\mathbf{\Omega} := \left(\omega_{ij}\right)_{m_k \times m_k},$$

where $\mathbf{\Omega}$ *is a Gaussian Orthogonal Ensemble (GOE), i.e., an* m_k*-dimensional symmetric Gaussian random matrix with independent (up to symmetry) entries* $\omega_{ii} \sim N(0, 2)$ *and* $\omega_{ij} \sim N(0, 1)$ *for* $i \neq j$.

Denote the ordered eigenvalues of $\widetilde{\boldsymbol{S}}_1$ be

$$l_1^{\widetilde{\boldsymbol{S}}_1} \geq l_2^{\widetilde{\boldsymbol{S}}_1} \geq \cdots \geq l_p^{\widetilde{\boldsymbol{S}}_1}. \tag{21}$$

Then we have the following limits for these eigenvalues.

Theorem 2 *Suppose that Assumptions 1–3 hold. For any* $k \in \{1, \ldots, K\}$ *satisfying* $\lim_{n\to\infty} a_k^{\mathbf{T}} > \sqrt{c_1/c_2}$, *we have that*

$$\frac{l_j^{\widetilde{\boldsymbol{S}}_1}}{\psi_{\widetilde{\boldsymbol{S}}_1}(a_k^{\mathbf{T}})} - 1 \xrightarrow{a.s.} 0. \quad j \in \mathcal{J}_k, \tag{22}$$

where

$$\psi_{\widetilde{\boldsymbol{S}}_1}(a_k^{\mathbf{T}}) = \left(a_k^{\mathbf{T}} + c_1/c_2\right)\left(a_k^{\mathbf{T}} + 1\right)/a_k^{\mathbf{T}}. \tag{23}$$

Remark 2 This theorem can be easily verified by Lemmas 1–2 and Theorem 2.2 in Ding (2020). Thus, we omit the proof in this paper.

Now, we are in a position to present the CLT for the sample spiked eigenvalues of matrix $\widetilde{\boldsymbol{S}}_1$ and its proof is postponed to Sect. 4.

Theorem 3 *Suppose Assumptions 1–3 hold. For any* $k \in \{1, \ldots, K\}$ *satisfying* $\lim_{n\to\infty} a_k^{\mathbf{T}} > \sqrt{c_1/c_2}$, *then the* m_k*-dimensional random vector*

$$\boldsymbol{\gamma}_k^{\widetilde{\boldsymbol{S}}_1} = \sqrt{q}\left\{\frac{l_j^{\widetilde{\boldsymbol{S}}_1}}{\psi_{n,\widetilde{\boldsymbol{S}}_1}(a_k^{\mathbf{T}})} - 1, \quad j \in \mathcal{J}_k\right\}$$

converge weakly to the joint distribution of the m_k *eigenvalues of Gaussian random matrix*

$$\boldsymbol{\Omega}\left(\theta_1^{-2}\right),$$

where $\psi_{n,\widetilde{\boldsymbol{S}}_1}(\cdot)$ *is a substitute of* $\psi_{\widetilde{\boldsymbol{S}}_1}(\cdot)$ *with* c_1 *and* c_2 *replaced by* c_{1n} *and* c_{2n} *and* $\boldsymbol{\Omega}(\theta_1^{-2})$ *is a GOE matrix with a scale parameter* θ_1^{-2}, *i.e.,* $\theta_1\boldsymbol{\Omega}(\theta_1^{-2})$ *is a GOE, and*

$$\theta_1^2 := \left(\theta_1^{(k)}\right)^2 = \frac{\left(a_k^{\mathbf{T}}\right)^4\left(a_k^{\mathbf{T}} + c_1/c_2\right)^2\left(a_k^{\mathbf{T}} + 1\right)^2}{\left(a_k^{\mathbf{T}}\right)^4\left(\left(a_k^{\mathbf{T}}\right)^2 - c1/c2\right)\left(a_k^{\mathbf{T}} + 1 + c_1/c_2\right) + c_2\left(\left(a_k^{\mathbf{T}}\right)^2 - c_1/c_2\right)^2}.$$

Remark 3 As the limits defined in (22) may converge very slow, to guarantee the existence of limiting distribution, here and in the sequel, we need to use the nonasymptotic parameters c_{n1}, c_{n2} and $a_k^{\mathbf{T}}$ in the CLTs.

4 Limits and Fluctuations for the Eigenvalues of $\boldsymbol{F}(\boldsymbol{\Xi})$

Recall the noncentral Fisher matrix $\boldsymbol{F}(\boldsymbol{\Xi})$ defined in (14),

$$\boldsymbol{F}(\boldsymbol{\Xi}) = \widetilde{\boldsymbol{S}}_1\widetilde{\boldsymbol{S}}_2^{-1} \tag{24}$$

and its eigenvalues

$$l_1 \geq l_2 \geq \cdots \geq l_p. \tag{25}$$

Then we have the following theorems and their proof are postponed to the Sect. 4.

Theorem 4 *Suppose that Assumptions 1–3 hold. For any* $k \in \{1, \ldots, K\}$ *satisfying*

$$\lim_{n\to\infty} a_k^{\mathbf{T}} > \frac{c_1c_2 + \sqrt{c_1^2c_2^2 + c_1c_2(1-c_1-c_2)}}{c_2(1-c_1-c_2)}, \tag{26}$$

then we have

$$\frac{l_j}{\psi(a_k^{\mathbf{T}})} - 1 \xrightarrow{a.s.} 0, \quad j \in \mathcal{J}_k,$$

where

$$\psi(a_k^{\mathbf{T}}) = \frac{(1-c_2)(a_k^{\mathbf{T}} + c_1)(a_k^{\mathbf{T}} + 1)}{(1-c_1-c_2)a_k^{\mathbf{T}} - c_1}. \tag{27}$$

Theorem 5 *If Assumptions 1–3 hold, then the m_k-dimensional random vector*

$$\boldsymbol{\gamma}_k^F = \sqrt{n-q}\left\{\frac{l_j - \psi_n(a_k^{\mathbf{T}})}{\psi_n(a_k^{\mathbf{T}})}, \quad j \in \mathcal{J}_k\right\}$$

converge weakly to the joint distribution of the m_k eigenvalues of the following Gaussian random matrix

$$\boldsymbol{\Omega}\left(\theta_2^{-2}\right),$$

where

$$\psi_n(a_k^{\mathbf{T}}) = \frac{(1-c_{2n})(a_k^{\mathbf{T}} + c_{1n})(a_k^{\mathbf{T}} + 1)}{(1-c_{1n}-c_{2n})a_k^{\mathbf{T}} - c_{1n}}$$

and

$$\theta_2^2 := \left(\theta_2^{(k)}\right)^2 = \frac{1}{(1-c_2)(a_k^{\mathbf{T}})^2(a_k^{\mathbf{T}}c_2+1)\left(c_2^2(a_k^{\mathbf{T}})^2 + ((c_1-1)a_k^{\mathbf{T}} + 2c_1)c_2a_k^{\mathbf{T}} + c_1\right)} \times \frac{c_2(a_k^{\mathbf{T}}+1)^2(a_k^{\mathbf{T}}c_2+c_1)^2(a_k^{\mathbf{T}}c_2 + (c_1-1)a_k^{\mathbf{T}} + c_1)^2}{\left(c_2^2a_k^{\mathbf{T}} + ((c_1-2)a_k^{\mathbf{T}} + 2c_1 - 1)c_2 - c_1\right)}.$$

5 Limits and Fluctuations for the Sample Canonical Correlation Coefficients

As Theorem 1 has established the one-to-one relation between the square of the sample canonical correlation coefficients and the eigenvalues of the noncentral Fisher matrix. Thus, by the results introduced in last subsection, we can easily obtain the

limits and fluctuations of the sample canonical correlation coefficients, which are presented as the following two theorems.

Theorem 6 *Suppose that Assumptions 1–3 hold. For any $k \in \{1, \ldots, K\}$ satisfying*

$$a_k = \lim_{n\to\infty} \frac{c_2 a_k^{\mathbf{T}}}{c_2 a_k^{\mathbf{T}} + 1} > \sqrt{\frac{c_1 c_2}{(1-c_1)(1-c_2)}}, \tag{28}$$

then we have that for any $i \in \mathcal{J}_k$, the square of sample canonical correlation coefficient λ_i^2 almost surely converges to $\phi(a_k)$, where

$$\phi(a_k) = (a_k(1-c_1)+c_1)\,(a_k(1-c_2)+c_2)/a_k. \tag{29}$$

Theorem 7 *If Assumptions 1–3 hold, then the m_k-dimensional random vector*

$$\boldsymbol{\gamma}_k = \sqrt{n}\left\{\lambda_i^2 - \phi_n(a_k), \quad i \in \mathcal{J}_k\right\}$$

converges weakly to the joint distribution of the m_k eigenvalues of Gaussian random matrix

$$\boldsymbol{\Omega}(\theta_3^2),$$

where

$$\phi_n(a_k) = (a_k(1-c_{1n})+c_{1n})\,(a_k(1-c_{2n})+c_{2n})/a_k$$

and

$$\theta_3^2 := (\theta_3^{(k)})^2 = \frac{(1-a_k)^2(2va_k + c_1 + c_2 - 2w)(va_k^2 - w)}{a_k^2} \tag{30}$$

$w = c_1c_2$ *and* $v = (1-c_1)(1-c_2)$.

Remark 4 Noted that Theorems 6, Theorem 7 agree with the results in Bao et al. (2019). Thus, this paper can be viewed as a different approach from Bao et al. (2019), but achieving the same destination.

Remark 5 This theorem can be proved by Theorems 1, 5 and Delta method. As the calculation is mechanical and tedious, so we omit the details in this paper.

Remark 6 In order to verify the performance of Theorem 7, we present the following numerical studies (Fig. 2). We compare the empirical density (the blue histogram) of λ_1^2 or λ_2^2 with standard normal density curve (the red line) with 4,000 repetitions.

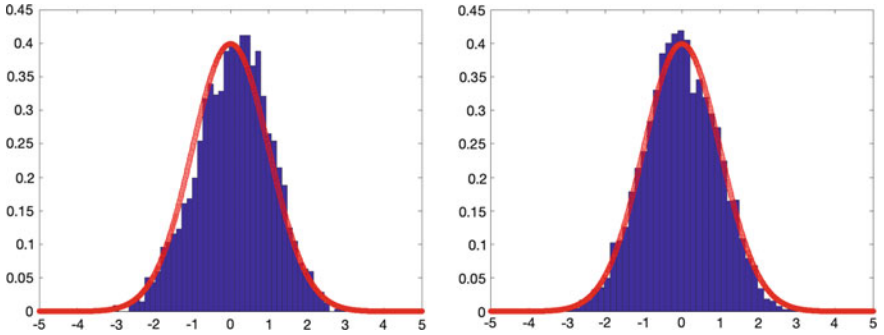

Fig. 2 The asymptotic normality of λ_1^2 (the left panel) and λ_2^2 (the right panel) with $(\rho_1^2, \rho_2^2, \ldots, \rho_5^2, \ldots, \rho_p^2) = (0.8, 0.7, \ldots, 0.4, 0, \ldots, 0)$, $(p, q, n) = (200, 600, 1000)$

6 Technical Proofs

In this section, we give the technical proofs of Theorems 1, 3–6. Note that we may also use c_1, c_2 to denote c_{1n}, c_{2n} respectively in the proofs of CLTs for simplicity. The context will be clear enough that there is no risk of ambiguity.

6.1 Proof of Theorem 1

Recall the notation

$$\widetilde{\mathbf{X}} = (\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_n)_{p\times n}, \quad \widetilde{\mathbf{Y}} = (\tilde{\mathbf{y}}_1, \ldots, \tilde{\mathbf{y}}_n)_{q\times n}, \quad \widetilde{\mathbf{W}} = (\tilde{\mathbf{w}}_1, \ldots, \tilde{\mathbf{w}}_n)_{p\times n}.$$

we define the sample covariance matrix of $(\widetilde{\mathbf{X}}^T, \widetilde{\mathbf{Y}}^T)^T$ be

$$\tilde{\mathbf{S}}_n \begin{pmatrix} \tilde{\mathbf{x}}_i \\ \tilde{\mathbf{y}}_i \end{pmatrix} = \frac{1}{n} \begin{pmatrix} \widetilde{\mathbf{X}}\widetilde{\mathbf{X}}^T & \widetilde{\mathbf{X}}\widetilde{\mathbf{Y}}^T \\ \widetilde{\mathbf{Y}}\widetilde{\mathbf{X}}^T & \widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{S}}_{xx} & \tilde{\mathbf{S}}_{xy} \\ \tilde{\mathbf{S}}_{yx} & \tilde{\mathbf{S}}_{yy} \end{pmatrix}. \tag{31}$$

It is easy to check that under Assumption 1, $\tilde{\mathbf{S}}_{xy}\tilde{\mathbf{S}}_{yy}^{-1}\tilde{\mathbf{S}}_{yx}\tilde{\mathbf{S}}_{xx}^{-1}$ and $\mathbf{S}_{xy}\mathbf{S}_{yy}^{-1}\mathbf{S}_{yx}\mathbf{S}_{xx}^{-1}$ share the same eigenvalues. In addition, by the notation

$$\boldsymbol{\Delta} = \widetilde{\mathbf{Y}}^T(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{-1/2}, \quad \mathbf{I}_n - \widetilde{\mathbf{Y}}^T(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{-1}\widetilde{\mathbf{Y}} = \boldsymbol{\Theta}\boldsymbol{\Theta}^T.$$

We have that

$$\tilde{\mathbf{S}}_{xy}\tilde{\mathbf{S}}_{yy}^{-1}\tilde{\mathbf{S}}_{yx}\tilde{\mathbf{S}}_{xx}^{-1}(\mathbf{I}_p - \tilde{\mathbf{S}}_{xy}\tilde{\mathbf{S}}_{yy}^{-1}\tilde{\mathbf{S}}_{yx}\tilde{\mathbf{S}}_{xx}^{-1})^{-1} = \widetilde{\mathbf{X}}\boldsymbol{\Delta}\boldsymbol{\Delta}^T\widetilde{\mathbf{X}}^T(\widetilde{\mathbf{X}}\boldsymbol{\Theta}\boldsymbol{\Theta}^T\widetilde{\mathbf{X}}^T)^{-1}, \tag{32}$$

$$\mathbf{\Delta}^T\widetilde{\mathbf{X}}^T = (\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2}\mathbf{\Lambda}^T + \mathbf{\Delta}^T\widetilde{\mathbf{W}}^T\mathbf{\Gamma}^T \tag{33}$$

and

$$\mathbf{\Theta}^T\widetilde{\mathbf{X}}^T = \mathbf{\Theta}^T(\mathbf{\Lambda}\widetilde{\mathbf{Y}} + \mathbf{\Gamma}\widetilde{\mathbf{W}})^T = \mathbf{\Theta}^T\widetilde{\mathbf{Y}}^T\mathbf{\Lambda}^T + \mathbf{\Theta}^T\widetilde{\mathbf{W}}^T\mathbf{\Gamma}^T = \mathbf{\Theta}^T\widetilde{\mathbf{W}}^T\mathbf{\Gamma}^T. \tag{34}$$

Write $\mathbf{B} = \widetilde{\mathbf{W}}\mathbf{\Delta}$ and $\mathbf{C} = \widetilde{\mathbf{W}}\mathbf{\Theta}$. As $\mathbf{\Delta}\mathbf{\Delta}^T$ and $\mathbf{\Theta}\mathbf{\Theta}^T$ are projection matrices with $\mathbf{\Delta}^T\mathbf{\Theta} = \mathbf{0}$, thus we have $\mathbf{B}$ and $\mathbf{C}$ are independent random matrices with i.i.d standard normal entries, which implies

$$(32) = \mathbf{\Gamma}(\mathbf{\Gamma}^{-1}\mathbf{\Lambda}(\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2} + \mathbf{B})((\widetilde{\mathbf{Y}}\widetilde{\mathbf{Y}}^T)^{1/2}\mathbf{\Lambda}^T\mathbf{\Gamma}^{-1} + \mathbf{B}^T)(\mathbf{C}\mathbf{C}^T)^{-1}\mathbf{\Gamma}^{-1},$$

which has the same eigenvalues of $\frac{q}{n-q}\boldsymbol{F}(\mathbf{\Xi}) := \frac{q}{n-q}\widetilde{\boldsymbol{S}}_1\widetilde{\boldsymbol{S}}_2^{-1}$. Thus, the ordered eigenvalues of $\tilde{\mathbf{S}}_{xy}\tilde{\mathbf{S}}_{yy}^{-1}\tilde{\mathbf{S}}_{yx}\tilde{\mathbf{S}}_{xx}^{-1}$ and that of the noncentral Fisher matrix have the following relation

$$l_i = g(\lambda_i^2) = k_{n,q}\frac{\lambda_i^2}{1-\lambda_i^2},$$

where $k_{n,q} = \frac{n}{q} - 1$. Then we complete the proof of Theorem 1.

6.2 *Proof of Theorem 3*

We start to consider the conditional limiting distribution of $\boldsymbol{\gamma}_k^{\widetilde{S}_1}$ given $\widetilde{\mathbf{Y}}$, denoted by $\boldsymbol{\gamma}_k^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}$ in the following. For simplicity, we let $\lambda_k^{\widetilde{S}_1} = (a_k^{\mathbf{T}} + c_1/c_2)(a_k^{\mathbf{T}} + 1)/a_k^{\mathbf{T}}$ stand for the limits of $l_i^{\widetilde{S}_1}$.

As $\mathbf{\Xi}$ has finite rank, thus we can decompose $\mathbf{\Xi}_{1/2}$ as

$$\mathbf{\Xi}_{1/2} = \mathbf{O}_1\mathbf{D}\mathbf{O}_2 = \mathbf{O}_1\begin{pmatrix}\mathbf{D}_1\\ \mathbf{0}\end{pmatrix}\mathbf{O}_2 = \mathbf{O}_1\begin{pmatrix}\mathbf{D}_{11} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\mathbf{O}_2, \tag{35}$$

where $\mathbf{D}$ is a $p \times q$ matrix, $\mathbf{D}_1$ is the first M rows of $\mathbf{D}$, $\mathbf{D}_{11}$ is the first M columns of $\mathbf{D}_1$, $\mathbf{O}_1$ and $\mathbf{O}_2$ are two orthogonal matrices. Suppose λ solve the following equation

$$\begin{aligned}0 &= |\lambda\mathbf{I} - \widetilde{\boldsymbol{S}}_1| = |\lambda\mathbf{I} - \mathbf{O}_1^T(\mathbf{\Xi}_{1/2} + q^{-1/2}\mathbf{B})(\mathbf{\Xi}_{1/2} + q^{-1/2}\mathbf{B})^T\mathbf{O}_1|\\ &= |\lambda\mathbf{I} - (\mathbf{D} + q^{-1/2}\mathbf{O}_1^T\mathbf{B}\mathbf{O}_2^T)(\mathbf{D} + q^{-1/2}\mathbf{O}_1^T\mathbf{B}\mathbf{O}_2^T)^T|.\end{aligned}$$

Since $\mathbf{B}$ is Gaussian distributed, we have $\mathbf{O}_1^T\mathbf{B}\mathbf{O}_2^T \overset{d}{=} \mathbf{B}$, where $\overset{d}{=}$ stands for identically distributed. Thus, without loss of generality, we can assume that the matrix $\mathbf{\Xi} = \mathbf{D}\mathbf{D}^T$. Similar to $\mathbf{D}$, we decompose $\mathbf{B}$ as

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_1 \\ \mathbf{B}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{B}_{11}\ \mathbf{B}_{12} \\ \mathbf{B}_{21}\ \mathbf{B}_{22} \end{pmatrix}.$$

Thus for the sample spiked eigenvalues $l_i^{\widetilde{S}_1}$, $i \in \mathcal{J}_k$, $k = 1, \ldots, K$, we have that

$$\begin{aligned} 0 &= \left| l_i^{\widetilde{S}_1}\mathbf{I}_p - (\mathbf{D} + \frac{1}{\sqrt{q}}\mathbf{B})(\mathbf{D} + \frac{1}{\sqrt{q}}\mathbf{B})^T \right| \\ &= \left| \begin{matrix} l_i^{\widetilde{S}_1}\mathbf{I}_M - (\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1)(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1)^T & -(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1)\frac{1}{\sqrt{q}}\mathbf{B}_2^T \\ -\frac{1}{\sqrt{q}}\mathbf{B}_2(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1)^T & l_i^{\widetilde{S}_1}\mathbf{I}_{p-M} - \frac{1}{\sqrt{q}}\mathbf{B}_2\frac{1}{\sqrt{q}}\mathbf{B}_2^T \end{matrix} \right|. \end{aligned} \tag{36}$$

Since $|l_i^{\widetilde{S}_1}\mathbf{I}_{p-M} - \frac{1}{q}\mathbf{B}_2\mathbf{B}_2^T| \neq 0$, we can rewrite (36) as

$$0 = \left| l_i^{\widetilde{S}_1}\mathbf{I}_M - \left(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1\right)\left[\mathbf{I}_q + \frac{1}{q}\mathbf{B}_2^T\left[l_i^{\widetilde{S}_1}\mathbf{I}_{p-M} - \frac{1}{q}\mathbf{B}_2\mathbf{B}_2^T\right]^{-1}\mathbf{B}_2\right]\left(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1\right)^T \right|,$$

which is equivalent to

$$0 = \left| \mathbf{I}_M - \left(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1\right)\left(l_i^{\widetilde{S}_1}\mathbf{I}_q - \frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2\right)^{-1}\left(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1\right)^T \right| \tag{37}$$

when $l_i^{\widetilde{S}_1} \neq 0$. Then we let

$$\begin{aligned} \mathbf{\Omega}_q^{\widetilde{S}_1} &= \mathbf{I}_M - \left(\mathbf{D}_1 + \frac{1}{\sqrt{q}}\mathbf{B}_1\right)\left(l_i^{\widetilde{S}_1}\mathbf{I}_q - \frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2\right)^{-1}\left(\mathbf{D}_1^T + \frac{1}{\sqrt{q}}\mathbf{B}_1^T\right) \\ &= \mathbf{I}_M + \frac{1}{q}\mathrm{tr}\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}\mathbf{I}_M + \frac{\mathbf{D}_1\mathbf{D}_1^T}{l_i^{\widetilde{S}_1}(1 + c_{3n}m_{2n}(l_i^{\widetilde{S}_1}))} + \mathbf{\Omega}_0^{\widetilde{S}_1}, \end{aligned} \tag{38}$$

where $c_{3n} = (p - M)/q$,

$$\begin{aligned} \mathbf{\Omega}_0^{\widetilde{S}_1} &= \frac{1}{q}\mathbf{B}_1\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}\mathbf{B}_1^T - \frac{1}{q}\mathrm{tr}\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}\mathbf{I}_M \\ &\quad + \frac{1}{\sqrt{q}}\left(\mathbf{B}_1\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}\mathbf{D}_1^T + \mathbf{D}_1\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}\mathbf{B}_1^T\right) \\ &\quad + \mathbf{D}_{11}^T\left[\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)_{MM}^{-1} + \frac{\mathbf{I}_M}{l_i^{\widetilde{S}_1}(1 + c_{3n}m_{2n}(l_i^{\widetilde{S}_1}))}\right]\mathbf{D}_{11}, \end{aligned} \tag{39}$$

and

$$m_{2n}(l_i^{\widetilde{S}_1}) = \frac{1}{p - M}\mathrm{tr}\left[\frac{1}{q}\mathbf{B}_{22}\mathbf{B}_{22}^T - l_i^{\widetilde{S}_1}\mathbf{I}_{p-M}\right]^{-1}.$$

Note that $c_{3n} = (p - M)/q \to c_3 := c_1/c_2$ and $m_{2n}(z)$ is the Stieltjes transform of the ESD of $q^{-1}\mathbf{B}_{22}\mathbf{B}_{22}^T$, which almost surely tends to the Stieltjes transform $m_2(z)$ of the M-P law. For using later, we denote the Stieltjes transform of the ESD of $q^{-1}\mathbf{B}_{22}^T\mathbf{B}_{22}$ by $\underline{m}_{2n}(z)$. Then, it follows that $\underline{m}_{2n}(z) \to \underline{m}_2(z) = -(1 - c_3)/z + c_3 m_2(z)$.

Next, we will consider the limiting distribution of $\sqrt{q}\boldsymbol{\Omega}_0^{\widetilde{S}_1}$ defined in (39). As stated above, by classical CLT, it is not difficult to obtain that the $M \times M$ matrix $\frac{1}{\sqrt{q}}\mathbf{B}_1(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}\mathbf{B}_1^T - \frac{1}{\sqrt{q}}\mathrm{tr}(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}\mathbf{I}_M$ converge weakly to a GOE matrix with a scale parameter $\underline{m}_2'(\lambda_k^{\widetilde{S}_1})$.

For $\mathbf{B}_1(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}\mathbf{D}_1^T + \mathbf{D}_1(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}\mathbf{B}_1^T$, we denote its (i, j)-th $(i \le M, j \le M)$ entry by $d_j\mathbf{b}_i\mathbf{a}_j + d_i\mathbf{a}_i^T\mathbf{b}_j^T$, where $\mathbf{b}_i$ is the i-th row of $\mathbf{B}_1$ and $\mathbf{a}_j$ is the j-th column of $(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}$. Since $\mathbf{B}_1$ and $(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}$ are independent, thus $(d_j\mathbf{b}_i\mathbf{a}_j + d_i\mathbf{a}_i^T\mathbf{b}_j^T, 1 \le i \le j \le M)$ are asymptotically independent and normally distributed with variances

$$\sigma_n^2(i, j) = \begin{cases} 4d_i^2\mathbb{E}(\mathbf{a}_i^T\mathbf{a}_i) & \text{if } i = j \\ d_i^2\mathbb{E}(\mathbf{a}_i^T\mathbf{a}_i) + d_j^2\mathbb{E}(\mathbf{a}_j^T\mathbf{a}_j), & \text{if } i \ne j \end{cases}. \tag{40}$$

Here we use the fact that for $i \ne j$, $\mathbb{E}(\mathbf{a}_i^T\mathbf{a}_j) \to 0$ when $n \to \infty$, which can be verified from the following calculation.

Let $\mathbf{a}_j = (\mathbf{a}_{1j}', \mathbf{a}_{2j}')'$, where $\mathbf{a}_{1j}$ is the first M components of $\mathbf{a}_j$. Then by the inverse matrix formula, we have that

$$\mathbf{a}_j^T\mathbf{a}_j = \mathbf{a}_{1j}^T\mathbf{a}_{1j} + \mathbf{a}_{1j}^T\frac{1}{q}\mathbf{B}_{21}^T\frac{1}{q}\mathbf{B}_{22}\left(\frac{1}{q}\mathbf{B}_{22}^T\mathbf{B}_{22} - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-2}\mathbf{B}_{22}^T\mathbf{B}_{21}\mathbf{a}_{1j}.$$

Notice that

$$\begin{aligned} & 1 + \frac{1}{q}\mathrm{tr}\left(\frac{1}{\sqrt{q}}\mathbf{B}_{22}\left(\frac{1}{q}\mathbf{B}_{22}^T\mathbf{B}_{22} - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-2}\frac{1}{\sqrt{q}}\mathbf{B}_{22}^T\right) \\ = \; & 1 + \frac{1}{q}\mathrm{tr}\left(\frac{1}{q}\mathbf{B}_{22}^T\mathbf{B}_{22} - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1} + \frac{l_i^{\widetilde{S}_1}}{q}\mathrm{tr}\left(\frac{1}{q}\mathbf{B}_{22}^T\mathbf{B}_{22} - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-2} \\ = \; & 1 + \underline{m}_{2n}(l_j^{\widetilde{S}_1}) + l_j^{\widetilde{S}_1}\underline{m}_{2n}'(l_j^{\widetilde{S}_1}) \end{aligned}$$

and

$$\left(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q\right)^{-1}_{MM}$$
$$= \left(\frac{1}{q}\mathbf{B}_{21}^T\mathbf{B}_{21} - l_i^{\widetilde{S}_1}\mathbf{I}_M - \frac{1}{q}\mathbf{B}_{21}^T\frac{1}{\sqrt{q}}\mathbf{B}_{22}\left[\frac{1}{q}\mathbf{B}_{22}^T\mathbf{B}_{22} - l_i^{\widetilde{S}_1}\mathbf{I}_{q-M}\right]^{-1}\frac{1}{\sqrt{q}}\mathbf{B}_{22}^T\mathbf{B}_{21}\right)^{-1}$$
$$= \left(-l_i^{\widetilde{S}_1}\mathbf{I}_M - \frac{l_i^{\widetilde{S}_1}}{q}\mathrm{tr}\left[\frac{1}{q}\mathbf{B}_{22}\mathbf{B}_{22}^T - l_i^{\widetilde{S}_1}\mathbf{I}_{p-M}\right]^{-1}\mathbf{I}_M - \mathbf{\Omega}_1^{\widetilde{S}_1}\right)^{-1}, \tag{41}$$

where

$$\mathbf{\Omega}_1^{\widetilde{S}_1} = \frac{l_i^{\widetilde{S}_1}}{q}\mathbf{B}_{21}^T\left(\frac{1}{q}\mathbf{B}_{22}\mathbf{B}_{22}^T - l_i^{\widetilde{S}_1}\mathbf{I}_{p-M}\right)^{-1}\mathbf{B}_{21} - \frac{l_i^{\widetilde{S}_1}}{q}\left[\mathrm{tr}\left(\frac{1}{q}\mathbf{B}_{22}\mathbf{B}_{22}^T - l_i^{\widetilde{S}_1}\mathbf{I}_{p-M}\right)^{-1}\right]\mathbf{I}_M.$$

Thus, from Theorem 2 and notation $\lambda_k^{\widetilde{S}_1}$ we have

$$\mathbb{E}(\mathbf{a}_j^T\mathbf{a}_j) \to \frac{1 + \underline{m}_2(\lambda_j^{\widetilde{S}_1}) + \lambda_j^{\widetilde{S}_1}\underline{m}_2'(\lambda_j^{\widetilde{S}_1})}{(\lambda_j^{\widetilde{S}_1})^2(1 + c_3 m_2(\lambda_j^{\widetilde{S}_1}))^2}. \tag{42}$$

Similarly, by Eq. (41), we can find that

$$\sqrt{q}\left[(\frac{1}{q}\mathbf{B}_2^T\mathbf{B}_2 - l_i^{\widetilde{S}_1}\mathbf{I}_q)^{-1}_{m_k m_k} + \frac{1}{l_i^{\widetilde{S}_1}(1 + c_{3n}m_{2n}(l_i^{\widetilde{S}_1}))}\mathbf{I}_{m_k}\right]$$

converges weakly to the $m_k \times m_k$ GOE matrix with scale parameter $\frac{c_3 m_2'(\lambda_k^{\widetilde{S}_1})}{(\lambda_k^{\widetilde{S}_1})^2(1+c_3 m_2(\lambda_k^{\widetilde{S}_1}))^4}$. As the three parts of (39) are asymptotically independent, thus we conclude that $\sqrt{q}\mathbf{\Omega}_0^{\widetilde{S}_1}$ converges weakly to the $M \times M$ random matrix

$$\mathbf{\Omega}_1(\underline{m}_2'(\lambda_k^{\widetilde{S}_1})) + \mathbf{D}_{11}\mathbf{\Omega}_2\left(\frac{\left(1+\underline{m}_2(\lambda_k^{\widetilde{S}_1}) + \lambda_k^{\widetilde{S}_1}\underline{m}_2'(\lambda_k^{\widetilde{S}_1})\right)\left(1+c_3 m_2(\lambda_k^{\widetilde{S}_1})\right)^4 + c_3 m_2'(\lambda_k^{\widetilde{S}_1})}{(\lambda_k^{\widetilde{S}_1})^2(1+c_3 m_2(\lambda_k^{\widetilde{S}_1}))^4}\right)\mathbf{D}_{11},$$

where $\mathbf{\Omega}_1$ and $\mathbf{\Omega}_2$ are two independent GOEs.

Let $a_k^{\widetilde{S}_1}$ stand for the sample spiked eigenvalues of $\mathbf{\Xi}$ given $\widetilde{\mathbf{Y}}$, $\gamma_{ki}^{\widetilde{S}_1}|\widetilde{\mathbf{Y}} = \sqrt{q}\frac{l_i^{\widetilde{S}_1} - \lambda_k^{\widetilde{S}_1}}{\lambda_k^{\widetilde{S}_1}}|\widetilde{\mathbf{Y}}$,

$$\varepsilon_1 = \underline{m}_{2n}(l_i^{\widetilde{S}_1}) - \underline{m}_{2n}(\lambda_k^{\widetilde{S}_1}) = \frac{\gamma_{ki}^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}}{\sqrt{q}}\lambda_k^{\widetilde{S}_1}\underline{m}_2'(\lambda_k^{\widetilde{S}_1}) + \frac{\gamma_{ki}^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}}{\sqrt{q}}o_p(1)$$

and

$$\varepsilon_2 = \left(\frac{-1}{l_i^{\widetilde{S}_1} + l_i^{\widetilde{S}_1}\frac{p-M}{q}m_{2n}(l_i^{\widetilde{S}_1})}\right) - \left(\frac{-1}{\lambda_k^{\widetilde{S}_1} + \lambda_k^{\widetilde{S}_1}c_{3n}m_{2n}(\lambda_k^{\widetilde{S}_1})}\right)$$
$$= \frac{\gamma_{ki}^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}}{\sqrt{q}}\frac{1 + c_3m_2(\lambda_k^{\widetilde{S}_1}) + c\lambda_k^{\widetilde{S}_1}m_2'(\lambda_k^{\widetilde{S}_1})}{\lambda_k^{\widetilde{S}_1}[1 + c_3m_2(\lambda_k^{\widetilde{S}_1})]^2} + o_p\left(\frac{1}{\sqrt{q}}\right).$$

Then, from the above argument, we have that the matrix $\mathbf{\Omega}_q^{\widetilde{S}_1}$ becomes

$$(1 + \underline{m}_2(\lambda_k^{\widetilde{S}_1}))\mathbf{I}_{mk} - \frac{\mathbf{D}_1\mathbf{D}_1^*}{\lambda_k b(\lambda_k)} + \mathbf{\Omega}_0^{\widetilde{S}_1}(\lambda_k^{\widetilde{S}_1}) + \varepsilon_1\mathbf{I}_M + \varepsilon_2\mathbf{D}_1\mathbf{D}_1^* + o_p(\frac{1}{\sqrt{q}}),$$

where $b(\lambda_k^{\widetilde{S}_1}) = 1 + c_3m_2(\lambda_k^{\widetilde{S}_1})$. And from Theorem 2, we have

$$1 + \underline{m}_2(\lambda_k) - \frac{a_k^{\widetilde{S}_1}}{\lambda_k b(\lambda_k)} = 0.$$

By Skorokhod strong representation theorem (see Skorokhod 1956 or Hu and Bai 2014 for more details), on an appropriate probability space, one may redefine the random variables such that $\sqrt{q}\mathbf{\Omega}_0^{\widetilde{S}_1}$ tends to the normal variables with probability one. Then, the eigen-equation (37) becomes

$$0 = \begin{vmatrix} \frac{a_k^{\widetilde{S}_1}}{\lambda_k^{\widetilde{S}_1}b(\lambda_k^{\widetilde{S}_1})}(1 - \frac{a_1^{\widetilde{S}_1}}{a_k^{\widetilde{S}_1}}) + O(\frac{1}{\sqrt{q}}) & O(\frac{1}{\sqrt{q}}) & O(\frac{1}{\sqrt{q}}) \\ O(\frac{1}{\sqrt{q}}) & \cdots & O(\frac{1}{\sqrt{q}}) \\ O(\frac{1}{\sqrt{q}}) & [\mathbf{\Omega}_0^{\widetilde{S}_1}]_{kk} + \varepsilon_1\mathbf{I}_{m_k} + \varepsilon_2 a_k^{\widetilde{S}_1}\mathbf{I}_{m_k} + o(\frac{1}{\sqrt{q}}) & \cdots \\ O(\frac{1}{\sqrt{q}}) & \cdots & O(\frac{1}{\sqrt{q}}) \\ O(\frac{1}{\sqrt{q}}) & \cdots & \frac{a_k^{\widetilde{S}_1}}{\lambda_k^{\widetilde{S}_1}b(\lambda_k^{\widetilde{S}_1})}(1 - \frac{a_k^{\widetilde{S}_1}}{a_k^{\widetilde{S}_1}}) + O(\frac{1}{\sqrt{q}}) \end{vmatrix},$$

where $[\mathbf{\Omega}_0^{\widetilde{S}_1}]_{kk}$ is k-th diagonal block of $\mathbf{\Omega}_0^{\widetilde{S}_1}$.

One can find that all non-diagonal elements tend to zero and all the diagonal entries are bounded away from zero, except the k-th block. By multiplying $q^{1/4}$ to the k-th row block and k-th column block of the determinant of the eigen-equation above, and making $q \to \infty$, we have that $\gamma_k^{\widetilde{S}_1}$ tends to a solution of

$$|[\sqrt{q}\mathbf{\Omega}_0^{\widetilde{S}_1}]_{kk} + \sqrt{q}\varepsilon_1\mathbf{I}_{m_k} + \sqrt{q}\varepsilon_2 a_k^{\widetilde{S}_1}\mathbf{I}_{m_k}| = 0.$$

In fact, the limit of $\sqrt{q}(\varepsilon_1 + \varepsilon_2 a_k^{\widetilde{S}_1})/\gamma_k^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}$ satisfies

$$\frac{1 + c_3m_2(\lambda_k^{\widetilde{S}_1}) + c_3\lambda_k^{\widetilde{S}_1}m_2'(\lambda_k^{\widetilde{S}_1})}{\lambda_k^{\widetilde{S}_1}[1 + c_3m_2(\lambda_k^{\widetilde{S}_1})]^2}a_k^{\widetilde{S}_1} + \lambda_k^{\widetilde{S}_1}\underline{m}_2'(\lambda_k^{\widetilde{S}_1}).$$

By basic calculation, we have the limit distribution of $\frac{\boldsymbol{\gamma}_k^{\widetilde{S}_1}|\widetilde{\mathbf{Y}}}{\sqrt{q}(\varepsilon_1+\varepsilon_2 a_k^{\mathbf{T}})}\boldsymbol{\Omega}_0^{\widetilde{S}_1}$ is $\frac{1}{\theta_{11}}\boldsymbol{\Omega}_1$, where $\boldsymbol{\Omega}_1$ is a GOE and

$$\theta_{11}=\frac{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}{\sqrt{((a_k^{\mathbf{T}})^2-c_3)(2a_k^{\mathbf{T}}+1+c_3)}}.$$

Thus, for general $\widetilde{\mathbf{Y}}$, we have that

$$\begin{aligned}\gamma_k^{\widetilde{S}_1}&=\sqrt{q}\frac{l_i^{\widetilde{S}_1}-\lambda_k^{\widetilde{S}_1}}{\lambda_k^{\widetilde{S}_1}}=\sqrt{q}\frac{l_i^{\widetilde{S}_1}-\psi_{n,\widetilde{S}_1}(a_k^{\widetilde{S}_1})}{\lambda_k^{\widetilde{S}_1}}|\widetilde{\mathbf{Y}}+\sqrt{q}\frac{\psi_{n,\widetilde{S}_1}(l_i^{\boldsymbol{\Xi}})-\lambda_k^{\widetilde{S}_1}}{\lambda_k^{\widetilde{S}_1}}\\&=\sqrt{q}\frac{l_i^{\widetilde{S}_1}-\psi_{n,\widetilde{S}_1}(a_k^{\widetilde{S}_1})}{\lambda_k^{\widetilde{S}_1}}|\mathbf{Y}+\sqrt{\frac{q}{n}}\psi'_{\widetilde{S}_1}(a_k^{\mathbf{T}})\sqrt{n}\frac{l_i^{\boldsymbol{\Xi}}-a_k^{\mathbf{T}}}{a_k^{\mathbf{T}}}\frac{a_k^{\mathbf{T}}}{\lambda_k^{\widetilde{S}_1}},\end{aligned}$$

where $\psi_{n,\widetilde{S}_1}(\cdot)$ is defined in Theorem 3 and $\psi'_{\widetilde{S}_1}(\cdot)$ is its derivatives. It follows from Lemma 2 that, $\sqrt{\frac{q}{n}}\psi'_{\widetilde{S}_1}(a_k^{\mathbf{T}})\frac{a_k^{\mathbf{T}}}{\lambda_k^{\widetilde{S}_1}}\boldsymbol{\gamma}_k$ converges weakly to $\frac{1}{\theta_{12}}\boldsymbol{\Omega}_2$, where $\boldsymbol{\Omega}_2$ is a GOE and independent of $\boldsymbol{\Omega}_1$, and

$$\theta_{12}=\frac{(a_k^{\mathbf{T}})^2(a_k^{\mathbf{T}}+c_1/c_2)(a_k^{\mathbf{T}}+1)}{\sqrt{c_2}[(a_k^{\mathbf{T}})^2-c_1/c_2]}.$$

Thus, we conclude that $\boldsymbol{\gamma}_k^{\widetilde{S}_1}$ converges weakly to

$$\frac{1}{\theta_1}\boldsymbol{\Omega}, \tag{43}$$

where

$$\begin{aligned}\frac{1}{\theta_1^2}&=\frac{1}{\theta_{11}^2}+\frac{1}{\theta_{12}^2}\\&=\frac{(a_k^{\mathbf{T}})^4\left((a_k^{\mathbf{T}})^2-c1/c2\right)\left(a_k^{\mathbf{T}}+1+c_1/c_2\right)+c_2\left((a_k^{\mathbf{T}})^2-c_1/c_2\right)^2}{(a_k^{\mathbf{T}})^4\left(a_k^{\mathbf{T}}+c_1/c_2\right)^2\left(a_k^{\mathbf{T}}+1\right)^2}.\end{aligned}$$

Then, we complete the proof of Theorem 3.

6.3 *Proof of Theorem 4*

According the contents of the previous section, we let the eigenvalues of $\widetilde{\boldsymbol{S}}_1$ be sorted as

$$l_1^{\widetilde{\boldsymbol{S}}_1} \geq l_2^{\widetilde{\boldsymbol{S}}_1} \geq \cdots \geq l_p^{\widetilde{\boldsymbol{S}}_1}, \tag{44}$$

and the spectral decomposition of $\widetilde{\boldsymbol{S}}_1$ be

$$\widetilde{\boldsymbol{S}}_1 = \mathbf{U}\begin{pmatrix} \boldsymbol{\Sigma}_1 & 0 \\ 0 & \boldsymbol{\Sigma}_2 \end{pmatrix}\mathbf{U}^T, \tag{45}$$

where $\boldsymbol{\Sigma}_1 = diag(l_1^{\widetilde{\boldsymbol{S}}_1}, \ldots, l_M^{\widetilde{\boldsymbol{S}}_1})$ is an $M \times M$ diagonal matrix, $\mathbf{U}$ is a orthogonal matrix. In addition, let the sample eigenvalues for noncentral Fisher matrix $\boldsymbol{F}(\boldsymbol{\Xi})$ be sorted as

$$l_1 \geq l_2 \geq \cdots \geq l_p. \tag{46}$$

Recall that

$$\widetilde{\boldsymbol{S}}_2 = \frac{1}{n-q}\mathbf{C}\mathbf{C}^T = \frac{1}{n-q}\begin{pmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{pmatrix}(\mathbf{C}_1^T \ \mathbf{C}_2^T) = \frac{1}{n-q}\begin{pmatrix} \mathbf{C}_1\mathbf{C}_1^T & \mathbf{C}_1\mathbf{C}_2^T \\ \mathbf{C}_2\mathbf{C}_1^T & \mathbf{C}_2\mathbf{C}_2^T \end{pmatrix},$$

where $\mathbf{C}_1$ is the first M rows of $\mathbf{C}$. Then we have that the eigen-equation

$$\left|\widetilde{\boldsymbol{S}}_1\widetilde{\boldsymbol{S}}_2^{-1} - \lambda\mathbf{I}\right| = 0$$

equals

$$\left|\begin{pmatrix} \boldsymbol{\Sigma}_1 & 0 \\ 0 & \boldsymbol{\Sigma}_2 \end{pmatrix} - \frac{\lambda}{n-q}\mathbf{U}^T\mathbf{C}\mathbf{C}^T\mathbf{U}\right| = 0. \tag{47}$$

According to the facts that the entries of $\mathbf{C}$ are standard normally distributed and $\frac{1}{n-q}\tilde{\mathbf{C}}\tilde{\mathbf{C}}^T := \frac{1}{n-q}\mathbf{U}^T\mathbf{C}\mathbf{C}^T\mathbf{U} \overset{d}{=} \frac{1}{n-q}\mathbf{C}\mathbf{C}^T$, the eigen-equation (47) can be rewritten as

$$\left|\begin{pmatrix} \boldsymbol{\Sigma}_1 & 0 \\ 0 & \boldsymbol{\Sigma}_2 \end{pmatrix} - \frac{\lambda}{n-q}\tilde{\mathbf{C}}\tilde{\mathbf{C}}^T\right| = \left|\begin{pmatrix} \boldsymbol{\Sigma}_1 & 0 \\ 0 & \boldsymbol{\Sigma}_2 \end{pmatrix} - \lambda\begin{pmatrix} \frac{1}{n-q}\tilde{\mathbf{C}}_1\tilde{\mathbf{C}}_1^T & \frac{1}{n-q}\tilde{\mathbf{C}}_1\tilde{\mathbf{C}}_2^T \\ \frac{1}{n-q}\tilde{\mathbf{C}}_2\tilde{\mathbf{C}}_1^T & \frac{1}{n-q}\tilde{\mathbf{C}}_2\tilde{\mathbf{C}}_2^T \end{pmatrix}\right| = 0.$$

If we only consider the sample spiked eigenvalues $l_i, i \in \mathcal{J}_k, k = 1, \ldots, K$, then we have that almost surely $|\boldsymbol{\Sigma}_2 - l_i\frac{1}{n-q}\tilde{\mathbf{C}}_2\tilde{\mathbf{C}}_2^T| \neq 0$ for large enough n, which implies

$$\left|\boldsymbol{\Sigma}_1 - l_i\frac{1}{n-q}\tilde{\mathbf{C}}_1\tilde{\mathbf{C}}_1^T - l_i^2\frac{1}{(n-q)^2}\tilde{\mathbf{C}}_1\tilde{\mathbf{C}}_2^T(\Sigma_2 - l_i\frac{1}{n-q}\tilde{\mathbf{C}}_2\tilde{\mathbf{C}}_2^T)^{-1}\tilde{\mathbf{C}}_2\tilde{\mathbf{C}}_1^T\right| = 0,$$

or equivalently

$$\left|\mathbf{\Sigma}_1+\tfrac{1}{n-q}\mathrm{tr}(\tfrac{1}{n-q}\tilde{\mathbf{C}}_2^T\mathbf{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2-l_i^{-1}\mathbf{I})^{-1}\mathbf{I}+\mathbf{\Omega}_q^{\mathbf{F}}(l_i^{-1})\right|=0.$$

Here

$$\begin{aligned}\mathbf{\Omega}_q^{\mathbf{F}}(l_i^{-1})=&\frac{1}{n-q}\tilde{\mathbf{C}}_1\left[\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\mathbf{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2-l_i^{-1}\mathbf{I}\right]^{-1}\tilde{\mathbf{C}}_1^T\\&-\frac{1}{n-q}\mathrm{tr}\left(\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\mathbf{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2-l_i^{-1}\mathbf{I}\right)^{-1}\mathbf{I}.\end{aligned}\tag{48}$$

By the strong law of large numbers and the Stietjes transformation equation of M-P law, we have that

$$\mathbf{\Omega}_q^{\boldsymbol{F}}(l_i^{-1})\xrightarrow{a.s.}\mathbf{0},\tag{49}$$

and

$$\tfrac{1}{n-q}\mathrm{tr}\left(\tfrac{1}{n-q}\tilde{\mathbf{C}}_2^T\mathbf{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2-l_i^{-1}\mathbf{I}\right)^{-1}\xrightarrow{a.s.}\underline{m}_{\mathbf{\Sigma}_2^{-1}}(l_i^{-1}),\tag{50}$$

where $\underline{m}_{\mathbf{\Sigma}_2^{-1}}(l_i^{-1})$ satisfies the following equation:

$$l_i^{-1}=-\frac{1}{\underline{m}_{\mathbf{\Sigma}_2^{-1}}(l_i^{-1})}+c_4\int\frac{t}{1+t\underline{m}_{\mathbf{\Sigma}_2^{-1}}(l_i^{-1})}dF^{\mathbf{\Sigma}_2^{-1}}(t),\tag{51}$$

where $c_4=c_1/(1-c_2)$ and $F^{\mathbf{\Sigma}_2}$ is the LSD of the matrix $\mathbf{\Sigma}_2$ defined in (45). Thus, let $n\to\infty$ and solve the eigen-equation, we have that

$$a_k^{\boldsymbol{F}}+\underline{m}_{\mathbf{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1})=0,$$

which implies

$$\lambda_k^{\boldsymbol{F}}=\psi_{\mathbf{F}}(a_k^{\mathbf{F}}):=\frac{a_k^{\mathbf{F}}}{1+c_4a_k^{\mathbf{F}}m_2(a_k^{\mathbf{F}})}.\tag{52}$$

Thus, by Lemma 1 and Theorem 2, we obtain that

$$\psi_{\mathbf{F}}(a_k^{\boldsymbol{F}})=\psi_{\mathbf{F}}(\psi_{\tilde{\mathbf{S}}_1}(\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}}))),$$

where

$$\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}})=a_k^{\mathbf{T}},\qquad\psi_{\tilde{\mathbf{S}}_1}(\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}}))=\frac{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}{a_k^{\mathbf{T}}}.$$

Then we conclude that

$$\psi(a_k^{\mathbf{T}}) := \psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}}) = \frac{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}{a_k^{\mathbf{T}}} \frac{1}{1-c_4(1+1/a_k^{\mathbf{T}})} = \frac{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}{a_k^{\mathbf{T}}-c_4(a_k^{\mathbf{T}}+1)},$$

which completes the proof of Theorem 4.

6.4 *Proof of Theorem 5*

We first show the proof of the CLT of the random vector $\gamma_k^{\boldsymbol{F}} = \{\sqrt{n-q}(l_i - \lambda_k^{\boldsymbol{F}})/\lambda_k^{\boldsymbol{F}}, i \in \mathcal{J}_k\}$ when given $\widetilde{\boldsymbol{S}}_1$. In the sequel, we let $\lambda_k^{\boldsymbol{F}}$ stand for the limit of l_i. Recall the eigen-equation

$$\left|\boldsymbol{\Sigma}_1 + \frac{1}{n-q}\mathrm{tr}\left(\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\boldsymbol{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2 - l_i^{-1}\mathbf{I}\right)^{-1}\mathbf{I} + \boldsymbol{\Omega}_q^{\boldsymbol{F}}(l_i^{-1})\right| = 0,$$

or equivalently

$$\left|\boldsymbol{\Sigma}_1 + \frac{1}{n-q}\mathrm{tr}(\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\boldsymbol{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2 - (\lambda_k^{\boldsymbol{F}})^{-1}\mathbf{I})^{-1}\mathbf{I} + \boldsymbol{\Omega}_q^{\boldsymbol{F}}((\lambda_k^{\boldsymbol{F}})^{-1}) + \varepsilon_3\right| = 0, \quad (53)$$

where

$$\varepsilon_3 = \frac{1}{n-q}\mathrm{tr}\left(\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\boldsymbol{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2 - l_i^{-1}\mathbf{I}\right)^{-1}\mathbf{I} - \frac{1}{n-q}\mathrm{tr}\left(\frac{1}{n-q}\tilde{\mathbf{C}}_2^T\boldsymbol{\Sigma}_2^{-1}\tilde{\mathbf{C}}_2 - (\lambda_k^{\boldsymbol{F}})^{-1}\mathbf{I}\right)^{-1}\mathbf{I} + \boldsymbol{\Omega}_q^{\boldsymbol{F}}(l_i^{-1}) - \boldsymbol{\Omega}_q^{\boldsymbol{F}}((\lambda_k^{\boldsymbol{F}})^{-1}).$$

By the same proof procedure in Sect. 6.2, we have that

$$\varepsilon_3 = \tilde{\varepsilon}_3\mathbf{I} + o_p(\frac{1}{\sqrt{n-q}})\mathbf{1}\mathbf{1}' = -\frac{\gamma_k^{\boldsymbol{F}}|\widetilde{\boldsymbol{S}}_1}{\sqrt{n-q}}\frac{\underline{m}'_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\mathbf{F}})^{-1})}{\lambda_k^{\mathbf{F}}}(1+o_p(1))\mathbf{I} + o_p(\frac{1}{\sqrt{n-q}})\mathbf{1}\mathbf{1}',$$

where $\underline{m}'_{\boldsymbol{\Sigma}_2^{-1}}(\cdot)$ is the derivative of $\underline{m}_{\boldsymbol{\Sigma}_2^{-1}}(\cdot)$. Then, by (51), we have that

$$\frac{1}{\underline{m}'_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1})} = \frac{1}{\underline{m}^2_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1})} - c_4 m_2'(-\underline{m}_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1}))$$

which implies

Table 1 Definition

Matrices type	Sample spikes	Limit	Population spikes
$\boldsymbol{\Xi}$	$l_i^{\boldsymbol{\Xi}}$	$a_k^{\mathbf{T}} = \psi_{\boldsymbol{\Xi}}(a_k^{\mathbf{T}})$	$a_k^{\mathbf{T}}$
$\widetilde{\boldsymbol{S}}_1 \vert \boldsymbol{\Xi}$	$l_i^{\widetilde{\boldsymbol{S}}_1}$	$\lambda_k^{\widetilde{\boldsymbol{S}}_1} = \psi_{\widetilde{\boldsymbol{S}}_1}(a_k^{\widetilde{\boldsymbol{S}}_1})$	$a_k^{\widetilde{\boldsymbol{S}}_1}$
$\boldsymbol{F}(\boldsymbol{\Xi}) \vert \widetilde{\boldsymbol{S}}_1 = \widetilde{\boldsymbol{S}}_1(\widetilde{\boldsymbol{S}}_2)^{-1} \vert \widetilde{\boldsymbol{S}}_1$	l_i	$\lambda_k^{\boldsymbol{F}} = \psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})$	$a_k^{\boldsymbol{F}}$

$$\underline{m}'_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1}) = \frac{(a_k^{\boldsymbol{F}})^2}{1 - c_4(a_k^{\boldsymbol{F}})^2 m_2'(a_k^{\boldsymbol{F}})}.$$

Denote

$$\theta_{\boldsymbol{F}} := \frac{\underline{m}'_{\boldsymbol{\Sigma}_2^{-1}}((\lambda_k^{\boldsymbol{F}})^{-1})}{(\lambda_k^{\boldsymbol{F}})^2} = \frac{[1 + c_4 a_k^{\boldsymbol{F}} m_2(a_k^{\boldsymbol{F}})]^2}{1 - c_4(a_k^{\boldsymbol{F}})^2 m_2'(a_k^{\boldsymbol{F}})}.$$

By Theorem 7.1 in Bai and Yao (2008), we have $(1/\lambda_k^{\boldsymbol{F}})\sqrt{n-q}\boldsymbol{\Omega}_q^{\boldsymbol{F}}((\lambda_k^{\mathbf{F}})^{-1})$ when given $\widetilde{\boldsymbol{S}}_1$ tends to a GOE matrix with a scale parameter $\theta_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})$. As mentioned above, $l_i \to \lambda_k^{\boldsymbol{F}}$ as $n \to \infty$. Therefore, if $i \in \mathcal{J}_k$, then the eigen-equation becomes

$$0 = \begin{vmatrix} a_1^{\boldsymbol{F}} - a_k^{\boldsymbol{F}} + O((n-q)^{-\frac{1}{2}}) & O((n-q)^{-\frac{1}{2}}) & O((n-q)^{-\frac{1}{2}}) \\ O((n-q)^{-\frac{1}{2}}) & \cdots & O((n-q)^{-\frac{1}{2}}) \\ O((n-q)^{-\frac{1}{2}}) & [\boldsymbol{\Omega}_q^{\boldsymbol{F}}]_{kk} + \tilde{\varepsilon}_3 \mathbf{I}_{m_k} + o((n-q)^{-\frac{1}{2}}) & \cdots \\ O((n-q)^{-\frac{1}{2}}) & \cdots & O((n-q)^{-\frac{1}{2}}) \\ O((n-q)^{-\frac{1}{2}}) & \cdots & a_M^{\boldsymbol{F}} - a_k^{\boldsymbol{F}} + O((n-q)^{-\frac{1}{2}}) \end{vmatrix},$$

where $[\boldsymbol{\Omega}_q^{\boldsymbol{F}}]_{kk}$ is k-th diagonal block of $\boldsymbol{\Omega}_q^{\boldsymbol{F}}((\lambda_i^{\boldsymbol{F}})^{-1})$. By Skorokhod strong representation theorem, and analogous discussion in last subsection, we have that

$$(1/\lambda_k^{\boldsymbol{F}})\sqrt{n-q}[\boldsymbol{\Omega}_q^{\boldsymbol{F}}]_{kk} - \gamma_k^{\boldsymbol{F}} \vert \widetilde{\boldsymbol{S}}_1 \times \theta_{\boldsymbol{F}}(a_i^{\boldsymbol{F}})\mathbf{I}_{m_k} \xrightarrow{a.s.} 0,$$

which implies $\gamma_k^{\boldsymbol{F}} \vert \widetilde{\boldsymbol{S}}_1$ converges weakly to the jointed eigenvalues of the matrix

$$\frac{1}{\sqrt{\theta_{\boldsymbol{F}}}}\boldsymbol{\Omega},$$

where

$$\theta_{\boldsymbol{F}} = \frac{(1 - c_1 - c_2 - c_1/a_k^{\mathbf{T}})^2(1 - c_3/(a_k^{\mathbf{T}})^2)}{(1 - c_2)[1 - c_1 - c_2 - 2c_1/a_k^{\mathbf{T}} - c_3/(a_k^{\mathbf{T}})^2]}.$$

Next, we present the proof of Theorem 5, by applying the previous results. We first recall the relative definition in the Table 1.

By the notation in this table, we have the following results:

$$\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}}) = a_k^{\mathbf{T}}, \qquad \psi_{\widetilde{\mathbf{S}}_1}(\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}})) = \frac{(a_k^{\mathbf{T}} + c_3)(a_k^{\mathbf{T}} + 1)}{a_k^{\mathbf{T}}}$$

$$\begin{aligned}\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}}) &= \frac{(a_k^{\mathbf{T}} + c_3)(a_k^{\mathbf{T}} + 1)}{a_k^{\mathbf{T}}} \frac{1}{1 - c_4(1 + 1/a_k^{\mathbf{T}})} \\ &= \frac{(a_k^{\mathbf{T}} + c_3)(a_k^{\mathbf{T}} + 1)}{a_k^{\mathbf{T}} - c_4(a_k^{\mathbf{T}} + 1)},\end{aligned}$$

where $c_3 = c_1/c_2$ and $c_4 = c_1/(1 - c_2)$. Recall the three CLTs above,

$$\begin{aligned}\sqrt{n}\frac{l_i^{\mathbf{\Xi}} - \psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}})}{\psi_{\mathbf{\Xi}}(a_k^{\mathbf{T}})} &\xrightarrow{d} \text{the eigenvalues of } \mathbf{\Omega}_{kk} \\ \sqrt{q}\frac{l_i^{\widetilde{\mathbf{S}}_1} - \psi_{\widetilde{\mathbf{S}}_1}(a_k^{\widetilde{\mathbf{S}}_1})}{\psi_{\widetilde{\mathbf{S}}_1}(a_k^{\widetilde{\mathbf{S}}_1})}\Big|\mathbf{Y} &\xrightarrow{d} \text{the eigenvalues of } \frac{1}{\theta_1}\mathbf{\Omega}_{kk} \\ \sqrt{n-q}\frac{l_i - \psi_{\boldsymbol{F}}(\alpha_i^{\boldsymbol{F}})}{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}\Big|\mathbf{Y}, \mathbf{B} &\xrightarrow{d} \text{the eigenvalues of } \frac{1}{\sqrt{\theta_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}}\mathbf{\Omega}_{kk},\end{aligned}$$

where

$$\begin{aligned}\theta_1 &= \frac{(a_k^{\mathbf{T}} + c_3)(a_k^{\mathbf{T}} + 1)}{\sqrt{((a_k^{\mathbf{T}})^2 - c_3)(2a_k^{\mathbf{T}} + 1 + c_3)}} \\ \theta_{\boldsymbol{F}} &= \frac{(1 - c_1 - c_2 - c_1/a_k^{\mathbf{T}})^2(1 - c_3/(a_k^{\mathbf{T}})^2)}{(1 - c_2)[1 - c_1 - c_2 - 2c_1/a_k^{\mathbf{T}} - c_3/(a_k^{\mathbf{T}})^2]}.\end{aligned}$$

Noted that $a_k^{\widetilde{\mathbf{S}}_1} = l_i^{\mathbf{\Xi}}$ given $\widetilde{\mathbf{Y}}$ and $a_k^{\boldsymbol{F}} = l_i^{\widetilde{\mathbf{S}}_1}$ given $\widetilde{\mathbf{Y}}$ and $\mathbf{B}$, we have

$$\begin{aligned}&\sqrt{n-q}\frac{l_i - (\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{T}})}{(\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{T}})} \\ =\ &\sqrt{n-q}\frac{l_i - \psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}\frac{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}{(\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{\Xi}})}\Bigg|(\mathbf{Y}, \mathbf{B}) \\ &+\sqrt{n-q}\frac{\psi_{\boldsymbol{F}}(l_i^{\widetilde{\mathbf{S}}_1}) - \psi_{\boldsymbol{F}}(\psi_{\widetilde{\mathbf{S}}_1}(a_k^{\widetilde{\mathbf{S}}_1}))}{(\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{T}})}\Bigg|\mathbf{Y} \\ &+\sqrt{n-q}\frac{\psi_{\boldsymbol{F}}(\psi_{\widetilde{\mathbf{S}}_1}(l_i^{\mathbf{\Xi}})) - (\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{T}})}{(\psi_{\boldsymbol{F}} \circ \psi_{\widetilde{\mathbf{S}}_1} \circ \psi_{\mathbf{\Xi}})(a_k^{\mathbf{T}})},\end{aligned}$$

where $\circ$ stands for the symbol for the function composition. For the second and third parts, by the Delta method we obtain that

$$
\begin{aligned}
&\sqrt{n-q}\frac{\psi_{\boldsymbol{F}}(\psi_{\widetilde{\boldsymbol{S}}_1}(l_i^{\boldsymbol{\Xi}}))-\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}(a_k^{\mathbf{T}})}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}\\
=\ &\sqrt{\frac{n-q}{n}}(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1})'(a_k^{\mathbf{T}})\sqrt{n}\frac{l_i^{\boldsymbol{\Xi}}-a_k^{\mathbf{T}}}{a_k^{\mathbf{T}}}\frac{a_k^{\mathbf{T}}}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}+o_p(1),\\
&\sqrt{n-q}\frac{\psi_{\boldsymbol{F}}(l_i^{\widetilde{\boldsymbol{S}}_1})-\psi_{\boldsymbol{F}}(\lambda_k^{\widetilde{\boldsymbol{S}}_1})}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}\Bigg|\mathbf{Y}\\
=\ &\sqrt{\frac{n-q}{q}}(\psi_{\boldsymbol{F}})'(\lambda_k^{\widetilde{\boldsymbol{S}}_1})\sqrt{q}\frac{l_i^{\widetilde{\boldsymbol{S}}_1}-\lambda_k^{\widetilde{\boldsymbol{S}}_1}}{\lambda_k^{\widetilde{\boldsymbol{S}}_1}}\frac{\lambda_k^{\widetilde{\boldsymbol{S}}_1}}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}\Bigg|\mathbf{Y}+o_p(1).
\end{aligned}
$$

Because the matrix $\mathbf{B}$ and $\mathbf{C}$ are independent when given $\widetilde{\mathbf{Y}}$, by rewriting the first part we have

$$
\sqrt{n-q}\frac{l_i-\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}\Bigg|(\mathbf{Y},\mathbf{B})\overset{d}{=}\sqrt{n-q}\frac{l_i-\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}\Bigg|\mathbf{Y}.
$$

Now we have the limits of the above terms,

$$
\begin{aligned}
&\frac{\psi_{\boldsymbol{F}}(a_k^{\boldsymbol{F}})}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\boldsymbol{\Xi}})}\Bigg|(\mathbf{Y},\mathbf{B})\xrightarrow{p}1,\\
&\frac{a_k^{\mathbf{T}}}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}\xrightarrow{p}\frac{a_k^{\mathbf{T}}[a_k^{\mathbf{T}}-c_4(a_k^{\mathbf{T}}+1)]}{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)},\\
&\frac{\lambda_k^{\widetilde{\boldsymbol{S}}_1}}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}\Bigg|\mathbf{Y}\xrightarrow{p}1+c_4a_k^{\mathbf{F}}m_2(a_k^{\mathbf{F}})\\
&\psi'_{\mathbf{F}}(a_k^{\mathbf{F}})=\frac{1}{\theta_{\mathbf{F}}},\quad(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1})'(a_k^{\mathbf{T}})=\frac{1}{\theta_{\mathbf{F}}}\frac{(a_k^{\mathbf{T}})^2-c_3}{(a_k^{\mathbf{T}})^2}.
\end{aligned}
$$

As the mean and covariance of the limiting distribution of the first and second parts are not related to $\widetilde{\mathbf{Y}}$, we conclude that the three parts are asymptotically independent. Then we have that

$$
\sqrt{n-q}\frac{l_i-(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}{(\psi_{\boldsymbol{F}}\circ\psi_{\widetilde{\boldsymbol{S}}_1}\circ\psi_{\boldsymbol{\Xi}})(a_k^{\mathbf{T}})}
$$

converges weakly to the joint distribution of the eigenvalues of Gaussian random matrix

$$
\frac{\boldsymbol{\Omega}_1}{\sqrt{\theta_{\boldsymbol{F}}}}+\frac{\sqrt{1-c_2}}{\sqrt{c_2}}\frac{a_k^{\mathbf{T}}-c_4(a_k^{\mathbf{T}}+1)}{a_k^{\mathbf{T}}\sqrt{\theta_{\boldsymbol{F}}}\theta_1}\boldsymbol{\Omega}_2+\frac{\sqrt{1-c_2}}{\theta_{\boldsymbol{F}}a_k^{\mathbf{T}}}\frac{[(a_k^{\mathbf{T}})^2-c_3][a_k^{\mathbf{T}}-c_4(a_k^{\mathbf{T}}+1)]}{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}\boldsymbol{\Omega}_3
$$

By simplifying the above formula, we obtain that the above matrix is identically distributed as $\frac{1}{\theta_2}\boldsymbol{\Omega}$, where

$$\frac{1}{\theta_2^2} = (1-c_2)(a_k^{\mathbf{T}})^2(a_k^{\mathbf{T}}c_2+1)\left(c_2^2(a_k^{\mathbf{T}})^2+((c_1-1)a_k^{\mathbf{T}}+2c_1)c_2a_k^{\mathbf{T}}+c_1\right)$$
$$\times \frac{\left(c_2^2a_k^{\mathbf{T}}+((c_1-2)a_k^{\mathbf{T}}+2c_1-1)c_2-c_1\right)}{c_2(a_k^{\mathbf{T}}+1)^2(a_k^{\mathbf{T}}c_2+c_1)^2(a_k^{\mathbf{T}}c_2+(c_1-1)a_k^{\mathbf{T}}+c_1)^2},$$

which completes the proof of Theorem 5.

6.5 *Proof of the Theorem 6*

From (18), we have $a_k^{\mathbf{T}} = \frac{1}{c_2}\frac{a_k}{1-a_k}$ and $a_k^{\widetilde{\mathbf{S}}_1} = a_k^{\mathbf{T}} = \frac{1}{c_2}\frac{a_k}{1-a_k} = \frac{1}{c_2}t$. Then from (27), we have

$$\psi(a_k^{\mathbf{T}}) = \frac{(a_k^{\mathbf{T}}+c_3)(a_k^{\mathbf{T}}+1)}{a_k^{\mathbf{T}}-c_4(a_k^{\mathbf{T}}+1)}$$
$$= \frac{(1+c_1t^{-1})(1+c_2t^{-1})}{c_2t^{-1}(1-\frac{c_1}{1-c_2}(1+c_2t^{-1}))}.$$

Thus by (15), we obtain

$$\lambda_i^2 = \frac{\frac{c_2}{1-c_2}\psi(a_k^{\mathbf{T}})}{1+\frac{c_2}{1-c_2}\psi(a_k^{\mathbf{T}})} = \frac{(1+c_1t^{-1})(1+c_2t^{-1})}{1+t^{-1}}$$
$$= a_k(1-c_1+c_1a_k^{-1})(1-c_2+c_2a_k^{-1}).$$

Then we complete the proof of Theorem 6.

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Contributions to Multivariate Analysis Due to C. R. Rao and Associated Developments

Yasunori Fujikoshi

Abstract C. R. Rao has made various significant contributions to multivariate analysis. Among them, we consider the following topics: (i) Rao's U-statistic in discriminant analysis, (ii) MANOVA tests, (iii) Asymptotic expansion and Rao's F approximation for Λ statistic, (iv) Growth curve analysis, and (v) Information criteria for the selection of variables. Some of these were introduced at the dawn of multivariate analysis. Under topic (v), we also discuss recent developments on the selection of variables in discriminant analysis.

Keywords Additional information · Growth curve analysis · MANOVA tests · Model selection - Rao's F approximation · Rao's U-statistic

1 Introduction

In this paper, we consider some important contributions to multivariate analysis due to C. R. Rao, and overview associated developments. In Sect. 2, we focus on Rao's U-statistic for additional information in two-group discriminant analysis. This research leads to a development of statistical methods for the selection of variables. In Sect. 3, multivariate analysis of variance (MANOVA) problems are discussed, based on Rao (1948). We note that Rao developed various types of tests based on real data, which are essentially LR tests. One of these is to test an additional information hypothesis for a set of response variables. Section 4 considers the distribution of a Lambda statistic, $\Lambda_p(q, n-q)$, which appears as the null distribution for various tests, including a MANOVA test. It is noted that an asymptotic expansion of $T = -\{n-(p+q+1)/2\}\Lambda_p(q, n-q)$ was first obtained by Rao (1948). Afterwards,

Abbreviated title: Contributions to Multivariate Analysis due to Rao

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Box (1949) gave an asymptotic expansion for a class of statistics including T. Rao (1952) proposed a highly accurate F approximation for a transformed version of $\Lambda_p(q, n-q)$. Section 5 is concerned with analysis of growth curve data. Rao (1965) introduced two types of models for such data and developed statistical inference of the growth curve models.

It is important to examine whether a set of variables has additional information in the presence of a given set of variables. Such notions were discussed by Rao and others in various models. Applying information criteria such as AIC and BIC to such models, variable selection methods have been proposed. After explaining these, in Sect. 6, we provide more detail on discriminant analysis.

We note that there have been many other important contributions to multivariate analysis due to Rao that are not covered in this paper, some of which are concerned with topics in the following areas: (a) Factor analysis (Rao 1955, etc.). (b) Principal component analysis (Rao 1964, etc.). (c) Correspondence analysis (Rao 1997, etc.). (d) Separation theorems and reduction of dimensionality (Rao 1979, etc.).

2 Rao's U-Statistic in Discriminant Analysis

In two-group discriminant analysis, Rao (1946) investigated whether some variables can be dropped without losing discriminative information. One of his motivations was to reduce computational problems, in addition to enabling efficient discrimination. He proposed the following test of an additional information hypothesis, which determines whether augmenting a given set of p variables with another set of q variables provides additional discrimination between two populations. Suppose that there are n_i samples from $(p+q)$-variate populations, and let D^2_{p+q} and D^2_p be the squared Mahalanobis distances based on the $(p+q)$ variate and the p variate. He proposed a test statistic

$$U = \frac{n-(p+q)-1}{q} \frac{n_1 n_2 (D^2_{p+q} - D^2_p)}{n(n-2) + n_1 n_2 D^2_p}. \tag{1}$$

whose null distribution is an F-distribution with degrees of freedom q and $n-(p+q)-1$, where $n = n_1 + n_2$. The statistics U or $c(D^2_{p+q} - D^2_p)/\{n-2+cD^2_p\}$, where $c = n_1 n_2/n$, were named Rao's U-statistic by Kshirsagar (1972). The test based on U-statistic is called U-test.

The above additional information hypothesis can be formulated as follows. In two-group discriminant analysis, we have two populations Π_i, $i = 1, 2$, and n_i observations from Π_i of p-dimensional variate $\boldsymbol{Y}$. The mean vectors of $\boldsymbol{Y}$ when $\boldsymbol{Y} \in \Pi_i$ are

$$\mathrm{E}(\boldsymbol{Y} \mid \Pi_i) = \boldsymbol{\mu}^{(i)}, \quad i = 1, 2,$$

where it is assumed that the covariance matrices are the same, i.e., $\mathrm{Var}(\boldsymbol{Y} \mid \Pi_i) = \boldsymbol{\Sigma}$. In discriminant analysis, we are interested in which set of variables are important, or which set of variables are redundant. Let $\boldsymbol{Y}$ be decomposed as $\boldsymbol{Y} = (\boldsymbol{Y}_1', \boldsymbol{Y}_2')'$, where $\boldsymbol{Y}_i$; $p_i \times 1$. Let us formulate the notion that $\boldsymbol{Y}_2$ provides no additional information for the discriminant analysis in the presence of $\boldsymbol{Y}_1$, or simply that $\boldsymbol{Y}_1$ is sufficient or $\boldsymbol{Y}_2$ is redundant. We refer to such a notion as the sufficiency of $\boldsymbol{Y}_1$ or the redundancy of $\boldsymbol{Y}_2$.

When the parameters are known, it is natural to classify a new observation $\boldsymbol{Y}$ into Π_1 if

$$(\boldsymbol{Y} - \boldsymbol{\mu}^{(1)})'\boldsymbol{\Sigma}^{-1}(\boldsymbol{Y} - \boldsymbol{\mu}^{(1)}) < (\boldsymbol{Y} - \boldsymbol{\mu}^{(2)})'\boldsymbol{\Sigma}^{-1}(\boldsymbol{Y} - \boldsymbol{\mu}^{(2)}) \tag{2}$$

and otherwise classify $\boldsymbol{Y}$ into Π_2. This expression (2) is equivalent to $L(\boldsymbol{Y}, \boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}) > 0$, where

$$L(\boldsymbol{Y}, \boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \boldsymbol{\Sigma}) = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)'\boldsymbol{\Sigma}^{-1}\boldsymbol{Y} - \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)'\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2), \tag{3}$$

which is called the population discriminant function. The coefficients of the population discriminant function are given by

$$\boldsymbol{\beta} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}^{(1)} - \boldsymbol{\mu}^{(2)}) = (\boldsymbol{\beta}_1', \boldsymbol{\beta}_2')',$$

where $\boldsymbol{\beta}_1 : p_1 \times 1$ and $\boldsymbol{\beta}_2 : p_2 \times 1$. One way to define the redundancy of $\boldsymbol{Y}_2$ is to define it as $\boldsymbol{\beta}_2 = \boldsymbol{0}$. Let δ and δ_1 be the population Mahalanobis distances between Π_1 and Π_2 based on $\boldsymbol{Y}$ and $\boldsymbol{Y}_1$, respectively. Then,

$$\begin{aligned}\delta^2 &= (\boldsymbol{\mu}^{(1)} - \boldsymbol{\mu}^{(2)})'\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}^{(1)} - \boldsymbol{\mu}^{(2)}),\\ \delta_1^2 &= (\boldsymbol{\mu}_1^{(1)} - \boldsymbol{\mu}_1^{(2)})'\boldsymbol{\Sigma}_{11}^{-1}(\boldsymbol{\mu}_1^{(1)} - \boldsymbol{\mu}_1^{(2)}),\end{aligned}$$

where $\boldsymbol{\mu}^{(i)}$ and $\boldsymbol{\Sigma}$ are partitioned as

$$\boldsymbol{\mu}^{(i)} = \begin{pmatrix}\boldsymbol{\mu}_1^{(i)}\\ \boldsymbol{\mu}_2^{(i)}\end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix}\boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12}\\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22}\end{pmatrix}, \tag{4}$$

$\boldsymbol{\mu}_i^{(g)} : p_i \times 1$, $g = 1, 2$ and $\boldsymbol{\Sigma}_{ij} : p_i \times p_j$. It is also reasonable to define the redundancy of $\boldsymbol{Y}_2$ as $\delta^2 = \delta_1^2$. Note that we have

$$\delta^2 = \delta_1^2 + \delta_{2\cdot 1}^2, \tag{5}$$

where

$$\begin{aligned}\delta_{2\cdot 1}^2 &= (\boldsymbol{\mu}_{2\cdot 1}^{(1)} - \boldsymbol{\mu}_{2\cdot 1}^{(2)})'\Sigma_{22\cdot 1}^{-1}(\boldsymbol{\mu}_{2\cdot 1}^{(1)} - \boldsymbol{\mu}_{2\cdot 1}^{(2)}),\\ \boldsymbol{\Sigma}_{22\cdot 1} &= \boldsymbol{\Sigma}_{22} - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12},\\ \boldsymbol{\mu}_{2\cdot 1}^{(i)} &= \boldsymbol{\mu}_2^{(i)} - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\mu}_1^{(i)}, \quad i = 1,\ 2.\end{aligned}$$

This relation is obtained by substituting a well-known inverse matrix formula

$$\boldsymbol{\Sigma}^{-1} = \begin{pmatrix} \boldsymbol{\Sigma}_{11}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{pmatrix} + \begin{pmatrix} -\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12} \\ \mathbf{I}_{p-k} \end{pmatrix} \boldsymbol{\Sigma}_{22\cdot 1}^{-1} \begin{pmatrix} -\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1} & \mathbf{I}_{p-k} \end{pmatrix}$$

for $\boldsymbol{\Sigma}^{-1}$ in δ^2. On the other hand, the coefficient vector of the linear discriminant function is expressed as

$$\boldsymbol{\beta}_1 = \boldsymbol{\Sigma}_{11}^{-1}(\boldsymbol{\mu}_1^{(1)} - \boldsymbol{\mu}_1^{(2)}) - \boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\beta}_2, \quad \boldsymbol{\beta}_2 = \boldsymbol{\Sigma}_{22\cdot 1}^{-1}(\boldsymbol{\mu}_{2\cdot 1}^{(1)} - \boldsymbol{\mu}_{2\cdot 1}^{(2)}).$$

From these results, we can see that, as proved by Rao (1970), the following three statements are equivalent:

$$\text{(i) } \delta^2 = \delta_1^2, \quad \text{(ii) } \boldsymbol{\mu}_{2\cdot 1}^{(1)} = \boldsymbol{\mu}_{2\cdot 1}^{(2)}, \quad \text{(iii) } \boldsymbol{\beta}_2 = 0.$$

The second statement is related to the equality of conditional means. In fact,

$$\begin{aligned} \mathrm{E}(\boldsymbol{Y}_2^{(i)} \mid \boldsymbol{Y}_1^{(i)}) &= \boldsymbol{\mu}_2^{(i)} + \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}(\boldsymbol{Y}_1^{(i)} - \boldsymbol{\mu}_1^{(i)}) \\ &= \boldsymbol{\mu}_{2\cdot 1}^{(i)} + \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{Y}_1^{(i)}, \quad i = 1, 2. \end{aligned} \tag{6}$$

Statements (i) and (iii) help in understanding that $\boldsymbol{Y}_2$ provides no additional information for the discriminant analysis in the presence of $\boldsymbol{Y}_1$. Statement (iii) is used for obtaining a likelihood ratio test for (i) or (iii), which is equivalent to a U-test. Statements (i), (ii), and (iii) and their equivalence were extended to the case of several groups by Fujikoshi (1982). Gupta et al. (2006) derive a large sample asymptotic expansion of Rao's U-statistic under nonnormality. Pynnönen (1987) extended the notion of redundancy to the case where the covariance matrices are different.

In general, it is important to formulate that a subset of response or explanatory variables is sufficient, or the set of remainder variables has no additional information or redundant, as in discriminant analysis. It is also important to extend statistical inferences for such formulations. For some of such results, see Fujikoshi (1989, 1992). In Sect. 6, we see that such formulations are used in variable selection methods.

3 MANOVA Tests

Rao made many important contributions to MANOVA through the analysis of various real data. First, we note that he gives an example in his book (1952) where Mahalanobis D^2 (or Hotelling T^2) based on two variables showed no significance between the two populations; whereas two sample t-tests based on each of the variables were highly significant. This is the first example of what is called the "curse of dimensionality" in multivariate analysis, which was named as Rao's paradox by Healy (1969) and Rencher (2002, p.116). Rencher (2002) explained this paradox in

detail, and also showed the situation that, conversely, the multivariate test is more powerful in some situations, despite the univariate tests are not being significant. In general, the "curse of dimensionality" phrase was introduced by Bellman (1957) for describing the problem caused by the exponential increase in volume associated with adding extra dimensions to the Euclidean space. When we are concerned with the analysis of a p variate, we might be concerned with the analysis of various subsets of the p variate. Related to this problem, Rao (1966a) gave conditions under which additional variables are useful in tests of significance.

As in a typical MANOVA model, consider a multivariate one-way analysis of variance model, in which we measure p dependent variables on each experimental unit instead of just one variable. We consider q treatments and assign n_i subjects to the ith treatment. It is assumed that all of the n $(= n_1 + \cdots + n_q)$ observations are normally distributed with the common covariance matrix $\boldsymbol{\Sigma}$. Let $\boldsymbol{Y}_{i1}, \ldots, \boldsymbol{Y}_{in_i}$ be samples from the ith treatment group $\mathrm{N}_p(\boldsymbol{\mu}^{(i)}, \boldsymbol{\Sigma})$. For testing the equality of the mean vectors, i.e., $H_0 : \boldsymbol{\mu}^{(1)} = \cdots = \boldsymbol{\mu}^{(q)}$, let $\mathsf{B}$and$\mathsf{W}$ be the matrices of sums of squares and products due to treatments (between groups) and errors (within groups), respectively. These matrices are defined by

$$\mathsf{B} = \sum_{i=1}^{q} n_i(\bar{\boldsymbol{Y}}_{i\cdot} - \bar{\boldsymbol{Y}}_{\cdot\cdot})(\bar{\boldsymbol{Y}}_{i\cdot} - \bar{\boldsymbol{Y}}_{\cdot\cdot})', \quad \mathsf{W} = \sum_{i=1}^{q}\sum_{j=1}^{n_i}(\boldsymbol{Y}_{ij} - \bar{\boldsymbol{Y}}_{i\cdot})(\boldsymbol{Y}_{ij} - \bar{\boldsymbol{Y}}_{i\cdot})'$$

where $\bar{\boldsymbol{Y}}_{i\cdot} = (1/n_i)\sum_{j=1}^{n_i} \boldsymbol{Y}_{ij}$ and $\bar{\boldsymbol{Y}}_{\cdot\cdot} = (1/n)\sum_{i=1}^{q}\sum_{j=1}^{n_i} \boldsymbol{Y}_{ij}$. Then, under H_0, B and W are independently distributed as Wishart distributions $\mathrm{W}_p(q-1, \boldsymbol{\Sigma})$ and $\mathrm{W}_p(n-q, \boldsymbol{\Sigma})$, respectively. Letting $\mathsf{T} = \mathsf{B} + \mathsf{W}$, an LR test for H_0 is based on $\Lambda = |\mathsf{W}|/|\mathsf{T}|$, whose null distribution does not depend on $\boldsymbol{\Sigma}$ and is denoted by $\Lambda_p(q-1, n-q)$. Such Λ was called Wilks Lambda in Rao (1948), based on the underlying theory of Λ due to Wilks (1932).

In MANOVA, there are two types of problems. One is the problem of comparing the mean vectors as in the above one-way MANOVA model. The other is the problem of comparing within the mean vectors. Rao (1948) gave various types of MANOVA methods through real data, most of which can also be formulated as a general testing problem in a multivariate linear model. A multivariate linear model is given by

$$\mathsf{Y} = \mathbf{A}\boldsymbol{\Theta} + \mathsf{E}, \tag{7}$$

where $\mathbf{A}$ is an $n \times k$ given matrix and $\boldsymbol{\Theta}$ is a $k \times p$ unknown parameter matrix. It is assumed that the rows of the error matrix E are independently distributed as a p-variate normal distribution with mean zero and unknown covariance matrix $\boldsymbol{\Sigma}$, i.e., $\mathrm{N}_p(\mathbf{0}, \boldsymbol{\Sigma})$. Various hypotheses are expressed as

$$H_g : \ \mathbf{C}\Theta\mathbf{D} = \mathbf{O}, \tag{8}$$

where $\mathbf{C}$ and $\mathbf{D}$ are given matrices of $c \times k$ and $p \times d$ with ranks c and d, respectively. In fact, a relation between the row vectors of $\boldsymbol{\Theta}$ and a relation within the row vectors

of $\boldsymbol{\Theta}$ are expressed by, respectively, defining $\mathbf{C}$ and $\mathbf{D}$, as appropriate. The likelihood ratio test is based on

$$\Lambda = \frac{|\mathsf{S}_e|}{|\mathsf{S}_e + \mathsf{S}_h|} = \frac{|\mathsf{S}_e|}{|\mathsf{S}_t|}, \tag{9}$$

whose null distribution is $\Lambda_d(c, n-k)$, where

$$\begin{aligned}
\mathsf{S}_h &= \{\mathbf{C}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathsf{Y}\mathbf{D}\}'\{\mathbf{C}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{C}'\}^{-1}\mathbf{C}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathsf{Y}\mathbf{D}, \\
\mathsf{S}_e &= \mathbf{D}'\mathsf{Y}'(\mathbf{I}_n - \mathbf{P}_{\mathbf{A}})\mathsf{Y}\mathbf{D}, \\
\mathsf{S}_t &= \mathsf{S}_h + \mathsf{S}_w.
\end{aligned}$$

Rao (1948) proposed a test for whether $\boldsymbol{Y}_2 = (Y_{k+1}, \ldots, Y_p)'$ brings out further differences in q populations when the differences due to $\boldsymbol{Y}_1 = (Y_1, \ldots, Y_k)'$ are removed. Let us consider this problem in a multivariate one-way MANOVA or multi-group discriminant model. Such an additional information hypothesis may be defined as

$$\boldsymbol{\mu}_{2\cdot 1}^{(1)} = \cdots = \boldsymbol{\mu}_{2\cdot 1}^{(q)}, \tag{10}$$

where $\boldsymbol{\mu}_{2\cdot 1}^{(i)} = \boldsymbol{\mu}_2^{(i)} - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\mu}_1^{(i)}$, $i = 1, \ldots, q$. Here, $\boldsymbol{\mu}^{(i)}$ and $\boldsymbol{\Sigma}$ have been decomposed as in (4). Let us decompose B and W as

$$\mathsf{B} = \begin{pmatrix} \mathsf{B}_{11} & \mathsf{B}_{12} \\ \mathsf{B}_{21} & \mathsf{B}_{22} \end{pmatrix}, \quad \mathsf{W} = \begin{pmatrix} \mathsf{W}_{11} & \mathsf{W}_{12} \\ \mathsf{W}_{21} & \mathsf{W}_{22} \end{pmatrix},$$

and decompose T similarly. Then, the LR test is based on

$$\Lambda_{2\cdot 1} = \frac{|\mathsf{W}|/|\mathsf{W}_{11}|}{|\mathsf{T}|/|\mathsf{T}_{11}|} = \frac{|\mathsf{W}_{22\cdot 1}|}{|\mathsf{T}_{22\cdot 1}|}, \tag{11}$$

where $\mathsf{W}_{22\cdot 1} = \mathsf{W}_{21} - \mathsf{W}_{21}\mathsf{W}_{11}^{-1}\mathsf{W}_{21}$ and $\mathsf{T}_{22\cdot 1} = \mathsf{T}_{21} - \mathsf{T}_{21}\mathsf{T}_{11}^{-1}\mathsf{T}_{21}$. The null distribution is $\Lambda_{p-k}(q-1, n-q-k)$. For a proof of the result, see, for example, Fujikoshi et al. (2010), Theorem 3.3.2.

4 Asymptotic Expansion and Rao's F Approximation for Λ Statistic

We consider the lambda distribution, defined as the distribution of

$$\Lambda = \frac{|\mathsf{W}|}{|\mathsf{W} + \mathsf{B}|} \sim \Lambda_p(q, n-q), \tag{12}$$

where B and W are independently distributed and follow the Wishart distributions $\mathrm{W}_p(q, \boldsymbol{\Sigma})$ and $\mathrm{W}_p(n-q, \boldsymbol{\Sigma})$, respectively. Such Λ appears, for example, as a likelihood ratio test for testing the equality of mean vectors $\boldsymbol{\mu}_i, i = 1, \ldots, q+1$, based on an N_i sample from $\mathrm{N}_p(\boldsymbol{\mu}_i, \boldsymbol{\Sigma})$. In this case, $N = N_1 + \cdots + N_{q+1}$ and $n = N - 1$. When we consider the distribution of Λ, we may assume $\boldsymbol{\Sigma} = \mathbf{I}_p$. The likelihood ratio criterion is based on $\lambda = \Lambda^{n/2}$. The hth moment of Λ is given by

$$\mathrm{E}[\Lambda^h] = \prod_{j=1}^{p} \frac{\Gamma[\frac{1}{2}(n-q-j+1)+h]\Gamma[\frac{1}{2}(n-j+1)]}{\Gamma[\frac{1}{2}(n-q-j+1)]\Gamma[\frac{1}{2}(n-j+1)+h]}. \tag{13}$$

We consider an asymptotic expansion of the distribution of $-2\rho \log \Lambda^{n/2}$ with a Bartlett correction factor ρ under a large sample framework:

$$p, q; \text{ fixed}, \quad n \to \infty.$$

Here, ρ is chosen as $1 - (p+q+1)/(2n)$, and we set

$$m = n\rho = n - \frac{1}{2}(p+q+1). \tag{14}$$

Then, the characteristic function of $V = -m \log \Lambda$ is expressed as

$$\begin{aligned} C(t) &= \mathrm{E}\left[\Lambda^{-mit}\right] \\ &= \prod_{j=1}^{p} \frac{\Gamma[\frac{1}{2}m(1-2it) + \frac{1}{4}(p-q+1) - \frac{1}{2}(j-1)]}{\Gamma[\frac{1}{2}m + \frac{1}{4}(p-q+1) - \frac{1}{2}(j-1)]} \\ &\quad \times \frac{\Gamma[\frac{1}{2}m + \frac{1}{4}(p+q+1) - \frac{1}{2}(j-1)]}{\Gamma[\frac{1}{2}m(1-2it) + \frac{1}{4}(p+q+1) - \frac{1}{2}(j-1)]}. \end{aligned} \tag{15}$$

We can derive an expansion for $C(t)$ by using the generalized version of Stirling's formula for the gamma function

$$\begin{aligned} \log \Gamma(z+h) = \log \sqrt{2\pi} + \left(z + h - \frac{1}{2}\right) \log z - z \\ - \sum_{r=1}^{m} (-1)^r \frac{B_{r+1}}{r(r+1)z^r} + R_{m+1}(z), \end{aligned}$$

where $R_{m+1}(z) = \mathrm{O}\left(z^{-(m+1)}\right)$ and $B_r(h)$ is the Bernoulli polynomial of degree r defined by

$$\frac{\tau \mathrm{e}^{h\tau}}{\mathrm{e}^{\tau} - 1} = \sum_{r=0}^{\infty} \frac{\tau^r}{r!} B_r(h).$$

The first three of these are $B_0(h) = 1$, $B_1(h) = h - \frac{1}{2}$, $B_2(h) = h^2 - h + \frac{1}{6}$. The final result is given as follows:

$$C(t) = (1-2it)^{-f/2}\left[1 + \frac{\gamma_2}{m^2}\{(1-2it)^{-2} - 1\} + \frac{1}{m^4}\left\{\gamma_4((1-2it)^{-4} - 1) - \gamma_2^2((1-2it)^{-2} - 1)\right\}\right] + \mathrm{O}(m^{-5}), \tag{16}$$

where $f = pq$, $\gamma_2 = pq(p^2 + q^2 - 5)/48$, and

$$\gamma_4 = pq\{3p^4 + 3q^4 + 10p^2q^2 - 50(p^2 + q^2) + 159\}/1920.$$

Inverting the above characteristic function formally, we have an asymptotic expansion:

$$\mathrm{P}(-m\log\Lambda \le x) = G_f(x) + \frac{\gamma_2}{m^2}[G_{f+4}(x) - G_f(x)] + \frac{1}{m^4}[\gamma_4\{G_{f+8}(x) - G_f(x)\} - \gamma_2^2\{G_{f+4}(x) - G_f\}] + \mathrm{O}(m^{-5}), \tag{17}$$

where $G_f(x)$ is the distribution function of χ_f^2.

It may be noted that result (17) was first derived by Rao (1948), based on an expression due to Wald and Brookner (1941). On the other hand, Box (1949) obtained the result as a special case of a general asymptotic expansion of the distribution of a random variable whose moments belong to a class of Box-type moments.

Rao (1951) proposed a better F approximation of the distribution of another function of $\Lambda = \Lambda_p(q, n-q)$. The approximation is to consider

$$\frac{1 - \Lambda^{1/s}}{\Lambda^{1/s}} \cdot \frac{ms + 2\lambda}{pq} \tag{18}$$

as an F approximation with pq and $ms + 2\lambda$ degrees of freedom, where

$$\lambda = -\frac{1}{4}pq + \frac{1}{2}, \quad s = \left(\frac{p^2q^2 - 4}{p^2 + q^2 - 5}\right)^{1/2}. \tag{19}$$

For $p = 1$ or 2 (or $q = 1$ or 2), the F-distribution is exactly as given. If $ms + 2\lambda$ is not an integer, interpolation between two integer values can be used. The F approximation may be also written as a beta approximation $\beta(\frac{1}{2}(ms + 2\lambda), \frac{1}{2}pq)$ for $Y = \Lambda^{1/s}$ which was obtained in Rao (1951) as follows. From (17), the density function of $V = -m\log\Lambda$ can be expressed as

$$f_V(v) = g_r(v)\left[1 + \frac{\gamma_2}{m^2}\left\{\frac{v^2}{r(r+2)} - 1\right\} + \mathrm{O}(m^{-3})\right], \tag{20}$$

where $r = pq$ and $g_r(v)$ is the density function of χ_r^2, by using $g_{r+2}(v) = (v/r)g_r(v)$. Rao considered a better approximation for

$$Y = \Lambda^{1/s} = \mathrm{e}^{-V/(sm)}, \tag{21}$$

introducing a constant s. The density function of Y is expressed as

$$\begin{aligned} f_Y(y) &= f_V(sm(-\log y))\frac{sm}{y} \\ &= \frac{1}{\Gamma(r/2)2^{r/2}}(ms)^{r/2}y^{(ms)/2+\lambda-1}y^{-\lambda}(-\log y)^{r/2-1} \\ &\times \left\{1 + \frac{\gamma_2 s^2}{r(r+2)}(-\log y)^2 + \mathrm{o}(m^{-2}) + \mathrm{o}((1-y)^2)\right\}, \end{aligned} \tag{22}$$

introducing a constant λ. Now, we use

$$\begin{aligned} y^{-\lambda} &= \{1-(1-y)\}^{-\lambda} \\ &= 1 + \lambda(1-y) + \frac{1}{2}\lambda(1+\lambda)(1-y)^2 + \cdots, \\ (-\log y)^{r/2-1} &= \left[-\log\{1-(1-y)\}\right]^{r/2-1} \\ &= (1-y)^{r/2-1}\left[1 + \frac{1}{2}\left(\frac{1}{2}r-1\right)(1-y)\right. \\ &\left. + \left\{\frac{1}{3}\left(\frac{1}{2}r-1\right) + \frac{1}{8}\left(\frac{1}{2}r-1\right)\left(\frac{1}{2}r-2\right)\right\}(1-y)^2 + \cdots\right]. \end{aligned}$$

Substituting the above expansions to the density of Y given by (22), we have

$$\begin{aligned} f_Y(y) &= \frac{1}{\Gamma(r/2)2^{r/2}}(ms)^{r/2}y^{(ms)/2+\lambda-1}(1-y)^{r/2-1} \\ &\times \left\{1 + a_1(1-y) + a_2(1-y)^2 + \mathrm{o}(m^{-2}) + \mathrm{o}((1-y)^2)\right\}, \end{aligned} \tag{23}$$

where

$$\begin{aligned} a_1 &= \lambda + \frac{1}{2}\left(\frac{1}{2}r-1\right), \\ a_2 &= \frac{1}{2}\lambda(1+\lambda) + \left(\frac{1}{2}r-1\right)\left\{\frac{1}{2}\lambda + \frac{1}{3} + \frac{1}{8}\left(\frac{1}{2}r-2\right) + \frac{\gamma_2 s^2}{r(r+2)}\right\}. \end{aligned}$$

Here, we note that defining s and λ as in (19) is equivalent to equating a_1 and a_2 to zero. Further, using the generalized version of Stirling's formula for the gamma function, we can see that

$$\frac{\Gamma(\frac{1}{2}ms+\lambda+\frac{1}{2}r)}{\Gamma(\frac{1}{2}ms+\lambda)\Gamma(\frac{1}{2}r)}=\frac{1}{\Gamma(\frac{1}{2}r)2^{r/2}}(ms)^{r/2}+\mathrm{O}(m^{-1}).$$

This shows that the distribution of $Y=\Lambda^{1/s}$ has an expansion whose leading term is a Beta distribution $\beta(\frac{1}{2}(ms+2\lambda),\frac{1}{2}pq)$ with a smaller error.

Now we note there have been developments related to asymptotic approximations of Λ. A computable error bound for large-sample approximations was derived based on an error bound in the L_1-norm for a multivariate-scale mixture; see Fujikoshi and Ulyanov (2006). A high-dimensional approximation and its error bound have been studied under $p/n\to c\in(0,1)$ by Fujikoshi et al. (2010) and Wakaki (2007). The distribution of Λ is called the nonnull distribution of Λ when B is distributed as a noncentral Whishart distribution $\mathrm{W}_p(q,\boldsymbol{\Sigma};\boldsymbol{\Omega})$. An extension of (17) up to the order m^{-2} to the nonnull case was given by Sugiura and Fujikoshi (1969). Kulp and Nagarsenker (1984) gave an asymptotic expansion of the nonnull distribution of $Y=\Lambda^{1/s}$.

5 Growth Curve Analysis

Research of growth curve analysis dates back to Wishart (1938), who compared the growth curves of animals under different treatments. In particular, the weight of each animal under each treatment was ascertained each week for a number of weeks. For the original measurements of weekly weights $(y_1,\ldots,y_p)$, Wishart (1938) fitted orthogonal polynomials, for example,

$$a+b_1\phi_1(t)+b_2\phi_2(t)$$

to each growth curve dataset and replaced the original measurements of weekly weights $(y_1,\ldots,y_p)$ by (y_1,b_1,b_2). Then, a univariate analysis of variance on b_1 or b_2 was considered, using y_1 as a concomitant.

Rao (1959) proposed to analyze such growth curve data by considering a multivariate structure in addition to a growth curve structure. In general, suppose that a single variable Y is measured at p time points $t_1,\ldots,t_p$ (or different conditions) on n subjects, chosen at random from a group. One way to analyze such repeated measures is to specify a polynomial regression for Y on the time variable t, and to assume that the covariance matrix of $\boldsymbol{Y}=(Y_1,\ldots,Y_p)'$ is unknown and positive definite.

Let the observations $Y_{i1},\ldots,Y_{ip}$ of the ith subject be denoted by

$$\boldsymbol{Y}_i=(Y_{i1},\ldots,Y_{ip})',\quad i=1,\ldots,n.$$

Then, in the growth curve model, it is assumed that for $i=1,\ldots,n$,

$$\mathrm{E}(\boldsymbol{Y}_i) = \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\theta}, \tag{24}$$

and $\mathrm{Var}(\boldsymbol{Y}_i) = \boldsymbol{\Sigma}$, where $\mathbf{X}$ is a given $p \times q$ matrix with rank q, $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_q)'$ is an unknown parameter vector, and $\boldsymbol{\Sigma}$ is unknown positive and definite. The matrix $\mathbf{X}$ is called a within-design matrix. In the growth curve model (24), Rao (1959) proposed and developed the following theory:

(1) Is the specification (24) adequate?
(2) How can estimators of $\theta_1, \ldots, \theta_q$ be obtained and the precision of the estimators be expressed?
(3) How can general linear hypotheses concerning $\theta_1, \ldots, \theta_q$ be tested?
(4) How can simultaneous confidence limits for a class of linear functions of $\theta_1, \ldots, \theta_q$ be obtained?

In addition, Rao (1987) proposed approaches to the following problem.

(5) Suppose that the measurements of growth at the time points $t_1, \ldots, t_p, t_{p+1}$ are available for n individuals and only at $t_1, \ldots, t_p$ for an $(n+1)-$th individual. How do we predict the measurement at t_{p+1} for the $(n+1)-$th individual?

The growth curve model for above one-group data was extended by Potthoff and Roy (1964) as follows. Suppose that the rows of Y are independently distributed as p-dimensional normal distributions with a common covariance matrix $\boldsymbol{\Sigma}$, and

$$\mathrm{E}(\mathsf{Y}) = \mathbf{A}\boldsymbol{\Theta}\mathbf{X}', \tag{25}$$

where $\mathbf{A}$ is the $n \times k$ between-group design matrix, $\mathbf{X}$ is the $p \times q$ within design matrix, and $\boldsymbol{\Theta}$ is the $k \times q$ unknown parameter matrix. A general testing problem is to test

$$H_g : \mathbf{C}\boldsymbol{\Theta}\mathbf{D} = \mathbf{O}, \text{ against } K_g : \mathbf{C}\boldsymbol{\Theta}\mathbf{D} \neq \mathbf{O}. \tag{26}$$

Here, $\mathbf{C}$ is a given $c \times k$ matrix with rank c, and $\mathbf{D}$ is a given $q \times d$ matrix with rank d. The growth curve model (25) is reduced to a MANOVA model when the within-individual design matrix $\mathbf{X}$ is $\mathbf{I}_p$. In this sense, the growth curve model is a generalized MANOVA model.

In order to relate the growth curve model to a multivariate linear model, consider the transformation from Y to $(\mathsf{U}\ \mathsf{V})$:

$$(\mathsf{U}\ \mathsf{V}) = \mathsf{Y}(\mathbf{G}_1\ \mathbf{G}_2), \tag{27}$$

where $\mathbf{G}_1$ and $\mathbf{G}_2$ are the same matrices as in the group, $\mathbf{G}_1 = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$, $\mathbf{G}_2 = \tilde{\mathbf{X}}$, and $\tilde{\mathbf{X}}$ is a $p \times (p-q)$ matrix satisfying $\tilde{\mathbf{X}}'\mathbf{X} = \mathbf{O}$ and $\tilde{\mathbf{X}}'\tilde{\mathbf{X}} = \mathbf{I}_{p-q}$. Then, the rows of $(\mathsf{U}\ \mathsf{V})$ are independently distributed as p-dimensional normal distributions with means

$$\mathrm{E}[(\mathsf{U}\ \mathsf{V})] = (\mathbf{A}\Theta\ \mathbf{O})$$

and the common covariance matrix

$$\boldsymbol{\Psi} = \mathbf{G}'\boldsymbol{\Sigma}\mathbf{G} = \begin{pmatrix} \mathbf{G}_1'\boldsymbol{\Sigma}\mathbf{G}_1 & \mathbf{G}_1'\boldsymbol{\Sigma}\mathbf{G}_2 \\ \mathbf{G}_2'\boldsymbol{\Sigma}\mathbf{G}_1 & \mathbf{G}_2'\boldsymbol{\Sigma}\mathbf{G}_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Psi}_{11} & \boldsymbol{\Psi}_{12} \\ \boldsymbol{\Psi}_{21} & \boldsymbol{\Psi}_{22} \end{pmatrix},$$

where $\mathbf{G} = (\mathbf{G}_1\ \mathbf{G}_2)$. This transformation can be regarded as one from $\boldsymbol{Y} = (Y_1, \ldots, Y_p)'$ to a q-dimensional main variable $\boldsymbol{U} = (U_1, \ldots, U_q)'$ and a $(p-q)$-dimensional auxiliary variable $\boldsymbol{V} = (V_1, \ldots, V_{p-q})'$. The growth curve model is equivalent to the following two models:

(1) The conditional distribution of U given V is

$$\mathsf{U} \mid \mathsf{V} \sim N_{n\times q}(\mathsf{A}^*\boldsymbol{\Xi},\ \boldsymbol{\Psi}_{11\cdot 2}). \tag{28}$$

(2) The marginal distribution of V is

$$\mathsf{V} \sim \mathrm{N}_{n\times(p-q)}(\mathbf{O},\ \boldsymbol{\Psi}_{22}), \tag{29}$$

where

$$\mathsf{A}^* = (\mathbf{A}\ \mathsf{V}), \quad \boldsymbol{\Xi} = \begin{pmatrix} \boldsymbol{\Theta} \\ \boldsymbol{\Gamma} \end{pmatrix},$$
$$\boldsymbol{\Gamma} = \boldsymbol{\Psi}_{22}^{-1}\boldsymbol{\Psi}_{21},\ \boldsymbol{\Psi}_{11\cdot 2} = \boldsymbol{\Psi}_{11} - \boldsymbol{\Psi}_{12}\boldsymbol{\Psi}_{22}^{-1}\boldsymbol{\Psi}_{21}.$$

Rao (1965) also gave the above reduction, and called V the observation matrix of concomitant variables. Statistical methods based on likelihood were introduced by Rao (1959, 1965), Khatri (1966), Gleser and Olkin (1970), and others. The LR test was first given by Khatri (1966). Gleser and Olkin (1970) gave the LR test based on a canonical for the testing problem (26). The LR test is based on

$$\Lambda = |\mathsf{S}_e|/|\mathsf{S}_e + \mathsf{S}_h|,$$

where

$$\mathsf{S}_e = \mathbf{D}'(\mathbf{X}'\mathsf{S}^{-1}\mathbf{X})^{-1}\mathbf{D}, \quad \mathsf{S}_h = (\mathbf{C}\hat{\Theta}\mathbf{D})(\mathbf{C}\mathsf{R}\mathbf{C}')^{-1}\mathbf{C}\hat{\Theta}\mathbf{D}$$

and

$$\mathsf{R} = (\mathbf{A}'\mathbf{A})^{-1} + (\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'\mathsf{Y}\mathsf{S}^{-1}\{\mathsf{S} - \mathbf{X}'(\mathbf{X}\mathsf{S}^{-1}\mathbf{X}')^{-1}\mathbf{X}\}$$
$$\times\, \mathsf{S}^{-1}\mathsf{Y}'\mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}.$$

Here, $\hat{\boldsymbol{\Theta}}$ and S are given by

$$\hat{\boldsymbol{\Theta}} = \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'\mathsf{Y}\mathsf{S}^{-1}\mathbf{X}(\mathbf{X}'\mathsf{S}^{-1}\mathbf{X})^{-1},$$
$$\mathsf{S} = \frac{1}{m}\mathsf{Y}'(\mathbf{I}_n - \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}')\mathsf{Y}, \quad m = n - k.$$

Further, the null distribution of Λ is $\Lambda_d(c, n-k-(p-q))$.

Rao (1965) and Grizzle and Allen (1969) discuss the possibility of using fewer than $p - q$ covariables. Fujikoshi and Rao (1991) proposed two types of formulation for the hypotheses of redundancy of a given set of covariables. The likelihood ratio criteria were obtained for testing these hypotheses. Further, using these results, they proposed information criteria such as for selection of the best subset of covariables.

In the growth curve models as in (24) and (25), it is necessary that the observations be observed at the same time points for each of the subjects, and that each of the groups have the same within-design matrix $\mathbf{X}$. In order to resolve the latter assumption, a general growth curve model was proposed by Rosen (1987), Verbyla and Venables (1988), etc., as follows:

$$\mathrm{E}(\mathrm{Y}) = \sum_{i=1}^{r} \mathbf{A}_i \boldsymbol{\Theta}_i \mathbf{X}_i', \tag{30}$$

which is called the sum-of-profiles model. On the other hand, in order to incorporate individual effects fully, the following random coefficients model or mixed effects model was considered:

$$\begin{aligned} \boldsymbol{Y}_i &= \mathbf{X}_i \boldsymbol{\beta}_i + \boldsymbol{e}_i, \quad i = 1, \ldots, n, \\ \boldsymbol{\beta}_i &= \boldsymbol{\theta} + \boldsymbol{b}_i, \quad i = 1, \ldots, n, \end{aligned}$$

where $\mathbf{X}_i$ is a $p_i \times k$ known matrix,

$$\begin{aligned} &\boldsymbol{b}_1, \ldots, \boldsymbol{b}_n \sim \text{i.i.d. } \mathrm{N}_k(\mathbf{0}, \boldsymbol{\Delta}), \boldsymbol{\Delta} \geq \mathbf{O}, \\ &\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n \text{ are independent, } \boldsymbol{e}_i \sim \mathrm{N}_{p_i}(\mathbf{0}, \sigma^2 \mathbf{I}_{n_i}), \\ &\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n\} \text{ and } \{\boldsymbol{b}_1, \ldots, \boldsymbol{b}_n\} \text{ are independent.} \end{aligned}$$

This model is a special case of mixed effects and random coefficients models (see Laird and Ware 1982, and Vonesh and Carter 1987). Rao (1965) considered the above model in the case $\mathbf{X}_1 = \cdots = \mathbf{X}_r$, and developed its statistical inference.

At the end of this section, we consider some topics on discriminant analysis of growth curve data. Such problems were first discussed by Burnaby (1966). The paper pointed out a need for a general procedure of eliminating either a single growth factor or several nuisance factors from discriminant functions or generalized distances between numbers of populations. Some results were given with the help of Rao's comments. Rao (1966b) and, in his book, Rao (1973) treated this problem in a more general form which was called discrimination between composite hypotheses, as follows. Let $\boldsymbol{Y}$ be a p-variate random vector depending on a parameter vector $\boldsymbol{\theta} \in \boldsymbol{\Theta}$. Let H_1 be the hypothesis that $\boldsymbol{\theta} \in \boldsymbol{\Theta}_1$ and H_2 that $\boldsymbol{\theta} \in \boldsymbol{\Theta}_2$, where $\boldsymbol{\Theta}_1$ and $\boldsymbol{\Theta}_2$ are two disjoint subsets of $\boldsymbol{\Theta}$. The problem involves choosing between H_1 and H_2 on the basis of an observed value of $\boldsymbol{Y}$. More concretely, let $\boldsymbol{Y}$ be a p-variate normal vector such that

$$\mathrm{E}(\boldsymbol{Y} \mid \boldsymbol{\theta}_i, H_i) = \boldsymbol{a}_i + \mathbf{X}\boldsymbol{\theta}_i, \quad \mathrm{Var}(\boldsymbol{Y} \mid \boldsymbol{\theta}_i, H_i) = \boldsymbol{\Sigma}, \quad i = 1, 2.$$

Here, $\mathbf{X}$ is a given $p \times k$ matrix of rank k. Let $\mathbf{Z}$ be a $p \times (p-k)$ matrix of rank $p-k$ such that $\mathbf{X}'\mathbf{Z} = \mathbf{O}$. Then,

$$\mathrm{E}(\mathbf{Z}'\boldsymbol{Y} \mid H_i) = \mathbf{Z}'\boldsymbol{a}_i, \quad \mathrm{Var}(\mathbf{Z}'\boldsymbol{Y} \mid H_i) = \mathbf{Z}'\boldsymbol{\Sigma}\mathbf{Z}', \quad i = 1, 2.$$

From (3), the discriminant function based on $\mathbf{Z}'\boldsymbol{Y}$ is given by

$$(\mathbf{Z}'\boldsymbol{a}_1 - \mathbf{Z}'\boldsymbol{a}_2)'(\mathbf{Z}'\boldsymbol{\Sigma}\mathbf{Z})^{-1}\mathbf{Z} = (\boldsymbol{a}_1 - \boldsymbol{a}_2)'\mathbf{Z}(\mathbf{Z}'\boldsymbol{\Sigma}\mathbf{Z})^{-1}\mathbf{Z}'\boldsymbol{Y},$$

which is reduced as

$$(\boldsymbol{a}_1 - \boldsymbol{a}_2)'\{\boldsymbol{\Sigma}^{-1} - \boldsymbol{\Sigma}^{-1}\mathbf{X}(\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Sigma}^{-1}\}\boldsymbol{Y}. \tag{31}$$

Further, it was shown that

$$\sup_{\mathbf{X}'\boldsymbol{\ell}=\mathbf{0}} \frac{[\mathrm{E}(\boldsymbol{\ell}'\boldsymbol{Y} \mid H_1) - \mathrm{E}(\boldsymbol{\ell}'\boldsymbol{Y} \mid H_2)]^2}{2^{-1}[\mathrm{Var}(\boldsymbol{\ell}'\boldsymbol{Y} \mid H_1) + \mathrm{Var}(\boldsymbol{\ell}'\boldsymbol{Y} \mid H_2)]} \tag{32}$$

is attained at

$$\boldsymbol{\ell}_* = \{\boldsymbol{\Sigma}^{-1} - \boldsymbol{\Sigma}^{-1}\mathbf{X}'(\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}\boldsymbol{\Sigma}^{-1}\}(\boldsymbol{a}_1 - \boldsymbol{a}_2). \tag{33}$$

The result follows by using the fact that, under the condition $\mathbf{X}'\boldsymbol{\ell} = \mathbf{0}$, expression (32) is reduced to

$$\sup_{\mathbf{X}'\boldsymbol{\ell}=\mathbf{0}} \frac{[\mathrm{E}\{\boldsymbol{\ell}'(\boldsymbol{a}_1 - \boldsymbol{a}_2)\}^2]}{\boldsymbol{\ell}'\boldsymbol{\Sigma}\boldsymbol{\ell}}. \tag{34}$$

The discriminant function (31) is $\boldsymbol{\ell}_*'\boldsymbol{Y}$, where $\boldsymbol{\ell}_*$ is as defined in (33).

On the other hand, the usual discriminant method and its modifications have been studied for some growth curve models. For example, assume that $\boldsymbol{Y}$ is observed at two populations Π_i, $i = 1, 2$, and

$$\boldsymbol{Y} \mid \Pi_i \sim \mathrm{N}_p(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}), \ i = 1, 2,$$

where $\boldsymbol{\mu}^{(i)} = \mathbf{X}\boldsymbol{\theta}_i$, $i = 1, 2$. Further, let $\widehat{\boldsymbol{\theta}}_i$, $i = 1, 2$ and $\widehat{\boldsymbol{\Sigma}}$ be the MLEs of $\boldsymbol{\theta}_i$, $i = 1, 2$ and $\boldsymbol{\Sigma}$, based on n_i samples from Π_i, $i = 1, 2$. Then, there is a situation to decide which a new observation $\boldsymbol{Y}$ belongs to Π_1 and Π_2. A natural method is to discriminate $\boldsymbol{Y}$ based on the discriminant function $L(\boldsymbol{Y}, \widehat{\boldsymbol{\mu}}^{(1)}, \widehat{\boldsymbol{\mu}}^{(2)}, \widehat{\boldsymbol{\Sigma}})$ in (3). As another example, Lee (1982) considered the classification of growth curves from a non-Bayesian and Baysian viewpoint, under the case where $\boldsymbol{\Sigma}$ is arbitrary positive definite and is of Rao's simple structure (Rao 1967). In some cases, it will be necessary to evaluate the expected probabilities of misclassification. However, this subject has not been much well researched.

6 Information Criteria for Selection of Variables

Related to the selection of variables in multivariate analysis, Rao (1977) stated the following in the foreword of Multivariate Analysis IV (P. R. Krishnaiah, ed., 1977, North-Holland Publishing Company):

"While refinement of Fisherian methods continue to be made, relatively few new lines of investigations are started. New extensions of univariate methods to multiple measurement are being made, which are no doubt useful, but there has not been adequate discussion of the number or choice of variables. In spite of the enormous increase in the multivariate methods, they do not seem to be rich enough to meet all practical demands..."

As we have seen in Sect. 2, Rao proposed a U-statistic for testing a hypothesis that $\boldsymbol{Y}_2$ provides no additional information to a discriminant analysis in the presence of $\boldsymbol{Y}_1$, where $\boldsymbol{Y} = (\boldsymbol{Y}_1', \boldsymbol{Y}_2)'$ and $\boldsymbol{Y} : p_i \times 1$. However, if several other specifications are considered, we need to decide upon the best specification. One approach is to apply model selection criteria such as AIC, BIC, and C_p. In order to represent these approaches, it is standard to formulate the notions of sufficiency or redundancy of a subset of variables such that its likelihood is obtained in a computable form. Before describing it in detail in the case of two-group discriminant analysis, here we note that such an approach has been extended for the selection of variables in various multivariate models. Corresponding results have been obtained for, for example, the selection of the response variables and the explanatory variables in multivariate linear models, the selection of the main variables and the covariables in growth curve models, the selection of variables in canonical correlation analyses, and the selection of dimensionality in principal component analyses.

In the following, we state a more detailed two-group discriminant analysis, following Fujikoshi and Sakurai (2019) and Oda et al. (2020). Suppose that $\boldsymbol{j}$ denotes a subset of $\boldsymbol{\omega} = \{1, \ldots, p\}$ containing p_j elements, and $\boldsymbol{Y}_j$ denotes the p_j vector consisting of the elements of $\boldsymbol{Y}$, indexed by the elements of $\boldsymbol{j}$. We use the notation D_j and $D_{\boldsymbol{\omega}}$ for D based on $\boldsymbol{Y}_j$ and $\boldsymbol{Y}_{\boldsymbol{\omega}} (= \boldsymbol{Y})$, respectively. Let M_j be a variable selection model, defined by

$$M_j : \ \beta_i \neq 0 \text{ if } i \in \boldsymbol{j}, \text{ and } \beta_i = 0 \text{ if } i \notin \boldsymbol{j}. \tag{35}$$

The model M_j is equivalent to $\Delta_j = \Delta_{\boldsymbol{\omega}}$, i.e., the Mahalanobis distance based on $\boldsymbol{Y}_j$ is the same as the one based on the full set of variables, $\boldsymbol{Y}$. We identify the selection of M_j with the selection of $\boldsymbol{Y}_j$. Let AIC_j be the AIC for M_j. Then, it is known (see, e.g., Fujikoshi 1985) that

$$\begin{aligned} \mathrm{A}_j &= \mathrm{AIC}_j - \mathrm{AIC}_{\boldsymbol{\omega}} \\ &= n \log \left\{ 1 + \frac{g^2 (D_{\boldsymbol{\omega}}^2 - D_j^2)}{n - 2 + g^2 D_j^2} \right\} - 2(p - p_j), \end{aligned} \tag{36}$$

where $g = \sqrt{(n_1 n_2)/n}$. Similarly, let BIC_j be the BIC for M_j, and we have that $\mathrm{B}_j = \mathrm{BIC}_j - \mathrm{BIC}_{\boldsymbol{\omega}}$ is the one replaced 2 in A_j by $\log n$.

The variable selection methods based on AIC and BIC are given as $\min_j \mathrm{AIC}_j$ and $\min_j \mathrm{BIC}_j$, respectively. Therefore, such criteria become computationally onerous when p is large. To circumvent this issue, we can use a test-based method (TM, see 2020) or KOO method (Zhao et al. 1986; Nishii et al. 1988; Bai et al. 2018), drawing on the significance of each variable. A critical region for "$\beta_i = 0$" based on the likelihood ratio principle is expressed (see, e.g., Rao 1946, 1973) as

$$\mathrm{T}_{d,i} = n \log \left\{ 1 + \frac{g^2 (D^2_{\boldsymbol{\omega}} - D^2_{(-i)})}{n - 2 + g^2 D^2_{(-i)}} \right\} - d > 0, \tag{37}$$

where $(-i)$, $i = 1, \ldots, p$ is the subset of $\boldsymbol{\omega} = \{1, \ldots, p\}$ obtained by omitting the i from $\boldsymbol{\omega}$, and d is a positive constant that may depend on p and n. Note that

$$\mathrm{T}_{2,i} > 0 \iff \mathrm{AIC}_{(-i)} - \mathrm{AIC}_{\boldsymbol{\omega}} > 0.$$

A test-based method or KOO method is defined by selecting the set of suffixes or the set of variables given by

$$\mathrm{TM}_d = \{i \in \boldsymbol{\omega} \mid \mathrm{T}_{d,i} > 0\}, \tag{38}$$

or $\{Y_i \in \{Y_1, \ldots, Y_p\} \mid \mathrm{T}_{d,i} > 0\}$. The notation $\widehat{\boldsymbol{j}}_{\mathrm{TM}_d}$ is also used for TM_d.

In general, if d is large, a small number of variables are selected. On the other hand, if d is small, a large number of variables are selected. Ideally, we want to select only the true variables whose discriminant coefficients are not zero. Consistency properties of AIC, BIC, and TM_d have been studied under a large-sample framework ($n \to \infty$) and a high-dimensional framework ($n/p \to c \in (0, 1)$); see Fujikoshi (1985), Nishii et al. (1988), Fujikoshi and Sakurai (2019) and Oda et al. (2020). In general, we note that the conclusions of asymptotic consistencies of model selection criteria may be reversed. For example, in the selection of the explanatory variables in a multivariate regression model, it is known (Nishii et al. 1988) that under a large-sample framework, BIC is consistent, but AIC is not consistent. On the other hand, it is known (Fujikoshi and Sakurai 2014; Yanagihara et al. 2015; Bai et al. 2018) that under a high-dimensional framework, AIC is consistent, but BIC is not consistent.

For high-dimensional data such that $p > n$, Lasso and other regularization methods have been extended. For such studies, see, e.g., Clemmensen et al. (2011), Witten and Tibshirani (2011), and Hao et al. (2015).

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On Testing Structures of the Covariance Matrix: A Non-normal Approach

Tõnu Kollo and Marju Valge

Abstract Test-statistics for testing covariance structures are examined for non-normal p-dimensional populations with the finite fourth-order mixed moments. Special attention has been paid to the sphericity and uncorrelatedness hypotheses. For the sphericity test, test-statistics based on trace functions are examined. A χ^2-statistic is constructed for the uncorrelatedness test. In a special case when all the fourth-order moments are equal, the results are simplified. Taylor expansions of the test-statistics have been derived, asymptotic normal and chi-square distributions have been established and their behaviour examined in the situation when both, sample size n and the number of variables p are growing when $\frac{p}{n} < 1$. A simulation experiment was carried out to investigate empirically speed of convergence to the asymptotic distributions depending on the sample size, the number of variables and the parameters of the population distribution.

Keywords Asymptotic normality · Chi-square statistic · Covariance structure · Sphericity hypothesis · Uncorrelatedness hypotheses

1 Set-Up of the Problem

Let $\mathcal{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ be a sample of size n from a p-dimensional population $\mathbf{x} \sim \mathbf{x}_i \sim P_{\mathbf{x}}$ with

$$E\mathbf{x} = \boldsymbol{\mu}; \quad D\mathbf{x} = \boldsymbol{\Sigma},$$

and the finite fourth-order mixed moments.

Denote

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i; \quad \mathbf{S} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})'.$$

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We are interested in testing some basic hypotheses about the covariance structure

$$H_0 : \mathbf{\Sigma} = \mathbf{\Sigma}_0, \tag{1}$$

with a special interest to the hypotheses

$$H_{01} : \mathbf{\Sigma} = \mathbf{I}_p, \tag{2}$$
$$H_{02} : \mathbf{\Sigma} = \sigma^2 \mathbf{I}_p, \tag{3}$$
$$H_{03} : \mathbf{\Sigma} = \mathbf{\Lambda}, \quad \mathbf{\Lambda} - \text{diagonal}. \tag{4}$$

Test H_{02} is called the sphericity test while H_{03} is the uncorrelatedness test. The first tests for detection covariance structures under normality go back to 1940s. Wald (1943) suggested a score test based on the information matrix, Rao (1948) proposed another score test using score function and information matrix. In practice maximum likelihood ratio (MLR) test (see Rao 1973, § 6e), for instance) is the most popular one, but it is known that when the number of parameters to be tested is large, the test will almost always reject the null hypothesis. In Kollo et al. (2016), it is shown for the normal population that instead of MLR test the Rao's score test should be used when the number of variables is growing. In 1970s, new tests were constructed where instead of information matrix trace functions were used. This approach became later fruitful in the high-dimensional set-up. John (1971, 1972) proved that the test based on

$$U = \frac{1}{p}\text{tr}\left[\left(\frac{\mathbf{S}}{(1/p)\text{tr}\,\mathbf{S}} - \mathbf{I}_p\right)^2\right]$$

is locally most powerful invariant test for sphericity H_{02}. Nagao (1973) suggested test statistics for H_{02}

$$T_2 = \frac{p^2}{2}\text{tr}\left[\left(\frac{\mathbf{S}}{\text{tr}\,\mathbf{S}} - \frac{1}{p}\mathbf{I}_p\right)^2\right]$$

and H_{03}

$$T_3 = \frac{n}{2}\text{tr}\left[\left(\mathbf{S}\mathbf{S}_d^{-1} - \mathbf{I}_p\right)^2\right],$$

where $\mathbf{S}_d$ is the diagonalized matrix $\mathbf{S}$. In high-dimensional set-up ($p \geq n$), several papers were published in the beginning of 2000s for a normal population. Ledoit and Wolf (2002) suggested for H_{01} the statistic

$$W = \frac{1}{p}\text{tr}\left[(\mathbf{S} - \mathbf{I}_p)^2\right] - \frac{p}{n}\left(\frac{1}{p}\text{tr}\,\mathbf{S}\right)^2 + \frac{p}{n}.$$

For the hypotheses (2)–(4) Kapetanios (2004), modified Ledoit–Wolf test and applied it to normalized data from normal population. Srivastava (2005, 2006) constructed test statistics in high-dimensional set-up for a normal population. For H_{01} he sug-

gested a test, which is based on non-zero eigenvalues of the sample covariance matrix $\mathbf{S}$. For H_{02}, he proposed the statistic

$$T_2^* = \frac{n^2}{(n-1)(n+2)} \frac{\frac{1}{p}\left[\mathrm{tr}\mathbf{S}^2 - \frac{1}{n}(\mathrm{tr}\mathbf{S})^2\right]}{\left[\frac{\mathrm{tr}\mathbf{S}}{p}\right]^2} - 1$$

In Srivastava (2006), there are two test-statistics for the uncorrelatedness test H_{03}:

– one is based on Fisher's z-transformation of correlation coefficients;

– another one – T_3^*—is an analogue of T_2^*, but involves beside trace functions the fourth order moments of the coordinates of $\mathbf{x}$.

Ahmad and von Rosen (2015b) modified Nagao's statistics to test H_{01} and H_{02} under normality in high-dimensional situation when $p > n$ and proved asymptotic normality of the tests using U-statistics.

We are going to construct test statistics for non-normal populations in the situation when both, the number of variables p and the sample size n are growing, $p, n \to \infty$, $p/n < 1$. The last assumption makes it possible to rely on asymptotic normality and asymptotic chi-square distributions. Non-normal case has got much attention in recent years. Shapiro and Browne (1987) consider the maximum likelihood test about covariance structure for elliptical distributions when some mildscale invariance conditions are fulfilled. Yuan and Bentler (1999) study robustness of the likelihood ratio statistic for two non-normal populations, including elliptical distributions. Srivastava and Reid (2012) test covariance structures under normality when P≥n, Srivastava et al. (2011) consider some tests for the covariance matrices with fewer observations than the dimension under non-normality, Harrar (2009) examines asymptotic for several tests under non-normality. Chen et al. (2010) develop tests for high-dimensional covariance matrices modifying Ledoit–Wolf test for elliptical distributions. Ahmad and von Rosen (2015a) proved asymptotics normality for trace-based statistics, introduced in Ahmad and von Rosen (2015b) for H_{01} and H_{02} using U-statistics when normality assumption is replaced by certain mild assumptions on the trace of the covariance matrix. Srivastava and Singull (2017) also consider sphericity test in high-dimensional set-up, using U-statistics. We derive expressions of test-statistics for sphericity and uncorrelatedness tests and examine empirically speed of convergence to the asymptotic distributions in simulation experiments.

2 Some Notation and Preliminary Results

Derivations in the paper utilize matrix technique which is based on vec-operator, Kronecker product, commutation matrix and matrix derivative. For deeper insight into this technique, an interested reader is referred to Magnus and Neudecker (1999), Harville (1997), Rao and Rao (1998) or Kollo and von Rosen (2010). From properties of vec-operator, the following two are frequently used

$$\text{vec}\,(\mathbf{ABC}) = (\mathbf{C}' \otimes \mathbf{A})\text{vec}\,\mathbf{B};$$

$$\text{tr}\,(\mathbf{AB}) = \text{vec}\,'(\mathbf{A})'\text{vec}\,\mathbf{B}$$

where tr denotes the trace function.

Later on we shall use matrix derivatives repeatedly, and the definition of Kollo and von Rosen (2010), p. 127 is applied.

Definition 1 Let the elements of $\mathbf{Y} \in \mathbb{R}^{r\times s}$ be functions of $\mathbf{X} \in \mathbb{R}^{p\times q}$. The matrix $\frac{d\mathbf{Y}}{d\mathbf{X}} \in \mathbb{R}^{pq\times rs}$ is called matrix derivative of $\mathbf{Y}$ by $\mathbf{X}$ in a set A, if all the partial derivatives $\frac{\partial y_{kl}}{\partial x_{ij}}$ exist, are continuous in A, and

$$\frac{d\mathbf{Y}}{d\mathbf{X}} = \frac{d}{d\text{vec}\,\mathbf{X}}\text{vec}\,'\mathbf{Y}$$

where

$$\frac{d}{d\text{vec}\,\mathbf{X}} = \Big(\frac{\partial}{\partial x_{11}}, \ldots, \frac{\partial}{\partial x_{p1}}, \frac{\partial}{\partial x_{12}}, \ldots, \frac{\partial}{\partial x_{p2}}, \ldots, \frac{\partial}{\partial x_{1q}}, \ldots, \frac{\partial}{\partial x_{pq}}\Big)'$$

and vec $(\cdot)$ is the usual vectorization operator.

Further, the following properties of the matrix derivative are used (Kollo and von Rosen 2010, p. 149)

1. $\frac{d\mathbf{X}}{d\mathbf{X}} = \mathbf{I}_{pq}$;
2. $\frac{d(\mathbf{Y}+\mathbf{Z})}{d\mathbf{X}} = \frac{d\mathbf{Y}}{d\mathbf{X}} + \frac{d\mathbf{Z}}{d\mathbf{X}}$;
3. $\frac{d(\mathbf{AXB})}{d\mathbf{X}} = \mathbf{B} \otimes \mathbf{A}'$;
4. When $\mathbf{Z} = \mathbf{Z}(\mathbf{Y})$, $\mathbf{Y} = \mathbf{Y}(\mathbf{X})$, then $\frac{d\mathbf{Z}}{d\mathbf{X}} = \frac{d\mathbf{Y}}{d\mathbf{X}}\frac{d\mathbf{Z}}{d\mathbf{Y}}$;
5. When $\mathbf{W} = \mathbf{YZ}$, $\mathbf{Z} \in \mathbb{R}^{s\times t}$, then $\frac{d\mathbf{W}}{d\mathbf{X}} = \frac{d\mathbf{Y}}{d\mathbf{X}}(\mathbf{Z} \otimes \mathbf{I}_r) + \frac{d\mathbf{Z}}{d\mathbf{X}}(\mathbf{I}_t \otimes \mathbf{Y}')$;
6. When $\mathbf{X} \in \mathbb{R}^{p\times p}$ then $\frac{d\mathbf{X}^{-1}}{d\mathbf{X}} = -\mathbf{X}^{-1} \otimes (\mathbf{X}')^{-1}$;
7. When $\mathbf{X} \in \mathbb{R}^{p\times p}$, then $\frac{d|\mathbf{X}|}{d\mathbf{X}} = |\mathbf{X}|\text{vec}\,(\mathbf{X}^{-1})'$, where $|\cdot|$ denotes the determinant;
8. $\dfrac{d\,\text{tr}\,(\mathbf{A}'\mathbf{X})}{d\mathbf{X}} = \text{vec}\,\mathbf{A}$.

We shall use moments of a random vector $\mathbf{x}$ in the following matrix representation

$$M_k(\mathbf{x}) = E\big[\underbrace{\mathbf{x} \otimes \mathbf{x}' \otimes \mathbf{x} \otimes \mathbf{x}' \otimes \ldots}_{k \text{ times}}\big] = E\left[\mathbf{x}\mathbf{x}' \otimes \mathbf{x}\mathbf{x}' \otimes \ldots\right], \; k = 1, 2, \ldots.$$

The corresponding kth central moment is

$$\overline{M}_k(\mathbf{x}) = M_k(\mathbf{x} - E\mathbf{x}).$$

Denote convergence in probability by $\xrightarrow{P}$ and in distribution by $\xrightarrow{\mathcal{D}}$. We are going to use the following convergence result (see Kollo and von Rosen (2010), p. 285, for

instance):

$$\sqrt{n}\ \mathrm{vec}\,(\mathbf{S}-\boldsymbol{\Sigma}) \xrightarrow{\mathcal{D}} N_{p^2}(\mathbf{0}, \boldsymbol{\Pi}) \tag{5}$$

where

$$\boldsymbol{\Pi} = \overline{M}_4(\mathbf{x}) - \mathrm{vec}\,\boldsymbol{\Sigma}\ \mathrm{vec}'\boldsymbol{\Sigma}. \tag{6}$$

Also we use a convergence theorem (Anderson 2003, pp. 132–133).

Theorem 1 *Assume that for* $\{\mathbf{x}_n\}$ *and a constant vector* $\mathbf{a}$

$$\sqrt{n}\ (\mathbf{x}_n - \mathbf{a}) \xrightarrow{\mathcal{D}} N_p(\mathbf{0}, \boldsymbol{\Sigma})$$

where

$$\mathbf{x}_n \xrightarrow{P} \mathbf{a}$$

when $n \to \infty$. *Let the function* $g(\mathbf{x}) : \mathbb{R}^p \to \mathbb{R}^q$ *have continuous partial derivatives in a neighbourhood of* $\mathbf{a}$. *Then, if* $n \to \infty$,

$$\sqrt{n}\,(g(\mathbf{x}_n) - g(\mathbf{a})) \xrightarrow{\mathcal{D}} N_q(\boldsymbol{\xi}'\boldsymbol{\Sigma}\boldsymbol{\xi}),$$

where

$$\boldsymbol{\xi} = \frac{dg(\mathbf{x})}{d\mathbf{x}}\Big|_{\mathbf{x}=\mathbf{a}} \neq \mathbf{0}$$

is the matrix derivative

$$\frac{dg(\mathbf{x})}{d\mathbf{x}} = \frac{d}{d\mathbf{x}}\,(g(\mathbf{x}))'\,.$$

We are going to examine later a special case when dependence between coordinates of $\mathbf{x}$ is determined by a linear transformation. This is a traditional assumption in Independent Component Analysis (Hyvärinen et al. 2001). Let $\mathbf{y} = (Y_1, \ldots, Y_p)'$ be a random p-vector with independent coordinates Y_i and let

$$E\mathbf{y} = \mathbf{0}; \quad D\mathbf{y} = \mathbf{I}_p.$$

Assume that the first four moments of $\mathbf{y}$ exist. Consider the equality

$$\mathbf{x} = \mathbf{A}\mathbf{y} + \boldsymbol{\mu} \tag{7}$$

with non-singular $\mathbf{A} : p \times p$. Then

$$E\mathbf{x} = \boldsymbol{\mu}; \quad D\mathbf{x} = \mathbf{A}\mathbf{A}' = \boldsymbol{\Sigma}.$$

Assume the initial sample $\mathbf{x}_1, \ldots, \mathbf{x}_n$ comes from this population. Then we can represent $\overline{\mathbf{x}}$ and $\mathbf{S}$ via the independent copies of $\mathbf{y}$:

$$\mathbf{S} = \mathbf{A}\left(\frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{y}_i - \overline{\mathbf{y}})(\mathbf{y}_i - \overline{\mathbf{y}})'\right)\mathbf{A}'. \tag{8}$$

Denote

$$\mathbf{S}_{\mathbf{y}} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{y}_i - \overline{\mathbf{y}})(\mathbf{y}_i - \overline{\mathbf{y}})', \tag{9}$$

then (8) has the form

$$\mathbf{S} = \mathbf{A}\mathbf{S}_{\mathbf{y}}\mathbf{A}', \tag{10}$$

And, from (10), we get

$$D(\operatorname{vec}\mathbf{S}) = D[(\mathbf{A}\otimes\mathbf{A})\operatorname{vec}\mathbf{S}_{\mathbf{y}}] = (\mathbf{A}\otimes\mathbf{A})D[\operatorname{vec}\mathbf{S}_{\mathbf{y}}](\mathbf{A}\otimes\mathbf{A})'.$$

After opening brackets in (9), we have

$$\mathbf{S}_{\mathbf{y}} = \frac{1}{n-1}\sum_{i=1}^{n}\mathbf{y}_i\mathbf{y}_i' - \frac{n}{n-1}\overline{\mathbf{y}}\overline{\mathbf{y}}'.$$

In the following, we need expression of $D[\operatorname{vec}(\mathbf{y}\mathbf{y}')]$. From Kollo and von Rosen (2010), p. 285, we get the representation via the fourth order moments

$$D\operatorname{vec}(\mathbf{y}\mathbf{y}') = E\left[\mathbf{y}\mathbf{y}'\otimes\mathbf{y}\mathbf{y}'\right] - \operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p. \tag{11}$$

Because of independence of Y_i, $i = 1,\ldots,p$, the fourth-order mixed moments in (11) have a simple form

$$E(Y_jY_kY_lY_m) = \begin{cases} 1, & \text{when there are two different pairs of equal indices;} \\ m_4(Y_j), & \text{when } j=k=m=l; \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

Taking into account the block-structure of the Kronecker product, we have the j-th diagonal block of the $E[(\mathbf{y}\mathbf{y}')\otimes(\mathbf{y}\mathbf{y}')]$ by using (12) in the form

$$E\left[Y_j^2\begin{pmatrix} Y_1^2 & Y_1Y_2 & \cdots & Y_1Y_p \\ \cdots & \cdots & \cdots & \cdots \\ Y_pY_1 & Y_pY_2 & \cdots & Y_p^2 \end{pmatrix}\right] = \begin{bmatrix} 1 & & & 0 \\ & \ddots & & \\ & & m_4(Y_j) & \\ & & & \ddots \\ 0 & & & 1 \end{bmatrix} = \mathbf{m}_4(Y_j).$$

If $j \neq k$, in the partitioned matrix (11), we have in the jk-th block the jk-th and kj-th elements equal to one and all the other elements are zeros. Denote the diagonal matrix of the fourth-order moments $m_4(Y_j)$ of the random variables Y_i as $(\mathbf{m}_4)_{[d]}$

$$(\mathbf{m}_4)_{[d]} = \begin{pmatrix} m_4(Y_1) & & 0 \\ & \ddots & \\ 0 & & m_4(Y_p) \end{pmatrix}. \tag{13}$$

Using the commutation matrix $\mathbf{K}_{p,p}$, we can present $E(\mathbf{yy}' \otimes \mathbf{yy}')$ as a sum

$$E(\mathbf{yy}' \otimes \mathbf{yy}') = \mathbf{I}_{p^2} + \mathbf{K}_{p,p} + \text{vec}\,\mathbf{I}_p \text{vec}'\mathbf{I}_p + \left[\left((\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p\right) - 3\mathbf{I}_{p^2}\right](\mathbf{K}_{p,p})_d. \tag{14}$$

Here, $(\mathbf{K}_{p,p})_d$ denotes the diagonalized matrix $\mathbf{K}_{p,p}$. For results on partitioned matrices, the reader is referred to Kollo and von Rosen (2010) or Magnus and Neudecker (1999), for example.

In a special case when $m_4(Y_j) = \gamma$, $j = 1, \ldots, p$, the equality (14) is simplified

$$E(\mathbf{yy}' \otimes \mathbf{yy}') = \mathbf{I}_{p^2} + \mathbf{K}_{p,p} + \text{vec}\,\mathbf{I}_p \text{vec}'\mathbf{I}_p + (\gamma - 3)(\mathbf{K}_{p,p})_d. \tag{15}$$

From here,

$$\begin{aligned} \mathbf{\Pi}_{\mathbf{A}} &= (\mathbf{A} \otimes \mathbf{A}) D[\text{vec}\,\mathbf{yy}'](\mathbf{A}' \otimes \mathbf{A}') \\ &= (\mathbf{I}_{p^2} + \mathbf{K}_{p,p})(\mathbf{\Sigma} \otimes \mathbf{\Sigma}) + (\mathbf{A} \otimes \mathbf{A})\left[\left((\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p\right) - 3\mathbf{I}_{p^2}\right](\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})'. \end{aligned} \tag{16}$$

In the special case $m_4(Y_j) = \gamma$ (elliptical distributions, for example), $j = 1, \ldots, p$, we get from (15) and (16)

$$\begin{aligned} \mathbf{\Pi}_{\mathbf{A}}^{\gamma} &= (\mathbf{A} \otimes \mathbf{A}) D\left[\text{vec}\,\mathbf{yy}'\right](\mathbf{A} \otimes \mathbf{A})' \\ &= \left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right)(\mathbf{\Sigma} \otimes \mathbf{\Sigma}) + (\gamma - 3)(\mathbf{A} \otimes \mathbf{A})(\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})'. \end{aligned} \tag{17}$$

In the case of i.i.d. normal variables Y_i, $i = 1, \ldots, p$, the equality (17) turns into the well-known asymptotic covariance matrix for $\mathbf{S}$:

$$\left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right)(\mathbf{\Sigma} \otimes \mathbf{\Sigma}).$$

Due to the asymptotic normality of the sample covariance matrix (see Kollo and von Rosen 2010) p. 285, for example), we can formulate the following theorem.

Theorem 2 *Let* $\mathbf{y} = (Y_1, \ldots, Y_p)$ *be a* p*-vector with i.i.d. coordinates and* $E\mathbf{y} = \mathbf{0}$*;* $D\mathbf{y} = \mathbf{I}_p$*. Let random* p*-vector* $\mathbf{x}$ *be represented via* $\mathbf{y}$ *by the formula* (7)*. Then, if* $n \to \infty$*,*

$$\sqrt{n}\,\text{vec}\,(\mathbf{S} - \mathbf{\Sigma}) \xrightarrow{\mathcal{D}} N_p(0, \mathbf{\Pi}_{\mathbf{A}})$$

where $\mathbf{\Pi}_{\mathbf{A}}$ *is given by* (16)*. In a special case when* $m_4(Y_j) = \gamma$*,* $j = 1, \ldots, p$*, the asymptotic covariance matrix is of the form*

$$\Pi_{\mathbf{A}}^{\gamma} = (\mathbf{I}_{p^2} + \mathbf{K}_{p,p})(\mathbf{\Sigma} \otimes \mathbf{\Sigma}) + (\gamma - 3)(\mathbf{A} \otimes \mathbf{A})(\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})'.$$

3 Ratio of Trace Functions

In Sect. 1, most of the statistics for testing covariance structures are based on the ratios of trace functions. Consider the statistic

$$T_2(\mathbf{S}) = \frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^2}.$$

Values of $T_2(\mathbf{S})$ close to 1 refer to the null hypothesis H_{02} and critical region is of the form $T_2(\mathbf{S}) > c_\alpha$. Let us examine the asymptotic behaviour of T_2 under H_0 in (1) when $n \to \infty$. Expand $T_2(\mathbf{S})$ into the Taylor series at $T_2(\boldsymbol{\Sigma})$. The first terms in the expansion are (Kollo and von Rosen 2010, p. 152)

$$T_2(\mathbf{S}) = T_2(\boldsymbol{\Sigma}) + \left(\frac{dT_2}{d\mathbf{S}}\right)'_{S=\boldsymbol{\Sigma}} \operatorname{vec}(\mathbf{S}-\boldsymbol{\Sigma}) + \frac{1}{2}\operatorname{vec}'(\mathbf{S}-\boldsymbol{\Sigma})\left(\frac{d^2T_2}{d\mathbf{S}^2}\right)_{\mathbf{S}=\boldsymbol{\Sigma}} \operatorname{vec}(\mathbf{S}-\boldsymbol{\Sigma}) + \ldots \quad (18)$$

The first derivative is

$$\begin{aligned}
\frac{dT_2}{d\mathbf{S}} &= \frac{d}{d\mathbf{S}}\left[\operatorname{tr}\mathbf{S}^2(\operatorname{tr}\mathbf{S})^{-2}\right] = \frac{d\operatorname{tr}\mathbf{S}^2}{d\mathbf{S}}(\operatorname{tr}\mathbf{S})^{-2} + \frac{d(\operatorname{tr}\mathbf{S})^{-2}}{d\mathbf{S}}\operatorname{tr}\mathbf{S}^2 \\
&= \frac{d\mathbf{S}^2}{d\mathbf{S}}\frac{d\operatorname{tr}\mathbf{S}^2}{d\mathbf{S}^2}(\operatorname{tr}\mathbf{S})^{-2} + \frac{d\operatorname{tr}\mathbf{S}}{d\mathbf{S}}\frac{d(\operatorname{tr}\mathbf{S})^{-2}}{d\operatorname{tr}\mathbf{S}}\operatorname{tr}\mathbf{S}^2 \\
&= (\mathbf{S}\otimes\mathbf{I}+\mathbf{I}\otimes\mathbf{S})\operatorname{vec}\mathbf{I}_p(\operatorname{tr}\mathbf{S})^{-2} - 2(\operatorname{tr}\mathbf{S})^{-3}\operatorname{tr}\mathbf{S}^2\operatorname{vec}\mathbf{I}_p \\
&= 2\operatorname{vec}\mathbf{S}(\operatorname{tr}\mathbf{S})^{-2} - 2\frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^3}\operatorname{vec}\mathbf{I}_p.
\end{aligned}$$

We obtained

$$\frac{dT_2}{d\mathbf{S}} = 2\operatorname{vec}\left(\mathbf{S} - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right)\frac{1}{(\operatorname{tr}\mathbf{S})^2}. \quad (19)$$

From Theorems 1 and 2, follows next result.

Theorem 3 *Let $T_2(\mathbf{S}) = \frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^2}$ where $\mathbf{S}$ is the sample covariance matrix (8). Then we have the following convergence under $H_0 : \boldsymbol{\Sigma} = \boldsymbol{\Sigma}_0$ when the sample size $n \to \infty$ and $\boldsymbol{\Sigma}_0 \neq \frac{\operatorname{tr}\boldsymbol{\Sigma}_0^2}{(\operatorname{tr}\boldsymbol{\Sigma}_0)^2}\mathbf{I}_p$*

$$\sqrt{n}(T_2(\mathbf{S}) - T_2(\boldsymbol{\Sigma}_0)) \xrightarrow{\mathcal{D}} N(0, \sigma^2_{\mathbf{A}_0}),$$

where

$$\sigma^2_{\mathbf{A}_0} = \frac{4}{(\operatorname{tr}\boldsymbol{\Sigma}_0)^4}\operatorname{vec}'(\boldsymbol{\Sigma}_0 - T_2(\boldsymbol{\Sigma}_0)\mathbf{I}_p)\boldsymbol{\Pi}_{\mathbf{A}_0}\operatorname{vec}(\boldsymbol{\Sigma}_0 - T_2(\boldsymbol{\Sigma}_0)\mathbf{I}_p),$$

$\boldsymbol{\Pi}_{\mathbf{A}_0}$ is given by (16) with $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_0$ and $\boldsymbol{\Sigma}_0 = \mathbf{A}_0\mathbf{A}_0'$. When $m_4(Y_j) = \gamma$, $j = 1, \ldots, p$, then in the expression of the asymptotic covariance matrix $\boldsymbol{\Pi}_{\mathbf{A}_0}$ is replaced by $\boldsymbol{\Pi}^{\gamma}_{\mathbf{A}_0}$ from (17).

Remark 1 Under $H_{02}: \mathbf{\Sigma} = \sigma^2 \mathbf{I}_p$, the first derivative in (19)

$$\frac{dT_2}{d\mathbf{S}}\Big|_{\mathbf{S}=\sigma^2\mathbf{I}_p} = \mathbf{0}.$$

Therefore, asymptotic normality does not hold for $T_2(\mathbf{S})$ under the null hypothesis H_{02}. The asymptotic behaviour under H_{02} is determined by the second term in the Taylor expansion which includes the second-order derivative of $T_2(\mathbf{S})$. The same time under the two-sided alternative hypothesis $H_{12}: \mathbf{\Sigma} \neq \sigma^2 \mathbf{I}_p$ asymptotic normality holds.

Let us find the second-order derivative

$$\begin{aligned}
\frac{d^2T_2}{d\mathbf{S}^2} &= \frac{d}{d\mathbf{S}}\left[\operatorname{vec}\left(\mathbf{S} - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right)\frac{2}{(\operatorname{tr}\mathbf{S})^2}\right] \\
&= 2\frac{d}{d\mathbf{S}}\left[\operatorname{vec}\left(\mathbf{S} - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right)\right]\frac{1}{(\operatorname{tr}\mathbf{S})^2} + 2\frac{d}{d\mathbf{S}}\left[\frac{1}{(\operatorname{tr}\mathbf{S})^2}\right]\operatorname{vec}'\left(\mathbf{S} - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right) \\
&= 2\left[\mathbf{I}_{p^2} - \frac{d}{d\mathbf{S}}\left(\frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\right)\operatorname{vec}'\mathbf{I}_p\right]\frac{1}{(\operatorname{tr}\mathbf{S})^2} + 2\left[-2\frac{1}{(\operatorname{tr}\mathbf{S})^3}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\left(\mathbf{S} - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right)\right] \\
&= 2\left\{\mathbf{I}_{p^2} + \left[-2\operatorname{vec}\mathbf{S}\frac{1}{\operatorname{tr}\mathbf{S}} + \frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^2} + \operatorname{vec}\mathbf{I}_p\right]\operatorname{vec}'\mathbf{I}_p\right\}\frac{1}{(\operatorname{tr}\mathbf{S})^2} \\
&\quad -4\frac{1}{(\operatorname{tr}\mathbf{S})^3}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\left(S - \frac{\operatorname{tr}\mathbf{S}^2}{\operatorname{tr}\mathbf{S}}\mathbf{I}_p\right) \\
&= \frac{2}{(\operatorname{tr}\mathbf{S})^2}\left[\mathbf{I}_{p^2} - \frac{2}{\operatorname{tr}\mathbf{S}}\operatorname{vec}\mathbf{S}\operatorname{vec}'\mathbf{I}_p + 3\frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^2}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p - \frac{2}{\operatorname{tr}\mathbf{S}}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{S}\right].
\end{aligned}$$

The final expression is

$$\frac{d^2T_2}{d\mathbf{S}^2} = \frac{2}{(\operatorname{tr}\mathbf{S})^2}\left[\mathbf{I}_{p^2} - \frac{2}{\operatorname{tr}\mathbf{S}}\left(\operatorname{vec}\mathbf{S}\operatorname{vec}'\mathbf{I}_p + \operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{S}\right) + 3\frac{\operatorname{tr}\mathbf{S}^2}{(\operatorname{tr}\mathbf{S})^2}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p\right]. \tag{20}$$

Under H_{02} the second-order derivative (20)

$$\begin{aligned}
\frac{d^2T_2}{d\mathbf{S}^2}\Big|_{\mathbf{S}=\sigma^2\mathbf{I}} &= \frac{2}{p^2\sigma^4}\left[\mathbf{I}_{p^2} - \frac{4}{p}\left(\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p\right) + 3\,\frac{p}{p^2}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p\right] \\
&= \frac{2}{p^2\sigma^4}\left[\mathbf{I}_{p^2} - \frac{1}{p}\operatorname{vec}\mathbf{I}_p\operatorname{vec}'\mathbf{I}_p\right].
\end{aligned}$$

The second term in the Taylor expansion under H_{02} equals

$$\frac{1}{2}\operatorname{vec}'(\mathbf{S} - \sigma^2\mathbf{I}_p)\frac{d^2T_2}{d\mathbf{S}^2}\Big|_{\mathbf{S}=\sigma^2\mathbf{I}_p}\operatorname{vec}(\mathbf{S} - \sigma^2\mathbf{I}_p) = \frac{1}{p^2\sigma^4}\left[\operatorname{tr}\mathbf{S}^2 - \frac{1}{p}(\operatorname{tr}\mathbf{S})^2\right].$$

The asymptotic behaviour of T_2 under H_{02} is determined by the last expression. If $p \to \infty$ then this term tends to zero when H_{02} is true.

Corollary 1 *Under the null hypothesis*

$$H_{02} : \boldsymbol{\Sigma} = \sigma^2 \mathbf{I},$$

the expansion (18) has the following form

$$T_2^0(\mathbf{S}) = \frac{1}{p} + \frac{1}{p^2\sigma^4}\operatorname{tr}\mathbf{S}^2 - \frac{1}{p^3\sigma^4}(\operatorname{tr}\mathbf{S})^2 + \ldots \tag{21}$$

Proof Equality (21) is obtained straightforwardly from (18) when $\boldsymbol{\Sigma}$ is replaced by $\sigma^2\mathbf{I}$ and we take into account that $\operatorname{tr}\boldsymbol{\Sigma} = \sigma^2 p$; $\operatorname{tr}\boldsymbol{\Sigma}^2 = \sigma^4 p$. Consider instead of $T_2(\mathbf{S})$ the following modified version

$$T_2^*(\mathbf{S}) = p \cdot T_2(\mathbf{S}) = \frac{\frac{\operatorname{tr}\mathbf{S}^2}{p}}{\left(\frac{\operatorname{tr}\mathbf{S}}{p}\right)^2}.$$

From (21), we get under $H_{02} : \boldsymbol{\Sigma} = \sigma^2\mathbf{I}_p$ the expansion for $T_2^*(\mathbf{S})$

$$T_2^*(\mathbf{S}) = 1 + \frac{1}{\sigma^4}\left(\frac{\operatorname{tr}\mathbf{S}^2}{p} - \left(\frac{\operatorname{tr}\mathbf{S}}{p}\right)^2\right) + \ldots \tag{22}$$

When $p, n \to \infty$, the asymptotic behaviour of $T_2^*(\mathbf{S})$ in (22) is determined by $\frac{\operatorname{tr}\mathbf{S}^2}{p}$.

We investigate in a simulation experiment behaviour of the statistic $T_2^*(\mathbf{S})$ under H_{02} at different sample sizes. In Fig. 1, graphs of $T_2^*(\mathbf{S})$ at $n = 50,\ 100,\ 250,\ 500,\ 750,\ 1000$ are presented. We see that starting from the sample size 250 values of the statistic are very close to 1.

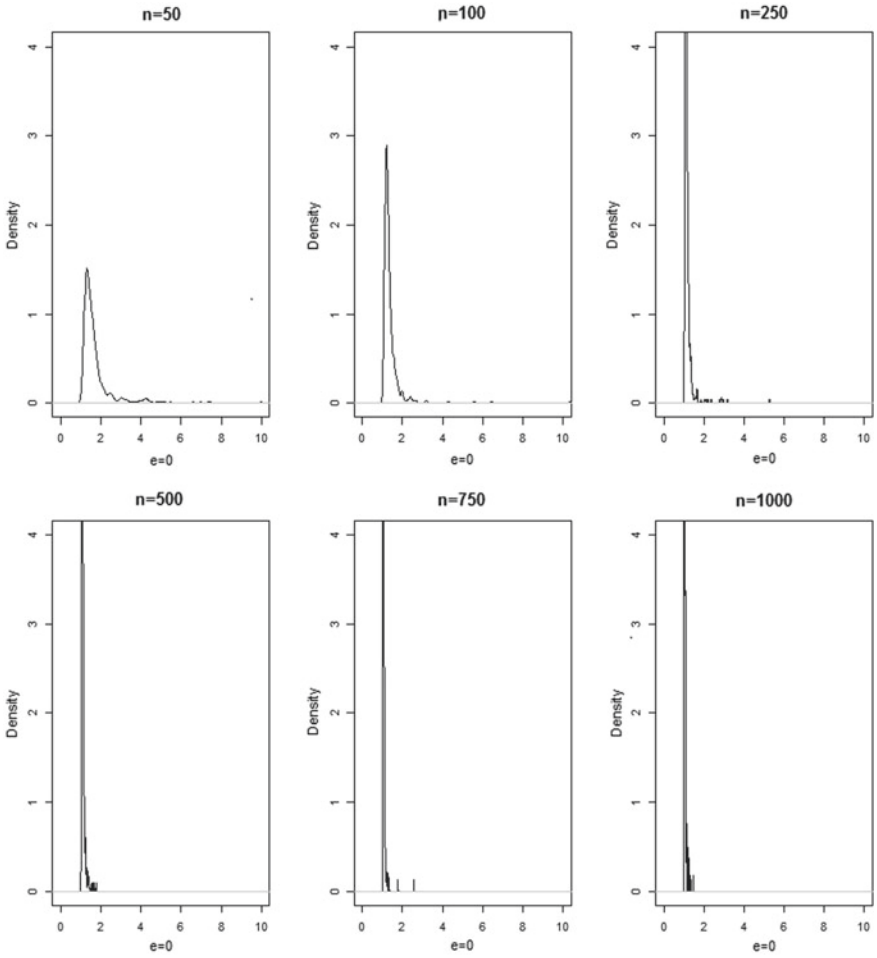

Fig. 1 Simulation of $T_2^{*0}(\mathbf{S})$: H_0: $\boldsymbol{\Sigma} = \sigma^2\mathbf{I}_5$, $\sigma^2 = 4$

To examine behaviour of $T_2^*(\mathbf{S})$, we simulated also values of $n(T_2^*(\mathbf{S}) - 1)$ under H_{02} at the same sample sizes. The resulting distribution is skewed, the best fit with empirical distribution was obtained by the chi-distribution (Fig. 2).

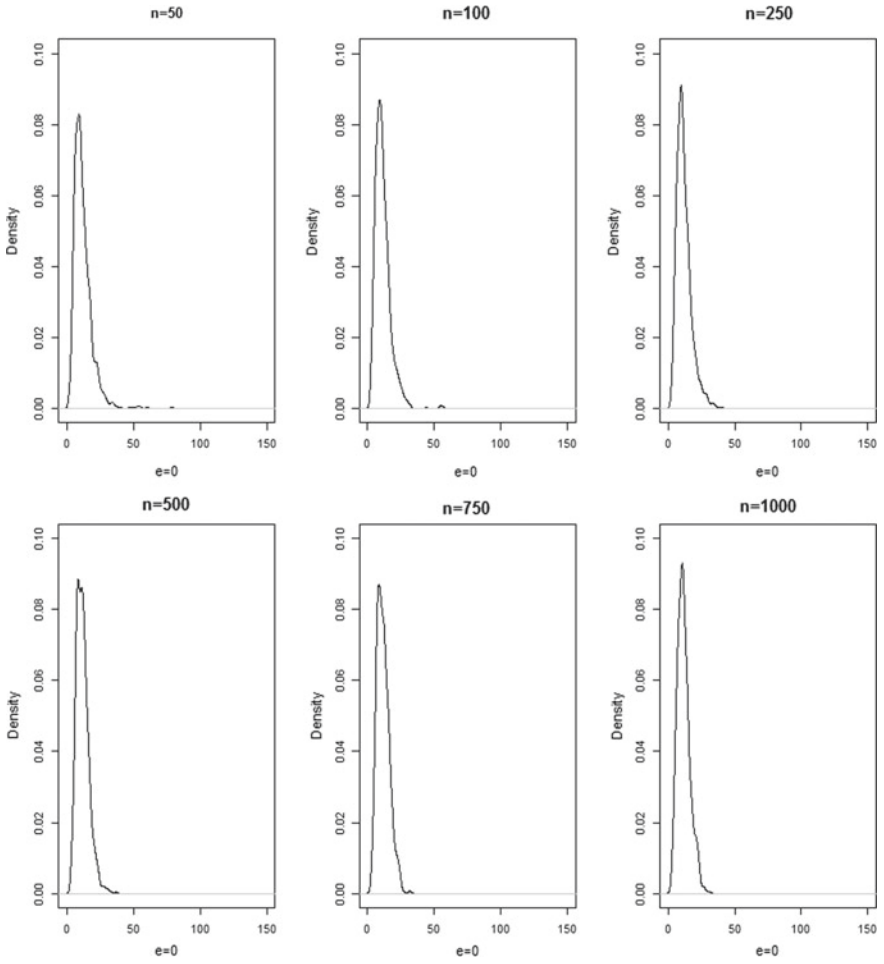

Fig. 2 Simulation of $n(T_2^{*0}(\mathbf{S}) - 1)$: H_0: $\mathbf{\Sigma} = \sigma^2\mathbf{I}_5$, $\sigma^2 = 4$

We also examined the behaviour of $T_2^*(\mathbf{S})$ under the alternative hypothesis H_{12}. In Fig. 3, the simulated values of the statistic are presented for the covariance matrix where the elements outside the main diagonal were equal to $e = 0.1,\ 0.5,\ 1.0,\ 2.0$, while diagonal elements were taken equal to 4. We see that, when $e = 0.1$, the graph is still close to the null hypothesis but very quickly the shape of the empirical distribution changes when value of e is growing.

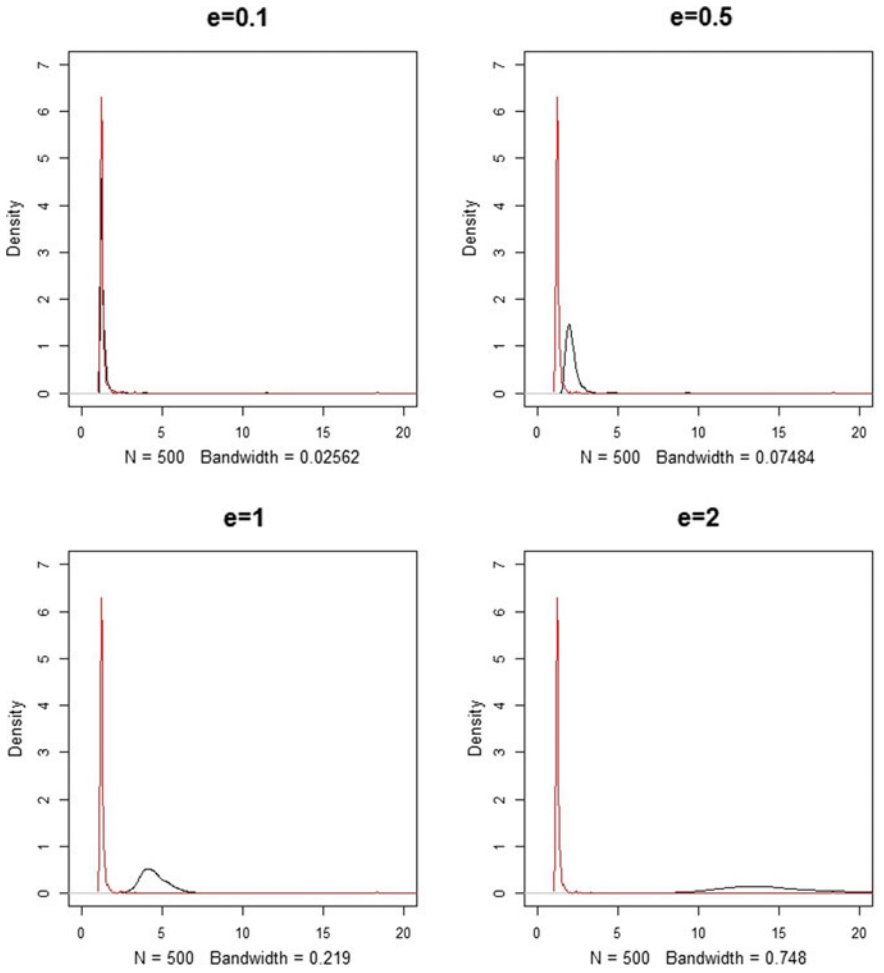

Fig. 3 Simulation of $T_2^{*0}(\mathbf{S})$: H_1: $\boldsymbol{\Sigma} \neq \sigma^2\mathbf{I}_5$, $(\Sigma)_{ij} = e, i \neq j, \sigma^2 = 4$

4 Test for Uncorrelatedness

4.1 Null Hypothesis

Let $H_{03} : \boldsymbol{\Sigma} = \boldsymbol{\Lambda}$, $\boldsymbol{\Lambda}$ diagonal, $\boldsymbol{\Lambda} \neq \sigma^2\mathbf{I}_p$, be the null hypothesis of interest under the alternative

$$H_{13} : \boldsymbol{\Sigma} \neq \boldsymbol{\Lambda}.$$

Under H_{03}, we have $\sigma_{ij} = 0, i, j = 1, \ldots, p; i \neq j$. Under H_{03}, the first derivative of T_2 is

$$\frac{dT_2}{d\mathbf{S}}\Big|_{\mathbf{S}=\mathbf{\Lambda}} = 2\mathrm{vec}\left(\mathbf{\Lambda} - \frac{\mathrm{tr}\,\mathbf{\Lambda}^2}{\mathrm{tr}\,\mathbf{\Lambda}}\right)\frac{1}{(\mathrm{tr}\,\mathbf{\Lambda})^2}.$$

We could apply now Theorem 3 in a special case $\mathbf{\Sigma}_0 = \mathbf{\Lambda}$, with $\mathbf{A}_0\mathbf{A}_0' = \mathbf{\Lambda}$, get an asymptotically normal test-statistic for testing H_{03} and repeat the study in the same way as we did for the sphericity test.

Instead, let us construct a chi-square statistic to test H_{03}. As

$$\left(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d\right)\left(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d\right) = \mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d\,,$$

we have the chi-square statistic of the form

$$T_3 = n\mathrm{vec}'\mathbf{S}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\widehat{\mathbf{\Sigma}}_{as}^{-}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{S} \tag{23}$$

where $\widehat{\mathbf{\Sigma}}_{as}^{-}$ is an estimate of a generalized inverse of the asymptotic covariance matrix of $\mathrm{vec}\,\mathbf{S}$. As shown in Moore (1977), the statistic is invariant under the choice of generalized inverses.

From (5)–(6), we get the statistic (23) of the form

$$T_3 = n\mathrm{vec}'(\mathbf{S})(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\widehat{\mathbf{\Pi}}^{-}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{S}. \tag{24}$$

By $\widehat{\mathbf{\Pi}}$, the estimate of $\mathbf{\Pi}$ is denoted where the fourth-order moments are replaced by their sample estimates and $\mathbf{\Sigma}$ with the sample covariance matrix $\mathbf{S}$.

Following Moore (1977)

$$T_3 \xrightarrow{\mathcal{D}} \chi^2_{\frac{1}{2}p(p-1)} \tag{25}$$

as we have $\frac{1}{2}p(p-1)$ nonrepeated elements in $(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{S}$.

Assumptions for the convergence (25) are fulfilled as $(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{S}$ belongs to the column space of

$$(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\widehat{\mathbf{\Pi}}^{-}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d).$$

Under H_{03}, the matrix $\mathbf{\Sigma}$ in the asymptotic covariance matrix $\mathbf{\Pi}$ in (6) is diagonal, $\mathbf{\Sigma} = \mathbf{\Lambda}$. In a special case when the fourth-order moments are determined by the linear transformation (7), $\mathbf{x} = \mathbf{A}\mathbf{y}$, we have $\overline{M}_4(\mathbf{x})$ in a simpler form.

$$\overline{M}_4(\mathbf{x}) = (\mathbf{A}\otimes\mathbf{A})M_4(\mathbf{y})(\mathbf{A}\otimes\mathbf{A})' \tag{26}$$

where $M_4(\mathbf{y})$ is given in (14). If all univariate fourth-order moments $m_4(Y_i)$ are equal

$$m_4(Y_i) = \gamma\,,$$

$\overline{M}_4(\mathbf{x})$ takes the form (15).

Structure of the asymptotic covariance matrix $\mathbf{\Pi_A}$ in this case is simplified under H_{03}.

Theorem 4 *Under H_{03}, the asymptotic covariance matrix $\mathbf{\Pi}$ has the form*

$$\mathbf{\Pi_A} = (\mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 3(\mathbf{K}_{p,p})_d)(\mathbf{\Lambda} \otimes \mathbf{\Lambda}) + (\mathbf{A} \otimes \mathbf{A})((\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p)(\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})' \tag{27}$$

where the diagonal matrix $(\mathbf{m}_4)_{[d]} : p \times p$ is defined in (13).

Proof Under H_{03}, taking into account (26), the asymptotic covariance matrix in (6) takes the form

$$\mathbf{\Pi_A} = (\mathbf{A} \otimes \mathbf{A}) M_4(\mathbf{y})(\mathbf{A} \otimes \mathbf{A})' - \operatorname{vec} \mathbf{\Lambda} \operatorname{vec}' \mathbf{\Lambda}.$$

After taking into account (16), we have

$$\begin{aligned}\mathbf{\Pi_A} &= (\mathbf{A} \otimes \mathbf{A}) \left\{ \mathbf{I}_{p^2} + \mathbf{K}_{p,p} + \operatorname{vec} \mathbf{I}_p \operatorname{vec}' \mathbf{I}_p + \left[(\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p - 3\mathbf{I}_{p^2} \right] (\mathbf{K}_{p,p})_d \right\} (\mathbf{A} \otimes \mathbf{A})' \\ &\quad - \operatorname{vec} \mathbf{\Lambda} \operatorname{vec}' \mathbf{\Lambda} \\ &= \left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} \right) (\mathbf{\Lambda} \otimes \mathbf{\Lambda}) + (\mathbf{A} \otimes \mathbf{A}) \left[(\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p - 3\mathbf{I}_{p^2} \right] (\mathbf{K}_{p,p})_d (\mathbf{A} \otimes \mathbf{A})',\end{aligned}$$

as under H_{03}

$$(\mathbf{A} \otimes \mathbf{A}) \operatorname{vec} \mathbf{I}_p \operatorname{vec}' \mathbf{I}_p (\mathbf{A} \otimes \mathbf{A})' = \operatorname{vec} \mathbf{\Lambda} \operatorname{vec}' \mathbf{\Lambda}.$$

When we open square brackets in the expression of $\mathbf{\Pi_A}$,

$$\begin{aligned}\mathbf{\Pi_A} &= \left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} \right) (\mathbf{\Lambda} \otimes \mathbf{\Lambda}) + (\mathbf{A} \otimes \mathbf{A})((\mathbf{m}_4)_{[d]} \otimes \mathbf{I}_p)(\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})' \\ &\quad - (\mathbf{A} \otimes \mathbf{A}) 3\mathbf{I}_{p^2} (\mathbf{K}_{p,p})_d (\mathbf{A} \otimes \mathbf{A})'.\end{aligned},$$

The second term can be simplified

$$(\mathbf{A} \otimes \mathbf{A}) 3\mathbf{I}_{p^2} (\mathbf{K}_{p,p})_d (\mathbf{A} \otimes \mathbf{A})' = 3(\mathbf{K}_{p,p})_d (\mathbf{A} \otimes \mathbf{A})(\mathbf{A} \otimes \mathbf{A})' = 3(\mathbf{K}_{p,p})_d (\mathbf{\Lambda} \otimes \mathbf{\Lambda})$$

and we have got the expression of $\mathbf{\Pi_A}$ as stated in the theorem .

In Theorem 5, we present our test-statistic under H_{03} in this particular case.

Theorem 5 *Let* $\mathbf{x}$ *be as defined in* (7). *Then the test-statistic T_3 in* (24) *has the form*

$$\begin{aligned}T_3^{\mathbf{A}} &= n \operatorname{vec}' \mathbf{S} (\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d) \\ &\quad \times \left\{ \mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 3(\mathbf{K}_{p,p})_d + (\mathbf{A} \otimes \mathbf{A}) \left[(\widehat{\mathbf{m}}_4)_{[d]} \otimes \mathbf{I}_p \right] (\mathbf{K}_{p,p})_d (\mathbf{A} \otimes \mathbf{A}) \left(\mathbf{S}_d^{-1} \otimes \mathbf{S}_d^{-1} \right) \right\}^{-} \\ &\quad \times \left(\mathbf{S}_d^{-1} \otimes \mathbf{S}_d^{-1} \right) (\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d) \operatorname{vec} \mathbf{S}.\end{aligned} \tag{28}$$

Proof From (24) and (27), it follows that we have to examine the product

$$
\begin{aligned}
&(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\widehat{\mathbf{\Pi}}_{\mathbf{A}}^{-}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d) \\
&= (\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d) \\
&\quad \times \left\{(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 3(\mathbf{K}_{p,p})_d) + (\mathbf{A} \otimes \mathbf{A})\left[(\widehat{\mathbf{m}}_4)_{[d]} \otimes \mathbf{I}_p\right](\mathbf{K}_{p,p})_d(\mathbf{A} \otimes \mathbf{A})'(\widehat{\mathbf{\Lambda}} \otimes \widehat{\mathbf{\Lambda}})^{-1}\right\}^{-} \\
&\quad \times (\widehat{\mathbf{\Lambda}} \otimes \widehat{\mathbf{\Lambda}})^{-1}(\mathbf{I} - (\mathbf{K}_{p,p})_d) \\
&= (\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d) \\
&\quad \times \left\{\mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 3(\mathbf{K}_{p,p})_d + (\mathbf{A} \otimes \mathbf{A})\left[(\widehat{\mathbf{m}}_4)_{[d]} \otimes \mathbf{I}_p\right](\mathbf{K}_{p,p})_d)(\mathbf{A} \otimes \mathbf{A})'(\widehat{\mathbf{\Lambda}}^{-1} \otimes \widehat{\mathbf{\Lambda}}^{-1})\right\}^{-} \\
&\quad \times (\widehat{\mathbf{\Lambda}}^{-1} \otimes \widehat{\mathbf{\Lambda}}^{-1})(\mathbf{I} - (\mathbf{K}_{p,p})_d),
\end{aligned}
$$

When we replace $\widehat{\mathbf{\Lambda}}$ by an estimate $\mathbf{S}_d$ — obtained from the sample covariance matrix, we get the final form of $T_3^{\mathbf{A}}$ in (28).

Corollary 2 *In assumptions of Theorem 5 when all the fourth-order moments of* $\mathbf{y}$ *are equal,* $m_4(Y_i) = \gamma$, $i = 1, \ldots, p$, *test-statistic* T_3^{γ} *has a simple form*

$$T_3^{\gamma} = \frac{n}{2}\mathrm{vec}'\mathbf{R}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{R},$$

where $\mathbf{R}$ *is the sample correlation matrix.*

Proof Under our assumptions, $M_4(\mathbf{x}_i)$ takes form (15) and $\mathbf{\Pi}_{\mathbf{A}}$ can be simplified. Denote the asymptotic covariance matrix now by $\mathbf{\Pi}_{\mathbf{A}}^{\gamma}$

$$\mathbf{\Pi}_{\mathbf{A}}^{\gamma} = (\mathbf{I}_{p^2} + \mathbf{K}_{p,p} + (\gamma - 3)(\mathbf{K}_{p,p})_d)(\mathbf{\Lambda} \otimes \mathbf{\Lambda}).$$

Then

$$
\begin{aligned}
T_3^{\gamma} &= n\mathrm{vec}'\mathbf{S}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\left\{(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} + (\gamma - 3)(\mathbf{K}_{p,p})_d)(\widehat{\mathbf{\Lambda}} \otimes \widehat{\mathbf{\Lambda}})\right\}^{-} \\
&\qquad \times (\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{S} \\
&= n\mathrm{vec}'\mathbf{S}(\widehat{\mathbf{\Lambda}} \otimes \widehat{\mathbf{\Lambda}})^{-\frac{1}{2}}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\left\{(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} + (\gamma - 3)(\mathbf{K}_{p,p})_d)\right\}^{-} \\
&\qquad \times (\mathbf{I} - (\mathbf{K}_{p,p})_d)(\widehat{\mathbf{\Lambda}} \otimes \widehat{\mathbf{\Lambda}})^{-\frac{1}{2}}\mathrm{vec}\,\mathbf{S}.
\end{aligned}
$$

When we replace $\widehat{\mathbf{\Lambda}}$ by its estimate $\mathbf{S}_d$, we have

$$T_3^{\gamma} = n\mathrm{vec}'\mathbf{R}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\left\{\mathbf{I}_{p^2} + \mathbf{K}_{p,p} + (\gamma - 3)(\mathbf{K}_{p,p})_d\right\}^{-}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\mathrm{vec}\,\mathbf{R}.$$

The generalized inverse in curly brackets can be expressed as a sum of two matrices. Direct calculation shows that the following representation satisfies the necessary and sufficient condition of the generalized inverse $\mathbf{A} = \mathbf{A}\mathbf{A}^{-}\mathbf{A}$

$$\left\{\mathbf{I} + \mathbf{K}_{p,p} + (\gamma - 3)(\mathbf{K}_{p,p})_d\right\}^{-} = \frac{1}{4}(\mathbf{I} + \mathbf{K}_{p,p}) + \left[c(\mathbf{K}_{p,p})_d\right].$$

where

$$c = -\frac{\gamma^2 - 5\gamma + 6}{\gamma^2 - 2\gamma + 1}.$$

As $(\mathbf{K}_{p,p})_d(\mathbf{I} - (\mathbf{K}_{p,p})_d) = \mathbf{0}$, the second term vanishes in the expression of T_3^γ.

Note that $\frac{1}{4}\left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right)$ is the Moore–Penrose generalized inverse of $\mathbf{I}_{p^2} + \mathbf{K}_{p,p}$,

$$\left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right)^+ = \frac{1}{4}\left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right).$$

As $(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\left(\mathbf{I}_{p^2} + \mathbf{K}_{p,p}\right) = \mathbf{I} - (\mathbf{K}_{p,p})_d + \mathbf{K}_{p,p} - (\mathbf{K}_{p,p})_d = \mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 2(\mathbf{K}_{p,p})_d$, we have

$$\begin{aligned} T_3^\gamma &= \frac{n}{4}\text{vec}'\mathbf{R}(\mathbf{I}_{p^2} + \mathbf{K}_{p,p} - 2(\mathbf{K}_{p,p})_d)(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\text{vec}\,\mathbf{R} \\ &= \frac{n}{2}\text{vec}\,\mathbf{R}(\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d)\text{vec}\,\mathbf{R}, \end{aligned}$$

as $\mathbf{I}_{p^2} - (\mathbf{K}_{p,p})_d$ is an idempotent matrix.

So we have established that if all the fourth-order moments of the random variables Y_i equal to γ, the statistic T_3^γ does not depend on this constant γ and

$$T_3^\gamma = \frac{n}{2}\sum_{\substack{i,j=1 \\ i \neq j}}^{p} r_{ij}^2.$$

To examine the convergence to the limiting chi-square distribution when all the fourth-order moments are equal, a simulation experiment was carried out. We considered sample sizes from $n = 100$ to $n = 1000$ in the situation when the number of variables was growing from $p = 5$ to $p = 50$; the number of replications $k = 500$. We see that fit with the asymptotic chi-square distribution is very good even for the relatively small sample size 100 and the goodness of fit does not depend on the dimensionality (Fig. 4).

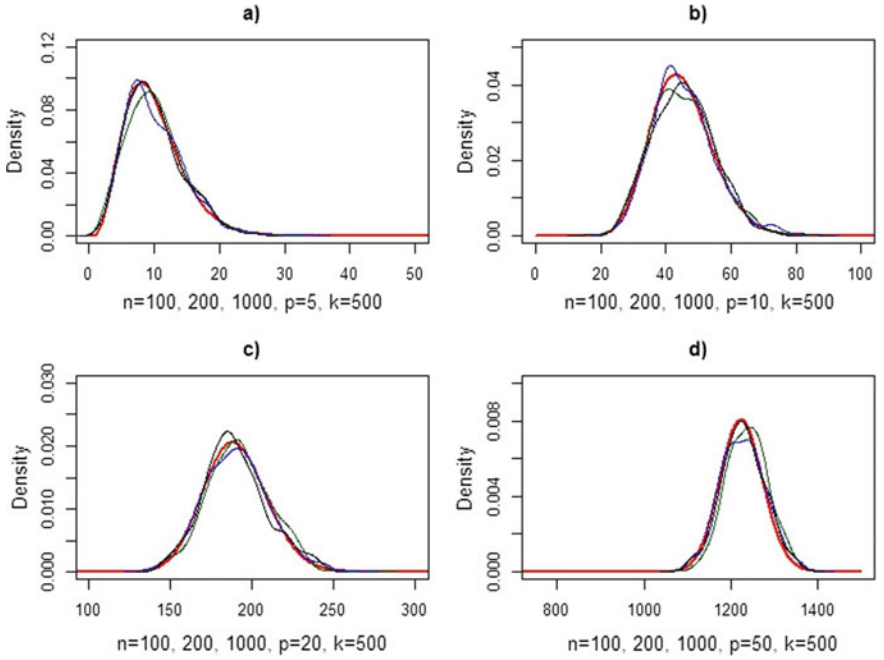

Fig. 4 Simulation results under H_{03}: $\mathbf{\Sigma} = \mathbf{\Lambda}$, $\lambda_i = p - i,\ i = 0, \ldots, p-1$

5 Conclusions and Discussion

We have studied covariance structures under the null hypothesis H_0: $\mathbf{\Sigma} = \mathbf{\Sigma}_0$, while special attention has been paid to the sphericity test H_{02}: $\mathbf{\Sigma} = \sigma^2\mathbf{I}_p$ and the uncorrelatedness test H_{03}: $\mathbf{\Sigma} = \mathbf{\Lambda}$. Dependence between the coordinates of a random vector under consideration, $\mathbf{x}$, has been introduced by the linear transformation $\mathbf{x} = \mathbf{A}\mathbf{y}$, where the coordinates Y_i of $\mathbf{y}$ are i.i.d. random variables with $EY_i = 0$, $DY_i = 1$. This is the typical situation in the Independent Component Analysis, for instance.

For the sphericity test, a ratio of trace functions was examined. It came out that the considered statistic did not converge under H_{02} to the normal distribution, instead chi-distribution gave the best fit. The same time under the two-sided alternative asymptotic normality holds.

For the uncorrelatedness test, a chi-square test statistic was designed. It came out that when the fourth-order moments are equal, $m_4(Y_i) = \gamma,\ i = 1, \ldots, p$, the statistic did not depend on γ and was expressed through the sum of squared correlation coefficients.

There are several problems to study in future. Asymptotic distributions for test-statistics have been obtained in two special cases for simple covariance structures under null-hypothesis. Study of asymptotic behaviour of other structures (compound symmetry, Toeplitz structure, autocorrelation structure, etc.) is of interest. Additional

simulation experiments have to be carried out when the fourth order moments $m_4(Y_i)$ are different. For the sphericity test further theoretical work is needed. In derivations, we assumed that the sample size $n > p$. In high-dimensional set-up, $n \leq p$ behaviour of the considered statistics will be different and a new approach to the problem has to be worked out.

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Design and Sampling

The Existence of Perpendicular Multi-arrays

Kazuki Matsubara and Sanpei Kageyama

Abstract As a generalization of perpendicular arrays defined by C. R. Rao in 1961, Li et al. have newly introduced a combinatorial array, called a perpendicular multi-array, in 2018 for constructions of splitting authentication codes having some perfect t-fold secrecy. Moreover, several classes of perpendicular multi-arrays have been constructed in the literature. In this paper, necessary conditions for the existence of a perpendicular multi-array are discussed, and fundamental/useful results for the existence of perpendicular multi-arrays are provided by use of the results on combinatorial designs. As a main result, it is shown that the necessary conditions are also sufficient for the existence of a perpendicular multi-array with block size 3×2 with the only one exception. Finally, the asymptotic existence of perpendicular multi-arrays with a cyclic automorphism is presented.

Keywords Perpendicular multi-array · Perpendicular array · Splitting-balanced block design · Group divisible

1 Introduction

A *perpendicular multi-array* of size $N \times k$, denoted by $\mathrm{PMA}_\lambda(k \times c, v)$, is an $N \times k$ multi-array, $\mathcal{A} = (A_{ij})$, on a set V of v points, which satisfies the following conditions:

(P1) each entry A_{ij} ($|A_{ij}| = c$) is a c-subset of V and kc distinct points occur in k entries of each row of $\mathcal{A}$, and

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(P2) for any pair of columns of $\mathcal{A}$ and for any pair of points x_1, x_2 in V, there are exactly λ rows of $\mathcal{A}$ such that each of the rows contains the points x_1, x_2 in the different entries of the two columns.

Here it holds that $N = \lambda v(v-1)/(2c^2)$.

Let us illustrate the definition of a PMA.

Example 1 A $\mathrm{PMA}_4(2 \times 4, 8)$ on $\mathbb{Z}_8$ by giving an example:

$$\left(\begin{array}{cc|cc} 0,1,2,4 & & 3,5,6,7 \\ 0,2,3,5 & & 4,6,7,1 \\ 0,3,4,6 & & 5,7,1,2 \\ 0,4,5,7 & & 6,1,2,3 \\ 0,5,6,1 & & 7,2,3,4 \\ 0,6,7,2 & & 1,3,4,5 \\ 0,7,1,3 & & 2,4,5,6 \end{array}\right)$$

with $k = 2$, $c = 4$, $N = 7$, $A_{11} = \{0, 1, 2, 4\}$, $A_{12} = \{3, 5, 6, 7\}$, etc.

From now on, each row of a $\mathrm{PMA}_\lambda(k \times c, v)$ is separately displayed in the form of

$$(a_{11}, a_{12}, \ldots, a_{1c} \mid a_{21}, a_{22}, \ldots, a_{2c} \mid \ldots \mid a_{k1}, a_{k2}, \ldots, a_{kc})$$

by use of kc points on V or $(A_{i1} \mid A_{i2} \mid \ldots \mid A_{ik})$ by use of k entries A_{ij} $(1 \le i \le N)$. Furthermore, let $\mathcal{R}$ be a set of N rows and $\mathcal{P}_i(j_1, j_2)$ be the multi-set of pairs of the points from the j_1th and the j_2th entries of the ith row as follows:

$$\mathcal{P}_i(j_1, j_2) = \left\{\{v, v'\} \mid v \in A_{ij_1}, v' \in A_{ij_2}\right\}. \tag{1}$$

Note that the condition (P2) implies that $\bigcup_{1 \le i \le N} \mathcal{P}_i(j_1, j_2)$ contains every pair of two points in V exactly λ times for any j_1, j_2 with $1 \le j_1 < j_2 \le k$.

The PMA has been newly introduced in Li et al. (2018) with some applications for constructing c-splitting authentication and secrecy codes with k source states and v messages, where c messages can be used to communicate a source state under the same encoding rule. Actually, Li et al. (2018) focused on the PMAs with the following additional condition in essence:

(P3) for any pair of points x_1 and x_2, in the subarray that consists of the rows of $\mathcal{A}$ that contain x_1 and x_2 in different columns, each of the two points appears equally often in all columns.

The $\mathrm{PMA}_\lambda(k \times c, v)$ satisfying the condition (P3) is called an *authentication perpendicular multi-array*, denoted by $\mathrm{APMA}_\lambda(k \times c, v)$. It is shown in Li et al. (2018) that (i) the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$ implies the existence of a c-splitting authentication code with perfect 2-fold secrecy and (ii) the existence of an $\mathrm{APMA}_\lambda(k \times c, v)$ implies the existence of a c-splitting authentication code with

perfect 2-fold secrecy and 1-fold secure against spoofing. Especially, a c-splitting authentication code obtained from an $\mathrm{APMA}_1(k \times c, v)$ has an optimality in some sense (see also Li et.al 2018). Furthermore, the existence of an $\mathrm{APMA}_1(3 \times 2, v)$ is shown in the literature.

Theorem 1 (Li et.al 2018) *There exists an* $APMA_1(3 \times 2, v)$ *if and only if* $v \equiv 1$ (*mod* 8) *with seven possible exceptions* $v \in \{9, 17, 41, 65, 113, 161, 185\}$.

Note that, by taking u copies of each row of $\mathcal{A}$, it is clear that the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$ (or an $\mathrm{APMA}_\lambda(k \times c, v)$) implies the existence of a $\mathrm{PMA}_{\lambda u}(k \times c, v)$ (or an $\mathrm{APMA}_{\lambda u}(k \times c, v)$).

In this paper, the $\mathrm{PMA}_\lambda(k \times c, v)$ (not necessarily with the condition (P3)) is considered. It is clear that the $\mathrm{PMA}_\lambda(k \times 1, v)$ coincides with the perpendicular array, denoted by $\mathrm{PA}_\lambda(k, v)$, defined in Rao (1961), who call the perpendicular array by the other name "an orthogonal array of Type II". The review of results on the existence of PAs is found in Bierbrauer (2007). Especially, the following result will be useful for the construction of PMAs given in Sect. 4.

Lemma 1 (Bierbrauer 2007) *There exists a* $PA_1(k, k)$ *for any odd prime power* k.

A PMA is regarded as a pair $(V, \mathcal{R})$ of a point set V and a row set $\mathcal{R}$. When $V = \mathbb{Z}_v$ and $\mathcal{R} = \{\boldsymbol{R} + t \mid \boldsymbol{R} \in \mathcal{R}\}$ with $\boldsymbol{R} + t = (a_{11} + t, \ldots, a_{1c} + t \mid \ldots \mid a_{k1} + t, \ldots, a_{kc} + t)$ for any $t \in \mathbb{Z}_v$, the array is said to be *cyclic*. Then a *row orbit* of $\boldsymbol{R} \in \mathcal{R}$ is defined by $\{\boldsymbol{R} + t \mid t \in \mathbb{Z}_v\}$. Choose an arbitrary row from each row orbit and call it a *base row*. Hence, for a cyclic $\mathrm{PMA}_\lambda(k \times c, v)$, the array can be represented by displaying base rows.

Example 2 A cyclic $\mathrm{PMA}_1(3 \times 2, 17)$ on $\mathbb{Z}_{17}$ is given by two base rows:

$$(0, 13 \mid 3, 9 \mid 2, 12)\,, (0, 16 \mid 1, 11 \mid 7, 13) \mod 17.$$

For two points x and y in the j_1th and the j_2th ($1 \le j_1 < j_2 \le k$) entries, respectively, of each base row, $x - y \equiv d \pmod v$ implies that in the orbit of the base row there exists a row containing x' and y' in the j_1th and the j_2th entries, respectively, for any distinct points x', y' in $\mathbb{Z}_v$ with $x' - y' \equiv d \pmod v$. Hence, it is seen that the array obtained from orbits of m base rows $(A^*_{i1} \mid \ldots \mid A^*_{ik})$, $1 \le i \le m$, satisfies the condition (P2) of a $\mathrm{PMA}_\lambda(k \times c, v)$ if

$$\bigcup_{1 \le i \le m} \{\pm(d - d') \mid d \in A^*_{ij_1}, d' \in A^*_{ij_2}\} = \lambda\,(\mathbb{Z}_v \backslash \{0\}) \tag{2}$$

holds for any j_1, j_2 with $1 \le j_1 < j_2 \le k$, where λS means a multi-set containing each element of the set S exactly λ times.

Since any $\mathrm{APMA}_\lambda(k \times c, v)$ is a $\mathrm{PMA}_\lambda(k \times c, v)$, Theorem 1 shows the existence of a $\mathrm{PMA}_1(3 \times 2, v)$ for any $v \equiv 1 \pmod 8$ with seven possible exceptions $v \in \{9, 17, 41, 65, 113, 161, 185\} = E$. In this paper, the remaining cases for the

existence of a $\mathrm{PMA}_\lambda(3 \times 2, v)$, i.e., $v \in E$, $\lambda = 1$ and $v \geq 6$, $\lambda \geq 2$, are mainly discussed. In Sect. 2, several combinatorial designs are introduced and some existence results of them are given for constructions of a $\mathrm{PMA}_\lambda(k \times c, v)$. In Sect. 3, necessary conditions for the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$ and some existence (or non-existence) results are provided. In Sect. 4, two methods of construction are presented by use of the combinatorial designs. In Sect. 5, as a main result of this paper, it is shown that the necessary conditions for the existence of a $\mathrm{PMA}_\lambda(3 \times 2, v)$ are sufficient with a definite exception of $(v, \lambda) = (9, 1)$. This kicks out $v = 9$ from Theorem 1. Finally, in Sect. 6, the asymptotic existence on cyclic PMAs is discussed.

2 Preliminaries

In this section, some types of combinatorial designs which play an important role for constructions of PMAs are mainly described.

Let v, k, c, λ be positive integers. A *splitting-balanced block design*, denoted by $(v, k \times c, \lambda)$-SBD, is a pair $(V, \mathcal{B})$, where V is a set of v points and $\mathcal{B}$ ($|\mathcal{B}| = b$) is a family of subsets (called blocks) of size kc each of V such that

(S1) the ith block $B_i \in \mathcal{B}$ is expressed as a disjoint union of k subblocks of size c, $B_i = B_{i1} \cup \cdots \cup B_{ik}$ for $1 \leq i \leq b$, and
(S2) every pair of distinct points $x, y \in V$ occurs in exactly λ blocks with x and y being in different subblocks.

In a $(v, k \times c, \lambda)$-SBD $(V, \mathcal{B})$ with b blocks, it is seen that every point is contained in exactly r blocks, where

$$b = \frac{\lambda v(v-1)}{c^2 k(k-1)}, \quad r = \frac{\lambda(v-1)}{c(k-1)} \tag{3}$$

hold (cf. Ogata et al. 2004). The parameter r is called a *replication number* of the design. The blocks in $\mathcal{B}$ is displayed in the form of

$$\{v_{11}, v_{12}, \ldots, v_{1c} \mid v_{21}, v_{22}, \ldots, v_{2c} \mid \ldots \mid v_{k1}, v_{k2}, \ldots, v_{kc}\}.$$

by use of kc points on V or $\{B_{i1} \mid B_{i2} \mid \ldots \mid B_{ik}\}$ by use of k subblocks B_{ij} $(1 \leq i \leq b)$.

This has been called a splitting balanced incomplete block design (splitting BIBD) in Du (2004, 2005), Ge et al. (2005), Liang (2018), Ogata et al. (2004), Wang and Su (2010) since 2004. However, this naming may not be proper, because of the fact that for only $c = 1$ a $(v, k \times 1, \lambda)$-SBD coincides with the traditional notion of a balanced incomplete block (BIB) design $(V, \mathcal{B})$, denoted by (v, k, λ)-BIBD (cf. Raghavarao 1988). Hence, we have called the structure a splitting-balanced block design (SBD) in Matsubara et al. (2017) instead.

A (v, k, λ)-BIBD is said to be *resolvable* if b blocks can be grouped into r sets (called *resolution sets*) of b/r $(= v/k)$ blocks each such that every point appears in each resolution set exactly once. Moreover, a resolvable (v, k, λ)-BIBD with $b = v + r - 1$ is said to be *affine resolvable* (cf. Abel et al. 2007; Raghavarao 1988).

A necessary condition for the existence of a $(v, k \times c, \lambda)$-SBD is given as follows.

Lemma 2 (Matsubara et al. 2017) *In a* $(v, k \times c, \lambda)$*-SBD with* b *blocks,*

$$b \geq \frac{v-1}{k-1} \tag{4}$$

holds. Furthermore, the existence of a $(v, k \times c, \lambda)$*-SBD with* $b = (v-1)/(k-1)$ *blocks is equivalent to the existence of an affine resolvable* (v, c, λ^*)*-BIBD with* $v = kc$ *and* $\lambda^* = r - \lambda$*, where* r *is a common replication number of both designs.*

The existence of several classes of the $(v, k \times c, \lambda)$-SBD is discussed in literature (e.g., Du 2004, 2005; Ge et al. 2005; Liang 2018; Matsubara et al. 2017; Ogata et al. 2004; Wang and Su 2010). Especially, the following result will be useful to construct a $\mathrm{PMA}_\lambda(3 \times 2, v)$.

Lemma 3 (Du 2004) *There exists a* $(v, 3 \times 2, \lambda)$*-SBD if and only if*

$$\lambda(v-1) \equiv 0 \pmod 4, \ \ \lambda v(v-1) \equiv 0 \pmod{24}$$

with a definite exception $(v, \lambda) = (9, 1)$.

If each of families $\mathcal{B}_1, \ldots, \mathcal{B}_k$ consisting of c-subsets in each column of a $\mathrm{PMA}_\lambda(k \times c, v)$ yields a (v, c, λ^*)-BIBD with some λ^*, then a set of the k BIB designs $(V, \mathcal{B}_1), \ldots, (V, \mathcal{B}_k)$ is known to be *k-pairwise additive BIB designs* (cf. Matsubara and Kageyama 2015; Sawa et al. 2007). Especially, in k-pairwise additive (v, c, λ^*)-BIBDs, any pair of two BIB designs yields a $(v, 2c, \lambda^{**})$-BIBD with $\lambda^{**} = \lambda + 2\lambda^*$ (cf. Sawa et al. 2007). Moreover, the existence of a 3-pairwise additive $(v, 2, 1)$-BIBD is given as the following shows.

Lemma 4 (Matsubara and Kageyama 2015) *There exists a* 3*-pairwise additive* $(v, 2, 1)$*-BIBD for any* $v \geq 6$.

Lemma 4 provides the existence of a $\mathrm{PMA}_4(3 \times 2, v)$ for any $v \geq 6$ which corresponds with the case $\lambda = 4$ of the main result (Theorem 8) in Sect. 5.

Let v, k, λ be positive integers. A *group divisible design*, denoted by (k, λ)-GDD, is a triplet $(V, \mathcal{G}, \mathcal{B})$, where V is a set of v points, $\mathcal{G}$ is a partition of V into subsets (called groups) and $\mathcal{B}$ $(|\mathcal{B}| = b)$ is a family of subsets (called blocks) of size k each of V such that

(G1) every pair of distinct points $x, y \in V$ in different groups occurs in exactly λ blocks, and

(G2) every pair of distinct points $x, y \in V$ in the same group does not occur in any block.

The *group type* of a (k, λ)-GDD is a multi-set $\{|G| \mid G \in \mathcal{G}\}$. The usual exponential notation is used to describe group types. Thus the notation $h_1^{t_1} h_2^{t_2} \cdots h_n^{t_n}$ means that there are t_i groups of size h_i for $1 \leq i \leq n$ (cf. Ge 2007).

The following proposition on GDDs is shown.

Lemma 5 (Ge 2007) *Let g, u and m be non-negative integers. Then there exists a $(3, 1)$-GDD of type $g^u m^1$ if and only if the following conditions are all satisfied:*

1. *if $g > 0$, then $u \geq 3$, or $u = 2$ and $m = g$, or $u = 1$ and $m = 0$, or $u = 0$;*
2. *$m \leq g(u - 1)$ or $gu = 0$;*
3. *$g(u - 1) + m \equiv 0 \pmod 2$ or $gu = 0$;*
4. *$gu \equiv 0 \pmod 2$ or $m = 0$; and*
5. *$\frac{1}{2}g^2u(u - 1) + gum \equiv 0 \pmod 3$.*

The following results of GDDs are obtained by checking that the parameters satisfy the conditions described in Lemma 5.

Corollary 1 *There exists a $(3, 1)$-GDD of type $12^u 8$ for any $u \geq 3$.*

Corollary 2 *There exists a $(3, 1)$-GDD of type 8^4.*

Corollary 3 *There exists a $(3, 1)$-GDD of type $6^{2u+1} 8$ for any $u \geq 1$.*

The combinatorial designs given in this section will be utilized for constructions of PMAs discussed in Sect. 5.

3 Some Necessary Conditions and Existence Results

In this section, the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$ is considered by taking account into some results on the other combinatorial structures.

At first, the necessary conditions for the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$ are considered. It is obvious by the conditions (P1) and (P2) that for any $\mathrm{PMA}_\lambda(k \times c, v)$ of size $N \times k$

$$kc \leq v \tag{5}$$

holds and

$$N = \frac{\lambda v(v - 1)}{2c^2} \tag{6}$$

is a positive integer.

When $k \geq 3$, since any two rows of a $\mathrm{PMA}_\lambda(k \times c, v)$ yield a $(v, 2 \times c, \lambda)$-SBD, every point must occur equally $(cN/v$ times) in each column. Hence it is seen that

$$\frac{cN}{v} = \frac{\lambda(v - 1)}{2c} \tag{7}$$

is a positive integer.

The sufficiency of these necessary conditions (5), (6), (7) for the case of $(k, c) = (3, 2)$ will be proved as in Theorem 8 of Sect. 5.

Regarding the number of rows in an array, Lemma 2 provides the following necessary condition for the existence of a $\mathrm{PMA}_\lambda(k \times c, v)$.

Theorem 2 *In a $PMA_\lambda(k \times c, v)$ of size $N \times k$,*

$$N = \frac{\lambda v(v-1)}{2c^2} \geq v - 1$$

holds. In particular, $N = v - 1$ implies $v = 2c$.

Proof Any pair of two columns of a $\mathrm{PMA}_\lambda(k \times c, v)$ yields a $(v, 2 \times c, \lambda)$-SBD by regarding N rows of the two columns as b blocks of the design. Since the number of blocks of the $(v, 2 \times c, \lambda)$-SBD is equal to the number of rows of the $\mathrm{PMA}_\lambda(k \times c, v)$, Lemma 2 implies that $N \geq v - 1$ holds. Moreover, Lemma 2 also shows that the existence of a $(v, 2 \times c, \lambda)$-SBD with $b = v - 1$ obtained from a $\mathrm{PMA}_\lambda(k \times c, v)$ with $N = v - 1$ leads $v = 2c$. □

Now, the existence of PMAs with $N = v - 1, v$ is discussed. At first, the case of $k = 2$ is considered. Since the existence of a $\mathrm{PMA}_\lambda(2 \times c, v)$ is equivalent to the existence of a $(v, 2 \times c, \lambda)$-SBD, it is seen that the existence results on $(v, 2 \times c, \lambda)$-SBDs given in Du (2005), Ge et al. (2005), Liang (2018), Matsubara et al. (2017) show the existence of some classes of a $\mathrm{PMA}_\lambda(2 \times c, v)$. Especially, for the case of $(N, k) = (v - 1, 2)$, Lemma 2 implies that the existence of a $\mathrm{PMA}_\lambda(2 \times c, v)$ with $N = v - 1$ is equivalent to the existence of the affine resolvable $(2c, c, \lambda^*)$-BIBD, that is, an Hadamard matrix of order $2c$ (cf. Abel et al. 2007), where $\lambda = c$ and $\lambda^* = c - 1$. Note that, in an Hadamard matrix, the smallest unknown order is 668 $(= 2c)$ (Kharaghani and Tayfeh-Rezaie 2005). Hence, the existence of PMAs with $N = v - 1$ is presented as follows.

Theorem 3 *There exists a $PMA_c(2 \times c, 2c)$ with $N = v - 1$ $(= 2c - 1)$ for any even $c < 334$.*

The $\mathrm{PMA}_4(2 \times 4, 8)$ given in Example 1 is the case $c = 4$ of Theorem 3.

On the other hand, for the case of $(N, k) = (v, 2)$, the existence of a $(2c^2 + 1, 2 \times c, 1)$-SBD with $b = v$ and a $(c^2 + 1, 2 \times c, 2)$-SBD with $b = v$ is given for any $c \geq 2$ in Ge et al. (2005). Hence, the existence of PMAs with $N = v$ is presented as follows.

Theorem 4 *There exist a $PMA_1(2 \times c, 2c^2 + 1)$ with $N = v$ $(= 2c^2 + 1)$ and a $PMA_2(2 \times c, c^2 + 1)$ with $N = v$ $(= c^2 + 1)$ for any $c \geq 2$.*

Furthermore, the following results are given by Matsubara et al. (2017) [Theorems 6 and 7].

Theorem 5 *When $c \geq 3$ and $t \geq 1$ are both odd, there does not exist a $PMA_{tc}(2 \times c, 2c)$.*

Theorem 6 *For given c, a PMA$_c(2 \times c, 2c+1)$ exists only if $2c+1$ is the sum of two squares.*

Note that Theorems 5 and 6 give the results of the cases $N = t(v-1)$ with $t \geq 1$ and $N = v$, respectively. For example, Theorem 6 shows the following result.

Corollary 4 *A PMA$_{10}(2 \times 10, 21)$ and a PMA$_{16}(2 \times 16, 33)$ do not exist.*

Next, the case of $k \geq 3$ is considered.

Theorem 7 *There does not exist a PMA$_\lambda(k \times c, v)$ with $N = v-1$ and $k \geq 3$.*

Proof Theorem 2 implies that $v = 2c$ holds for any $\mathrm{PMA}_\lambda(k \times c, v)$ with $N = v-1$. Hence, $k \geq 3$ implies that $kc > 2c = v$, which is a contradiction to (5). □

On the other hand, a $\mathrm{PMA}_\lambda(k \times c, v)$ with $N = v$ and $k = 3$ can be constructed by use of a computer as follows.

Example 3 A cyclic $\mathrm{PMA}_2(3 \times 6, 37)$ on $\mathbb{Z}_{37}$ is given by

$$(0, 13, 15, 17, 20, 35 \mid 3, 5, 11, 19, 28, 34 \mid 9, 14, 22, 27, 32, 33) \mod 37.$$

To the best of the authors' knowledge, any $\mathrm{PMA}_\lambda(k \times c, v)$ with $N = v$ and $k \geq 3$ is not available except for the $\mathrm{PMA}_2(3 \times 6, 37)$ in Example 3.

4 Constructions from Combinatorial Designs

In this section, two methods of constructing PMAs through the combinatorial designs given in Sect. 2 are provided.

At first, the construction by use of a $(v, k \times c, \lambda)$-SBD is considered. When k is an odd prime, useful constructions of APMAs has been found in Li et al. (2018). Similarly, we can obtain other two constructions for the PMAs.

Lemma 6 *The existence of a $(v, k \times c, \lambda)$-SBD and a PA$_1(k, k)$ implies the existence of a PMA$_\lambda(k \times c, v)$.*

Proof Let the ith block of a $(v, k \times c, \lambda)$-SBD $(V, \mathcal{B})$ be

$$\{B_{i1} \mid B_{i2} \mid \ldots \mid B_{ik}\}, \ 1 \leq i \leq b,$$

where $B_{i1}, \ldots, B_{ik}$ are c-subsets of V. Also let the jth row of a $\mathrm{PA}_1(k, k)$ on $\{1, 2, \ldots, k\}$ be

$$(a_{j1}, a_{j2}, \ldots, a_{jk}), \ 1 \leq j \leq \frac{1}{2}k(k-1).$$

Then, since there uniquely exists a j $(1 \le j \le k(k-1)/2)$ for any $\{x, y\} \subset \{1, 2, \ldots, k\}$ and any h_1, h_2 with $1 \le h_1 < h_2 \le k$ such that $\{x, y\} = \{a_{jh_1}, a_{jh_2}\}$, the following rows yield the required multi-array:

$$\left(B_{ia_{j1}} \mid B_{ia_{j2}} \mid \ldots \mid B_{ia_{jk}}\right)$$

with $1 \le i \le b$ and $1 \le j \le k(k-1)/2$. □

Lemma 7 *The existence of a (k, λ)-GDD of type $h_1^{t_1} h_2^{t_2} \cdots h_n^{t_n}$, a $PA_1(k, k)$ and a $PMA_\lambda(k \times c, h_i c + 1)$ for each i $(1 \le i \le n)$ implies the existence of a $PMA_\lambda(k \times c, v^*)$ with $v^* = c(h_1 t_1 + \cdots + h_n t_n) + 1$.*

Proof Let G_ℓ $(1 \le \ell \le t_1 + t_2 + \cdots + t_n)$ be groups of a (k, λ)-GDD of type $h_1^{t_1} h_2^{t_2} \cdots h_n^{t_n}$ on $\mathbb{Z}_v$ with $v = \sum_{i=1}^{n} h_i t_i$. Then, we take the direct product $\mathbb{Z}_v \times \mathbb{Z}_c$ and let $(\mathbb{Z}_v \times \mathbb{Z}_c) \cup \{\infty\}$ be a point set of the required multi-array.

Let the ith block of the (k, λ)-GDD of type $h_1^{t_1} h_2^{t_2} \cdots h_n^{t_n}$ be

$$\{v_{i1}, v_{i2}, \ldots, v_{ik}\},\ 1 \le i \le b,$$

where b is the number of blocks of the (k, λ)-GDD. Let the jth row of a $\mathrm{PA}_1(k, k)$ on $\mathbb{Z}_k$ be

$$(a_{j1}, a_{j2}, \ldots, a_{jk}),\ 1 \le j \le \frac{1}{2}k(k-1).$$

Then, by replacing each point $v_{ii'} \in \mathbb{Z}_v$ with a subset $B_{ii'} = \{(v_{ii'}, e) \mid e \in \mathbb{Z}_c\}$ for $1 \le i \le b$ and $1 \le i' \le k$, the following row set $\mathcal{R}_0$ is at first considered:

$$\left(B_{ia_{j1}} \mid B_{ia_{j2}} \mid \ldots \mid B_{ia_{jk}}\right)$$

with $1 \le i \le b$ and $1 \le j \le k(k-1)/2$.

Furthermore, let $\mathcal{R}_\ell$ on $(G_\ell \times \mathbb{Z}_c) \cup \{\infty\}$ with $1 \le \ell \le t_1 + \cdots + t_n$ be the row sets obtained from a $\mathrm{PMA}_\lambda(k \times c, |G_\ell|c + 1)$ with $|G_\ell| = h_i$ for some i $(1 \le i \le n)$ by the assumption. Then the $1 + t_1 + \cdots + t_n$ row sets $\mathcal{R}_0$ and $\mathcal{R}_\ell$ $(1 \le \ell \le t_1 + \cdots + t_n)$ can yield the required multi-array. □

5 Existence of a $\mathrm{PMA}_\lambda(3 \times 2, v)$

In this section, the existence of a $\mathrm{PMA}_\lambda(3 \times 2, v)$ is shown through individual examples and the construction results given in Sect. 4. For such existence, from the necessary conditions (5), (6) and (7) with $(k, c) = (3, 2)$, i.e., $v \ge 6$, $N = \lambda v(v-1)/8$ and $cN/v = \lambda(v-1)/4$, it is sufficient to show the existence of a $\mathrm{PMA}_\lambda(3 \times 2, v)$ for the following cases:

(I) $v \equiv 1 \pmod 8$ when $\lambda \ge 1$,

(II) $v \equiv 5 \pmod 8$ when $\lambda \equiv 0 \pmod 2$,
(III) $v \equiv 0, 2, 3 \pmod 4$ when $\lambda \equiv 0 \pmod 4$.

At first, two individual examples are provided by use of a computer.

Example 4 A cyclic $\mathrm{PMA}_1(3 \times 2, 41)$ on $\mathbb{Z}_{41}$ is given by

$$(0, 24 \mid 1, 15 \mid 33, 36),\ (0, 21 \mid 28, 33 \mid 2, 35),\ (0, 27 \mid 3, 25 \mid 17, 20),$$
$$(0, 1 \mid 22, 37 \mid 26, 38),\ (0, 17 \mid 11, 27 \mid 30, 40) \mod 41.$$

Example 5 A cyclic $\mathrm{PMA}_2(3 \times 2, 29)$ on $\mathbb{Z}_{29}$ is given by

$$(1 \cdot 4^d, -1 \cdot 4^d \mid 2 \cdot 4^d, -2 \cdot 4^d \mid 4 \cdot 4^d, -4 \cdot 4^d) \mod 29$$

with $0 \le d \le 6$.

For both of Examples 4 and 5, it can be checked that the base rows satisfy the condition (2). Hence, it is seen that the arrays obtained from the base rows satisfy the conditions (P1) and (P2).

Next, the non-existence result can be presented.

Lemma 8 *There does not exist a PMA*$_1(3 \times 2, 9)$.

Proof Assume that there exists a $\mathrm{PMA}_1(3 \times 2, 9)$ on $\mathbb{Z}_9$, i.e., 9×3 multi-array $\mathcal{A} = (A_{ij})$ with $|A_{ij}| = 2$. For convenience, A_{ij} is denoted by A_i^j here.

Let a set of entries in the first column of $\mathcal{A}$ be $\mathcal{A}_1 = \{A_i^1 \mid 1 \le i \le 9\}$. Then, since $(\lambda, k, c, v) = (1, 3, 2, 9)$ implies that each point is contained in exactly two of the entries in $\mathcal{A}_1$, there exists a set $\mathcal{S} = \{A_{i_1}^1, A_{i_2}^1, \ldots, A_{i_d}^1\} \subset \mathcal{A}_1$ for some d $(2 \le d \le 9)$ such that

$$A_{i_h}^1 \cap A_{i_{h+1}}^1 \ne \phi\ (1 \le h \le d-1),\ A_{i_d}^1 \cap A_{i_1}^1 \ne \phi. \tag{8}$$

Since any permutation of points and any permutation of rows are both allowed in a PMA, it can be assumed without loss of generality that

$$\mathcal{S} = \{A_1^1, A_2^1, \ldots, A_d^1\},\ A_i^1 = \{i-1, i\},\ 1 \le i \le d, \tag{9}$$

where $A_d^1 = \{d-1, 0\}$. Note that each point of $\mathbb{Z}_d$ is not contained in any entry in $\mathcal{A}_1 \backslash \mathcal{S}$.

Hereafter A_i^j and $\mathcal{P}_i(j_1, j_2)$ defined by (1) are considered for $1 \le i \le d \le 9$, $1 \le j \le 3$ and $1 \le j_1 < j_2 \le 3$, where A_{i+d}^j and $\mathcal{P}_{i+d}(j_1, j_2)$ are regarded as A_i^j and $\mathcal{P}_i(j_1, j_2)$, respectively. Then, in the PMA with $\lambda = 1$ each of $\binom{d}{2}$ pairs of two distinct points in $\mathbb{Z}_d$ is contained in $\bigcup_{1 \le i \le d} \mathcal{P}_i(j_1, j_2)$ exactly once for each $(j_1, j_2) = (1, 2), (1, 3)$. Since both elements of A_i^1 $(1 \le i \le d)$ are contained in $\mathbb{Z}_d$, it is seen that

$$\sum_{1 \le i \le d} \left| A_i^j \cap \mathbb{Z}_d \right| = \frac{d(d-1)}{4},\ j = 2, 3. \tag{10}$$

Since $d(d-1)/4$ must be a positive integer in (10) for $d \leq 9$, it is seen that $d = 4, 5, 8, 9$.

When $d = 4$, (9) implies that $A_i^1 = \{i-1, i\}$, $A_{i+1}^1 = \{i, i+1\}$, $A_{i+2}^1 = \{i+1, i+2\}$ $(1 \leq i \leq 4)$ on $\mathbb{Z}_4$. Since $\{i, i+1\}$ must be contained in both of $\bigcup_{1\leq i\leq 4} \mathcal{P}_i(1,2)$ and $\bigcup_{1\leq i\leq 4} \mathcal{P}_i(1,3)$ exactly once each, it holds that $i+1 \in A_i^2 \cup A_i^3$ and $i \in A_{i+2}^2 \cup A_{i+2}^3$ for each i of $1 \leq i \leq 4$. This implies $\sum_{1\leq i\leq 4} |A_i^2 \cap \mathbb{Z}_d| + \sum_{1\leq i\leq 4} |A_i^3 \cap \mathbb{Z}_d| = 8$, which is a contradiction to (10), i.e., $\sum_{1\leq i\leq 4} |A_i^2 \cap \mathbb{Z}_d| + \sum_{1\leq i\leq 4} |A_i^3 \cap \mathbb{Z}_d| = 6$.

When $d = 5$, it is seen that there exists a set $\mathcal{S}' = \{A_{i_1}^1, A_{i_2}^1, \ldots, A_{i_{d'}}^1\}$ consisting of the entries in $\mathcal{A}_1 \backslash \mathcal{S}$ for some d' $(2 \leq d' \leq 4)$ which satisfies (8). However, by the discussion similar to $\mathcal{S}$ with $2 \leq d \leq 4$, it can be shown that there does not exist an $\mathcal{S}'$ with $2 \leq d' \leq 4$. Hence it follows that $d \neq 5$.

When $d = 8$, (9) implies $A_9^1 = \{8, 8\}$, which is a contradiction.

When $d = 9$, (9) implies that $A_i^1 = \{i-1, i\}$, $A_{i+1}^1 = \{i, i+1\}$, $A_{i+2}^1 = \{i+1, i+2\}$ $(1 \leq i \leq 9)$ on $\mathbb{Z}_9$. Since $\{i, i+1\}$ must be contained in both of $\bigcup_{1\leq i\leq 9} \mathcal{P}_i(1,2)$ and $\bigcup_{1\leq i\leq 9} \mathcal{P}_i(1,3)$ exactly once each, it follows that

$$i+1 \in A_i^2 \cup A_i^3,\ i \in A_{i+2}^2 \cup A_{i+2}^3,\ 1 \leq i \leq 9. \tag{11}$$

Also, (9) implies that $A_i^1 = \{i-1, i\}$, $A_{i+1}^1 = \{i, i+1\}$, $A_{i+2}^1 = \{i+1, i+2\}$, $A_{i+3}^1 = \{i+2, i+3\}$, $A_{i+4}^1 = \{i+3, i+4\}$ $(1 \leq i \leq 9)$ on $\mathbb{Z}_9$. Moreover, (11) implies that $\{i, i+2\}$ appears in both of $\mathcal{P}_{i+1}(1,2) \cup \mathcal{P}_{i+1}(1,3)$ and $\mathcal{P}_{i+2}(1,2) \cup \mathcal{P}_{i+2}(1,3)$ for $1 \leq i \leq 9$. Hence, it is seen that $i \notin A_{i+3}^2 \cup A_{i+3}^3$ and $i+3 \notin A_{i+1}^2 \cup A_{i+1}^3$ for $1 \leq i \leq 9$. Since $\{i, i+3\}$ must be contained in both of $\bigcup_{1\leq i\leq 9} \mathcal{P}_i(1,2)$ and $\bigcup_{1\leq i\leq 9} \mathcal{P}_i(1,3)$ exactly once each, it follows that

$$i+3 \in A_i^2 \cup A_i^3,\ i \in A_{i+4}^2 \cup A_{i+4}^3,\ 1 \leq i \leq 9.$$

Thus, it is seen that $A_i^2 \cup A_i^3 = \{i+1, i+3, i+5, i+7\}$ $(1 \leq i \leq 9)$. However, the $\{i, i+1\}$ does not appear in $\bigcup_{1\leq i\leq 9} \mathcal{P}_i(2,3)$, which is a contradiction. □

Now, the main theorem of this paper will be established.

Theorem 8 *The necessary conditions (5), (6) and (7) are sufficient for the existence of a* $PMA_\lambda(3 \times 2, v)$ *with a definite exception* $(v, \lambda) = (9, 1)$.

Proof At first, for each of three cases (I) with $\lambda = 1$ and $v \neq 9$, (II) with $\lambda = 2$ and (III) with $\lambda = 4$ described at the beginning of this section, the required array is constructed.

Case (I): On account of Theorem 1 and Examples 2 and 4, it is sufficient to prove the existence of a $\mathrm{PMA}_1(3 \times 2, v)$ with $v \in \{65, 113, 161, 185\}$. Note that $v \equiv 17 \pmod{24}$ holds for every $v \in \{65, 113, 161, 185\}$.

Corollary 1 provides a $(3, 1)$-GDD of type $12^u 8$ with $12u + 8$ points and $u + 1$ groups for any $u \geq 3$. In addition, a $\mathrm{PMA}_1(3 \times 2, v)$ for $v = 17$ is given in Example 2. Furthermore, a $\mathrm{PA}_1(3, 3)$ and a $(25, 3 \times 2, 1)$-SBD can be obtained by Lemmas 1

and 3, respectively. Hence, a $\mathrm{PMA}_1(3 \times 2, 25)$ can be constructed by use of the construction in Lemma 6. Then, Lemma 7 with $c = 2$ shows that the (3, 1)-GDD of type $12^u 8$ and the $\mathrm{PMA}_1(3 \times 2, v)$ for $v = 17, 25$ yield a $\mathrm{PMA}_1(3 \times 2, 24u + 17)$ for any $u \geq 3$. Hence, there exists a $\mathrm{PMA}_1(3 \times 2, v)$ for $v = 113, 161, 185$.

On the other hand, Lemma 7 with $c = 2$ also shows that the (3, 1)-GDD of type 8^4 given in Corollary 2 and the $\mathrm{PMA}_1(3 \times 2, 17)$ yield a $\mathrm{PMA}_1(3 \times 2, 65)$.

Case (II): For $v \equiv 13, 21 \pmod{24}$, Lemma 6 with the $(v, 3 \times 2, 2)$-SBD given in Lemma 3 and the $\mathrm{PA}_1(3, 3)$ provide the required array. Hence, it is sufficient to prove the existence of a $\mathrm{PMA}_2(3 \times 2, v)$ for $v \equiv 5 \pmod{24}$.

Now, Example 5 is the case of $v = 29$. Lemma 7 with $c = 2$ also shows that a (3, 2)-GDD of type $6^{2u+1}8$ with $12u + 14$ points and $2u + 2$ groups obtained by taking copies of the design given in Corollary 3 and the $\mathrm{PMA}_2(3 \times 2, v)$ with $v = 13, 17$ yield a $\mathrm{PMA}_2(3 \times 2, v)$ for $v \equiv 5 \pmod{24}$ with $v \geq 53$.

Case (III): Lemma 4 provides the $\mathrm{PMA}_4(3 \times 2, v)$ for any $v \geq 6$.

Therefore, for larger λ in each of the three cases (I) with $v \neq 9$, (II) and (III), the required array can be constructed by taking copies of the array with $\lambda = 1$, $\lambda = 2$ and $\lambda = 4$, respectively. For $v = 9$, Lemma 6 with a $(9, 3 \times 2, \lambda)$-SBD given in Lemma 3 and the $\mathrm{PA}_1(3, 3)$ yields a $\mathrm{PMA}_\lambda(3 \times 2, 9)$ for any $\lambda \geq 2$. Furthermore, Lemma 8 shows the non-existence of a $\mathrm{PMA}_1(3 \times 2, 9)$. The proof is complete. □

Remark 1 Lemma 8 also shows the non-existence of an $\mathrm{APMA}_1(3 \times 2, 9)$ which improves Theorem 1 mentioned in Sect. 1.

6 Asymptotic Existence on a Cyclic $\mathrm{PMA}_1(4 \times 2, v)$

It does not seem to be easy to construct an infinite family of PMAs for some classes of $k \geq 4$ or $c \geq 3$. The asymptotic existence of such PMAs is here discussed. Regarding some cyclic combinatorial structures, asymptotic results have been obtained by using Weil's theorem (cf. Lidl and Niederreiter 2018) on multiplicative character sums (e.g., Buratti and Pasotti 2009; Chang and Ji 2004; Li et al. 2018). In this section, the asymptotic existence of a cyclic $\mathrm{PMA}_1(4 \times 2, p)$ is shown for a prime $p \equiv 1 \pmod 8$ with $p > 5 \times 10^9$ based on the result in Li et al. (2018, Theorem 3.16). Note that Theorem 3.16 in Li et al. (2018) shows the existence of an $\mathrm{APMA}_1(5 \times 2, p)$ for any prime $p \equiv 1 \pmod{40}$ with $p > 41$ by use of an asymptotic method and a computer search.

For $q \equiv 1 \pmod n$ and a primitive element $\alpha \in \mathrm{GF}(q)$, denote by C_0^n the unique multiplicative subgroup $\{\alpha^{in} \mid 0 \leq i \leq (q-1)/n\}$ of index n and order $(q-1)/n$, while C_j^n $(1 \leq j \leq n-1)$ denotes the multiplicative coset of C_0^n represented by α^j, i.e., $C_j^n = \alpha^j \cdot C_0^n$. The multiplicative cosets $C_0^n, C_1^n, \ldots, C_{n-1}^n$ of C_0^n are called *cyclotomic classes of index n* in $\mathrm{GF}(q)$. The following result can be obtained by using Weil's theorem.

Lemma 9 (Chang and Ji 2004) *Let $p \equiv 1 \pmod q$ be a prime satisfying the inequality*

$$p - \left[\sum_{0 \le i \le s-2} \binom{s}{i} (s-i-1)(q-1)^{s-i} \right] \sqrt{p} - sq^{s-1} > 0. \tag{12}$$

Then, for any given s-tuple $(j_1, j_2, \ldots, j_s) \in \{0, 1, \ldots, q-1\}^s$ *and any given s-tuple* $(c_1, c_2, \ldots, c_s)$ *of pairwise distinct elements of* $GF(p)$*, there exists an element* $x \in GF(p)$ *such that* $x + c_i \in C^q_{j_i}$ *for each* $i = 1, 2, \ldots, s$.

Now, for a cyclic $\mathrm{PMA}_1(4 \times 2, v)$, the following asymptotic existence result can be obtained.

Theorem 9 *Let* $p \equiv 1 \ (mod\ 8)$ *be an odd prime with* $p > 5 \times 10^9$*. Then there exists a cyclic* $PMA_1(4 \times 2, p)$.

Proof Let $p = 8m + 1$ be a prime, where m is a positive integer and $p > 5 \times 10^9$. Then, it is seen that the inequality (12) with $(q, s) = (4, 7)$ holds for any $p > 5 \times 10^9$, more precisely $p > 4.84881 \cdots \times 10^9$. Let α be a primitive element of $\mathrm{GF}(p)$ and $C^4_0, C^4_1, C^4_2, C^4_3$ be a cyclotomic classes of index 4. Then the following row is at first considered for some $x \in \mathrm{GF}(p)$:

$$\boldsymbol{R} = \left(\alpha, \alpha x \mid \alpha^2, \alpha^2 x \mid \alpha^3, \alpha^3 x \mid \alpha^4, \alpha^4 x\right).$$

Now, we can uniquely determine integers a_1, a_2 and a_3 in $\mathbb{Z}_4$ such that $\alpha - 1 \in C^4_{a_1}$, $\alpha^2 - 1 \in C^4_{a_2}$ and $\alpha^3 - 1 \in C^4_{a_3}$, respectively. Moreover, Lemma 9 with

$$(j_1, j_2, j_3, j_4, j_5, j_6, j_7) = (1, a_1 + 2, a_1 + 2, a_2 + 2, a_2 + 1, a_3 + 2, a_3)$$

on $\mathbb{Z}_4$ and

$$(c_1, c_2, c_3, c_4, c_5, c_6, c_7) = (0, -\alpha, -\alpha^{-1}, -\alpha^2, -\alpha^{-2}, -\alpha^3, -\alpha^{-3})$$

on $\mathrm{GF}(p)$ provides an element $x \in \mathrm{GF}(p)$ such that

$$\begin{aligned} &x \in C^4_1,\ x - \alpha \in C^4_{a_1+2},\ x - \alpha^{-1} \in C^4_{a_1+2},\ x - \alpha^2 \in C^4_{a_2+2}, \\ &x - \alpha^{-2} \in C^4_{a_2+1},\ x - \alpha^3 \in C^4_{a_3+2},\ x - \alpha^{-3} \in C^4_{a_3}. \end{aligned}$$

Then it follows that

$$\pm(\alpha^i - 1) \in C^4_{a_i},\ \pm x(\alpha^i - 1) \in C^4_{a_i+1},\ \pm(x - \alpha^i) \in C^4_{a_i+2},\ \pm\alpha^i(x - \alpha^{-i}) \in C^4_{a_i+3}.$$

for $i = 1, 2, 3$.

For $\boldsymbol{R}$ with the x, let the ith base row be $\boldsymbol{R}_i = \alpha^{4(i-1)}\boldsymbol{R} = (A_{i1} \mid A_{i2} \mid A_{i3} \mid A_{i4})$ for $1 \le i \le m$, where

$$A_{ij} = \left\{\alpha^{4(i-1)+j}, \alpha^{4(i-1)+j} x\right\},\ j = 1, 2, 3, 4.$$

Then, the j_1th and the j_2th entries of $\boldsymbol{R}_i$ $(1 \le i \le m)$ yield the following differences:

$$\bigcup_{1\le i\le m} \alpha^{4(i-1)+j_1}\left\{\pm(\alpha-1), \pm x(\alpha-1), \pm(x-\alpha), \pm\alpha(x-\alpha^{-1})\right\}$$

for $(j_1, j_2) = (1, 2), (2, 3), (3, 4)$,

$$\bigcup_{1\le i\le m} \alpha^{4(i-1)+j_1}\left\{\pm(\alpha^2-1), \pm x(\alpha^2-1), \pm(x-\alpha^2), \pm\alpha^2(x-\alpha^{-2})\right\}$$

for $(j_1, j_2) = (1, 3), (2, 4)$ and

$$\bigcup_{1\le i\le m} \alpha^{4(i-1)+j_1}\left\{\pm(\alpha^3-1), \pm x(\alpha^3-1), \pm(x-\alpha^3), \pm\alpha^3(x-\alpha^{-3})\right\}$$

for $(j_1, j_2) = (1, 4)$. Since $p = 8m + 1$ and $\{a_i, a_i + 1, a_i + 2, a_i + 3\} = \mathbb{Z}_4$ for $i = 1, 2, 3$, it is seen that the m base rows $\boldsymbol{R}_i$ with $1 \le i \le m$ satisfy the condition (2).

Thus, m row orbits of the base rows yield the required array. □

Remark 2 Similarly to Theorem 9, various asymptotic results of cyclic PMAs can be obtained. For example, it can be shown that there exists a cyclic $\mathrm{PMA}_1(k \times 2, p)$ for any $k \ge 3$ and any prime $p \equiv 1 \pmod 8$ satisfying the inequality (12) with $(q, s) = (4, 2k - 1)$.

7 Conclusions

As pointed out in Li et al. (2018), authentication and secrecy codes without splitting have been intensively studied in literature, but authentication and secrecy codes with splitting have been much less studied than their counterparts. To construct the codes with splitting, they newly defined the PMA and the APMA. In this paper, we made some progress on the results of the PMAs. However, not many PMAs with $N = v - 1, v$ are constructed except for the case of $k = 2$ as in Theorems 3 and 4. Although Theorem 7 shows the non-existence of a PMA with $N = v - 1, k \ge 3$, there possibly exists a PMA with $N = v, k \ge 3$. Unfortunately, the methods presented in this paper cannot provide the exact existence, even if the asymptotic existence, of any (cyclic) $\mathrm{PMA}_\lambda(k \times c, v)$ with $N = v$ and $k \ge 3$ except for $(\lambda, k, c, v) = (2, 3, 6, 37)$ and $(1, 3, 2, 9)$ given in Example 3 and Lemma 8, respectively.

To the best of our knowledge, any application of PMAs (or APMAs) has never been considered except for Li et al. (2018), and any other application is not also discussed in this paper. On the other hand, other types of combinatorial multi-arrays have been introduced in literature, for example, an orthogonal multi-array (OMA) (Brickell 1984) and a balanced orthogonal multi-array (BOMA) (Mukerjee 1998; Sitter 1993) which are generalizations of the orthogonal array. Especially, the OMA and the BOMA are multi-arrays allowed to have different sizes of entries in each row and each column, and statistical applications of the BOMA are given in Mukerjee

(1998); Sitter (1993). Furthermore, in Bailey and Cameron (2019), a special class of the BOMA is focused as multi-part balanced incomplete-block designs, and another statistical application of the designs is discussed. The "balanced" property of the BOMA implies that entries of each column yield a pairwise balanced design (PBD), where the PBD is a generalization of a BIB design by allowing various block sizes (see Raghavarao 1988). It is clear that the existence of a PMA $\mathcal{A} = (A_{ij})$ with the balanced property, i.e., $\{A_{ij} \mid 1 \leq i \leq N\}$ yields a BIB design for each j with $1 \leq j \leq k$, is equivalent to the existence of pairwise additive BIB designs discussed in Matsubara and Kageyama (2015), Sawa et al. (2007).

It is well known that perpendicular arrays can be used to construct orthogonal arrays. Furthermore, some relationship between the pairwise additive BIB designs and a special class of mutually orthogonal latin squares equivalent to the orthogonal array is discussed in Matsubara and Kageyama (2015), Sawa et al. (2007). However, it seems that any construction of the OMA (or the BOMA) by use of the PMA (or the pairwise additive BIB designs) has never been known.

Several generalizations of a PMA can be considered. One of the generalizations is to consider a strength of the PMA. Actually, the PMA with the strength t is defined for any $t \geq 2$ in Li et al. (2018). Another generalization is to allow different sizes of the entry for PMA. Moreover, since Rao (1961) introduced two types of orthogonal arrays, orthogonal arrays of type I (called ordered designs in Bierbrauer 2007) and orthogonal arrays of type II (called perpendicular arrays in Bierbrauer 2007), a generalization of the ordered design as an ordered multi-design (OMD) and its applications may be discussed. In fact, a PMA given in Example 5 is such an ordered multi-design.

The relationship among three types of the combinatorial multi-arrays (OMA, OMD, PMA), their generalizations and their applications to the design of experiments (or other fields) will be discussed in a forthcoming paper.

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Statistical Design Issues for fMRI Studies: A Beginner's Training Manual

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Abstract An experimental subject [patient] is presented with a mental stimulus such as a 1.5-second flickering checkerboard image or a painful heat stimulus at some of a total of n time points in the experiment. During this presentation, the patient absorbs a sequence of mental stimuli along with a provision for intermediate resting period as well. The measurement of a brain voxel at an instant is collected by an fMRI scanner. The purpose is to examine a collection of the response profiles to understand the nature and extent of local brain activity in response to the stimuli. Functional Magnetic Resonance Imaging (fMRI) is a technology for studying how our brains respond to mental stimuli. In recent times, researchers have paid attention to "modeling" the responses in terms of sequences of mental stimuli received during a given period including the "resting phase" as well. The simplest such model incorporates linear relation between mean response and the parameters describing the effects of the stimuli, applied at regularly spaced time points during the study period. There is a nuisance parameter and also those representing the unknown heights of the hemodynamic response function, HRF, at the stimulus onset time point and at some of the immediately preceding time points. Statistical design theorists have focused their attention to the study of design sequences for collecting most informative data in order to render most precise inference about these parameters under an assumed statistical model. We have noted that most experimental design researchers are not aware of this application of linear models and design considerations in fMRI studies. Accordingly, our primary consideration has been to introduce this application area and related concepts in simple terms. We have given illustrative examples at length. In the process, we have introduced the concept of "Clear Zero". We thought this would create enough interest among researchers in the broad areas of linear models and DoE. In this paper, we review the linear model and discuss estimation issues and related concepts such as "orthogonality" and "balance", as are applicable to fMRI research study. Incidentally, a concept termed "Clear 0" is introduced and studied at length. This is geared toward our understanding of comparison between two given design sequences from inferential aspects.

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1 Introduction

The key reference to this article is Cheng and Kao (2015) who carried out an investigation on the scope of study of optimal experimental designs in the context of fMRI studies.

In fMRI studies, each instant is defined as a compact duration of 4 seconds. According to the linear model envisaged in this context, at any instant, the brain voxel captures the cumulative effects of a "nuisance parameter" θ and the h-parameters at the current instant as well as at each of the immediate past ordered $(K-1)$ instants—for some K—whenever there has been an onset of active stimulus [coded by 1] at any of these instances. The h-parameters are said to represent the unknown heights of the hemodynamic response function, HRF, at the stimulus onset time point and at some of the immediately preceding time points. This is akin to the concept of "residual" or "carry-over" effects in the framework of Repeated Measurements Designs [RMDs]. Vide Shah and Sinha (1989).

In actual implementation of stimulus, "doses" may be administered at different activation levels and their effects may be studied. Here we consider only a $(1-0)$ situation, i.e., only two available codes which correspond to active phase or resting phase. We refer to Kao et al. (2008) for this and related considerations.

In real-life applications of fMRI studies, a design sequence is of sufficiently large length n and the number of h-parameters (K) is also substantially large. We have tried to keep the length of the design sequences quite general in most of the illustrations. However, we have confined to very small values of K in most examples to illustrate the concepts and also to highlight the difficulty levels with large values. It will be amply clear from the text that an analysis of the data accrued through a given design sequence is, most often, a routine exercise. It is only when we seek desirable properties of the parameter estimates that we run into complexities unless the number of non-negligible h-parameters is small or moderate.

The mean model formulation is developed as follows. An experimental design of length n, say $D(n)$, is a description of a sequence of 0s and 1s of total length n. For example, for $n = 8$, the following describes an eight-point design: $D(8) = [0, 1, 1, 0, 1, 0, 0, 1]$. The utility of the suggested design $D(8)$ is described below. For any n, $D(n)$ is very much like $D(8)$. The linear model to be described below is developed as a "circular" model—a well-known consideration in the context of RMDs or cross-over designs. Vide Kunert (1984) or Shah and Sinha (1989). To visualize a circular model, the same sequence (describing $D(8)$) is used as a "dummy" sequence and this is described as follows:

$< 0, 1, 1, 0, 1, 0, 0, 1 >$ $\rightarrow$ $[0, 1, 1, 0, 1, 0, 0, 1]$

Dummy Sequence followed by Data-generating Sequence

There are eight data/time points and as such we observe the responses y_1 to y_8 corresponding to the eight time points in the data-generating sequence [0, 1, 1, 0, 1, 0, 0, 1] going from left to right. The response at the uth time point corresponds to the measurement of a brain voxel collected by the fMRI scanner at that time point. According to the description in the linear model, the scanner also reads and incorporates the effects of the phases in the preceding $K-1$ time points. In the terminology of RMDs or cross-over designs, for the first time point, the "direct effect" [denoted by h_1] is to be captured along with the "carry-over effects" [h_2, h_3, ...] of the preceding time points as described in the Dummy Sequence—from right to left. Although, at each data point, only if the stimulus is active [denoted by 1], the corresponding h-parameter will be considered. Lastly, for n data/time points, we can incorporate at the most n "parameters"—including the constant parameter θ. This implies that we can incorporate in the model at the most $(n-1)$ h-parameters. Otherwise, identifiability/estimability issues creep in. In terms of K, it means that we assume—to start with—that $K \leq (n-1)$. In reality, the experimenter has a perfect knowledge about a "cap" on the number of h-parameters and accordingly he/she makes a choice of n, the number of data points.

We start with Table 1 describing the linear model underlying the design $D(8)$. We assume $K = 7$. Once for all, we may fix the notation as $DS(K, n)$ to denote a design sequence of length n, assuming that there are K h-parameters, besides the nuisance parameter θ. Naturally, for estimability, it is necessary that $n > K$. When K is not understood clearly from the context, we may simply write it as $DS(n)$.

Remark 1 Interestingly enough, one single design sequence of length n results in n responses and an underlying linear model with $((1, 0))$ elements. Cheng and Kao (2015) have rightly referred to "Biased (Spring Balance) Weighing Designs" with reference to the linear model described above. In the terminology of spring balance weighing designs with bias, the nuisance parameter θ represents the bias component and the h-parameters behave like "true (unknown) weight" parameters of a number of objects. The coefficients 0, 1 appearing in the linear model are also worth noting as in case of a spring balance weighing design framework. Our understanding of weighing designs—including the use of Hadamard Matrices—comes in handy to

Table 1 Linear model with positional carry-over effects

S1. No.	h_7	h_6	h_5	h_4	h_3	h_2	h_1	y	Mean model
1	1	0	1	0	0	1	0	y_1	$\theta + h_2 + h_5 + h_7$
2	0	1	0	0	1	0	1	y_2	$\theta + h_1 + h_3 + h_6$
3	1	0	0	1	0	1	1	y_3	$\theta + h_1 + h_2 + h_4 + h_7$
4	0	0	1	0	1	1	0	y_4	$\theta + h_2 + h_3 + h_5$
5	0	1	0	1	1	0	1	y_5	$\theta + h_1 + h_3 + h_4 + h_6$
6	1	0	1	1	0	1	0	y_6	$\theta + h_2 + h_4 + h_5 + h_7$
7	0	1	1	0	1	0	0	y_7	$\theta + h_3 + h_5 + h_6$
8	1	1	0	1	0	0	1	y_8	$\theta + h_1 + h_4 + h_6 + h_7$

address the question of formation of "optimal" sequences. Vide Raghavarao (1971) or Shah and Sinha (1989). However, there is a fundamental difference between the two design formulations. In case of weighing designs, each single weighing results in just one observation whereas in case of fMRI designs, each single design sequence of length n generates the full sequence of n observations. This explains the difficulty level in recommending design sequences with parameters (K, n) possessing nice properties. There is no sequential search of a design sequence in fMRI study.

In theory, in a study of fMRI design sequence, there is an inherent linear model $(\mathbf{Y}, \mathbf{X}^{(*)}\beta, \sigma^2\mathbf{I})$ where (i) coefficient matrix $\mathbf{X} = ((x_{ij}))$ consists of 0s and 1s, (ii) $\mathbf{X}^{(*)} = (\mathbf{1}, \mathbf{PX})$ and $\beta = (\theta, h_1, h_2, \ldots)'$. It may be noted that in the above table, the $\mathbf{X}$-matrix is shown in the reverse order. Multiplication by a permutation matrix $\mathbf{P}$ will bring it to the right/standard order. That explains the use of the matrix $\mathbf{P}$ above.

Remark 2 It may be noted that the "Dummy Sequence" displayed above forms the basis of what is known as a "Circular Model". One should realize the implication of "circular model" in this context. It implies that the columns $\mathbf{h}_1, \mathbf{h}_2, \ldots$. are circular in nature. That is, the columns of the matrix $\mathbf{X}$ are circular in nature.

Remark 3 We now discuss the implication of a non-circular model. First of all, there is no "Dummy Sequence" attached to a non-circular model. We straightaway have the "Data Generating Sequence", to be in operation from left to right. Therefore, model expectation of y_1 is θ or $\theta + h_1$, depending on the nature of onset of the phase at time point 1, i.e., resting or active. Next, model expectation of y_2 will involve θ and one of the four possible combinations of the h-parameters: $-, h_1, h_2, h_1 + h_2$, depending on the cases: $(0, 0)$; $(0, 1)$, $(1, 0)$, $(1, 1)$. This will continue until y_{K-1}. From y_K onward, all the K potential h-parameters qualify to enter the model. In a sense, under a non-circular model, the first $K - 1$ observations provide curtailed information about the h-parameters while the rest provide full information. For large n compared to K, as is usually the case, one recommendation is to discard the initial $K - 1$ observations and work with the rest. In other words, effective sample size is reduced from n to $n - K + 1$. Consideration of a non-circular model does not pose any problem for statistical analysis of the entire body of data. However, we do not expect any "nice" structural pattern of the $\mathbf{X}$-matrix. That may be the reason why such a model has not been studied in detail in fMRI research. We will not discuss this matter any further except for providing a general description of a $DS(K, n)$ which satisfies the rank condition for a non-circular model. We assume K to be even. This DS is composed of the first $K + 1$ members as $(1, 0, 1, 0, \ldots, 1, 0; 0)$ of length $K + 1$. Successive terms in the model expectation (in a non-circular model) are $\theta + h_1, \theta + h_2, \theta + h_1 + h_3, \ldots, \theta + h_2 + h_4 + \cdots + h_K; \theta + h_3 + h_5 + \ldots$.. It can be verified that θ and all the h-parameters are estimable from the $K + 1$ observations accrued from this DS of length $K + 1$.

Remark 4 In case it is believed that there are only $K^*[< K]$ h-parameters in the model, the understanding is that the initial set of K^* h-parameters, viz., $h_1, h_2, \ldots, h_{K^*}$ are important and the rest can be ignored from the mean model.

For $K = K^* = 7$, the model expectations of successive responses corresponding to the above design are already shown in the last column of the table. It is readily seen that $E(y_8 - y_3) = h_6 - h_2 = E(y_7 - y_4)$. Thus, the design layout corresponds to a singular model. We now assume that $h_7 = 0$ which amounts to saying that $K^* = 6$ and that the underlying $\mathbf{X}^{(*)}$ matrix is of order 8×7. In the final analysis, it turns out that the above design sequence entails one to estimate all the h-parameters only when there are four of them, viz., h_1, h_2, h_3, h_4 are non-negligible and the rest are negligible. In reality, one has to possess perfect knowledge about K^* [or, at least, a comfortable upper bound of it] and then look for appropriate design sequence to ensure estimability of all the non-negligible h-parameters.

The rest of the paper is organized as follows. In Sect. 2, we revisit the concepts of structurally balanced and orthogonal design sequences by using illustrative examples with small values of K and n. As mentioned before, our aim is to familiarize the readers with this area of application of linear models in fMRI studies, similar in context to that of biased spring balance weighing designs. In Sect. 3, we introduce the concept of "Clear Zero" sequence in fMRI studies. The purpose is to increase the efficiency of a given design sequence in terms of inference on the h-parameters. We deal with the special cases of $K = 2, 3$ while n is kept general. In most of the subsequent sections, we deal with possible applications of the notion of "Clear Zero" to derive modified and possibly "improved" design sequences. Our focus is more with an exposure to the topics with suitable illustrative examples.

2 Structurally Balanced and Orthogonal Design Sequences

For $K = 3$ h-parameters, the mean model generally involves expressions such as $\theta, \theta + h_i, i = 1, 2, 3; \theta + h_i + h_j, i \neq j$ and, finally, $\theta + h_1 + h_2 + h_3$. The underlying design sequence is said to be "Structurally Balanced Design Sequence [SBDS]" when frequency counts of $\theta + h_1, \theta + h_2, \theta + h_3$ are the same and also those of $\theta + h_1 + h_2, \theta + h_1 + h_3, \theta + h_2 + h_3$ are the same. In other words, for an SBDS with $K = 3$, in terms of the h-parameters, singletons are equally frequent and also doubletons are equally frequent. The notion generalizes naturally for higher values of K.

Before we proceed further, we must admit the inherent difficulty level in attaining structural balance of a design sequence. For arbitrary values of $K, n(> K)$, specification of a $DS(K, n)$ of length n attaining SB in the above sense is highly non-trivial. When SB obtains, there is "complete symmetry" in the information matrix of the h-parameters in the sense that it attains the form $p\mathbf{I} + \mathbf{qJ}$ for suitable scalars p, q.

Specifically, for $K = 3$ and for an $SBDS(3, n)$ of size n, let f_0, f_1, f_2, f_3 represent, respectively, the frequency counts of θ, each of the singletons, each of the doubletons and finally that of $\theta + h_1 + h_2 + h_3$. Then $n = f_0 + 3f_1 + 3f_2 + f_3$ and the 4×4 information matrix of the β-parameter vector is given by

$$[n, f_1+f_2+f_3, f_1+f_2+f_3, f_1+f_2+f_3]; [---, f_1+2f_2+f_3, f_2+f_3, f_2+f_3];$$

$$[---, ---, f_1+2f_2+f_3, f_2+f_3]; [---, ---, ---, f_1+2f_2+f_3].$$

We set $a = f_1 + 2f_2 + f_3$ and $b = f_2 + f_3$. Then, the 3×3 information matrix for the h-parameters has the representation

$$[(a(n-a), nb-a^2, nb-a^2), (nb-a^2, a(n-a), nb-a^2), (nb-a^2, nb-a^2, a(n-a)]$$

and it is completely symmetric (cs). Further, orthogonality of the estimates happens whenever $a^2 = nb$ which simplifies to

$$(f_0+f_1)(f_2+f_3) = (f_1+f_2)^2.$$

When this obtains, pairwise covariances of estimates of the h-parameters are zeros. Here is an example for $n = 8$, $K = 3$: $DS(3, 8) = [1, 1, 1, 0, 1, 0, 0, 0]$. It is structurally balanced with $f_0 = f_1 = f_2 = f_3 = 1$. Hence, orthogonality condition is trivially satisfied.

It is interesting to note that a design sequence can be structurally unbalanced but still it may turn out to be orthogonal ! Here is an example from Kao (2015).

$$n = 12, K^* = 4 : D(4, 12) = [1, 0, 1, 1, 1, 1, 0, 0, 0, 1, 0, 0].$$

Whereas each one of the coefficient vectors (involving the h-parameters)

$$[1000]'; [0100]', [0001]'$$

appears exactly once, $[0010]'$ appears twice in the model expectations of the observations. That explains structural imbalance of the design sequence. In spite of that, it turns out that $V(\hat{h}_i) = 3; Cov(\hat{h}_i, \hat{h}_j) = 0; i \neq j = 1, 2, 3, 4$.

Kao (2015) listed some orthogonal design sequences for $K = 3, 4, 5$ while n is a multiple of 4 and these were found using Hadamard matrices and the theory of quadratic residues. We list some of these sequences below.

Literature survey suggests that design sequences for very general design parameters K, n and possessing such structurally balanced and/or orthogonality properties are hard to find. A combinatorially challenging problem would be: For given K, to find out a balanced orthogonal design with smallest length n of design sequence! Another related problem would be to ascertain if an orthogonal/structurally balanced design sequence for a given value of K continues to be so for smaller/higher values of K.

It is well known that there is a close connection between Hadamard Matrices and Weighing Design Matrices [of both types: Chemical Balance and Spring Balance]. Vide Raghavarao (1971) and Shah and Sinha (1989). Researches have examined the possibility of starting with Hadamard Matrices and converting them into $((0, 1))$-matrices so as to examine their properties as Design Sequences for fMRI experiments.

We will come back to this aspect of orthogonality later in Sect. 4.

Table 2 Orthogonal design sequences

S1. No.	n	K	Sequence
1	8	3	1 1 1 0 1 0 0 0
2	12	4	1 0 1 1 1 1 0 0 0 1 0 0
3	20	5	1 0 0 1 1 1 1 1 0 1 0 1 0 0 0 0 1 1 0 0
4	24	5	1 1 1 1 1 0 1 0 1 1 0 0 1 1 0 0 1 0 1 0 0 0 0 0
5	32	5	1 1 0 1 1 0 1 1 1 1 1 1 0 0 0 1 0 1 0 1 1 1 0 0 0 0 1 0 0 1 0 0 0

3 Concept of "Clear Zero" Sequence

Suppose a design sequence contains a succession of 0s of length f. Further, assume that there are K non-negligible h-parameters in the model. Then there are $(f - K + 1)$ y-observations whose model expectations are θ each! As such there is no information on the h-parameters from these observations. What if all or a subset of these 0s are replaced by 1s? Would it provide increased precision for the estimates of the h-parameters? This and similar issues were raised by one of the authors in the form of "Clear 0s" and now we provide a systematic study of this concept below. Our goal is to introduce the concept using small illustrative examples, keeping the design sequence length n as general as possible. However, we confine to $K = 2, 3$. This area of research is just coming up and we hope the readers would be interested to pursue this topic.

3.1 Type I: $D(f + 3) = [1\ \ 0\ \ \mathbf{0}_f\ \ 1]$

We start with a design sequence called Type I: $D(f + 3) = [1\ \ 0\ \ \mathbf{0}_f\ \ 1]$ and invoke the "operation" of "Clear 0" to the collection of f 0s. Thus, the design sequence is transformed to $D^*(f + 3) = [1\ \ 0\ \ \mathbf{1}_f\ \ 1]$. Note that y-observations $y_1, y_2, \ldots, y_n$ correspond to the design points from left to right where $n = f + 3$. For the original design sequence, we separate out y_1, y_2, y_n from the rest. To start with, let us assume that there are only two h-parameters, viz., h_1, h_2. Then the model expectations are

$$E(y_1) = \theta + h_1 + h_2;\ E(y_2) = \theta + h_2;\ E(y_n) = \theta + h_1$$

while $E(y_i) = \theta$ for the rest of the observations.

Again, for the transformed sequence, we separate out y_1, y_2, y_3 from the rest. This time the model expectations are

$$E(y_1) = \theta + h_1 + h_2;\ E(y_2) = \theta + h_2;\ E(y_3) = \theta + h_1$$

while $E(y_i) = \theta + h_1 + h_2$, for the rest of the observations.

For two h-parameters and the constant parameter θ, the information matrix is of order 3×3. The first part of the information matrix is formed of the three observations separated out in the beginning. It is the same for both the structures and is given by

$$(3, 2, 2);\ (2, 2, 1);\ (2, 1, 2).$$

The other part is different for the two sequences. For the first choice, we have

$$(f, 0, 0);\ (0, 0, 0);\ (0, 0, 0).$$

For the second choice, we have $f\mathbf{J}$.

It turns out that for the first choice, we have determinant of the information matrix for (h_1, h_2) as

$$Det(\mathbf{I}) = (c_0 - d_0)[(c_0 + d_0) - 2\frac{b_0^2}{(a_0 + f)}].$$

Similarly, for the second choice, it is given by

$$Det(\mathbf{I}^*) = (c_0 - d_0)[2f + c_0 + d_o - 2\frac{(b_0 + f)^2}{(a_0 + f)}].$$

In the above, we have used the notations a_0, b_0, c_0, d_0 to represent the first part of the information matrix as

$$(a_0, b_0, b_0);\ (b_0, c_0, d_0);\ (b_0, d_0, c_0).$$

It follows that second choice would result in higher value of the Det(.) provided $a_0 > 2b_0$. In this example, $a_0 = 3$, $b_0 = 2$. Consequently, use of "Clear 0" operation does not help in this particular design sequence.

3.2 *Type II:* $D(f + 4) = [1\ 0\ 0_f\ 0\ 1]$ *Versus* $D^*(f + 4) = [1\ 0\ 1_f\ 0\ 1]$

For $f = 1, 2, 3$ and for $K = 2$, the second design sequence has a smaller value of the Det.(.) and hence it is not gainful. For $f = 4$, the two determinantal values are identical! And for $f > 4$, the second design sequence continues to show improvement in terms of higher determinantal value.

We also observe that the same phenomena hold for $K = 3$. We skip the details.

3.3 Type III: $D(2s + f + 2) = [1_s\ 0\ 0_f\ 0\ 1_s]$ Versus $D^*(2s + f + 2) = [1_s\ 0\ 1_f\ 0\ 1_s]$

For $K = 2$, we deduce that for the design sequence $D(2s + f + 2)$,

$$I(h) = [(2s(f + 2), 2s(f + 2) - n); (2s(f + 2) - n, 2s(f + 2)]$$

and hence $Det.(I) = (P + 2)(4sf + 6s - f - 2)$ where $P = 2s + f$.

Again, for the design sequence $D^*(2s + f + 2)$, we deduce that

$$I^*(h) = [(2(2s + f), -4); (-4, 2(2s + f))]$$

and hence $Det.(I^*) = 4(P + 2)(P - 2)$. Hence, the second design sequence has a larger value of the Det.(.) provided $4sf < 2s + 5f + 2$.

For $s = 1$, this holds for all f. For $s = 2$, it holds when $f = 1, 2$. For all other values of $s > 2$, there is no solution to f.

We will now study the case of $K = 3$. For the design sequence $D(2s + f + 2)$, the full information matrix of all the four parameters is given by

$$[(n, 2s, 2s, 2s); (2s, 2s, 2s - 1, 2s - 2); (2s, 2s - 1, 2s, 2s - 1); (2s, 2s - 2, 2s - 1, 2s)].$$

From this, we derive the form of the information matrix of the three h-parameters:

$$[(2s(f + 2), 2s(f + 2) - n, 2s(f + 2) - 2n); (2s(f + 2) - n, 2s(f + 2), 2s(f + 2) - n);$$

$$(2s(f + 2) - 2n, 2s(f + 2) - n, 2s(f + 2))].$$

From the above, we deduce that

$$Det.(I) = 4(2s + f + 2)^2[2s(f + 1) - f - 2].$$

Next, we take up the design sequence $D^*(2s + f + 2)$ and derive an expression for the information matrix of all the four parameters as

$$[(n, 2s + f, 2s + f, 2s + f); (2s + f, 2s + f, 2s + f - 2, 2s + f - 2);$$

$$(2s + f, 2s + f - 2, 2s + f, 2s + f - 2); (2s + f, 2s + f - 2, 2s + f - 2, 2s + f)].$$

From this, we derive the form of $Det.(I^*)$ as is given below. We use the notation $P = 2s + f$.

$$Det.[(2P, 2P - 2n, 2P - 2n), (2P - 2n, 2P, 2P - 2n), (2P - 2n, 2P - 2n, 2P)].$$

This simplifies to $Det.(I^*) = 8n^2(P - 4)$ and it fails to show improvement over the first design sequence whenever $s > 1$. Also for $s = 1$, improvement holds for $f > 4$.

3.4 *Type IV:* $D(f+5) = [1\ 0\ 0_f\ 0\ 1\ 0]$ *Versus* $D^*(f+5) = [1\ 0\ 1_f\ 0\ 1\ 0]$

In this case, after carrying out usual analysis for $K = 2$ and $n = f + 5$, we find that Det(I) = Det. $[(2n-4, -4); (-4, 2n-4)] = 4(f+1)(f+5)$ while Det(I^*) = Det. $[((f+2)(n-f-2), n(f-1)-(f+2)^2); (n(f-1)-(f+2)^2, (f+2)(n-f-2))] = 9(f-1)(f+5)$. For $f = 1$, second design sequence breaks down; for $f = 2$, again, second design fails to show any improvement. However, for all other values of f, it performs better.

Again, for $K = 3$, we find that when $f = 1$, second design sequence is singular.

For $f = 2$, we obtain

Det(I) = Det. $[(10, -4, 3); (-4, 10, -4); (3, -4, 10)] = 686$ while

$Det(I^*) = Det.[(12, -9, 5); (-9, 12, -9); (5, -9, 12)] = 294.$

So second design sequence does not serve our purpose.

We now continue our search for $f = 3$ and $K = 3$.

$Det(I) = Det.[(12, -4, 4); (-4, 12, -4); (4, -4, 12)] = 1280.$

Again, for $Det(I^*)$, we obtain

$Det(I^*) = Det.[(15, -9, 7); (-9, 15, -9); (7, -9, 15)] = 1344$. Therefore, for each $f \geq 3$, there is likely to be an improvement by adopting the second design sequence.

3.5 *Type V:* $D(f+6) = [0\ 1\ 0\ 0_f\ 0\ 1\ 0]$ *Versus* $D^*(f+6) = [0\ 1\ 0\ 1_f\ 0\ 1\ 0]$

First we study the case of $K = 2$.

Det(I) = Det. $[(2(n-2), -4); (-4, 2(n-2)] = 4n(n-4)$. Next, we compute $Det.(I^*) = [(4(f+2), f-10); (f-10, 4(f+2))] = 3n(5f-2)$. This shows that for all $f \geq 2$, second design sequence shows improvement over first design sequence.

Next, we study the case of $K = 3$. It follows that

Det(I) = Det. $[(2(n-2), -4, -4); (-4, 2(n-2), -4); (-4, -4, 2(n-2)] = 8n^2(n-6)$, where $n = f + 6$.

For $Det(I^*)$, we go case by case:

For the case of $f = 1, n = 7$, $Det(I^*) = Det[(12, -9, 5); (-9, 12, -9); (5, -9, 12)] = 294$ which is smaller than $Det(I)$ value of 392. Again, for the case of $f = 2, n = 8$, $Det(I^*) = Det[(16, -8, 0); (-8, 16, -8); (0, -8, 16)] = 2048$

Table 3 Ratio $Det.(I^*)/Det.(I)$ as a function of f

S1. No.	f	$Det.(I^*)/Det.(I)$
1	2	2
2	3	3.17
3	4	3.75
4	5	4.1
5	10	4.8

which doubles the value of $Det(I)$, i.e., 1024.

We tend to believe that such improvements will continue even further whenever $f > 2$.

As to the general case, we find as follows:
Det(I^*)=Det. $[(4(f+2), f-10, 2(f-2)); (f-10, 4(f+2), f-10); (2(f-2), f-10, 4(f+2))] = 12n(f+2)(5f-2) - 2(f+2)(f-10)^2 - 2(f-2)(7f^2+20f-132) = 44f^3 + 472f^2 + 912f - 2016$, upon simplification.

It follows that $Det.(I^*) > Det.(I)$ iff $36f^3 + 376f^2 + 624f - 2016 > 0$. This is obviously true whenever $f > 2$. Computation of the ratio of the two determinants $Det.(I^*)/Det.(I)$ is quite revealing as a function of f.

3.6 *Type VI:* $D(2s+f+4) = [0\ \ 1_s\ \ 0\ \ 0_f\ \ 0\ \ 1_s\ \ 0]$ *Versus* $D^*(2s+f+4) = [0\ \ 1_s\ \ 0\ \ 1_f\ \ 0\ \ 1_s\ \ 0]$

First we study the case of $K = 2$.

$Det.(I) = Det.[(2s(f+4), 2s(f+4) - 2n); (2s(f+4) - 2n, 2s(f+4)] = 2n[2f(2s-1) + 4(3s-2)]$.

Next, we compute

$$Det.(I^*) = Det.[(4(2s+f), 4(2s+f) - 3n); (4(2s+f) - 3n, 4(2s+f))] = 3n(5n-32).$$

This shows that for all $f \geq 2$, second design sequence shows improvement over first design sequence, irrespective of the value of s!

Now we take up the case of $K = 3$.

For the design sequence $D(2s+f+4)$ and the entire vector parameter of dimension 4, we derive the form of the Information Matrix as

$$[(n, 2s, 2s, 2s); (-, 2s, 2(s-1), 2(s-2)I_{s\geq 2}); (-, -, 2s, 2(s-1)I_{s\geq 2}); (-, -, -, 2s)].$$

Particular cases of $s = 1, 2$ are readily derivable. For $s = 1$, $Det.(I) = 8fn^2$ where $n = f + 6$. For $s = 2$, $Det.(I) = 32fn^2$ where $n = (f + 8)$.

For general $s \geq 2$, $Det.(I)$ is to be evaluated as

$$Det.[(2s(f+4), 2s(f+4)-2n, 2s(f+4)-4n); (-, 2s(f+4), 2s(f+4)-2n); (-, -, 2s(f+4)]$$

which simplifies to

$$Det.(I) = 8ns(f+4)[2s(f+4)-n] - 16n[s(f+4)-n]^2 + 8n^2[s(f+4)-2n].$$

This is a cubic function of s. We can simplify it further. Set $Q = s(f+4)$. Then

$$Det.(I) = 8nQ(2Q-n) - 16n(Q-n)^2 + 8n^2(Q-2n) = 32n^2(Q-n) = 32n^2[f(s-1)+2(s-2)],$$

upon simplification.

We now take up the case of $D^*(2s+f+4)$ which results in $Det.(I^*)$. We sort out the particular cases first.

(i) For $s = f = 1, n = 7$, $Det.(I^*) = Det.[(12, -9, 5); (-9, 12, -9); (5, -9, 12)] = 294$ while $Det.(I) = 192$.
(ii) For $s = 1, f = 2, n = 8$, $Det.(I^*) = Det.[(16, -8, 0); (-8, 16, -8); (0, -8, 16)] = 2048$ while $Det.(I) = 1024$
(iii) For $s = 2, f = 1, n = 9$, $Det.(I^*) = Det.[(20, -7, -7); (-7, 20, -7); (-7, -7, 20)] = 4374$ while $Det.(I) = 5132$.
(iv) For $s = f = 2, n = 10$, $Det.(I^*) = Det.[(24, -6, -16); (-6, 24, -6); (-16, -6, 24)] = 4800$ while $Det.(I) = 6400$.

Now we take up the general case. WOLG, we assume $s, f \geq 2$. As before, we first derive an expression for the information matrix of all the four parameters:

$$[(n; 2s+f, 2s+f, 2s+f); (-, 2s+f, 2s+f-3, 2s+f-4);$$

$$(-, -, 2s-f, 2s+f-3); (-, -, -, 2s+f)].$$

From this it follows that

$$I^*(h_1, h_2, h_3) = [(P, P-3n, P-4n); (-, P, P-3n); (-, -, P)]; P = 4(2s+f).$$

We now obtain

$$Det.(I^*) = 3nP(2P-3n)8n(P-3n) + (P-4n).(9n^2 - 2Pn) = 8n^2[7(2s+f) - 36],$$

upon simplification.

In the general case, for $K = 3$, we now refer to $Det.(I)$ and $Det.(I^*)$ and resolve that $Det.(I) < Det.(I^*)$ iff $4f(s-1) + 8(s-2) < 14s + 7f - 36$ which is equivalent to $4fs - 6s - 11f + 20 < 0$. For $s = 2$, this holds true whenever $f \geq 3$. However, for $s > 2$, this is not true for any $f > 1$.

We will take up some more aspects of comparison of design sequences later.

Remark 5 In the above, we have discussed at length various data structures (design sequences) to introduce and explore the concept of "Clear Zero" for improving information on the h-parameters. As we mentioned in the beginning, this is a new topic and we encourage the researchers/readers to take up this study seriously in general terms.

4 More on Orthogonal Design Sequences and Implementation of "Clear Zero"

We start with the design sequence for $N = 32$ observations given by Kao (2015) and listed in Table 2. We display it in the reverse order. Note that we are adopting a circular model so that the two orders are information-equivalent(Table 3).

$$DS(32) = [0(3)\ 1(1)\ 0(2)\ 1(1)\ 0(4)\ 1(3)\ 0(1)\ 1(1)\ 0(1)\ 1(1)\ 0(3)\ 1(5)\ 0(1)\ 1(2)\ 0(1)\ 1(2)].$$

To save space, we have used "frequency count" inside brackets. Thus, 0(3) means $(0, 0, 0)$. It is known that for $2 \leq K \leq 5$, this design sequence is orthogonal. The information matrix for all the six parameters $(\theta, h_1, h_2, \ldots, h_5)$ is given by

$$[(32, 16, 16, 16, 16, 16); (-, 16, 8, 8, 8, 8); (-, -, 16, 8, 8, 8);$$

$$(-, -, -, 16, 8, 8); (-, -, -, -, 16, 8); (-, -, -, -, -, 16)].$$

From this, orthogonality of estimates of h-parameters follows readily. Kao (2015) also developed design sequences for $N = 31$ and $N = 30$ which possess structural balance properties. We confine to $K = 3$ and note the following. First we take up the case of $N = 31$.

$$DS(3, 31) = [0(3)\ 1(1)\ 0(2)\ 1(1)\ 0(4)\ 1(3)\ 0(1)\ 1(1)\ 0(1)\ 1(1)\ 0(3)\ 1(4)\ 0(1)\ 1(2)\ 0(1)\ 1(2)].$$

We readily observe that the 4×4 information matrix is given by

$$[(31, 15, 15, 15); (-, 15, 7, 7); (-, -, 15, 7); (-, -, -, 15)].$$

It transpires that

$$I(h) = (8/31)[31I - J].$$

Next we take up the case of $N = 30$.

$$DS(3, 30) = [0(3)\ 1(1)\ 0(2)\ 1(1)\ 0(3)\ 1(3)\ 0(1)\ 1(1)\ 0(1)\ 1(1)\ 0(3)\ 1(4)\ 0(1)\ 1(2)\ 0(1)\ 1(2)].$$

Here again the 4×4 information matrix is given by

$$[(30, 15, 15, 15); (-, 15, 7, 7); (-, -, 15, 7); (-, -, -, 15)].$$

It transpires that

$$I(h) = (1/2)[16I - J].$$

We will now take up similar study after introducing "clear zero" concept in the above sequences. We recall that introduction of "clear zeros" is meant to replace zeros by ones in suitable positions. This is likely to enhance information on the h-parameters.

Kao (2015) design sequence for $N = 31$ displayed above is changed to an Alternative Design Sequence [ADS] as follows by using "clear zero" concept:

$$ADS(3, 31) = [0(3)\ 1(1)\ 0(2)\ 1(1)\ \mathbf{0}(\mathbf{3})\ 1(3)\ 0(1)\ 1(1)\ 0(1)\ 1(1)\ 0(3)\ \mathbf{1}(\mathbf{5})\ 0(1)\ 1(2)\ 0(1)\ 1(2)].$$

This time, the 4×4 information matrix is given by

$$[(31, 16, 16, 16); (-, 16, 8, 8); (-, -, 16, 8); (-, -, -, 16)].$$

It turns out that the 3×3 information matrix of the h-parameters is identical to that derived above.

Next, we take up the case of $N = 30$ and derive the form of ADS by using "clear zero" concept.

$$ADS(3, 30) = [0(3)\ 1(1)\ 0(2)\ 1(1)\ \mathbf{0}(\mathbf{2})\ 1(3)\ 0(1)\ 1(1)\ 0(1)\ 1(1)\ 0(3)\ \mathbf{1}(\mathbf{5})\ 0(1)\ 1(2)\ 0(1)\ 1(2)].$$

This time, the 4×4 information matrix is given by

$$[(30, 16, 16, 16); (-, 16, 8, 8); (-, -, 16, 8); (-, -, -, 16)].$$

It turns out that the 3×3 information matrix of the h-parameters is equal to $(8/15)[15I - J)$ and this is less than $(1/2)[16I - J]$ in the sense of nnd matrices.

We will continue with this topic further with some more examples.

5 On the Relative Status of Comparable Design Sequences

We start with a general n and $K < n$. Consider the following design sequences:

$$DS_1(K, n) = [1; 0, 0, \ldots, 0, 0];\ DS_2(K, n) = [1, 1; 0, 0, \ldots, , 0, 0];$$

$$DS_t(K, n) = [1, 1, \ldots, 1; 0, 0, \ldots, 0, 0];\ 1 \leq t \leq K.$$

Note that $DS_K(K, n)) = [1, 1, \ldots, 1; 0, 0, \ldots, 0, 0]$ has an active phase of length K for every choice of the pair $(n, K, K < n)$. Henceforth, we will deal with these K

design sequences only. Our aim is to provide estimates of the h-parameters, following each design sequence.

For a typical $1 \leq t \leq K$, model expectations of the observations underlying $DS_t(K, n)$ are given by

$$\theta + h_1; \theta + h_1 + h_2; \ldots, \theta + h_1 + h_2 + \cdots + h_t;$$

$$\theta + h_2 + h_3 + \cdots + h_{t+1}; \ldots, \theta + h_{K-t+1} + \cdots + h_K;$$

$$\theta + h_{K-t+2} + \cdots + h_K; \ldots, \theta + h_K; \theta; \theta; \ldots.$$

Specializing to $t = 1$,

$$\hat{h}_i = y_i - \hat{\theta}; i = 1, 2, \ldots, K; \hat{\theta} = \sum_{i=K+1}^{i=n} y_i/(n-K)$$

whence

$$V(\hat{h}_i) = 1 + (n-K)^{(-1)}, Cov(\hat{h}_i, \hat{h}_j) = (n-K)^{(-1)}.$$

On the other hand, for the other extreme case of $t = K$, we observe that for each h-parameter, there are two estimates available. These are given by

$$h_1 : y_1 - \hat{\theta}, y_K - y_{K+1}; h_2 : y_2 - y_1, y_{K+1} - y_{K+2}; \ldots;$$

$$h_{K-1} : y_{K-1} - y_{K-2}, y_{2K-2} - y_{2K-1}; h_K : y_K - y_{K-1}, y_{2K-1} - \hat{\theta}.$$

In the above, $\hat{\theta}$ is based on $n - 2K + 1$ observations—independent of the others. Note that pairs of estimates of each of the h-parameters are mutually uncorrelated. Hence, easily we can provide combined estimates and compute their variances.

In the general case, from the first set of t observations, we can estimate $h_1, h_2, \ldots, h_t$ [using $\hat{\theta}$ based on $n - K - t + 1$ observations at the end]. Likewise, estimates of $h_2, h_3, \ldots, h_{K-1}, h_K$ are derived from the observations $y_{t+1}, y_{t+2}, \ldots, y_{K+t-1}$. Estimates of each h-parameter are pairwise uncorrelated. So the two can be appropriately combined.

Remark 6 So long we have presented results related to the vector η of h-parameters. The determinantal value of the information matrix is known to serve as the reciprocal of the generalized variance. We have also undertaken a comparison of the design sequences w.r.t. the average variance for estimated η and derived parametric functions $\phi(1) = h_1, \phi(2) = h_1 + h_2, \phi(3) = h_1 + h_2 + h_3$. We skip the details.

6 Further Comparisons of Design Sequences: Case of $K = 3$

We consider a few more design sequences, still with $K = 3$.

$$DS_1(8) : [1, 0, 1, 0, 0, 1, 0, 1];\ DS_2(8) : [1, 1, 0, 0, 0, 0, 1, 1];$$

$$DS_3(8) : [1, 1, 1, 0, 0, 1, 1, 1];\ DS_4(8) : [1, 1, 1, 1, 0, 0, 0, 0].$$

Again "Clear 0" concept is applied to $DS(2)$ and $DS(4)$ to derive one from each as are shown below:

$$DS_2^*(8) : [1, 1, 0, 0, 1, 0, 1, 1];\ DS_4^*(8) : [1, 1, 1, 1, 0, 0, 1, 0].$$

Below we display information matrices for the h-parameters, assuming $K = 3$.

$$I(1) : [16, -8, 0); (-8, 16, -8); (0, -8, 16)];\ Det(I) = 2^{11}.$$

$$I(2) : [(16, 8, 0); (8, 16, 8); (0, 8, 16)];\ Det(I) = 2^{11}.$$

$$I(^*(2)) : [(15, -1, -1); (-1, 15, -1), (-1, -1, 15)];\ Det(I) = 2^8 \times 13.$$

$$I(3) : [(12, 4, -4); (4, 12, 4), (-4, 4, 12)];\ Det(I) = 2^{10}.$$

$$I(4) = I(DS(2)).$$

$$I(^*(4)) : [(15, -1, -4), (-1, 15, 4), (-4, 4, 16)];\ Det(I) = 3136 = 2^6 \times 49.$$

Observations

1. $DS_2^*(8)$ performs better than $DS_2(8)$! Also $DS_4^*(8)$ performs better than $DS_4(8)$! Moreover, $DS_2^*(8)$ fares better than $DS_4^*(8)$.

2. The above comparison may not be "fair" since the design sequences are based on unequal number of 1s. Note that every sequence comprises 1s and 0s and the understanding is that a 0-phase corresponds to "idle" phase while a 1-phase is "active". So the number of active phases should also be considered while examining relative performances. We may apply the usual concept of "Efficiency" and work out "Efficiency per active phase". For a single parameter, efficiency is directly related to and measured by [Fisher] Information. For $K = 3$ h-parameters, we can compute the determinant of the 3×3 information matrix and divide it by the cube of the number of active phases, for the criterion of maximization. If we go by comparison w.r.t. the average variance, the criterion is to minimize average variance multiplied by the number of active phases.

Below we take up a comparison of the above four design sequences—each of length n = 8.

We have already computed $Det.(I)$ for$K = 3$ [excluding the common divisor]. We again show them below for comparison purpose.

$$DS_1(8) : 2^{11}; DS_2(8) : 2^{11}; DS_3(8) : 2^{10}; DS_4(8) : 2^{11}.$$

Next, we divide each determinantal value by cube of the number of 1's in each design sequence. This amounts to comparison of

$$2^{11}/4^3, 2^{11}/4^3, 2^{10}/6^3, 2^{11}/4^3$$

in terms of maximization.

It transpires that, except $DS_3(8)$, all others are equivalent in terms of "per active phase" criterion.

Note that in the above, we have also introduced $DS_2^*(8)$ and $DS_4^*(8)$ as "action-taken" in the presence of "Clear Zero". Moreover, these have been compared with others—though without regard to the number of 1's, i.e., active phases in the DS. We revert back to the computations with the required modifications. We only take up $DS_2(8)$, $DS_2^*(8)$, and $DS_4^*(8)$ below. This amounts to comparison of

$$2^{11}/4^3, 2^8 \times 13/5^3, 2^6 \times 49/5^3$$

in terms of maximization. It follows that $DS_2(8)$ is the best of the lot.

7 Further Comparisons of Design Sequences: Focus on "Clear Zero" Feature

Consider the design sequence

$$DS(r, K; n) : [(1, 1, \ldots, 1)(freq.\, r)\ followed\ by\ (0, 0, \mathbf{0}, \ldots, 0(freq.\, n - r))]$$

Under the assumption that $(n - r) \geq (K - 1)$, the Information Matrix for the h-parameters for the case of $K = 3$ is given by

$$[(A, A - n, A - 2n); (A - n, A, A - n); (A - 2n, A - n, A)]\ where\ A = r(n - r).$$

Further, it is seen that [ignoring the common multiplier] $Det(I) = 4n^2[r(n - r) - n]$.

In the above, we have indicated the position of "Clear Zero" by **0**. We now replace this 0 by 1 and call the sequence D^*. For simplicity, we take $n \geq (r + 5)$.

For D^*, the Information Matrix changes to

$$[(B, B-2n, B-3n), (B-2n, B, B-2n), (B-3n, B-2n, B)] \; where \; B = (r+1)(n-r-1).$$

This time the determinant is given by $Det(I^*) = 3n^2(5B - 8n)$.

We now take up

$Case\ (i)\ : n = 2(r+1)$.

In that case, $B = n^2/4$ and $Det(I^*) = 3n^2(5n^2/4 - 8n) = 3n^3(5n - 32)/4$.

Recall the assumption $n - r \geq 5$. This means $r + 2 \geq 5$, i.e., $r \geq 3$. Hence, $n \geq 8$ so that $Det(I^*) > 0$.

Comparison of $Det(I)$ and $Det(I^*)$ is made below.

$$Det(I) = 4n^2[r(n-r) - n] = 4n^2[r(r+2) - 2(r+1)] = 4n^2(r^2 - 2).$$

$$Det(I^*) > Det(I) <=> 3n^3(5n - 32)/4 > 4n^2(r^2 - 2)$$

$$<=> 15n^2 - 96n > 4(n^2 - 4n - 4) <=> 11n^2 - 80n + 16 > 0,$$

which is true since $n \geq 8$.

$Case\ (ii)\ : n = 2r + 1$

Here, $Det(I)$ and $Det(I^*)$ come out as

$$Det(I) = n^2[(n-2)^2 - 5]; \; Det(I^*) = 3n^2[5n^2 - 32n - 5]/4.$$

Hence $Det(I^*)$ improves over $Det(I)$ iff, after simplification, we have $11n^2 - 80n - 11 > 0$ which is true for all $n \geq 8$.

This indicates that "Clear Zero" concept has an edge over the original sequence w.r.t. generalized variance criterion. Similarly, we can take up the study involving average variance.

Remark 7 It is desirable to "extend" this result and accommodate more "Clear Zeros" in the sequence. We will take up one more adjacent zero and consider the changed design sequence

$$DS^{**}(r, K, n) : [(1, 1, \ldots, 1)(freq.\, r) \; followed \; by \; (0, 0, 1, 1, 0, 0, \ldots, 0(freq.\, n - r))].$$

We assume $n - r \geq K$ and $K = 3$. The Information Matrix I^{**} for the h-parameters is given by

$$[(C, C-2n, C-4n); (C-2n, C, C-2n); (C-4n, C-2n, C)] \, where \, C = (r+2)(n-r-2).$$

Ignoring common multiplier,

$$Det(I^{**}) = 16n^2[(r+2)(n-r-2) - 2n].$$

Note that the choice of (n, r) should ensure that $Det.(I^{**})$ is positive. As before, we now consider two cases.
Case (i): n = 2(r + 1)

In this case,

$$Det(I^{**}) > Det(I) <=> 3r(n-r) - 16(r+1) + n <=> 3n^2 - 28n - 12 > 0,$$

which holds for $n \geq 10$.

A comparison between Det(I^{**}) and $Det(I^{*})$ shows that DS^{**} fares better than DS^{*} iff $n \geq 34$.
Case (ii): n = 2r + 1

In this case, we deduce

$$Det(I^{**}) > Det(I) <=> 3n^2 - 28n - 35 > 0,$$

which holds for $n \geq 11$.

Here again it is found that DS^{**} fares better than DS^{*} only when $n > 35$.

8 Comparisons of Symmetrized Design Sequences: More on "Clear Zero" Feature

In this section, we generalize the results of Sect. 7 for fairly general design sequences with symmetrized structures.

At first we note that the design sequences $[DS_1(8) - DS_4(8)]$ introduced in Sect. 7 are "symmetric" in nature. Each DS has length $n = 8$ and it exchanges the positions of 0s and 1s exactly from one half to the other half—preserving a symmetric structure from the middle on both sides. We will generalize this in a general form.

$$DS(r, K, n) < 1\,1\ \ldots r\ times;\ 0\,0\ \ldots (n-r)\ times;\ 0\,0\ \ldots (n-r)\ times;\ 1\,1 \ldots r\ times >$$

Assume $K = 3$. Further, assume $r \geq 2;\ n - r \geq 3$. It follows that

$$I(h) = [(A, A-2n; A-4n), (A-2n, A, A-2n); (A-4n, A-2n, A)],\ A = 4r(n-r).$$

Hence, $Det(I) = 32n^2[2r(n-r) - n]$.

We now define a "symmetrized version" of $DS(r, K, n)$ as $DS(t, r, K, n)$ where t is a new design parameter used as follows.

$$DS(t, r, K, n) < 1\,1\ \ldots r\ times;\ 0\,0\ \ldots t\ times;\ 1\,1\ \ldots (n-r-t)\ times;\ do\ symmetrization >$$

We study this $DS(t, r, K, n) = DS^{*}$ now. Assume $r \geq 2,\ t \geq 2,\ n - r - t \geq 2$ while $K = 3$.

Set $A = 4t(n-t)$.
Then

$$I^*(h) = [(A, A-4n, A-8n); (A-4n, A, A-4n); (A-8n, A-4n, A)].$$

It follows that $Det(I^*) = 256n^2[t(n-t)-n]$. We can now go for a comparison between $DS(r, K, n)$ and $DS^*(t, r, K, n)$.
$Case I : n = 2r$

$$Det.I = 256r^3(r-1);\ Det.I^* = 256n^2[t(n-t)-n].$$

Note that $n - r = r$ and this $n - r$ splits into t and $n - r - t$. Set $t = pr, 0 < p < 1$. Then

$$Det.I^*/Det.I = n^2[t(n-t)-n]/r^3(r-1) = [4pr^4(2-p) - 8r^3]/r^3(r-1).$$

This ratio is greater than 1 iff

$$[4pr(2-p) - 8] > (r-1) <=> r[4p(2-p) - 1] > 7.$$

For any given p, we can find a lower bound for r.
For example, $p = 1/4 => r \geq 10$; $p = 1/2 => r \geq 4$; $p = 3/4 => r \geq 3$.
Of course, pr must be an integer.
On the other hand, for any given r, we may choose a value of p so that pr is an integer, subject to satisfying the superiority condition which simplifies to

$$0 < p < 1 - \sqrt{[(3 - 7/r)]}/2.$$

For $r = 3, upper\ bound = 1 - 0.2357 => t = 2$; $r = 4, upper\ bound = 1 - 0.5590 => t = 2$; $r = 5, upper\ bound = 1 - 0.6324 => t = 2$. Therefore, we can make a choice of (r, t) with a pay-off, following "Clear Zero" policy.
Lastly, we can take up the comparison, incorporating "per active phase-adjusted" criteria. Recall the structures of $DS(n, r)$ and $DS^*(n, r, t)$. Consider the case: $n = 2r$.
We need to compare $Det(I)/(2r)^3$ and $Det(I^*)/[2(n-t)]^3$.

$$(1)\ Det.(I) = 256r^3(r-1);\ (2)\ Det.(I^*) = 256n^2[t(n-t)-n].$$

Note that $n - r = r$ and this $n - r$ splits into t and $n - r - t$. Set $t = pr, 0 < p < 1$. Then

$$Det(I)/(2r)^3 < Det(I^*)/[2(n-t)]^3 <=> (n-t)^3 Det(I) < r^3 Det(I^*).....(1)$$

Using the expressions for $Det(I)$ and $Det(I^*)$,

$$(1) <=> 256 \times (n-t)^3 \times r^3(r-1) < r^3 \times 256 \times n^2 \times [t(n-t) - n]$$

$$<=> (n-t)^3(r-1) < 4r^3[p(2-p)r - 2] <=> (2-p)^3(r-1) < 4[rp(2-p) - 2]$$

$$<=> r(2-p)(8p - 4 - p^2) > [8 - (2-p)^3].$$

This requires $8p > 4 + p^2 <=> p > 4 - 2\sqrt{(3)} = 0.5359$. Particular cases:

$$(i)\ p = 0.6 => r \geq 9, (ii)\ p = 0.7 => r \geq 4, (iii)\ p = 0.8 => r \geq 3.$$

$Case2 : n = 2r + 1$
The condition $Det(I^*)/Det(I) > 1$ turns out to be

$$8r^2.p^2 - 8(r+1)(2r+1)p + C < 0; t = rp,$$

where $C = 2r^2 + 16r + 7$. Particular cases:

$$r = 3 => p \geq 0.58; r = 4 => p \geq 0.446.$$

9 Concluding Remarks

Regarding potential applications of linear models in the analysis of design sequences for fMRI studies, we have explained the model in its simplest form—as is suggested in the literature. Having done this, we have discussed about estimability issues. Then the emphasis has been on relative comparison of design sequences. Inference questions center around what are called h-parameters. In the process, we have introduced what is termed as the concept of "Clear Zero". Efficiency comparisons are also made taking due regard to "per active phase" basis. Our objective has been to familiarize the readers to this fascinating area of research in the general framework of linear models and having similarity with spring balance weighing designs [with bias]. There is enough scope for generalizations and extensions in several directions.

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A Review of Rigorous Randomized Response Methods for Protecting Respondent's Privacy and Data Confidentiality

Tapan K. Nayak

Abstract Randomized response (RR) methods for protecting respondent's privacy when collecting data on sensitive characteristics have been proposed and discussed for over fifty years. The basic ideas of RR have also been used to develop the post-randomization method (PRAM) for protecting data confidentiality. Both RR and PRAM randomize true responses using specified probabilities and the choice of those probabilities is central to designing RR methods and PRAM. However, most papers do not give clear guidance on how to choose the transition probabilities. Some rigorous approaches have appeared only recently. This paper reviews the essential elements of RR and PRAM, some important differences between the two, and designing RR methods and PRAM for achieving certain precise privacy and confidentiality protection goals. In particular, we discuss (i) designing an RR survey to guarantee that a randomized response would not reveal much information about the respondent, in a precise sense, and (ii) devising PRAM to strictly control identification risks when releasing microdata.

Keywords Data utility · Identity disclosure · Minimaxity · Post-randomization · Privacy criteria · Transition probability

1 Introduction

The primary objective of randomized response (RR) methods is to protect respondent's privacy and thereby reduce false responses when collecting data on sensitive or stigmatizing characteristics, such as tax evasion, drug use, gambling, and abortion.

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The first RR method, introduced by Warner (1965), concerns interview surveys of a binary characteristic, where the population consists of a sensitive group A (e.g., drug users) and its complement A^c (e.g., not drug users). In Warner's method, a respondent answers one of the two questions: Q_1: Do you belong to A? and Q_2: Do you belong to A^c? Each respondent selects a question by performing a specified random experiment, unobserved by the interviewer, with a given device, e.g., a spinner or a shuffled deck of cards bearing the two questions. The respondent answers the selected question. Thus, the interviewer does not know the question that a respondent answers. The experiment imposes specific and known probabilities, say p and $1 - p$, of selecting Q_1 and Q_2. The value of p determines both the degree of privacy protection and the amount of statistical information loss due to randomization. Thus, to design Warner's method, one should first select p and then construct an experiment for implementing it.

Following the pioneering work of Warner (1965), numerous other RR methods with different mechanisms for randomizing the true responses have been proposed for both categorical and quantitative variables. We refer interested readers to the books Chaudhuri and Mukerjee (1988), Chaudhuri (2010) and Chaudhuri et al. (2016) for discussion of various methods and further references. In this article, we consider RR methods only for categorical variables. An RR method transforms the true responses probabilistically. For a true response, the RR output is generated from a predetermined probability distribution on an output space. In Sect. 2, we briefly review a general framework and some key theoretical results that are needed for later sections. RR methods for quantitative variables are structurally quite different and can generally be viewed as (additive or multiplicative) random noise infusion to the true values.

For many years, research on RR methods was done primarily by statisticians and for use in face-to-face interview surveys, which requires experiments that are easy to understand and perform correctly and randomization devices that are simple and portable. Various randomization devices and mechanisms have been proposed as different RR methods. Recently, Blair et al. (2015) stated that "our extensive search yields only a handful of published studies that use the randomized response method to answer substantive questions." Evidently, the theoretical advances in RR methods have not been used much in real surveys. Perhaps, one reason for that gap is the increasing adoption of mail, telephone and online surveys, replacing interview surveys, in the past several decades. Notably, Holbrook and Krosnick (2010) tested RR methods in one telephone and eight Internet surveys of American adults and found that respondents were either unable or unwilling to implement the RR mechanisms properly.

Interestingly, starting around the beginning of this century, interest in RR methods has grown tremendously among computer scientists and in new dimensions. The explosive growth of automated data capture by companies from business transactions, online searches, postings and other activities have raised much public awareness and concerns about privacy. Computer scientists have taken substantial interest in developing theory and methods for privacy-preserving data mining and data publishing; see, e.g., Aggarwal and Yu (2008), Chen et al. (2009) and Fung et al. (2019).

New privacy concepts and measures have been developed and RR methods have been implemented by leading companies such as Google, Apple and Microsoft; see Erlingsson et al. (2014), Ding et al. (2017) and Cormode et al. (2018). Perhaps, one impetus for this resurgence and expansion of interest in RR techniques is that in online data capturing, the actual randomization can be carried out easily and accurately by computer programs. Consequently, recent research on RR theory and methods has focused appropriately on the choice of the randomization probabilities, leaving aside ancillary features of possible physical mechanisms for implementing them.

Gouweleeuw et al. (1998) used the basic ideas of RR to introduce the post-randomization method (PRAM) for perturbing categorical data to protect data confidentiality. It also randomizes the true responses, similar to RR. But, the data agency performs randomization after data collection and so, the randomization probabilities may be chosen based on the data set. We discuss some important differences between RR and PRAM in Sect. 2. For both methods, the choice of the transition probabilities is critical. Intuitively, one should try to choose those to minimize data utility (or statistical information) loss while meeting privacy and confidentiality protection goals. Some precise and practical privacy and confidentiality protection goals have been proposed and investigated only recently. One primary objective of this article is to review some rigorous approaches to privacy and confidentiality protection via RR and PRAM. We also attempt to cover some important works that appeared in computer science literature.

In Sect. 2, we describe the essential elements of RR and PRAM and some basic mathematical results. We do not aim to give a comprehensive review of RR and PRAM, but attempt to highlight some important points that we think have not been appreciated well. In Sect. 3, we discuss a rigorous notion of privacy protection. The basic idea is that an RR procedure should guarantee that an output would not reveal much new information about the respondent's true value. A formal development of this idea compares prior and posterior probabilities. This criterion is closely connected to *local differential privacy*, which has received considerable attention in recent years. We also discuss a necessary and sufficient condition that an RR method must satisfy in order to guarantee such privacy. In Sect. 4, we discuss optimal RR methods for providing specified privacy. In particular, we describe an admissibility result under a very general view of data utility, and optimal methods under certain criteria. Section 5 relates to data confidentiality protection. Specifically, we consider identity disclosure control in microdata release and review a procedure that uses PRAM to guarantee an upper bound for the probability of correctly identifying any unit in perturbed microdata. Section 6 is devoted some concluding remarks.

2 Basic Elements of RR and PRAM

In this section, we describe the mathematical structures of RR and PRAM. Applying RR to multiple variables is equivalent to applying it to the cross-classification of those variables. Let X denote a categorical variable or cross-classification of several

variables that we want to subject to RR. Let $\mathcal{S}_X = \{c_1, \ldots, c_k\}$ denote the set of possible categories of X. Let $\pi_i = P(X = c_i), i = 1, \ldots, k$, and $\pi = (\pi_1, \ldots, \pi_k)'$, which is unknown. The goal of an RR survey is to obtain information about π while protecting respondent's privacy. The basic idea of RR is to collect a stochastic transformation of each respondent's true category. Let Z denote the output variable with output space $\mathcal{S}_Z = \{d_1, \ldots, d_m\}$. A special case is $\mathcal{S}_Z = \mathcal{S}_X$. In general, $\mathcal{S}_Z$ may be different from $\mathcal{S}_X$, with possibly $m \neq k$. For each input, the output is selected according to some probabilities specified by the RR method. Let $p_{ij} = P(Z = d_i | X = c_j), i = 1, \ldots, m, j = 1, \ldots, k$, denote the transition probabilities of an RR method. Obviously, $\sum_i p_{ij} = 1$ for $j = 1, \ldots, k$. The transition probability matrix (TPM), $P = ((p_{ij}))$, is chosen during the planning of an RR method.

For any given P, one can devise multiple physical experiments to implement it (see Nayak et al. 2016). Under the common assumption of truthful respondent participation, all statistical properties of an RR method depend solely on its TPM. The choice of the experiment for implementing a given P does not affect the mathematical properties of the method. Thus, formal assessments and comparisons of RR methods should be made via their TPMs, ignoring the randomization experiments. However, as Leysieffer and Warner (1976), Fligner et al. (1977), Nayak (1994) and others have noted, when comparing different RR methods some papers have incorrectly matched disparate features of the experiments and drawn false conclusions. We consider P as the *design* of an RR method and discuss the planning and analysis of an RR method in terms of P.

A common assumption for analyzing RR data is multinomial sampling, i.e., random sampling from an infinite population or simple random sampling with replacement if the population is finite. Let $\lambda_i = P(Z = d_i), i = 1, \ldots, m$, and $\lambda = (\lambda_1, \ldots \lambda_m)'$. Also, let S_i denote the frequency of $Z = d_i$ and $\mathbf{S} = (S_1, \ldots, S_k)'$. Then, $\mathbf{S}$ is multinomially distributed, $\mathbf{S} \sim Mult(n, \lambda)$, where

$$\lambda = P\pi \tag{1}$$

and n is the sample size. We can use $\mathbf{S}$ to make inferences about λ. If $m = k$ and P is nonsingular, from an estimator of λ one can obtain an estimator of π via (1). In particular, $\hat{\lambda} = \mathbf{S}/n$, which is the MLE (and UMVUE) of λ, yields $\hat{\pi} = P^{-1}\hat{\lambda} = P^{-1}(\mathbf{S}/n)$. It can be seen that $\hat{\pi}$ is an unbiased estimator of π and

$$Var(\hat{\pi}) = \frac{1}{n}(D_\pi - \pi\pi') + \frac{1}{n}[P^{-1}D_\lambda(P^{-1})' - D_\pi], \tag{2}$$

where D_π is a diagonal matrix with diagonal elements $\pi_1, \ldots, \pi_k$ and D_λ is defined similarly (see Chaudhuri and Mukerjee 1988, p. 43). The first term on the right side of (2) is the sampling variance and the last term is the additional variance due to randomization.

If $m < k$ or $\text{rank}(P) < k$, then the model for $\mathbf{S}$ is not identifiable with respect to π and hence π is not estimable from RR data. Thus, for estimability of π, one

should only consider $m \geq k$ and $\text{rank}(P) = k$. While $m = k$ is quite common, several methods with $m > k$ have also been proposed, e.g., Leysieffer and Warner (1976), Kuk (1990) and Christofides (2003). Also, we shall see in Sect. 4.2 that $m > k$ in some optimal designs. We should mention that while most authors discussed estimation of π under multinomial sampling, Padmawar and Vijayan (2000), Chaudhuri (2001, 2004) and Nayak and Adeshiyan (2009) derived estimators of π under general sampling designs.

Now we turn our attention to PRAM. Like RR, it randomizes the true responses with known probabilities. However, that is done after data collection and by data agencies. These two practical matters yield some important differences between RR and PRAM. Here, we state some special and helpful features of PRAM, which we believe have not been well recognized. First, in PRAM, the transition probabilities may be chosen based on the entire data set, containing all true responses (which is not possible in RR surveys as the responses are randomized during data collection). Indeed, unbiased PRAM, discussed below, requires the TPM to depend on the data. When the TPM is data dependent, it is a random matrix and mathematical results in RR for fixed P, e.g., (2), may not hold true. Second, randomization may be applied selectively only to the responses with high disclosure risks. Note that agencies remove all direct identifiers, such as name and address, before releasing data. So, a respondent's values (true or randomized) are not revealed directly. In contrast, in RR surveys, a respondent's identity is known to the data collector. Third, related to the previous point, one may partition the data into homogeneous sets and then apply PRAM separately within the partition sets with possibly different TPMs. One method that utilizes data partitioning and unbiased PRAM is described in Sect. 5. Fourth, the randomization is carried out by a computer program, without needing a physical experiment. Fifth, in PRAM $\mathcal{S}_Z = \mathcal{S}_X$ and thus $m = k$ and the original and perturbed data appear in the same format. Sixth, the transition probabilities may not be known publicly. In particular, the transition probabilities cannot be published conveniently or helpfully when those are chosen diversely using the observed data, as in Sect. 5. There, the data agency should use a carefully designed unbiased PRAM to well preserve data utility, so that the released data may practically be treated as original data for making inferences.

Next, to describe *unbiased* PRAM, let T_i and S_i denote the frequency of c_i in the original and perturbed data, respectively, and let $\mathbf{T} = (T_1, \ldots, T_k)'$ and $\mathbf{S} = (S_1, \ldots, S_k)'$. When the data are collected by multinomial sampling, a PRAM with TPM P is said to be unbiased (Gouweleeuw et al. 1998 called this invariant) if

$$P\mathbf{T} = \mathbf{T}. \tag{3}$$

It can be easily verified that the solution space of (3) is a convex set and a trivial solution is $P = I$. Gouweleeuw et al. (1998) gave two methods for finding nontrivial solutions.

Unbiased PRAM was motivated by the fact that (3) implies $E[\mathbf{S}|\mathbf{T}] = P\mathbf{T}$ and hence $\hat{\pi}_* = \mathbf{S}/n$ is an unbiased estimator of π. Also, $\hat{\pi}_*$ is always a probability vector and it can be calculated without using P or its inverse. Thus, π can be estimated easily

from perturbed data. Nayak et al. (2016) derived and explored the exact variance of $\hat{\pi}_*$. In particular, they gave a decomposition of the variance into sampling variance and added variance due to PRAM, similar to (2). They also discussed estimation of π under a general sampling plan and unbiased PRAM. There, P is called unbiased if $P\hat{\pi} = \hat{\pi}$, where $\hat{\pi}$ is an appropriately weighted (and usually unbiased) estimator of π based on the original data.

We refer interested readers to Gouweleeuw et al. (1998), Willenborg and De Waal (2001), Van den Hout and Van der Heijden (2002), Van den Hout and Elamir (2006) and Shlomo and Skinner (2010) for additional discussion and applications of PRAM. The main task of designing RR and PRAM is choosing the transition probabilities. Naturally, suitable choices should depend on privacy and confidentiality protection goals. In the following sections, we discuss some recently developed precise privacy and confidentiality protection goals and methods for achieving those goals.

3 Privacy Protection by RR

Most privacy measures in statistics literature were developed for the situation where the survey variable is binary with one sensitive category and the response is also binary, see, e.g., Leysieffer and Warner (1976), Lanke (1976), Fligner et al. (1977), Nayak (1994), and Zhimin and Zaizai (2012). Using common terminology, let A and A^c denote the two categories of X, of which A is sensitive, and let Y (for yes) and N (for no) denote the two response categories. The privacy measures in the binary case are mostly functions of the two posterior probabilities $P(A|Y)$ and $P(A|N)$, where the prior probabilities of A and A^c are their population proportions, say π_A and $1 - \pi_A$. For example, Lanke (1976) measure of the degree of privacy protection is $\max\{P(A|Y), P(A|N)\}$. This and most other measures for the binary case depend also on π_A, which is unknown. A common suggestion is choose the RR design parameters $P(Y|A)$ and $P(Y|A^c)$ such that a chosen privacy measure does not exceed a threshold at some π_A. Here, the designer of the survey selects the privacy measure, the threshold and π_A. For many privacy measures, this is equivalent to requiring

$$\max\left\{\frac{P(Y|A)}{P(Y|A^c)}, \frac{P(Y|A^c)}{P(Y|A)}\right\} \leq \gamma, \tag{4}$$

where γ is determined by the privacy measure, privacy threshold and π_A.

3.1 Strict Privacy Criteria

The preceding approaches do not consider an intruder's personal knowledge about respondents. The following approach, recently initiated by computer scientists, focuses on the basic goal of privacy protection, which is limiting the amount of information an intruder might gain about a respondent from his/her randomized response.

Informally, the main idea, due to Evfimievski et al. (2003), is that we should view a privacy breach as an intruder gaining much new information about a respondent and an RR design should guarantee that no such privacy breaches would occur. Furthermore, an intruder's information (or opinion) should be expressed precisely using subjective probability.

Formally, let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k)$ denote an intruder's (subjective) prior distribution for a respondent's true value of X, and for any $Q \subseteq \mathcal{S}_X$, let $P_\alpha(Q)$ and $P_\alpha(Q|d_i)$ denote, respectively, the intruder's prior and posterior probabilities of $\{X \in Q\}$, given $Z = d_i$. Here, Q represents a "property" of the respondent. Clearly,

$$P_\alpha(Q) = \sum_{j:c_j \in Q} \alpha_j \quad \text{and} \quad P_\alpha(Q|d_i) = \sum_{j:c_j \in Q} P_\alpha(X = c_j | Z = d_i),$$

where

$$P_\alpha(X = c_j | Z = d_i) = \frac{P_\alpha(X = c_j, Z = d_i)}{P_\alpha(Z = d_i)} = \frac{\alpha_j p_{ij}}{\sum_{l=1}^{k} \alpha_l p_{il}}.$$

One idea is that to protect respondent's privacy, we should guarantee that $P_\alpha(Q|d_i)$ would never be much higher or lower than $P_\alpha(Q)$, i.e., $P_\alpha(Q|d_i)$ would always be "close" to $P_\alpha(Q)$. This idea yields different privacy criteria for different specifications of desired closeness between prior and posterior probabilities.

Evfimievski et al. (2003) used a specific "closeness" criterion and introduced ρ_1-to-ρ_2 privacy as follows.

Definition 1 Let $0 < \rho_1 < \rho_2 < 1$ be two numbers. (a) An RR procedure is said to permit an upward ρ_1-to-ρ_2 privacy breach with respect to $Q \subseteq \mathcal{S}_X$ and a prior distribution α if

$$P_\alpha(Q) < \rho_1 \quad \text{and} \quad P_\alpha(Q|d_i) > \rho_2$$

for some $1 \leq i \leq m$ with $P_\alpha(Z = d_i) > 0$. Similarly, a procedure permits a downward ρ_2-to-ρ_1 privacy breach with respect to Q and α if $P_\alpha(Q) > \rho_2$ and $P_\alpha(Q|d_i) < \rho_1$ for some d_i with $P_\alpha(Z = d_i) > 0$.

(b) An RR procedure provides ρ_1-to-ρ_2 privacy protection if it does not permit an upward ρ_1-to-ρ_2 or a downward ρ_2-to-ρ_1 privacy breach with respect to any Q and α.

Using the ratio of posterior to prior probabilities as a measure of closeness between the two, Nayak et al. (2015) defined the following.

Definition 2 For a given $\beta > 1$, an RR procedure admits a β-factor privacy breach, with respect to $Q \subseteq \mathcal{S}_X$ and a prior α if $P_\alpha(Q) > 0$ and

$$\frac{P_\alpha(Q|d_i)}{P_\alpha(Q)} > \beta \quad \text{or} \quad \frac{P_\alpha(Q|d_i)}{P_\alpha(Q)} < \frac{1}{\beta}$$

for some d_i such that $P_\alpha(Z = d_i) > 0$. An RR procedure provides β-factor privacy if it does not allow a β-factor breach with respect to any Q and α.

Chai and Nayak (2018) developed and explored the preceding ideas generally and we review their main results below. A general criterion for considering two probabilities as sufficiently "close" gives (explicitly or implicitly) for each $0 < p < 1$, an interval $[l_p, u_p]$ that consists of all values that are considered sufficiently close to p (taking a closed interval for simplicity). So, if a prior probability is p, a privacy breach occurs if and only if a corresponding posterior probability falls outside the interval $[l_p, u_p]$. This yields two functions $h_l(p) \equiv l_p$ and $h_u(p) \equiv u_p$, which specify the lower and upper breach boundaries. Thus, a general criterion may be viewed as a pair of given functions $h_l(p)$ and $h_u(p)$. Considering this, Chai and Nayak (2018) introduced the following.

Definition 3 Let h_l and h_u be two functions from $[0, 1]$ to $[0, 1]$ such that $0 \leq h_l(a) \leq a \leq h_u(a) \leq 1$ for all $0 \leq a \leq 1$. An RR procedure is said to satisfy privacy with respect to h_l and h_u if

$$h_l(P_\alpha(Q)) \leq P_\alpha(Q|d_i) \leq h_u(P_\alpha(Q)) \tag{5}$$

for all α, $Q \subseteq \mathcal{S}_X$ and $i = 1, \ldots, m$.

This definition says that a posterior probability p_* is sufficiently close to the corresponding prior p if $h_l(p) \leq p_* \leq h_u(p)$. Geometrically, a (prior, posterior) pair (p, p_*) is a point in the unit square, of which the regions below h_l and above h_u constitute the privacy breach region (PBR) of the criterion in Definition 3. A privacy satisfying RR method must not yield any prior-posterior pair that falls in the PBR. Conversely, the PBR of an RR procedure P is the collection of all non-attainable (prior, posterior) pairs under P. The privacy holding region of P or the complement of the PBR (with respect to the unit square) is $\{(p, p_*), 0 \leq p, p_* \leq 1 : P_\alpha(Q) = p$ and $P_\alpha(Q|d_i) = p_*$ for some d_i, α and $Q \subseteq \mathcal{S}_X\}$.

3.2 Privacy Characterization

A natural question is for given h_l and h_u, how to find a TPM that satisfies (5)? The first $\leq$ in (5) is equivalent to $P_\alpha(Q^c|d_i)) \leq 1 - h_l(1 - P_\alpha(Q^c))$. Considering this for all $Q \subseteq \mathcal{S}_X$, and defining $h(a) = \min\{h_u(a), 1 - h_l(1 - a)\}$, for $0 \leq a \leq 1$, it follows that an RR procedure P satisfies (5) if and only if

$$P_\alpha(Q|d_i) \leq h(P_\alpha(Q)) \tag{6}$$

for all $i = 1, \ldots, m$ and all α and $Q \subseteq \mathcal{S}_X$ such that $0 < P_\alpha(Q) < 1$. Chai and Nayak (2018) gave a necessary and sufficient condition for satisfying (6) using the following concept.

Definition 4 (Nayak et al. 2015) The ith row parity of P is defined as

$$\eta_i(P) = \max\left\{\frac{p_{ij}}{p_{il}} \mid j, l = 1, \ldots, k\right\} = \frac{\max_j\{p_{ij}\}}{\min_j\{p_{ij}\}},$$

with the convention $0/0 = 1$ and $a/0 = \infty$ for any $a > 0$. The parity of P is defined as $\eta(P) = \max_i\{\eta_i(P)\}$.

Theorem 1 *For a given h, an RR procedure P satisfies (6) if and only if $\eta(P) \leq B(h)$, where*

$$B(h) = \inf_{0<p<1}\left(\frac{1-p}{p}\right)\left(\frac{h(p)}{1-h(p)}\right)$$

and $h(p)/[1-h(p)] = \infty$ when $h(p) = 1$.

The necessary and sufficient condition in Theorem 1 depends on h only through $B(h)$ and on P only through its parity $\eta(P)$. Thus, $B(h)$ quantifies the privacy demand of h and $\eta(P)$ quantifies the privacy level of P. These two measures are useful for comparing privacy demands of different PBRs and privacy levels of various RR procedures, respectively. Chai and Nayak (2018) also showed that an RR procedure P with $\eta(P) = \gamma > 1$ guarantees (6) for all h such that

$$h(p) \geq h_{(\gamma)}(p) \equiv \frac{\gamma p}{1+(\gamma-1)p}, \quad 0 < p < 1. \tag{7}$$

Thus, $h_{(\gamma)}(.)$ in (7) is the precise upper breach boundary of any P with parity γ. Choosing h_l and h_u in practical applications may appear a difficult task. But, the preceding discussions give helpful guidance. Specifically, we only need to consider the functions in $\mathcal{H} = \{h_{(\gamma)}(.); \gamma > 1\}$ and choose one of those for the upper breach boundary. The precise lower breach boundary corresponding to $h_{(\gamma)}(.)$ is $\tilde{h}_{(\gamma)}(p) = 1 - h_{(\gamma)}(1-p)$. In practice, the plots of the precise PBRs for various γ might be helpful in selecting an appropriate PBR.

Theorem 1 says that in order to satisfy the criterion in Definition 3, each row parity of P must not exceed an upper bound, determined by h_l and h_u. The privacy condition (4) in the binary case with one sensitive category is similar. It gives an upper bound for the parity of just one row, corresponding to the response Y. We should mention that under (4), Nayak (1994) showed that the transition probabilities of an optimal design are $P(Y|A) = 1$, $P(Y|A^c) = 1/\gamma$ and hence $P(N|A) = 0$ and $P(N|A^c) = 1 - 1/\gamma$. However, this optimal design asks all respondents in the sensitive group to answer "Yes," which might be uncomfortable for some respondents. It also implies $P(A|N) = 0$, which might encourage some respondents to give the innocuous answer "No." Thus, the (mathematically) optimal design may not be suitable in real surveys. This indicates that (4) is inadequate and we should impose additional restrictions on the transition probabilities.

We also want to mention the following criterion that has received considerable attention in recent years, especially from computer scientists; see, e.g., Kairouz et al. (2016), Wang et al. (2016), Duchi et al. (2018), and Ye and Barg (2018).

Definition 5 An RR design provides ϵ-local differential privacy (ϵ-LDP), for $\epsilon > 0$, if

$$\sup_{Q \subseteq \mathcal{S}_Z} \sup_{c_i, c_j \in \mathcal{S}_X} \frac{P(Z \in Q | X = c_i)}{P(Z \in Q | X = c_j)} \leq e^{\epsilon}.$$

Chai and Nayak (2018) proved that an RR procedure provides ϵ-LDP if and only if

$$\frac{P_\alpha(Q)}{1 + (\gamma - 1)(1 - P_\alpha(Q))} \leq P_\alpha(Q|d_i) \leq \frac{\gamma P_\alpha(Q)}{1 + (\gamma - 1) P_\alpha(Q)}$$

for all α, Q and d_i, where $\gamma = e^{\epsilon}$. This shows that ϵ-LDP coincides with Definition 3, with $h_l(a) = a/[1 + (\gamma - 1)(1 - a)]$ and $h_u(a) = \gamma a/[1 + (\gamma - 1)a]$. This describes the PBR of ϵ-LPD, which may be used to communicate its privacy promises in terms of bounds on an intruder's possible information gain. It also follows that an RR design P provides ϵ-LDP if and only if $\eta(P) \leq \gamma = e^{\epsilon}$.

4 Comparison of RR Designs

We have seen that to satisfy the privacy requirement of either ϵ-LDP or Definition 3 we must use a design with $\eta(P) \leq \gamma$, for a given value of γ. For any given $\gamma > 1$, let $\mathcal{C}_\gamma = \{P_{m \times k} : \eta(P) \leq \gamma\}$, which is the class of all privacy-preserving designs at level γ. Typically, $\mathcal{C}_\gamma$ is large and a natural question is how should we choose a design from $\mathcal{C}_\gamma$ for practical application? As we noted earlier, for estimability of π, we should choose $P_{m \times k}$ with $m \geq k$ and full rank. Also, as Chai and Nayak (2018) discussed, P should not have any proportional rows, to be concise. Two designs are statistically equivalent if one can be obtained by merging the proportional rows of the other one. Intuitively, we should choose a P from $\mathcal{C}_\gamma$ that satisfies the preceding two conditions and maximizes data utility. However, data utility is a complex matter and it may be assessed in different ways. In the following, we first review an admissibility result under a broad view of data utility and then discuss design selection under certain optimality criteria.

4.1 Admissible Designs

Blackwell (1951, 1953) introduced a general criterion for comparing experiments, which in our context says the following.

Definition 6 An RR design $P_{m \times k}$ is said to be sufficient for (or at least as informative as) another RR design $A_{r \times k}$, to be denoted $P \succeq A$, if there exists a transition probability matrix $C_{r \times m}$ such that $A = CP$.

If $P \succeq A$ and also $A \succeq P$, then A and P are equivalent, and P is better than A if $P \succeq A$ but $A \not\succeq P$. Furthermore, P is said to be admissible if there does not exist another design that is better than P.

If $P \succeq A$, then applying A is equivalent to randomizing the true responses first using P and then randomizing the outputs of P using C. Intuitively, P should be more informative than A because the second randomization with C inflicts additional loss of statistical information. Formally, $P \succeq A$ implies that given any loss function and any inference rule δ based on the data from A, there exists a rule δ_* based on P whose risk function is no larger than the risk function of δ. In this sense, if $P \succeq A$, then P is universally at least as good as A. Chai and Nayak (2018) proved that two designs $P_{m\times k}$ and $A_{r\times k}$ in $\mathcal{C}_\gamma$ are equivalent if and only if $m = r$ and $A = CP$, where C is a permutation matrix, i.e., A can be obtained by permuting the rows of P, or just reordering the elements of the output space. Logically, we should use only admissible designs. Here, an important question is how do we know if a given design P is admissible or not? The following result of Chai and Nayak (2018) answers this question.

Theorem 2 *For any given γ, an RR design $P \in \mathcal{C}_\gamma$ is admissible if and only if (i) $\eta_i(P) = \gamma$ for all i (i.e., each row parity is γ) and (ii) each row of P contains exactly two distinct values.*

Now, we discuss an important RR method, viz., the RAPPOR algorithm, proposed recently by Erlingsson et al. (2014). Google, Apple, Microsoft, and other companies have been using it for online data capture; see, Ding et al. (2017) and Cormode et al. (2018). The basic method applies ϵ-LDP and works as follows. It represents all true responses with indicator vectors $X = (X_1, \ldots, X_k)$. Specifically, if the true response is c_i, then the ith component of X is 1 and all other components are 0. RAPPOR's randomization changes each component of $(X_1, \ldots, X_k)$ independently with probability $p = 1/(\sqrt{\gamma} + 1)$ and produces an output vector $Z = (Z_1, \ldots, Z_k)$.

The output space of RAPPOR is $\mathcal{S}_Z = \{z = (z_1, \ldots, z_k) : z_i = 0 \text{ or } 1 \text{ for } i = 1, \ldots, k\}$, which contains 2^k elements. So, RAPPOR's TPM is of order $2^k \times k$. The transition probabilities can be calculated easily. Let $x^{(i)}$ denote the indicator vector for true response c_i, i.e., $x^{(i)} = (x_1, \ldots, x_k)$, where $x_i = 1$ and $x_j = 0$ for all $j \neq i$. For any $z \in \mathcal{S}_z$, let $t_z = \sum_j z_j$. Then, it can be seen that

$$P((z_1, \ldots, z_k)|x^{(i)}) = \begin{cases} p^{t_z-1}(1-p)^{k-t_z+1}, & \text{if } z_i = 1 \\ p^{t_z+1}(1-p)^{k-t_z-1}, & \text{if } z_i = 0. \end{cases} \tag{8}$$

Let $\mathbf{1} = (1, \ldots, 1)$ and $\mathbf{0} = (0, \ldots, 0)$. From (8), we see that $P(\mathbf{1}|x^{(i)}) = p^{k-1}(1-p)$ and $P(\mathbf{0}|x^{(i)}) = p(1-p)^{k-1}$ for all i. So, the two rows of the RAPPOR's TPM, corresponding to $z = \mathbf{0}$ and $z = \mathbf{1}$, have parity 1 (not γ). This shows, in view of Theorem 2, the RAPPOR's design is not admissible.

We should mention that all other rows of RAPPOR's TPM satisfy the conditions of Theorem 2. So, the RAPPOR algorithm can be modified to make it admissible. Specifically, removing the two rows corresponding to $\mathbf{0}$ and $\mathbf{1}$ and normalizing the remaining matrix gives an admissible design. RAPPOR also gives a method for estimating π from perturbed data. The RAPPOR estimator is unbiased but not efficient. Chai and Nayak (2019) derived a better unbiased estimator that is also minimax under certain conditions.

4.2 Comparison of RR Designs

For $k = 2$, i.e., binary X, it follows from Theorem 2 that essentially only one design, given below, is admissible and hence it is the best design.

Theorem 3 *For binary X, an optimal RR design in $\mathcal{C}_\gamma$ is $P_{2\times 2}$ with $p_{11} = p_{22} = \gamma(\gamma+1)^{-1}$ and $p_{12} = p_{21} = (\gamma+1)^{-1}$.*

The optimal design in Theorem 3 is a Warner's design. For $k \geq 3$, many designs are admissible and choosing an optimal design requires additional criteria. In the following, we review some recent results.

Agrawal et al. (2009) presented the following optimality result in a special case. They required ρ_1-to-ρ_2 privacy. An RR design P satisfies ρ_1-to-ρ_2 privacy if and only if $\eta(P) \leq \gamma$, with $\gamma = [\rho_2(1-\rho_1)]/[\rho_1(1-\rho_2)]$. They considered the special case of $\mathcal{S}_Z = \mathcal{S}_X$. This implies that $m = k$. Additionally, they considered only symmetric P. Under these conditions, they proposed to take any P with the minimum condition number as an optimal design. The condition number of a symmetric positive definite matrix is defined as the ratio of its largest and smallest eigenvalues. To justify the criterion, they stated that the stability of numerical calculations with a matrix decreases as its condition number increases. They were mainly concerned with computing the inverse of P, which is often used for calculating an estimate of π and its variance. They proved that among all $P \in \mathcal{C}_\gamma$ that are also symmetric, the matrix P_0 with elements $p_{ii} = \gamma/(\gamma+k-1), i = 1, \ldots, k$, and $p_{ij} = 1/(\gamma+k-1)$ for $i \neq j$ has the minimum condition number. Thus, P_0 is the best design by their criterion.

Chai and Nayak (2018) also considered the special case of $\mathcal{S}_Z = \mathcal{S}_X$. Thus, the true values are randomized within the categories X. Here, the diagonal elements of P are the probabilities of keeping the true responses unchanged. Intuitively, we should change the true responses as little as possible to minimize data utility loss. This suggests to use a design $P \in \mathcal{C}_\gamma$ that has large diagonal values. One measure of "largeness" of the diagonal values of P is $\sum_i p_{ii}$, the trace of P. With this, a design $P \in \mathcal{C}_\gamma$ with the largest trace may be considered a best design at privacy level γ. Chai and Nayak (2018) proved that the optimal design P_0 of Agrawal et al. (2009), given above, is also the best design under the maximum trace criterion. Note that unlike Agrawal et al. (2009), this approach does not require P to be symmetric, although the optimal design P_0 is so.

Next, we review a minimax approach, recently investigated by Chai and Nayak (2019). Assuming multinomial sampling and squared error loss, they considered optimum determination of an RR *strategy*, which consists of a design P and an estimator $\hat{\pi} = (\hat{\pi}_1, \ldots, \hat{\pi}_k)$ of π. Under squared error loss, the risk function of an RR strategy $(P, \hat{\pi})$ is

$$R(P, \hat{\pi}; \pi) = E_{P,\pi}\Big[\|\hat{\pi} - \pi\|^2\Big] = E_{P,\pi}\Big[\sum_{i=1}^{k}(\hat{\pi}_i - \pi_i)^2\Big], \tag{9}$$

where the expectation is with respect to both sampling and randomization. They considered unbiased estimators of π that are also linear in $\mathbf{S}$, i.e., $\hat{\pi} = L\mathbf{S}/n$ for some matrix L, where $\mathbf{S}$ is the frequency vector of $d_1, \ldots, d_m$ and the divisor n is used for mathematical simplicity. As, $E(\mathbf{S}) = nP\pi$, $\hat{\pi} = L\mathbf{S}/n$ is unbiased if and only if $LP = I$. Recall that privacy protection requires that $P \in \mathcal{C}_\gamma$, for specified γ. Then, an RR strategy $(P_*, \tilde{\pi} = L_*S/n)$ is minimax among all privacy satisfying strategies if $P_* \in \mathcal{C}_\gamma$, $P_*L_* = I$ and

$$\sup_{\pi} E_{P_*,\pi}\Big[\| \frac{L_*S}{n} - \pi \|^2\Big] = \inf_{P \in \mathcal{C}_\gamma} \inf_{L:LP=I} \sup_{\pi} E_{P,\pi}\Big[\| \frac{LS}{n} - \pi \|^2\Big].$$

The RR design P_* is a minimax design.

To describe the minimax strategy, derived in Chai and Nayak (2019), for given $\gamma > 1$ and $k \geq 2$, define

$$f(x) = \frac{k^2(x\gamma^2 + k - x)}{(x\gamma + k - x)^2}, \quad x \geq 0, \tag{10}$$

and

$$q = \begin{cases} \lfloor \frac{k}{1+\gamma} \rfloor, & \text{if } f(\lfloor \frac{k}{1+\gamma} \rfloor) \geq f(\lceil \frac{k}{1+\gamma} \rceil) \text{ and } \lfloor \frac{k}{1+\gamma} \rfloor \geq 1 \\ \lceil \frac{k}{1+\gamma} \rceil, & \text{otherwise.} \end{cases} \tag{11}$$

Essentially, q is a maximizer of $f(.)$ over positive integers.

To describe how P_* randomizes the true categories, we represent the true responses with indicator vectors $X = (X_1, \ldots, X_k)$, as in RAPPOR. Then, for a true response $(x_1, \ldots, x_k)$, P_* generates an output $(z_1, \ldots, z_k)$ as follows. Suppose the true category is c_i, which implies $x_i = 1$ and $x_j = 0$ for $j \neq i$. Then, P_* assigns $z_i = 1$ with probability $p = (q\gamma)/(q\gamma + k - q)$ and $z_i = 0$ with probability $1 - p$. Next, if $z_i = 1$, P_* randomly selects $(q - 1)$ of the remaining $(k - 1)$ components of z and sets those to 1. If $z_i = 0$, P_* assigns 1 to q of the remaining components of z, selected at random. In both cases, all other components of z are 0. Thus, exactly q components of each output vector are 1 and the rest are 0. So, the output space of P_* is $\mathcal{S}_Z^* = \{(z_1, \ldots, z_k) : z_i \text{ is 0 or 1}, i = 1, \ldots, k, \text{ and } \sum z_i = q\}$ and it contains $m = \binom{k}{q}$ elements. As before, let $x^{(i)}$ denote the indicator vector for true response c_i. Then, it can be seen that the transition probabilities of the minimax design are

$$P((z_1, \ldots, z_k)|x^{(i)}) = \begin{cases} \gamma p_0, & \text{if } z_i = 1 \\ p_0, & \text{if } z_i \neq 1 \end{cases}$$

for $i = 1, \ldots, k$ and $(z_1, \ldots, z_k) \in \mathcal{S}_Z^*$, where $p_0 = k/[\binom{k}{q}(q\gamma + k - q)]$. So, each row of the TPM has two distinct values and parity γ, satisfying the conditions of Theorem 2.

As we describe next, the minimax estimator $\tilde{\pi}$ of π under P_* has a simple form and can be calculated easily. With vector representation, both the original and perturbed data under P_* appear as $n \times k$ matrices, with each row showing one respondent's data. Let $\mathbf{V}' = (V_1, \ldots, V_k)$ denote the vector of column sums of the perturbed data matrix. Then, the minimax estimator, derived in Chai and Nayak (2019), is

$$\tilde{\pi} = \frac{(k-1)(q\gamma + k - q)}{q(\gamma - 1)(k - q)}\left(\frac{\mathbf{V}}{n}\right) + \frac{1}{k}\left[\frac{(1-k)(q\gamma + k - q)}{(\gamma - 1)(k - q)} + 1\right]. \tag{12}$$

The minimax estimator is also a method of moments estimator based on $\mathbf{V}$. Here, we want to mention that the estimator in RAPPOR is similar to (12). It is based on method of moments and a linear function of the column sums of their perturbed data matrix. Naturally, $\tilde{\pi}$ in (12) is an unbiased estimator and it also follows that the risk function, as defined in (9), of the minimax strategy $(P_*, \tilde{\pi})$ is

$$R(P_*, \tilde{\pi}; \pi) = \frac{1}{n}\left[\frac{(k-1)^2}{f(q) - k} + \frac{1}{k} - 1\right] + \frac{1}{n}\sum_{i=1}^{k} \pi_i(1 - \pi_i), \tag{13}$$

where the function f and the quantity q are as defined in (10) and (11). Due to unbiasedness (13) also gives the trace of the variance-covariance matrix of $\tilde{\pi}$, i.e., $R(P_*, \tilde{\pi}; \pi) = \text{tr}[V(\tilde{\pi})] = \sum V(\tilde{\pi}_i)$. The last term of (13) is the risk of the MLE of π under no randomization. So, it reflects only the *sampling variation*. The first term in (13) is the *added variance* due to RR, which interestingly is independent of π, unlike the sampling variation.

We want to mention that Duchi et al. (2018) also investigated minimaxity of RR strategies and in a much broader setting. They considered a wider class of problems and loss functions. They derived bounds on minimax values and their convergence rates under ϵ-LDP. In particular, they obtained *rate optimal* methods for certain estimation problems. Naturally, those asymptotic results may not be useful in small samples. Also, rate optimality ignores the multipliers of convergence rates. So, a rate optimal procedure need not be asymptotically efficient because the minimax risks of two methods may converge to zero at the same (and optimal) rate, but with different multipliers. In contrast, the results of Chai and Nayak (2019) are exact, but for a specific problem.

5 Identification Risk Control by Post-randomization

Protecting data confidentiality is a difficult task because disclosure of personal information about survey participants may occur in various forms depending on the context, nature of released data and sensitivity of survey variables. Various types of disclosure and methods for their control are discussed in the books: Willenborg and De Waal (2001), Duncan et al. (2011) and Hundepool et al. (2012). In this article, we shall consider only identity disclosure in microdata release. Consider a complete

data set containing values of multiple variables for each of n sampled units. Data agencies commonly publish summaries of the data. But, researchers often want the full data set to explore different models and hypotheses. However, the original data may disclose the values of some sensitive variables for some of the survey participants or units, even if name, social security number and other direct identifiers are removed. In particular, one might be able to correctly identify the records of a target unit by matching gender, race, occupation, and other characteristics that can be obtained easily from other sources. Then, one can learn the identified unit's values for all other variables. This is called identity disclosure, which is also regarded as one of the most serious violations of data confidentiality.

5.1 Identification Risk Measures

The variables that an intruder might use for matching are called key (or pseudo-identifying) variables, which are usually categorical. For reducing identification risks, agencies perturb the true values of the key variables and then release the perturbed data. For choosing a suitable perturbation method, the agency should first determine its disclosure control goals. For that, the agency needs to select and specify the key variables. Thus, we assume that the key variables are given and all are categorical. As before, let X denote the cross-classification of all key variables and suppose X takes values in $\mathcal{S}_X = \{c_1, \ldots, c_k\}$. In this setting, Bethlehem et al. (1990), Skinner and Elliot (2002), Shlomo and De Waal (2008), Shlomo and Skinner (2010) and others have proposed and investigated different measures of identification risk.

Early works focused mainly on the units that are unique in the sample with respect to X. As agencies do not reveal which population units are in the sample, it is reasonable to assume that an intruder would not know if his target is in the sample or not. Such an intruder would correctly match a sample unique unit if it is also population unique with respect to X. Motivated by this, Bethlehem et al. (1990) defined identification risk as the probability that a unit is population unique, given that it is sample unique, both with respect to X. Obviously, this concerns only the sample unique units. Also, it ignores the effects of data perturbation. So, this measure is not useful for determining a suitable perturbation mechanism. Essentially, it aims to assess how much protection the sample unique units get from sampling. We refer to Skinner and Elliot (2002) for a discussion of similar measures and related references.

Shlomo and Skinner (2010) took a more relevant approach that focuses on correct matches in perturbed (and released) data. Naturally, they take data perturbation into account. However, they were concerned only with the unique matches in released data, presuming those to be the worst cases. Consequently, they defined a unit's identification risk as the probability that the unit is correctly identified given that it has a unique match in released data. This (conditional) probability is with respect to both sampling and data perturbation. This identification risk is unit specific and it varies over the sampled units.

There are some practical difficulties in using the preceding risk measure in finding a suitable perturbation mechanism. First, the risks of the sampled units involve the unknown population frequencies and hence those cannot be calculated from available information. Methods for estimating those have been proposed, but they require assumptions about the population distribution and data modeling. So, the estimates depend on the model assumptions. Second, the effectiveness of data perturbation is assessed using the average of the risks of all sampled units. That may not be appropriate because a small average risk does not imply that disclosure risks of all units are desirably small. Third, the search for a suitable perturbation procedure requires an iterative approach. One would need to assess the effectiveness of several procedures to select a procedure. For example, to apply data swapping, as described in Shlomo and Skinner (2010), one would need to evaluate the average risk measure for various swap rates to choose a suitable value for actual application.

Recently, Nayak et al. (2018), henceforth NZY, refined Shlomo and Skinner (2010) approach and introduced a strict identification risk control goal. They also developed a method for achieving that goal. To describe the NZY approach, consider an intruder J who wants to identify the records of a target unit B in the released perturbed data. Let $X_{(B)}$ denote B's value of X, and suppose $X_{(B)} = c_j$. NZY assumed that (a) J knows $X_{(B)}$, (b) J knows that B is in the sample and (c) J randomly selects one of the records in the released data that match $X_{(B)}$, and identifies those as B's data. If no records in released data match $X_{(B)}$, the intruder stops his search for B's data. While assumptions (a) and (c) are realistic, (b) is overly stringent because agencies do not disclose which population units are included in the sample.

Let T_j and S_j denote the frequencies of c_j in the original and perturbed data, respectively, and let $\mathbf{T} = (T_1, ..., T_k)'$ and $\mathbf{S} = (S_1, ..., S_k)'$. Note that if $X_{(B)} = c_j$, then S_j records in the released data match B on key variables. Intuitively, J's confidence in a declared match depends on S_j. Observing this, NZY considered the following to propose a strict disclosure control goal:

$$R_j(a) = P(CM|X_{(B)} = c_j, S_j = a), \quad j = 1, \ldots, k, a \geq 1$$

where CM denotes the event that B is *correctly matched* in the preceding setup. NZY proposed that the agency should select a suitable value ξ and guarantee, with appropriate data perturbation, that

$$R_j(a) \leq \xi \quad \text{for all } j = 1, \ldots, k, \text{ and all integers } a \geq 1. \tag{14}$$

Then, no unit's correct match probability would exceed ξ. This gives a clear and strong identification risk control goal.

Like all past identification risk measures, $R_j(a)$ also depends on the unknown population frequencies. So, we cannot calculate $R_j(a)$'s and thereby verify whether a data perturbation mechanism guarantees (14) or not. To avoid this difficulty, NZY considered

$$R_j(a, \mathbf{t}) = P(CM|X_{(B)} = c_j, S_j = a, \mathbf{T} = \mathbf{t}),$$

further conditioning on $\mathbf{t}$. Quite importantly, $R_j(a, \mathbf{t})$'s do not involve unknown parameters under PRAM and so, those can be assessed and controlled without estimating any parameter. Note that $R_j(a, \mathbf{t})$'s involve the original frequency vector $\mathbf{t}$, but that is available to the data agency. NZY suggested to satisfy (14) by using a data perturbation mechanism such that

$$R_j(a, \mathbf{t}) \leq \xi \quad \text{for } j = 1, \ldots, k, \text{ all } a > 0 \text{ and all } \mathbf{t}. \tag{15}$$

Effectively, (15) is their disclosure control goal, which readily implies (14).

5.2 A Post-randomization Method

Taking the preceding approach, NZY developed a class of unbiased PRAMs that can be used to satisfy (15) for $\xi > 1/3$. They give two reasons for choosing a $\xi > 1/3$ in practical situations. First, intruders should have strong evidence for declaring matches. To be credible, the correct match probability for a declared match should be substantial, perhaps larger than 0.5. Second, as noted earlier, assumption (b) is overly stringent. Usually, an intruder would not know if a target is in the sample or not. For such an intruder, a correct match probability is much smaller than $R_j(a)$, approximately $R_j(a)$ times the target's sample inclusion probability, which is usually quite small.

For any given $\xi > 1/3$, NZY developed an unbiased PRAM to satisfy (15) as follows. First, we should mention that any unbiased PRAM does not affect the empty categories. In other words, an unbiased PRAM does not change a true category to a category that was originally empty. Truly, $\mathcal{S}_Z$ consists of only the categories in $\mathcal{S}_X$ that have positive frequencies in the original data set, i.e., $\mathcal{S}_Z = \mathcal{S}_X^* = \{c_i : c_i \in \mathcal{S}_X \text{ and } t_i > 0\}$, which may be a proper subset of $\mathcal{S}_X$. Actually, $\mathcal{S}_X^*$ is also the input space as all observed values are in this set. For notational simplicity, we assume that all categories are nonempty and thus $\mathcal{S}_X^* = \mathcal{S}_X$.

The NZY method uses one specific class of unbiased PRAMs. Specifically, they use the transition probabilities

$$p_{ij} = P(Z = c_i | X = c_j) = \begin{cases} 1 - \frac{\theta}{t_j}, & \text{if } i = j; \\ \frac{\theta}{(k-1)t_j}, & \text{if } i \neq j, \end{cases} \tag{16}$$

where t_j is the original frequency of c_j and θ is a design parameter, chosen suitably to satisfy (15). Clearly, the TPM $P = ((p_{ij}))$ given by (16) is adaptive, viz., it depends on the observed data via the category frequencies. Also, P has a simple structure. It changes a true category c_j with probability θ/t_j, which is inversely proportional to the frequency of the unit's true category. If a true category is c_j, then it is kept unchanged with probability $1 - \theta/t_j$. When a true category is changed, the replacement is selected at random from the remaining categories. One helpful feature of

this P is that it is determined fully by a single parameter θ. So the effects of P on identification risks and statistical inferences can be studied in terms of θ only.

One key result of NZY is that for given $1/3 < \xi < 1$, the above P satisfies (15) if θ is chosen as the solution of $h(\theta) = \xi$, where

$$h(\theta) = \begin{cases} \frac{1-\theta}{1-\theta+\theta^2}, & \text{if } \theta \le \frac{2}{3}, \\ \frac{2-\theta}{4-2\theta+\theta^2}, & \text{if } \theta > \frac{2}{3}, \end{cases}$$

and $k \ge (1-\theta)^{-1}$. They also showed that $h(\theta)$ is a strictly decreasing function of θ, with $h(0) = 1$ and $h(1) = 1/3$ and thus for any $1/3 < \xi < 1$, $h(\theta) = \xi$ admits a unique solution for θ in $(0, 1)$. This result gives a theoretical basis for designing a post-randomization method for guaranteeing (15). Also, a suitable PRAM can be designed directly, without iterative calculations or adjustments, unlike previous approaches.

Actually, the method proposed by NZY applies the preceding result separately to subsets of the data set, which are formed by partitioning the data into homogeneous groups and then taking only the sensitive records in each group. That is done to better preserve data utility. While category and cell are synonymous, in the rest of this section we shall use cell for a cross-classified variable and category for individual variables, for additional clarity. So, we shall use cell for X, as it is the cross-classification of all key variables. For given $0 < \xi < 1$, a cell is considered *sensitive* if its frequency is less than $1/\xi$. A cell c_j is nonsensitive if $t_j \ge 1/\xi$ because in the original data, the probability of correctly identifying a unit falling in that cell is $1/t_j \le \xi$. The identification risks of all units in the nonsensitive cells are already sufficiently small. So, we only need to post-randomize X for all units in the sensitive cells. All sensitive cells in a partition set form a post-randomization block (PRB). The NZY method applies PRAM to the PRB's separately. More details of the method and some parts of an illustrative example are given below.

The main purpose of data partitioning is to control the nature and magnitude of possible changes due to PRAM, and even preserve selected parts and summaries of the data set. NZY gave several ideas for data partitioning. One simple approach is to partition the data by broader or generalized categories of the key variables. As an illustrative example, NZY applied the method to a data set publicly released by the U.S. Census Bureau. It contains values of several demographic and economic variables for 59,033 individuals. For illustration, NZY took gender (2), age (92), race (9), marital status (5), and public use microdata area (PUMA) (44) as the key variables, where the values in parentheses show the number of categories of the variables. The cross-classification of these key variables yields 364,320 cells.

In the example, NZY partitioned the data by gender, seven age intervals, viz., 0–17, 18–24, 25–34, 35–44, 45–54, 55–64, and 65 and above, and the three race categories: white, black, and "other races." That divided the data into 42 partition sets, corresponding to all possible combinations of gender, 7 age intervals, and 3 race classes. For example, all females of "other races" with age between 25 and 34 constitute one partition set. Similarly, all white males in the age interval 55–64 form

another partition set. Note, for example, that all individuals in a partition set are either male or female. As the method applies PRAM within each partition set, it will not alter the gender of any individual. Similarly, it will preserve race if the original category is white or black, which are the two major categories. Race may change only among the other races. Age will remain in the partitioning intervals. For example, if the true value is 38, the perturbed value will be between 35 and 44. It will preserve the counts of voting age (18 or above) and senior (65 and above) people, which are important in policy research. Also note that since marital status and PUMA were not used in data partitioning, those may change freely. This partition in one extreme fully preserves gender and on the other extreme permits unlimited changes of marital status and PUMA.

In the example, NZY took $\xi = 0.395$, for which only singleton and doubleton cells (with frequency 1 and 2, respectively) are sensitive. So, all singleton and doubleton cells of X in a partition set formed one PRB. In each of the 42 PRB's, the true X cells are post-randomized using the transition probabilities given by (16). For $\xi = 0.395$, it turns out that $\theta = 0.8$ and $(1-\theta)^{-1} = 5$. Earlier, we discussed (16) for one data set and assuming that all cells are nonempty. For applying post-randomization, we need to specialize (16) for each PRB. Specifically, we need to interpret k as the number of cells in the PRB, which changes from PRB to PRB. Also, $c_1, \ldots, c_k$ should represent the cells within a PRB. The theoretical results for guaranteeing (15) also require at least $(1-\theta)^{-1} (= 5$ for $\xi = 0.395)$ cells in each PRB. This was satisfied in the example. Actually, the number of cells in the 42 PRB's ranged between 124 and 1480. One should not partition the data overly finely into too many sets so that the condition $k \geq (1-\theta)^{-1}$ is satisfied.

We mention some other facts from the NZY example. The five key variables defined 364,320 cells. The data set, with sample size 59,033, showed only 25,406 nonempty cells, of which 13,662 are singleton and 4,777 are doubleton. As $\theta = 0.8$, the method changed the true cell of each singleton unit with probability 0.8 and each doubleton unit with probability 0.4. When a true cell was changed, the new cell was picked at random from the remaining cells within the PRB. The method kept the true values of all nonsensitive units unchanged.

Deriving methods for analyzing perturbed data, making appropriate adjustments for data perturbation, is burdensome to data users. Also, data users usually do not get full information about the perturbation mechanism that is needed for modeling the perturbation effects. So, it is important to perturb the data in such a way that standard inferential methods for the original data remain valid for the released data, at least approximately. Generally, we want perturbation methods that add a small (or negligible) variance and no bias. The NZY methods does quite well in that respect, largely due to data partitioning and using unbiased PRAM. The relative frequencies based on perturbed data are unbiased estimators of corresponding population probabilities. NZY examined the variance of these estimators and proved that the additional variance due to data perturbation is of order $1/n^2$, where n is sample size. That is negligible in comparison to sampling variance, which is of order $1/n$.

Consistent with the theoretical results, the NZY method exhibited very small effects on data distributions in their example. We reproduce the distributions of

Table 1 Frequency distributions of marital status

Marital status	Original data	Perturbed data	Difference
Married	24688 (0.4182)	24678 (0.4180)	10
Widowed	3156 (0.0535)	3180 (0.0539)	−24
Divorced	4742 (0.0803)	4704 (0.0797)	38
Separated	1040 (0.0176)	1039 (0.0176)	1
Never married	25407 (0.4304)	25432 (0.4308)	−25

Table 2 Frequency distribution of race

Race	Original data	Perturbed data	Difference
White	37201(0.6302)	37201 (0.6302)	0
Black	15239(0.2581)	15239(0.2581)	0
American Indian alone	97 (0.0016)	92(0.0015)	5
Alaska Native alone	1(0.00002)	0 (0)	1
American Indian and Alaska Native	42(0.0007)	46 (0.0008)	−4
Asian	3461(0.0586)	3445(0.0584)	16
Native Hawaiian and other Pacific Islander	20 (0.0004)	21(0.0004)	−1
Some other race alone	1349(0.0228)	1337(0.0227)	12
Two or more races	1623(0.0275)	1652(0.0280)	−29

marital status and race based on the original and perturbed data in Tables 1 and 2. There, columns 2 and 3 give the original and perturbed frequencies and the numbers in parentheses are relative frequencies. The last column gives the difference between the original and perturbed frequencies. Recall that marital status was allowed to change freely. Even then, the original and perturbed frequencies are very close. The differences between original and perturbed frequencies of race categories are also quite small. Note that the difference is 0 for white and black. That is not by coincidence, but due to the particular data partitioning, which forced to preserve race for those two groups. We refer interested readers to the NZY paper for more details about the method and the example.

6 Discussion

The idea of randomizing true responses for protecting respondent's privacy and data confidentiality has been around for a long time. But, it has not been used much in real surveys, perhaps due to lack of practical privacy measures and adequate guidance on choosing the transition probabilities. In recent years, RR methods have received

significant attention from companies and computer scientists in a new context, viz., for protecting privacy when recording data from various online activities. Recent research has yielded precise privacy concepts and measures and rigorous methods for determining the transition probabilities. We have reviewed some of those developments. In particular, we covered one approach to strict privacy protection (in Sects. 3 and 4) and one rigorous method for identification risk control in releasing microdata (in Sect. 5).

RR surveys and PRAM are similar in that both randomize true responses with predetermined probabilities and the transition probabilities govern their mathematical properties. But, one important difference is that in PRAM, the original data (containing true responses of all units) may be used to choose the transition probabilities, whereas in RR surveys, those must be determined before data collection. This implies that in PRAM, randomization may be applied after data partitioning and only to some selected units. The NZY method displays and utilizes these special features of PRAM.

Privacy and data confidentially are difficult but important topics and have been investigated for a long time. Also, research in these areas has increased significantly in recent years. New theories and methods are being developed by researchers in statistics, computer science, public policy, and other fields. Other concepts and methods such as grouping, data swapping, synthetic data, l-diversity, and differential privacy have been developed to mitigate disclosure risks. We consider response randomization as one of the most basic and promising tools for protecting privacy and data confidentiality. In particular, we believe that there is substantial scope for developing post-randomization methods, like the NZY method, for protecting data confidentiality.

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Shape and Circular Analysis

A Statistical Analysis of the Cardioid Radial Growth Model

John T. Kent, Kanti V. Mardia, Luigi Ippoliti, and Pasquale Valentini

Abstract A new two-parameter "full exponential cardioid" radial growth model for two-dimensional geometric objects is proposed and analyzed. The model depends additionally on two rotation parameters and on two seeds about which the growth is centered, plus a choice of three possible assumptions about statistical errors. If the seeds are assumed known, the remaining parameters can be estimated in closed form. Comparisons are given to earlier approaches. Two examples are given, one for a set of simulated data and one for a set of rat calvarial data.

Keywords Revised cardioid strain · Craniofacial growth · Deformation · Shape analysis · Outlines · Von mises distribution

1 Introduction

This paper revisits the Todd and Mark (1981a) "revised cardioid strain (RCS) radial growth model", a simple mechanistic model for craniofacial growth. Ramanathan et al. (2009) give a recent summary of its history and applications. A key property of the model is that the growth rate is greater near the bottom of the head than at the top so that it captures some of the key characteristics of real growth for humans and

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other animals. Further, the model gives a very simple description of growth, with only one growth parameter (plus 6 registration parameters, often treated as known) to fit.

The two key assumptions of the model are that (a) there is a "seed" inside the skull about which growth is centered, and (b) the rate of growth at a particular point on the head depends only on the angle from vertical. Various attempts have been made to justify the model in terms of physical principles. For example, Todd and Mark (1981a) motivate the model using hydrostatics and gravity.

The cardioid growth model can be considered as a very simplified version of the pattern theoretic growth model of Grenander et al. (2007) and Portman (2009, p. 19), which is based on infinitesimal growth patterns about a seed. However, the pattern theoretic growth model is much richer, albeit more complicated, because cumulative growth involves a series of iterated diffeomorphisms and many different seeds.

The use of the cardioid model as a "real" description of biological growth has been hugely controversial. See especially the Letter to the Editor by Bookstein (1981) in the same volume as Todd and Mark (1981a); there is also a rejoinder by the authors Todd and Mark (1981b). One of the main objections is the existence of a constant seed. Another is the simplistic assumption that growth depends on a single parameter. The full exponential cardioid (FEC) radial growth model developed below in (4) includes two parameters for growth.

The RCS model was firstly used to characterize craniofacial growth. However, this model has been also found useful to effectively approximate aging on frontal photographs of faces. See, for example, Miyoshi and Hyodo (2006); Ramanathan and Chellappa (2006); Ramanathan et al. (2009) and Yamaguchi and Oda (1999), especially for female faces and faces that appear childlike.

One of the main successful uses of the cardioid model has been in psychological experiments, where experimenters artificially age outlines or images of human heads using this model, with the aim of getting subjects to visually react to the perceived age; see, for example, Yamaguchi and Oda (1999). For this purpose it is not necessary for the model to be fully accurate biologically. It is only necessary that the subjects perceive appropriate differences in age as the image is altered.

The purpose of this paper is to develop statistical shape methodology to assess the strengths and weaknesses of the cardioid growth model. To facilitate the statistical analysis, we emphasize a modified version of the growth model, which differs from the original RCS model in three ways.

(a) Growth is modeled on a log scale rather than a linear scale.
(b) There are two parameters to model growth (essentially an intercept and slope parameter) instead of a single slope parameter in the original RCS model.
(c) Explicit assumptions are introduced to model the statistical error. Three possibilities are described.

It is a pleasure to include this paper in a volume dedicated to C R Rao's 100th birthday as it relates to two research areas where he has made substantial contributions. He did pioneering work in growth starting from Rao (1958) and subsequently he worked on shape analysis based on landmark data starting from Rao and Suryawanshi (1996).

2 Radial Growth Models for Two-Dimensional Objects

Let X and Y denote two geometric objects in the plane where every point $x'_j \in X$ has a unique counterpart $y'_j \in Y$, $j = 1, \ldots, J$. A radial growth model states that after appropriate centering and rotation, the X- and Y-configurations are related by a simple parametric transformation in polar coordinates.

It is convenient to represent points in the plane by complex numbers. Given "seeds" $\mu,\ \nu \in \mathbb{C}$ define "centered" points by

$$x_j = x'_j - \mu, \quad y_j = y'_j - \nu$$

with polar coordinates

$$x_j = x'_j - \mu = r_j \exp(i\theta_j), \quad y_j = y'_j - \nu = s_j \exp(i\phi_j). \tag{1}$$

Thus, $r_j,\ s_j$ are the radial components and $\theta_j,\ \phi_j$ are the angular components of the centered data.

For graphical purposes, let an angle θ be measured counterclockwise from vertical. Thus, $\theta = 0$ points upwards and $\theta = \pi/2$ points to the left. Thus, a complex number with positive real part lies in the upper half-plane and a complex number with positive imaginary part lies in the left half-plane.

Let a function $M(\theta) = \exp\{L(\theta)\}$, taking an angle to a positive number, be called a *radial deformation function*, following Grenander et al. (2007). The specific choice

$$M(\theta; a_0, b) = \exp\{L(\theta)\} = \exp(a_0 - b\cos\theta) \tag{2}$$

is called the *full exponential cardioid (FEC)* radial deformation function. The minus sign is chosen so that if b is positive, then $M(\theta; a_0, b) > M(0; a_0, b)$ for $\theta \neq 0$; in particular, the growth rate is smallest in the upwards vertical direction and largest in the downwards vertical direction.

Consider a two-dimensional side or sagittal view of a human head, with a seed inside the head but near the top of the skull. Suppose the head has been rotated so that the direction from the seed to the top of the head points upwards (the *preferred orientation*), with angle $\theta = 0$. Then, the FEC radial deformation function can capture the property that for babies and children, the growth rate is greater near the bottom of the head than at the top.

In general, the configurations X and Y may need to be rotated to their preferred orientations by angles α and β, say, before the deformation function can be applied. Given a radial deformation function, a general *radial growth model* from X to Y is defined by

$$e^{-i\beta} y_j = M(\theta_j - \alpha) e^{-i\alpha} x_j = M^*(\theta_j) e^{-i\alpha} x_j \tag{3}$$

where the angles α and β are nuisance orientation parameters and $M^*(\theta) = M(\theta - \alpha)$ is the *adapted* version of the M function.

For the FEC radial growth model, the adapted log radial deformation function can be written as

$$L^*(\theta) = L(\theta - \alpha) = a_0 - b\cos(\theta - \alpha) = a_0 - a_1\cos\theta - a_2\sin\theta, \text{ say.} \quad (4)$$

Note that

$$b = (a_1^2 + a_2^2)^{1/2} \text{ and } \alpha = \text{atan2}(a_2, a_1) \quad (5)$$

can be recovered from a_1 and a_2. Here atan2, a function found in many computing languages, is a version of the atan function, modified to ensure that the result is in the correct quadrant, so that $(a_1, a_2) = b(\cos\alpha, \sin\alpha)$.

For any radial growth model there are 6 *registration parameters* (two complex seeds and two orientation parameters). For the FEC radial growth model, there are additionally two *growth parameters*, a_0 and b. Under any radial growth model, the angular part does not change, $\phi_j - \beta = \theta_j - \alpha$; it is only the radial part that changes. That is, the angular part of $e^{-i\beta}y_j$ is the same as that of $e^{-i\alpha}x_j$; the radial part s_j of y_j depends on the radial part r_j of x_j through the radial deformation function. Although the phrase "growth" model is used for simplicity, shrinkage can occur when $M(\theta) < 1$.

If b is near 0, then the FEC radial growth model can be approximated by the *full linear cardioid (FLC)* radial growth model with deformation function

$$M_{\text{FLC}}(\theta; k_1, k_2) = k_1 - k_2\cos\theta, \quad (6)$$

with $k_1 = \exp(a_0)$, $k_2 = b\exp(a_0)$. If θ is allowed to range around the whole circle then the constraints $k_1 > 0$ and $k_1 + |k_2| > 0$ are needed to ensure that $M_{\text{FLC}}(\theta) = M_{\text{FLC}}(\theta; k_1, k_2)$ is always positive. However, in many applications the possible values of θ_j for points in X lie in a smaller arc $\theta^{(0)} < \theta < \theta^{(1)}$, say, and in such a situation the constraints on k_1 and k_2 can be relaxed somewhat.

The full linear cardioid radial growth model (6) includes two one-parameter special cases.

(a) The case $k_1 = 1$ and $k_2 = k_{\text{CS}}$ in (6), with parameter k_{CS}, is known as the *cardioid strain (CS)* model (Shaw et al. 1974). The analogous restriction for the FEC model (2) is $a_0 = 0$.
(b) The case $k_1 = 1 + k_{\text{RCS}}$ and $k_2 = k_{\text{RCS}}$, with parameter k_{RCS}, is known as the *revised cardioid strain (RCS)* model (Todd and Mark 1981a). The analogous restriction for the FEC model (2) is $a_0 = b$.

These models are called "strain" models because a physical justification can be attempted in terms of mechanical strain. For the other models, there is no claim of any physical motivation.

If growth is viewed as a continuous activity, then the growth model of Eq. (6) requires the choice of a unit time interval. After n time units with constant registration parameters, the model has overall radial deformation function $M_{\text{FLC}}(\theta; k_1, k_2)^n$ and it is not defined for non-integer values of time. On the other hand, a continuous

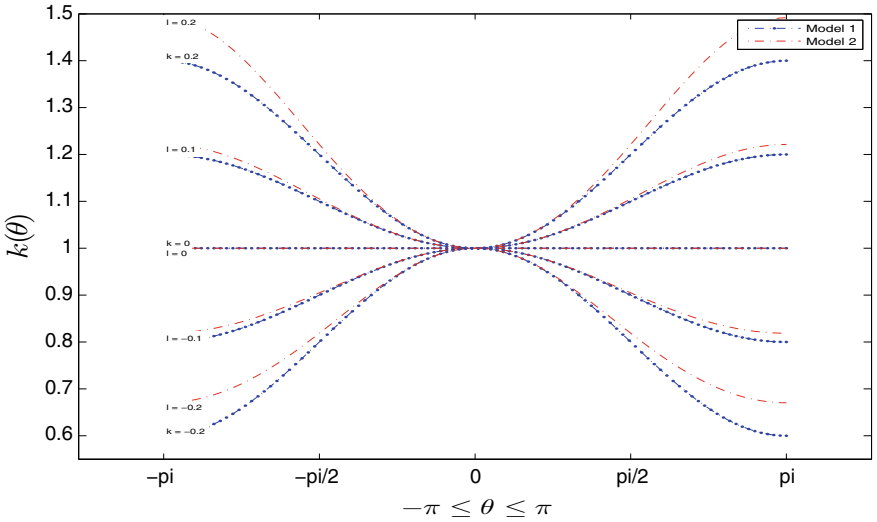

Fig. 1 Radial deformation functions with $k_{\mathrm{RCS}} = -0.2, -0.1, 0.0, 0.1, 0.2$. Model 1 = RCS model (blue); Model 2 = analogous FEC model (red)

version of (2) can be defined for all values of time $t \geq 0$ through a time-dependent radial deformation function $M_t(\theta) = \exp\{tL(\theta)\}$. Hence, the second model feels more natural when the choice of a unit time interval is arbitrary.

A comparison between radial deformation functions for the RCS and the FEC growth models is given in Fig. 1 for different choices of k_{RCS}, with $a_0 = b = k_{\mathrm{RCS}}$. The differences are small for small k_{RCS} and increase for larger k_{RCS}.

The choice of the model specification may be based on biological/scientific arguments. For example, the CS model shows no growth in the direction $\theta = 90°$ while the RCS shows no growth in the direction $\theta = 0°$. When there are no scientific reasons to prefer one version over the other, it can be more useful to work with the full model, either in continuous (2) or discrete (6) form. This paper emphasizes the continuous models.

The study of growth models can viewed as part of the subject of statistical shape analysis. Technically, the *shape* of an object consists of the information that remains after location, rotation, and size effects have been removed. However, in growth models it is important to retain information abut the size of an object. Hence, growth models can be more accurately described as examples of *size-and-shape* analysis (e.g., Dryden and Mardia 2016, p.66).

For convenience here is a reminder of the key abbreviations in the paper for various radial growth models:

CS : cardioid strain
RCS: revised cardioid strain

FLC: full linear cardioid, Eq. (6)
FEC: full exponential cardioid, Eq. (2).

3 Fitting the FEC Growth Model for Landmark Data

3.1 Landmark Data

In general, an object in the plane can be represented either by a finite set of landmarks or by a continuous outline. In this section, we focus on the landmark case. The outline case is covered below.

Thus, the two objects are described in terms of J landmarks, $X = \{x_1', \ldots, x_J'\}$ and $Y = \{y_1', \ldots, y_J'\}$ with x_j' known to correspond to y_j', $j = 1, \ldots, J$.

3.2 Statistical Models

There are several ways to introduce statistical errors into the FEC radial growth model. In each case the ϵ_j are assumed to follow independent complex normal distributions $CN(0, \sigma^2)$, so the real and imaginary parts are independent $N(0, \sigma^2)$. We assume σ^2 is "small" in each case. Recall the polar coordinates θ_j, ϕ_j for the centered landmarks are given in (1). In addition the notation $L_j^* = L^*(\theta_j) = L(\theta_j - \alpha)$ in (4) is used for the adapted log radial FEC value at the data points to simplify the formulas.

- (multiplicative errors)

$$e^{-i\beta} y_j = e^{-i\alpha} e^{L_j^*} x_j \left(1 + \epsilon_j\right). \tag{7}$$

- (additive-in-x errors)

$$e^{-i\beta} y_j = e^{-i\alpha} e^{L_j^*} \left(x_j + \epsilon_j\right). \tag{8}$$

- (additive-in-y errors)

$$e^{-i\beta} y_j = e^{-i\alpha} \left(e^{L_j^*} x_j + \epsilon_j\right). \tag{9}$$

  The model with additive-in-y errors is closest in character to a standard regression model.

To fit these models it is convenient to write complex numbers in polar coordinates and to look at the resulting models for the log radial and angular components. In particular, write $\epsilon_j = \epsilon_{j1} + i\epsilon_{j2}$ in terms of its real and imaginary components and note that the radial and angular components satisfy

$$|1+\epsilon_j| = \left\{\left(1+\epsilon_{j1}\right)^2 + \epsilon_{j2}^2\right\}^{1/2} \approx 1+\epsilon_{j1},$$

so that $\log|1+\epsilon_j| \approx \epsilon_{j1}$, and

$$\arg(1+\epsilon_j) = \text{atan2}(\epsilon_{j2}, 1+\epsilon_{j1}) \approx \epsilon_{j2},$$

where the error in the approximations is $O(|\epsilon_j|^2)$. Hence, the multiplicative error model can be written approximately as

$$\log(s_j/r_j) = L_j^* + \epsilon_{j1} \tag{10}$$

$$\phi_j - \theta_j = \psi + \epsilon_{j2} \tag{11}$$

where $\psi = \beta - \alpha$. In (10) the left-hand side of the equation can be viewed as the response variable in a linear regression and the right-hand side contains the regressor variables. Equation (11) involves angles with small random errors about a common mean. It is convenient to approximate the normal distribution for ϵ_{j2} by a von Mises distribution.

The von Mises distribution $VM(\psi, \kappa)$ with mean direction ψ and concentration parameter κ has density

$$f(\eta) = \frac{1}{2\pi I_0(\kappa)} \exp\{\kappa\cos(\eta-\psi)\}, \quad 0 \le \eta < 2\pi$$

(e.g., Mardia and Jupp 2000). The normalizing constant $I_0(\kappa)$ is a modified Bessel function. For large concentration parameter κ,

$$I_0(\kappa) \approx e^{\kappa}/(2\pi\kappa)^{1/2}, \tag{12}$$

and the von Mises distribution is approximately the same as a normal distribution with variance $\sigma^2 = 1/\kappa$. Hence, the angles $\phi_j - \theta_j$ are approximately i.i.d. $VM(\psi, \kappa)$, a von Mises distribution with mean direction ψ and concentration parameter $\kappa = 1/\sigma^2$.

The calculations for the additive models are similar but a bit more involved. Start with the additive-in-x error model. Since the complex normal distribution is invariant under rotations of the complex plane about the origin, $\epsilon_j' = \exp(-i\theta_j)\epsilon_j$ is also $CN(0, \sigma^2)$. Then,

$$|x_j+\epsilon_j| = |r_j+\epsilon_j'| = \left\{\left(r_j+\epsilon_{j1}'\right)^2 + \epsilon_{j2}'^2\right\}^{1/2} \approx r_j+\epsilon_{j1}',$$

so that $\log|r_j+\epsilon_j'| \approx \log r_j + \epsilon_{j1}'/r_j$, and

$$\arg(x_j+\epsilon_j) = \theta_j + \arg(r_j+\epsilon_j') = \theta_j + \text{atan2}(\epsilon_{j2}', r_j+\epsilon_{j1}') \approx \theta_j + \epsilon_{j2}'/r_j.$$

Hence, the additive-in-x error model can be written approximately as

$$\log(s_j/r_j) = L_j + \epsilon'_{j1}/r_j \tag{13}$$

$$\phi_j - \theta_j = \psi + \epsilon'_{j2}/r_j. \tag{14}$$

Thus, (13) represents a weighted regression model, where the jth term has variance σ^2/w_j in terms of the weights

$$w_j = r_j^2 = |x_j|^2. \tag{15}$$

Similarly, in (14), the angles $\phi_j - \theta_j$ are independently distributed from a von Mises distribution with a common mean direction ψ and with jth concentration parameter $\kappa_j = w_j/\sigma^2$.

The expansion for the additive-in-y error model is similar, except the weights are now given by $\left(e^{L_j^*}|x_j|\right)^2$. However, $e^{L_j^*}|x_j|$ is not observed, so it is approximated by $|y_j|$ to give the weights

$$w_j = s_j^2 = |y_j|^2 \tag{16}$$

which are used below for estimation.

Assuming for the moment that σ^2 is known, the parameters of both the radial and the angular models can be estimated by maximum likelihood. Details are given in the next section.

4 Estimation

In this section, details are given for estimating the parameters of the FEC model, either in its multiplicative or additive form. The estimation procedure takes the same form in all three cases, but with different "weight terms". Define

$$w_j^{(1)} = 1, \quad w_j^{(x)} = |x_j|^2 = r_j^2, \quad w_j^{(y)} = |y_j|^2 = s_j^2. \tag{17}$$

For the multiplicative model, the weight term is $w_j = w_j^{(1)}$. For the additive models in x and y, the weight terms are $w_j = w_j^{(x)}$ and $w_j = w_j^{(y)}$, respectively.

If the seeds μ and ν are known, the estimation can be carried out in closed form. The details for the radial and angular parts are given in the next two subsections, and combined in the following subsection. Finally, the estimation of the seeds is discussed.

4.1 Estimation for the Radial Model

The model for the log radial component is a linear regression model where the response variable $v_j = \log(s_j/r_j)$ has mean $L_j = a_0 + a_1 \cos\theta_j + a_2 \sin\theta_j$ and normally distributed $N(0, w_j^{-1}\sigma^2)$ error, $j = 1, \ldots, J$. Hence the parameters a_0, a_1, a_2 can be estimated by minimizing the weighted sum of squares

$$\sum w_j (v_j - L_j)^2.$$

The minimum sum of squares RSS_1, say, is given by

$$\mathrm{RSS}_1 = v^T (W - H) v.$$

Here, $H = WX(X^T WX)^{-1} X^T W$ is the weighted "hat" matrix based on the $J \times 3$ design matrix

$$X = \left[\mathbf{1}\ \boldsymbol{c}\ \boldsymbol{s}\right]$$

where $\mathbf{1}$ is a vector of ones, and $\boldsymbol{c}$ and $\boldsymbol{s}$ are vectors with entries $-\cos\theta_j$, $-\sin\theta_j$. The matrix $W = \mathrm{diag}(w_j)$ is a diagonal matrix containing the weights. The parameter estimates are given by

$$\begin{bmatrix} \hat{a}_0 \\ \hat{a}_1 \\ \hat{a}_2 \end{bmatrix} = (X^T WX)^{-1} X^T W \boldsymbol{v},$$

where $\boldsymbol{v}$ is a vector containing the v_j.

4.2 Estimation for the Angular Model

The angular differences $\phi_j - \theta_j = \eta_j$, say, can be modeled using a normal distribution

$$\eta_j = \phi_j - \theta_j \sim N(\psi, \sigma_j^2/w_j) \mod 2\pi.$$

However, since angles are only defined up to a multiple of 2π, it is more convenient, and nearly equivalent, to express the model in terms of the von Mises distribution

$$\eta_j \sim VM(\psi, \kappa_j),$$

with mean direction ψ and concentration parameter $\kappa_j = w_j \kappa$, where $\kappa = 1/\sigma^2$.

If the weights κ_j are treated as known, the log-likelihood for ψ becomes

$$\sum \kappa_j \cos(\eta_j - \psi) - K = \sum \kappa_j \{\cos \eta_j \cos \psi + \sin \eta_j \sin \psi\} - K$$
$$= (\sum \kappa_j)\{\overline{C} \cos \psi + \overline{S} \sin \psi\} - K,$$

where $K = \sum \log\{2\pi I_0(\kappa_j)\}$, and

$$\overline{C} = \sum (w_j \cos \phi_j) / \sum w_j, \quad \overline{S} = \sum (w_j \sin \phi_j) / \sum w_j.$$

The maximizing value of ψ is atan2$(\overline{S}, \overline{C})$. If we define

$$\mathrm{RSS}_2 = 2(\sum w_j)(1 - \overline{R}) = 2\sigma^2(\sum \kappa_j)(1 - \overline{R})$$

where $\overline{R} = \{\overline{C}^2 + \overline{S}^2\}^{1/2}$ is the weighted resultant length, then the maximized log-likelihood becomes

$$-\frac{1}{2\sigma^2}\mathrm{RSS}_2 - K + \sum \kappa_j.$$

Once ψ and α have been estimated, then β can be estimated using the identity $\psi = \beta - \alpha$.

4.3 Overall Estimation

Maximum likelihood estimation for the overall model requires several additional considerations.

(a) (Known seeds) Assume the seeds μ and ν are known. Define an overall "residual sum of squares"

$$\mathrm{RSS} = \mathrm{RSS}_1 + \mathrm{RSS}_2. \tag{18}$$

Then using the approximation (12), the log-likelihood maximized over the parameters a_0, a_1, a_2, ψ (or equivalently, over a_0, b, α, β) is given up to a constant term by

$$l = -\frac{1}{2}\{\mathrm{RSS}/\sigma^2 + 2J \log \sigma^2 - 2 \sum \log w_j\}. \tag{19}$$

Further, maximizing (19) over σ^2 yields a profile log-likelihood

$$l = l(\mu, \nu) = -\frac{1}{2}\{2J + 2J \log(\mathrm{RSS}/(2J)) - 2 \sum \log w_j\}, \tag{20}$$

depending just on the seeds μ and ν.

(b) (Standardization) Unfortunately, the log-likelihood in (20) is not suitable for comparing different seeds. The reason is that the response variables $v_j = \log(s_j/r_j)$ in (13) and $\eta_j = \phi_j - \theta_j$ in (14) measure changes in *relative* positions of the final landmark y_j with respect to the seed ν. To appreciate the problem for fixed data values x'_j, y'_j, $j = 1, \ldots, J$, let the seeds take the form $\mu = \nu = c > 0$, where for simplicity attention is restricted to the case c real. Then for large c, $v_j \approx (|y'_j| - |x'_j|)/c$ and $\eta_j \approx \mathrm{Im}(x'_j - y'_j)/c$. For the multiplicative model, $w_j = 1$ and so $\mathrm{RSS} = O(1/c)$ for large c. For both of the additive models, $w_j \approx c^2$ and $\mathrm{RSS} = O(1)$. In all three cases, (20) is approximately $-\frac{1}{2}\{-2J\log(c^2)\} = J\log(c^2) \to \infty$ as $c \to \infty$. That is, the likelihood is maximized at the singular solution $c = \infty$.
The solution is to scale the response variables v_j and η_j to $|y_j|v_j$ and $|y_j|\eta_j$ so that they measure changes in *absolute* positions instead of relative positions. The effect on the log-likelihood is to include an extra term. The profile log-likelihood for the scaled responses becomes

$$l^{\mathrm{scaled}} = l^{\mathrm{scaled}}(\mu, \nu) = -\frac{1}{2}\{2J + 2J\log(\mathrm{RSS}/(2J)) - 2\sum \log w_j + 2\sum \log w_j^{(y)}\}. \quad (21)$$

(c) (Regularization) However, there is additional problem that arises when using (21) to compare different seeds. If the seed ν converges to one of the y_j, then the corresponding log weight diverges, $\log w_j^{(y)} \to -\infty$. Thus for the multiplicative model and the additive-in-x model, the log-likelihood has a singular maximum at this limiting choice of seed.
The basic cause of the problem is that the polar decomposition of the error model breaks down when the radial value is close to 0. A simple way to resolve the problem is to "regularize" the log-likelihood by approximating $J^{-1}\sum \log w_j$, the log of the geometric mean of the weights, by $\log(J^{-1}\sum w_j)$, the log of the arithmetic mean. This substitution yields the "regularized" scaled log-likelihood

$$\begin{aligned} l^{\mathrm{scaled,reg}} &= l^{\mathrm{scaled,reg}}(\mu, \nu) \\ &= -\frac{1}{2}\left\{2J + 2J\log(\mathrm{RSS}/(2J)) - 2J\log(J^{-1}\sum w_j) + 2J\log(J^{-1}\sum w_j^{(y)})\right\}. \end{aligned} \quad (22)$$

This approach works for all three models. However, note that for the additive-in-y model, the final two terms in (21) cancel one another out and it does not matter whether or not the scaled log-likelihood is regularized. In this case Eqs. (21) and (22) are identical to one another.

(d) (Optimization) The value of $-l^{\mathrm{scaled,reg}}(\mu, \nu)$ can then be minimized numerically over the four parameters $\Re(\mu)$, $\Im(\mu)$, $\Re(\nu)$, $\Im(\nu)$, e.g., using the black-box minimizer `nlm` from R. Once μ and ν have been estimated, the regression parameters a_0, a_1, a_2 and the angular parameter ψ can be estimated using Sects. 4.1 and 4.2, respectively. Call the resulting estimator the approximate maximum likelihood estimator (AMLE).

(e) (Interpretation) Estimates of the regression and variance parameters are reported using the definitions in Sect. 4.2. That is, they are not affected by the scaling of the response variables introduced in (21). Further, since the FEC model has eight parameters, an "unbiased" estimate of the error variance can be defined by

$$\hat{\sigma}^2 = \frac{\text{RSS}}{2J - 8} \tag{23}$$

where RSS is defined by (18).

(f) (Standard errors) Once the parameters have been estimated by the AMLE, it is important to include standard errors. These can be obtained as follows. Sections 4.1 and 4.2 discuss optimization over the regression parameters a_0, a_1, a_2 and the angular parameter ψ, respectively. If these parameters are left in the model, then a version of the approximation (22) is obtained for the log-likelihood, where RSS depends on these parameters, as well as the four parameters in μ and ν. Differentiating this version of (22) twice numerically at the AMLE and changing the sign yields the 8×8 approximate observed Fisher information matrix, I_{obs}, say. Inverting I_{obs} gives the approximate variance matrix, $\hat{\Sigma}$, say for the AMLE. In particular, the square roots of the diagonal elements give the standard errors.
Further, the 2×2 submatrix of $\hat{\Sigma}$ for the real and imaginary parts of the seed μ can be used to construct a confidence ellipse for μ (and similarly for ν).

5 Outline Data

In general, an object in the plane can be represented either by a continuous outline or by a finite set of landmarks. So far the paper has focused on the landmark case.

Mathematically, an outline can be represented as a continuous curve $\{f(u) \in \mathbb{C} : u \in I\}$, where the index variable u ranges through an interval $I = [a, b]$. The curve is either open if $f(a) \neq f(b)$, or closed if $f(a) = f(b)$. We note that the index variable is a convenient tool to describe the curve, but is not an essential part of the curve. In particular, the curve can be re-parameterized by any monotone function $\Phi(u)$.

In general, given two curves, it is not possible to match a given point on the first curve to a particular point on the second curve. In Biology, matching points on the two objects are called *homologous* if they have the same biological interpretation. In the landmark case, it has been assumed above that the landmarks are homologous. However, in the outline setting, it is not assumed that any information about homology is available. Fortunately, under the growth model approximate matching can be carried out mathematically.

To proceed further, make the simplifying assumption that X and Y are "star-shaped" about their centers μ and ν respectively. A star-shaped curve can thus be written in polar coordinates with the angular part θ playing the role of the index

variable j. That is, for the X outline, there is a radial function $r(\theta)$ such that we can write

$$x(\theta) = e^{i\theta} r(\theta), \quad \theta \in [\theta^{(0)}, \theta^{(1)}].$$

The curve is closed if $\theta^{(0)} = 0,\ \theta^{(1)} = 2\pi$ and $r(0) = r(2\pi)$. The name "star-shaped" arises because the ray from the center μ at angle $\theta,\ \theta \in [\theta^{(0)}, \theta^{(1)}]$, intersects the X outline exactly once.

A similar representation is assumed to hold for the Y outline with radial function $s(\theta)$ and, for a given value of θ, we declare $x(\theta)$ and $y(\theta)$ to be matched. Of course this matching procedure assumes the registration parameters are known or at least estimated.

The fitting of growth models to outline data is left to future work.

6 Three-Dimensional Version of the Growth Model

It is straightforward to define a three-dimensional version of the growth model. If a direction on the unit sphere in $\mathbb{R}^d$ is represented by a unit vector $\boldsymbol{u}$, say, and if the standard basis directions are represented by the unit vectors

$$\boldsymbol{e}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{e}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{e}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

then, with $\boldsymbol{e}_3$ denoting the polar direction, the growth function L can be written as

$$L(\boldsymbol{u}) = a_0 - b\boldsymbol{u}^T \boldsymbol{e}_3 = a_0 - bu_3.$$

Unfortunately, the elegance of complex arithmetic is no longer available to simplify the fitting procedure.

7 Numerical Considerations

If the seeds μ and ν are known, the estimation of the remaining parameters is straightforward and can be computed using standard linear regression and directional statistics algorithms. However, the estimation of the seed is more challenging. Here are some preliminary recommendations. The objective function is given by changing the sign of the regularized scaled log-likelihood (22).

(a) Start by doing a grid search for the seeds, looking for the smallest value of the objective function.

(b) Then use a black-box optimizer to refine the estimate of the seeds. In this paper, the `nlm` function in R has been used to minimize the objective function. The log-likelihood given in (22), and the parameter is the 4-dimensional pair of seeds.

In general, there do not seem to be numerical problems using the regularized scaled log-likelihood, provided there is enough information in the data to estimate the seeds. However, as illustrated in the next section, there can be a high correlation between the estimates of the seeds μ and ν, making it difficult to estimate them individually.

8 Examples

8.1 Simulated Data

To illustrate the behavior of the fitting algorithm, consider the following simulated data set. The x values at some initial time are given by

$$x_j = (1 + (j-1)/7)\exp(\pi i(j-1)/7), \;\; j = 1, \ldots 8,$$

so that the angular pars are equally-spaced on a semi-circle and the radial parts increase in an arithmetic progression from 1 to 2. The y values at some final time follow the FEC model with $\alpha = \beta = 0$, $a_0 = 1.2, b = 0.2$, with $CN(0, \sigma^2)$ noise, $\sigma = 0.1$.

The additive-in-y FEC model has been fitted, with the results plotted in Fig. 2. In the figure, the two seeds have been shifted to lie at the origin and the configurations have been rotated by the fitted angles $\hat{\alpha}$ and $\hat{\beta}$. Growth is smallest in the vertically upwards direction and largest in the vertically downwards direction. The black numbers closest to the origin correspond to the x configuration. The gray lines show the direction of growth. The red numbers on the gray lines show the fitted y landmarks under the growth model and the green numbers show the actual y configuration.

The estimated regression and angular parameters (with standard errors) are given by $\hat{a}_0 = 1.230$ (0.022), $\hat{a}_1 = 0.163$ (0.027), $\hat{a}_2 = -0.012$ (0.013), $\hat{\psi} = -0.033$ (0.031). Also, $\hat{b} = 0.163$. These estimates are broadly compatible with the true values, though a_1 and b are somewhat under-estimated. The estimated value of a_2 is compatible with the true value $a_2 = 0$ (since $\alpha = 0$). Similarly, the estimated value of ψ is compatible with the true value $\psi = 0$.

Also plotted in Fig. 2 are 95% confidence ellipses for μ (the inner black ellipse) and ν (the outer red ellipse). The seeds are not very tightly determined by the data, even though the noise standard deviation is small. Note the estimated seeds are pushed to the left from their true values. In particular, if the true regression parameters were used in the plot, then landmarks 1 and 8 for x would lie on a vertical line and the true seed for x would lie midway between them. The reason that the seeds are not very accurately determined seems to be due to the high canonical correlations between

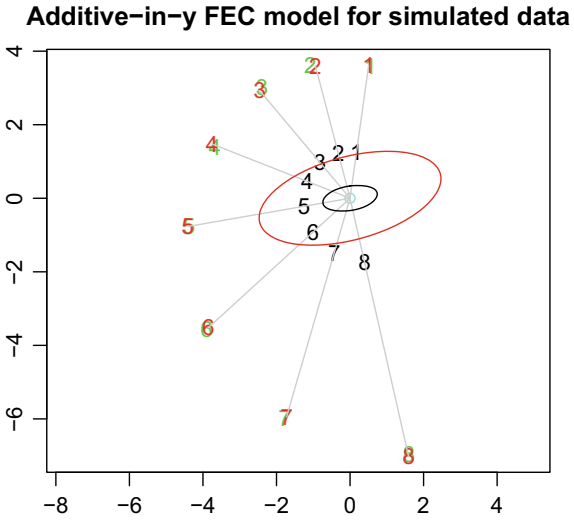

Fig. 2 Additive-in-y FEC model fitted to a simulated data set between an initial time and a final time. The data have been shifted and rotated so that the initial and final seeds are located at the origin and the polar direction is vertical. The black numbers nearest the origin are the initial landmark locations. The red numbers at the end of the gray lines radiating from the origin are the fitted final landmarks under the model. The green numbers are the final landmarks. The black ellipse about the origin represents a 95% confidence region for the initial seed. The larger red ellipse is the corresponding region for the final seed

the estimates of μ and ν (0.981 and 0.980). See, e.g., Mardia et al. (1979, Chap. 10) for a description of canonical correlation.

To save space only the fit from the additive-in-y model has been plotted. However, the figures for the multiplicative and the additive-in-x models are similar.

8.2 Rat Calvarial Data

The data set considered here consists of the position of $J = 8$ biological landmarks from a two-dimensional midsagittal section of the calvarium, (the skull without the lower jaw) from 18 different rats at 8 different ages from birth (7 d old) to adulthood (150 d old). Many researchers have investigated craniofacial growth laws using this data set, e.g., Moss et al. (1983, 1984, 1985), Bookstein (1991), Le and Kume (2000), Kent et al. (2001), Kent and Mardia (2002), Starke et al. (2003), Kenobi et al. (2010), Mardia et al. (2013), Dryden and Mardia (2016), Bookstein (2018).

A detailed description of the data is given in Bookstein (1991, Table 3.4.1) and Bookstein (2018, p. 122). The data can be found in, e.g., Dryden (2019). The landmarks, labeled 1–8, have the following definitions:

1: Bas, Basion 2: Opi, Opisthion
3: IPP, Interparietal Suture 4: Lam, Lambda
5: Brg, Bregma 6: SES, Spheno-ethmoid Synchondrosis
7: ISS, Intersphenoidal Suture 8: SOS, Spheno-occipital Synchondrosis

Landmark 1 lies at the back of the head and landmark 4 lies at the top of the head. The upper part of the jaw lies to the right of landmark 6. Note that landmarks 1, 8, 7, 6 are nearly collinear.

For the purposes of this paper, we ignore any differences between the individual rats and focus only on the changes in size and shape of the "average" configurations obtained by means of Generalized Procrustes analysis of the 18 configurations considered at each of the 8 times. In addition, the data at just the initial and final times are used to fit the FEC model. All three variants of the models (multiplicative, additive-in-x, and additive-in-y) have been fitted. A number of features can be noted.

(a) In each of Figs. 3, 4 and 5, the standardized data have been plotted. In particular, the two seeds lie at the origin and the configurations have been rotated by the fitted parameters $\hat{\alpha}$ and $\hat{\beta}$. Note that the top of the head points roughly upwards in each figure, confirming this aspect of intuition about growth models.

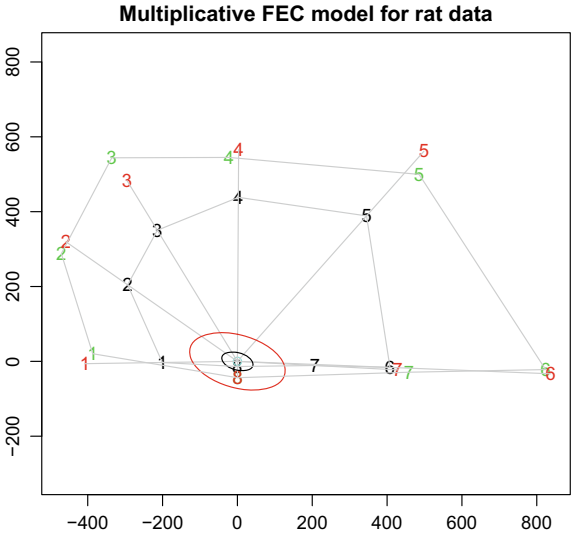

Fig. 3 Multiplicative FEC model fitted to rat data between the initial time and the final time. The data have been shifted and rotated so that the initial and final seeds are located at the origin and the polar direction is vertical. The black numbers nearest the origin are the initial landmark locations. The red numbers at the end of the gray lines radiating from the origin are the fitted final landmarks under the model. The green numbers are the final landmarks. The initial landmarks have been joined by a gray polygon; similarly for the final landmarks. The black ellipse about the origin represents a 95% confidence region for the initial seed. The larger red ellipse is the corresponding region for the final seed

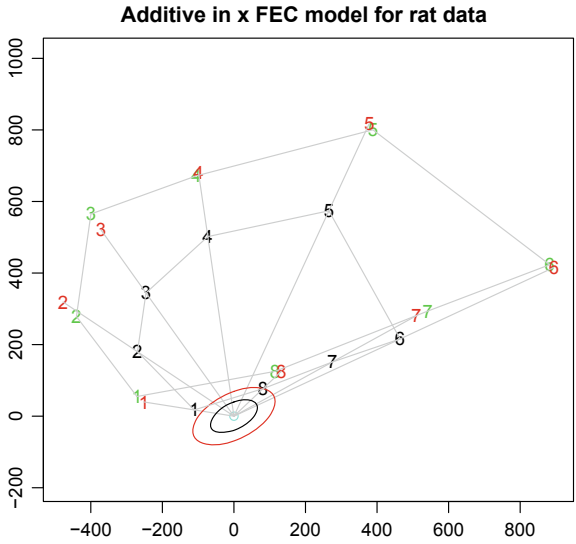

Fig. 4 Additive-in-x FEC model fitted to rat data between the initial time and the final time. See caption to Fig. 3 for more explanation

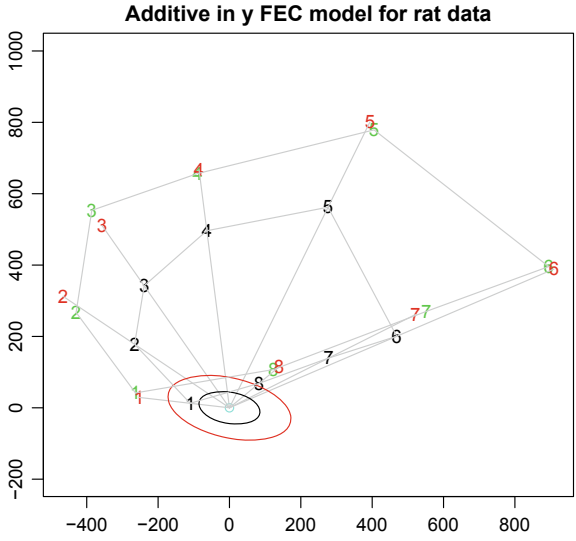

Fig. 5 Additive-in-y FEC model fitted to rat data between the initial time and the final time. See caption to Fig. 3 for more explanation

Growth is smallest in the vertically upwards direction and largest in the vertically downwards direction.

(b) The black numbers closest to the origin correspond to the initial configuration. The gray lines show the direction of growth. The red numbers on the gray lines show the fitted landmarks at the final time under the growth model and the green numbers show the final configuration.

Table 1 The fitted regression parameters (with standard errors and p-values) for the multiplicative, additive-in-x, and additive-in-y FEC models. Also given is the maximized log-likelihood for each model

Par	Mult	Add-x	Add-y
$\hat{a}_0$	0.702 (0.043)	0.916 (0.072)	0.903 (0.067)
$\hat{a}_1$	0.441 (0.055)	0.607 (0.068)	0.602 (0.067)
$\hat{a}_2$	0.071 (0.044)	−0.119 (0.060)	−0.106 (0.058)
$\hat{\psi}$	−0.041 (0.028)	−0.031 (0.024)	−0.037 (0.027)
log-lik	−61.85	−57.77	−58.21

(c) The estimated seeds for x and y lie just above landmark 8 for the multiplicative model, and below the line segment connecting landmarks 1 and 8 for both additive models. These locations (for rats) are broadly similar to one another, but they go against the intuition for human heads, where it is expected the seeds would lie nearer the top of the skull.

(d) At first sight the models appear to fit reasonably well. However, remember the model contains 8 parameters and the data contain $2J = 16$ degrees of freedom, where $J = 8$ is the number of landmarks. Hence, there is considerable scope for overfitting.

(e) Although the three models are non-nested, it is still interesting to compare their log-likelihoods. The multiplicative model has the smallest log-likelihood and the additive-in-x model the largest. In particular,

$$2(l_{\text{add-x}} - l_{\text{mult}}) = 8.16, \quad 2(l_{\text{add-x}} - l_{\text{add-y}}) = 0.88.$$

Hence, the additive models are similar to one another, and both are considerably better than the multiplicative model. (Taking χ^2_1 as an approximate benchmark distribution, note that $8.16 > 3.84$, the upper 5% critical value of χ^2_1.)

(f) By construction, the maximum growth rate in each figure is greatest in the vertically downwards direction. For the multiplicative model there is only one landmark below the seed (landmark 8). Since this landmark is very close to the seed for both x and y, the data provide only limited confirmation of the model in the downwards direction. The situation is even more extreme for the two additive models; there are no landmarks below the seeds.

(g) The fitted regression parameters (with standard errors) are given in Table 1. All three models have a similar interpretation. First $\hat{a}_2$ is compatible with a population value of 0, so no rotation of the x-configuration is needed to fit the growth model. Since $\hat{a}_0$ is significantly different from 0, there is no supporting evidence for an exponential version of the CS model. It is also reasonably clear in each case that $\hat{a}_0$ is significantly different from both $\hat{a}_1$ and $\hat{b}$. Hence, there is no supporting evidence for an exponential version of the RCS strain model. Finally, $\hat{\psi}$ is compatible with a population value of 0, so there is no need for a

rotation of the y-configuration (more specifically, there is no need to rotate the x- and y-configurations differently from one another).

(h) Also plotted in Figs. 3, 4 and 5 are 95% confidence ellipses for μ (the inner black ellipse) and ν (the outer red ellipse). Hence, the seeds are not very tightly determined by the data.

(i) Moss et al. (1983) fitted a similar growth model with an estimated seed between landmarks 7 and 8.

(j) In summary, at first sight the FEC growth model(s) seem to provide a plausible fit to the data. However, the argument for a biological interpretation of the seeds is not very convincing as the seeds lie near the boundary (multiplicative model) or even outside the convex hull of the landmarks (additive models). Further, it is important not to read too much into the fitted model. For data with a limited number of landmarks such as the rat data, there is a tendency to overfitting.

9 Conclusions

Mathematically, the FEC growth model proposed here is more elegant and tractable than earlier approaches. This paper has simplified one key aspect of the fitting process. If the seeds are known, then standard closed-form estimators can be used for the remaining parameters in the model. Thus, issues relating to the estimation of the seeds can be separated from the estimation of the remaining variables.

If a single model is to be used, then the additive-in-y model has several appealing features. It is closest in character to standard regression models since the errors are defined on the same scale as the response variable. Also, it is simpler to describe than the other models since the regularization step in Sect. 4.3 is not needed. That is, it makes no difference to the log-likelihood whether or not the weights are regularized. Further, for the examples considered here, the fit is as good as or better than the other two models.

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A Flexible Family of Mixed Distributions for Discrete Linear and Continuous Circular Random Variables

Ashis SenGupta, Kunio Shimizu, Seng Huat Ong, and Radhakanta Das

Abstract Probability distributions on the circle have been of long interest, see, e.g., Rao (1973). We extend this class of distributions to that for the joint distribution of a discrete linear and a continuous circular random variables, which is not in the support of a smooth manifold. The need of such distributions is widely recognized, for example, that for enhancing errors-in-variables regression models with count and circular variables. A new method of constructing these distributions is proposed and shown to produce simple analytical forms. Several properties of this family are established. Independence is elegantly characterized by the nullity of a linear-circular correlation coefficient and equivalently, by the nullity of a scalar dependency parameter. Relevant statistical inference procedures are derived. A real-life example with count data on traffic accidents over different times of the day, which necessitates a weighted distribution (Rao 1965) version of the proposed new distribution, is presented and analyzed.

Keywords Circular-linear distribution · Count data · Linear-circular correlation coefficient · Test of independence · Traffic accidents

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1 Introduction

Professor C.R. Rao in his seminal book Linear Statistical Inference and Its Application (Rao 1973, pp. 175–178) discusses "Distribution on a Circle". Such distributions are needed to model circular data. The recent emergence of circular, and more generally, directional data for which the observed random vector variable comprises both linear and circular components, has been phenomenal in a variety of modern areas of applied sciences. This has necessitated the development of probability distributions for directional data. The construction of bivariate linear and circular distributions which are not on a smooth manifold are of interest to model jointly linear and circular data in many disciplines. General methods of constructions for bivariate linear distributions are not directly applicable to circular distributions because of the difference in topologies between the line and the circle. SenGupta (2004, 2008, 2010) presented many methods to construct multivariate circular (hyper-toroidal) and cylindrical (see also Seal and SenGupta 2012) distributions. Ong and SenGupta (2012) considered mixture constructions of bivariate circular distributions. Recently, SenGupta and Ong (2014) presented a unified approach which is also based on the mixture method to construct bivariate linear and linear-circular models involving the exponential and the cardioid distributions with the truncated exponential distribution as the mixing distribution.

There exist many examples of bivariate linear and circular distributions in practical applications. For example, air pollution and wind direction data in environmental studies (Johnson and Wehrly 1977, 1978), height and time of arrivals of aphids (locusts) in agricultural research (SenGupta 1996), linear-circular time series model for wave height prediction (Hokimoto and Shimizu 2008), etc., are appropriately modeled by bivariate linear-circular, or cylindrical distributions. Further examples of such data in statistical machine learning are presented for classification of skulls (SenGupta and Ugwuowo 2011), asymmetric angular-linear multivariate regression models (SenGupta and Ugwuowo 2006), etc. In all of the above examples, the linear variables were continuous random variables.

Note, however, that there abound many real-life examples where there is need to study the joint behavior of a discrete linear (or count), X, and a continuous circular random variable, Θ. Such data arise with, e.g., number of arrivals of patients in a hospital, of amphibians in a mating location using lunar phase as a cue (Jarvis et al. 2021), of traffic accidents in a city (Laha et al. 2017), etc., in different time periods. In this paper, possibly as a maiden attempt, we construct a bivariate linear discrete and continuous circular distribution. The proposed bivariate distribution, based on a conditional distribution approach, has a joint pdf which has a basic simple form as a product of the conditional distribution of $X|\Theta$ and the marginal distribution of Θ. However, this form is generalized to generate a large family of flexible distributions. This also facilitates the estimation of parameters.

In Sect. 2, we introduce the new family of mixed bivariate distributions with discrete and circular marginal distributions. A connection with C.R. Rao's weighted distributions is also mentioned briefly. Analytic representation of the normalizing constant of the marginal density of Θ in terms of the Gauss hypergeometric function

${}_2F_1$ is presented. Also, the joint, the marginal, and the conditional densities are studied and further generalizations are discussed here. In Sect. 3, the marginal and the joint moments are derived. Linear-circular correlation and regression are presented in Sect. 4. Section 5 discusses parameter estimation and details the computational procedures and R subroutines needed. In Sect. 6, a result is proven relating a linear-circular correlation measure with the dependency parameter ρ. This in turn enhances a theorem on interesting and useful characterization of independence of the linear random variable X and the circular random variable Θ through ρ. Sect. 7 presents a real-life application of our distribution to the temporal behavior of traffic accidents in a growing industrial city in India. Finally, Sect. 8 gives some concluding remarks and research problems for future research.

2 Mixed Bivariate Distributions with Discrete and Circular Marginal Distributions

Let X and Θ be a discrete linear and a continuous circular random variable, respectively. We define the joint distribution of X and Θ with the mixed probability function

$$f_{X,\theta}(x,\theta) = e^{-\beta y}\frac{(\beta y)^x}{x!}C_r(\rho)y^r,\ x = 0, 1, 2, ...,\ \theta \in [0, 2\pi), \tag{1}$$

where $y = 1 + \rho\cos(\theta - \mu)$, $\beta > 0$, $\mu \in [0, 2\pi)$, $-1 < \rho < 1$, $r \in \mathbb{R}$ and

$$C_r^{-1}(\rho) = \int_0^{2\pi}[1 + \rho\ \cos\theta]^r d\theta.$$

Also for a given ρ, $1 - |\rho| \le y \le 1 + |\rho|$ so that $\forall\rho$, $0 < y < 2$. The role of β is thus to extend the support of the parameter βy of the conditional Poisson distribution to the full range of $(0, \infty)$.

2.1 Marginal Density of Θ

The marginal pdf of Θ is given by

$$f_\Theta(\theta) = C_r(\rho)(1 + \rho\ \cos\theta)^r = C_r(\rho)y^r,\ \theta \in [0, 2\pi),\ |\rho| < 1,\ r \in \mathbb{R}. \tag{2}$$

The above family of distributions may be viewed as a generalization of the cardioid density and was initially proposed by Arnold and SenGupta (2004). Also henceforth, unless otherwise specified, without loss of generality we will take the circular location parameter μ of this pdf of Θ as 0.

Normalizing Constant

The normalizing constant of $f_\Theta(\theta)$ is

$$C_r(\rho) = 1/[2\pi\, {}_2F_1(-r/2, (1-r)/2; 1; \rho^2)]\,,$$

where ${}_2F_1$ denotes the Gauss hypergeometric function. The hypergeometric series terminates if r is equal to a positive integer.

Note 1. If $r \leq 0$, it is obvious that ${}_2F_1(-r/2, (1-r)/2; 1; \rho^2) > 0$. If $r > 0$, it is not obvious that the value of ${}_2F_1$ is positive, but it follows from

$${}_2F_1(a, b; c; z) = (1-z)^{c-a-b}\, {}_2F_1(c-a, c-b; c; z)$$

that

$${}_2F_1(-r/2, (1-r)/2; 1; \rho^2) = (1-\rho^2)^{r+1/2}\, {}_2F_1(r/2+1, (r+1)/2; 1; \rho^2) > 0.$$

Modality

For $\rho = 0$ or $r = 0$, the distribution is a uniform distribution. Otherwise, the distribution is unimodal and symmetric about $\theta = 0$ and π. For $0 < \rho < 1$ $(-1 < \rho < 0)$, it has a unique mode at $\theta = 0$ (π) and an antimode at π (0) if $r > 0$, while if $r < 0$, then it has a unique mode at $\theta = \pi$ (0) and an antimode at 0 (π).

Special Cases

If $r = 0$, the distribution with probability density function (pdf) (2) reduces to a uniform distribution as ${}_2F_1(0, 1/2; 1; \rho^2) = 1$; if $r = 1$, to a cardioid distribution as ${}_2F_1(-1/2, 0; 1; \rho^2) = 1$; if $r = -1$, to a wrapped Cauchy distribution as ${}_2F_1(1/2, 1; 1; \rho^2) = {}_1F_0(1/2; \rho^2) = (1-\rho^2)^{-1/2}$; And if $\rho = \kappa/r$ $(\kappa > 0)$ and $r \to \infty$, the power cardioid density (2) converges to $e^{\kappa \cos\theta}/\{2\pi I_0(\kappa)\}$, which is the density of a von Mises distribution, because ${}_2F_1(-r/2, (1-r)/2; 1; (\kappa/r)^2)$ tends to $I_0(\kappa)$ as r goes to infinity, where $I_0(\cdot)$ denotes the modified Bessel function of the first kind and order zero. With the choice of $\rho = \tanh(\kappa\psi)$ and $r = 1/\psi$, $\kappa \geq 0$, $\psi \in \mathbb{R}$, the circular pdf studied by SenGupta (2010) also becomes yet another special case as a member of the power cardioid family.

2.2 Marginal Distribution of X

The joint distribution of X and Θ is

$$f_{X,\Theta}(x, \theta) = \frac{1}{x!} e^{-\beta(1+\rho\,\cos\theta)} \beta^x (1+\rho\,\cos\theta)^x C_r(\rho)(1+\rho\,\cos\theta)^r,$$

$$\theta \in [0, 2\pi),\ \beta > 0,\ |\rho| < 1,\ r \in \mathbb{R}.$$

Then, the marginal probability mass function (pmf) of X is

$$p_X(x) = \int_0^{2\pi} f_{X,\Theta}(x,\theta)d\theta$$
$$= \frac{C_r(\rho)}{x!}\int_0^{2\pi} e^{-\beta(1+\rho\,\cos\theta)}\beta^x(1+\rho\,\cos\theta)^x(1+\rho\,\cos\theta)^r d\theta.$$

Now writing $u = (1+\rho\,\cos\theta)$, $a(\rho) = 1-|\rho|$ and $b(\rho) = 1+|\rho|$, it is obvious that as θ covers $[0, 2\pi)$, u traverses $[a(\rho), b(\rho)]$ twice. The integrand is an even function. Also, $|\frac{d\theta}{du}| = \{\rho^2-(u-1)^2\}^{-\frac{1}{2}}$. Hence, after denoting the functions $G(\cdot)$ and $g(\cdot)$ as the cdf and pdf of Gamma $(x+r+1, \beta)$ distribution, respectively, we have

$$p_X(x) = \frac{2\beta^x C_r(\rho)}{x!}\int_{a(\rho)}^{b(\rho)} \{\rho^2-(u-1)^2\}^{-\frac{1}{2}} e^{-\beta u}u^{x+r}du$$
$$= \frac{2C_r(\rho)\Gamma(x+r+1)}{x!\beta^{r+1}}\int_{a(\rho)}^{b(\rho)} \{\rho^2-(u-1)^2\}^{-\frac{1}{2}} g(u)du$$
$$= \{G(b(\rho))-G(a(\rho))\}\frac{2C_r(\rho)\Gamma(x+r+1)}{x!\beta^{r+1}}\int_{a(\rho)}^{b(\rho)} \frac{g^T(u)}{\sqrt{\rho^2-(u-1)^2}}du,$$

where $g^T(u)$ denotes the pdf of a truncated Gamma $(x+r+1, \beta)$ distribution having support $[a(\rho), b(\rho)]$. Now writing

$$D_r(x;\rho,\beta) = E\left(\{\rho^2-(U-1)^2\}^{-\frac{1}{2}}|U\sim g^T(x+r+1,\beta)\right),$$

the marginal pmf of X can be expressed as

Result 1. $p_X(x) = 2\{G(b(\rho))-G(a(\rho))\}\frac{\Gamma(x+r+1)}{x!\beta^{r+1}}C_r(\rho)D_r(x;\rho,\beta)$,
$x = 0, 1, 2, \ldots$

2.3 Generalizations

We now discuss some interesting and useful aspects, including generalizations, of our proposed model given in (1) as itemized below.

1. β is used to get the full support of Poisson parameter on $(0,\infty)$, since $\forall\rho,\ y \in (0, 2)$.

2. Truncated Mixed distribution is often motivated by practical applications, e.g., number (count) of incidences exceeding a threshold such as with number of accidents, patients, migratory animals, etc., over time. We will analyze such a data set later.
3. Kernel of any circular pdf will work for the multiplier of β to yield the dependence between X and Θ through the Poisson parameter. The von Mises kernel may not be analytically attractive. However, we may replace the power cardioid kernel by $1 + \rho\ \cos[\theta + \lambda\ \cos\theta]$ to get an asymmetric family ($\rho \in (-1, 1), \neq 0$), with different peakedness by varying $\lambda \in [-1, 1]$. The kernel for Batschelet distributions (Batschelet 1981) is an attractive choice: $1 + \rho\ \cos[\theta + \lambda\ \sin\theta]$. It gives a flexible family with extended platy- and sharply lepto- kurtic / flat-topped and highly peaked unimodal symmetric distributions. Observe that these distributions can be constructed from a known circular density $f(\theta)$ by deriving the generated pdf $f^G(\theta) \equiv f(\psi(\theta))$, for some bijective function $\psi(\cdot)$. For example, our power cardioid kernel can be replaced by Batschelet's kernel,

$$K_\psi(\theta) = 1 + \rho\ \cos(\psi(\theta)), \quad \psi(\theta) = \theta + \lambda\ \sin\theta,$$

   to model a family of symmetric flat-topped circular densities. Note that here the number of parameters increases by 1 due to the inclusion of the parameter λ.
4. In practice, it may be meaningful or even necessary sometimes to consider a restricted support for X or θ. The concept of weighted distribution was enhanced by Prof. C.R. Rao through his pioneering works (Rao, 1965). Briefly, given the pdf $g(x; \eta)$ of a random variable X, a corresponding weighted distribution $f(x; \eta)$ for a properly defined weight function w(x) is obtained as

$$f(x; \eta) = w(x)g(x; \eta)/E_\eta(w(X)).$$

   As a special case, letting $w(x) = I(x \in \mathcal{C})$ where $I(\cdot)$ is the indicator function, we get $f(x; \eta)$ to be the truncated distribution of X defined on the support $\mathcal{C}$. Our joint distribution defined in (1) easily admits of such a truncated marginal distribution. The related computational details will be discussed in Sect. 5.1.
5. Asymmetric kernels, as mentioned above, can be useful in practice. However, this may require non-trivial computations. For example, even the estimation of the location parameter there will be more involved compared to our simple estimator of μ above as the sample mean direction in the symmetric case. Note that appealing results on marginal moments, e.g., Theorem 1(a) below, will not hold. Further, computation of the joint moments also, and hence the inference procedures, may not lead to elegant and conveniently implementable results. Thus, this case will be treated elsewhere to derive useful results.

Using the above notations and with known $f(\theta)$, our general approach is to use a bivariate model which may be represented as

$$g_{\Theta,X}(\theta, x) = Poi_X(x|\Theta = \theta; \beta K_*(\theta))\, f_\Theta(\psi(\theta); \boldsymbol{\delta}), \tag{3}$$

where K_* is the kernel and $\boldsymbol{\delta}$ is the parameter vector for the generated pdf $f_\Theta(\psi(\theta))$ obtained from the original pdf $f_\Theta(\theta)$ of Θ.

2.4 Conditional Distributions

Conditional pdf of Θ given $X = x$ is obtained as

$$f_\Theta(\theta|x) = \frac{\beta e^{-\beta y}(\beta y)^{x+r}}{2\{G(b(\rho)) - G(a(\rho)\}\Gamma(x+r+1)D_r(x;\beta,\rho)}\ ,\ \theta \in [0, 2\pi).$$

Conditional pmf of X given $\Theta = \theta$ is obtained as

$$f_X(x|\theta) = e^{-\beta y}(\beta y)^x/x!.$$

Independence

Independence occurs only under circular uniformity, i.e., $\rho = 0$, of Θ. Then, X reduces to a Poisson random variable (rv) with parameter β.

3 Moments

We present below both the marginal and joint moments of X and Θ under model (1). As will be seen from the latter section, these moments will play a pivotal role in developing inference procedures under this model.

3.1 Moments of $\boldsymbol{\Theta}$

The trigonometric moments of the circular random variable Θ are given in

Theorem 1 *(a) The qth sine moment of* Θ *is zero.*
(b) For a positive integer r,

$$E[\cos(q\Theta)] = \begin{cases} C_r(\rho)2\pi\left(\frac{\rho}{2}\right)^q \sum_{k=0}^{[(r-q)/2]} \binom{r}{k}\binom{r-k}{q+k}\left(\frac{\rho}{2}\right)^{2k}, & r \geq q, \\ 0, & r < q, \end{cases}$$

where $[z]$ *denotes the greatest integer less than or equal to z. For values of r different from a positive integer,*

$$E[\cos(q\Theta)] = \frac{(-r)_q\,(-\xi)^q}{q!}\,\frac{{}_2F_1(-r, q-r; q+1; \xi^2)}{{}_2F_1(-r, -r; 1; \xi^2)}$$
$$= \frac{(-r)_q\,(-\rho)^q}{2^r q!(1+\sqrt{1-\rho^2})^{q-r}}\,\frac{{}_2F_1(-r, q-r; q+1; \xi^2)}{{}_2F_1(-r/2, (1-r)/2; 1; \rho^2)}$$

with $\xi = \rho/(1+\sqrt{1-\rho^2})$, $q = 1, 2, \cdots$ *($(\cdot)_q$ denotes Pochhammer's symbol).*

Proof (a) This result follows by symmetry of the pdf around 0.
(b) From Eq. 3.616.4 of Gradshteyn and Ryzhik (2007), we have

$$\int_0^\pi (1-2a\cos x + a^2)^n \cos(mx)dx = \frac{1}{2}\int_0^{2\pi} (1-2a\cos x + a^2)^n \cos(mx)dx$$
$$= \begin{cases} \pi(-a)^m(1+a^2)^{n-m} \displaystyle\sum_{k=0}^{[(n-m)/2]} \binom{n}{k}\binom{n-k}{m+k}\left(\frac{a}{1+a^2}\right)^{2k}, & n \geq m, \\ 0, & n < m, \end{cases}$$

we have the result for a positive integer r. For the others, from Eq. 9.112 of Gradshteyn and Ryzhik (2007), we have

$${}_2F_1(p, p+n; n+1; x^2) = \frac{x^{-n}}{2\pi}\frac{\Gamma(p)n!}{\Gamma(p+n)}\int_0^{2\pi} \frac{\cos(nt)}{(1-2x\cos t + x^2)^p}\,dt$$

for $n = 0, 1, 2, \ldots;\ p \neq 0, -1, -2, \ldots;\ |x| < 1$ is used. Then,

$${}_2F_1(p, p+n; n+1; x^2) = \frac{x^{-n}}{2\pi}\frac{n!}{(p)_n}\int_0^{2\pi} \frac{\cos(nt)}{(1+x^2)^p[1-\{2x/(1+x^2)\}\cos t]^p}\,dt$$
$$= \frac{n!}{2\pi(p)_n x^n(1+x^2)^p}\int_0^{2\pi} \frac{\cos(nt)}{(1-z\cos t)^p}\,dt$$

with $z = 2x/(1+x^2)$, or $x = z/(1+\sqrt{1-z^2})$. Here, Pochhammer's symbol $(p)_n = p(p+1)\cdots(p+n-1) = \Gamma(p+n)/\Gamma(p)$. Thus,

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{\cos(nt)}{(1-z\cos t)^p}\,dt = \frac{(p)_n x^n(1+x^2)^p}{n!}\,{}_2F_1(p, p+n; n+1; x^2)$$
$$= \frac{2^p(p)_n z^n}{n!(1+\sqrt{1-z^2})^{p+n}}\,{}_2F_1(p, p+n; n+1; x^2).$$

When $n = 0$ as a special case, we have

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{1}{(1-z\cos t)^p}\,dt = (1+x^2)^p\,{}_2F_1(p, p; 1; x^2).$$

It follows from Eq. 9.134.2 of Gradshteyn and Ryzhik (2007)

$$ {}_2F_1(2\alpha, 2\alpha + 1 - \gamma; \gamma; x) = (1+x)^{-2\alpha}\, {}_2F_1(\alpha, \alpha + 1/2; \gamma; 4x/(1+x)^2), $$

that putting $2\alpha = p$ and $\gamma = 1$, we get

$$ {}_2F_1(p, p; 1; x^2) = (1+x^2)^{-p}\, {}_2F_1(p/2, (p+1)/2; 1; z^2). $$

Hence,

$$ \begin{aligned} \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{(1 - z\cos t)^p}\, dt &= (1+x^2)^p\, {}_2F_1(p, p; 1; x^2) \\ &= {}_2F_1(p/2, (p+1)/2; 1; z^2) \end{aligned} $$

with $z = 2x/(1+x^2)$, or $x = z/(1+\sqrt{1-z^2})$, and we finally have

$$ \begin{aligned} \frac{1}{2\pi}\int_0^{2\pi} (1 + \rho\cos\theta)^r\, d\theta &= (1+\xi^2)^{-r}\, {}_2F_1(-r, -r; 1; \xi^2) \\ &= {}_2F_1(-r/2, (1-r)/2; 1; \rho^2) \end{aligned} $$

with $\xi = \rho/(1+\sqrt{1-\rho^2})$.

Note 2. Equivalent expressions using associated Legendre functions for the normalizing constant and the qth cosine moment are obtainable as there exists the relationship (Gradshteyn and Ryzhik 2007, Eq. 8.772.3)

$$ \begin{aligned} P_\nu^\mu(z) = {} & \frac{1}{\Gamma(1-\mu)} \left(\frac{z-1}{z+1}\right)^{-\mu/2} \left(\frac{z+1}{2}\right)^\nu \\ & \times {}_2F_1\left(-\nu, -\nu - \mu; 1 - \mu; \frac{z-1}{z+1}\right), \quad \left|\frac{z-1}{z+1}\right| < 1 \end{aligned} $$

between the Gauss hypergeometric and associated Legendre functions.

3.2 Moments of X

Computation of marginal moments directly from the marginal distribution of X is inconvenient. However, use of the conditional distribution of X given $\Theta = \theta$ makes it quite convenient. A descending factorial is defined by

$$ n^{(k)} = n(n-1)\cdots(n-k+1) $$

for a nonnegative integer k with $n^{(0)} = 1$. Descending factorial moments for a Poisson distribution with parameter λ are well known. Then, the conditional kth descending factorial moment of X is

$$E[X^{(k)}|\theta] = \lambda^k = [\beta(1+\rho\cos\theta)]^k.$$

The corresponding unconditional moment is then easily given by

$$E[X^{(k)}] = \beta^k C_r(\rho)\int_0^{2\pi}(1+\rho\,\cos\theta)^{k+r}d\theta = \beta^k C_r(\rho)/C_{(k+r)}(\rho).$$

The power moments $E(X^k)$ can be easily obtained recursively from the above factorial moments $E[X^{(k)}]$.

3.3 Joint Moments

We show below that the joint moments of X and Θ, though somewhat involved, are available in analytic form as derived in

Result 2. *The $(k,q)-$th joint descending factorial-cosine moment of (X,Θ) is expressed as*

$$\begin{aligned}
&E[X^{(k)}\cos(q\Theta)]\\
&= \frac{\beta^k(-(k+r))_q\,(-\xi)^q(1+\xi^2)^{-k}}{q!}\,\frac{{}_2F_1(-(k+r),q-(k+r);q+1;\xi^2)}{{}_2F_1(-r,-r;1;\xi^2)}\\
&= \frac{\beta^k(-(k+r))_q\,(-\xi)^q(1+\xi^2)^{-(k+r)}}{q!}\,\frac{{}_2F_1(-(k+r),q-(k+r);q+1;\xi^2)}{{}_2F_1(-r/2,(1-r)/2;1;\rho^2)}.
\end{aligned}$$

Proof The $k-$th descending factorial moment for a Poisson distribution with parameter λ is easily computed as

$$E[X^{(k)}] = \lambda^k.$$

From the formula of the $q-$th cosine moment of the generalized cardioid distribution obtained earlier, the (k,q)th joint descending factorial-cosine moment is computed as follows:

$$\begin{aligned}
E[X^{(k)}\cos(q\Theta)] &= \sum_{x=0}^{\infty}\int_0^{2\pi} x^{(k)}\cos(q\theta)\,f_{X,\Theta}(x,\theta)d\theta\\
&= \beta^k C_r(\rho)\int_0^{2\pi}\cos(q\theta)(1+\rho\,\cos\theta)^{k+r}d\theta,
\end{aligned}$$

from which the first expression stated in the above Result 2 follows by definition of ${}_2F_1(.)$ and the second by a well-known property of it.

4 Linear-Circular Correlation and Regression

We next briefly discuss the correlation and regression measures associated with our model.

4.1 Linear-Circular Correlation

A correlation coefficient for linear-circular random variables motivated by the multiple correlation coefficient for linear variables is given by (see Jammalamadaka and SenGupta (2001)),

$$\eta^2(X, \Theta) = \frac{\rho_{xc}^2 + \rho_{xs}^2 - 2\rho_{xc}\rho_{xs}\rho_{cs}}{1 - \rho_{cs}^2},$$

where

$$\rho_{xc} = \text{Corr}(X, \cos\Theta),\ \rho_{xs} = \text{Corr}(X, \sin\Theta),\ \rho_{cs} = \text{Corr}(\cos\Theta, \sin\Theta).$$

Observe that η^2 greatly reduces to ρ_{xc}^2, since other terms in the above formula vanish due to the symmetry of the circular pdf.

4.2 Linear-Circular Regression

From the above, regression of X on Θ is given in an elegant form,

$$E(X|\theta) = \beta y = \beta(1 + \rho\ \cos\theta).$$

However, regression of Θ on X does not have such a simple form as that of X on Θ.

5 Parameter Estimation

Let (x_i, θ_i), $i = 1, 2, 3, ..., n$ be a random sample of size n from (1). The likelihood function is given by

$$L(\beta, \rho, r) = \prod_{i=1}^{n} \frac{(\beta(1 + \rho\ \cos\theta_i))^{x_i}}{x_i!} C_r(\rho)[1 + \rho\ \cos\theta_i]^r e^{-\beta(1+\rho\ \cos\theta_i)}.$$

The parameters (β, ρ, r) are estimated by numerically maximizing $L(\beta, \rho, r)$, the likelihood function. This will usually call for a set of initial values for the three parameters. Initial estimates $(\widehat{\rho}, \widehat{r})$ for (ρ, r) may be obtained from the marginal likelihood of Θ. Then, an initial estimate $\widehat{\beta}$ of β may be obtained by maximizing $L(\beta, \widehat{\rho}, \widehat{r})$ with respect to β. This set of estimated values $(\widehat{\rho}, \widehat{r}, \widehat{\beta})$ may then be used as an initial set of estimates to start the iterative process to obtain simultaneously the final maximum likelihood estimators (MLEs) of the three parameters. Since the parameter space is open and the likelihood function is regular, the resulting MLEs will be consistent and asymptotically normal (CAN) estimators. Small sample properties of these estimators may be studied separately.

5.1 Computational Details

Here, we consider the general situation where circular data are available in a grouped form and the linear data are censored at $x_0 - 1$. The cases of ungrouped (raw) and uncensored data easily follow from this treatment. The computation of the MLE of μ from the joint likelihood can be non-trivial. However, by noting that the $f(X, \Theta)$ is an even function, we get $E(\sin(\Theta - \mu)) = 0$, leading to the trigonometric moment estimator (TME) of μ as $\hat{\mu} = \bar{\theta}$, the sample mean direction of Θ. In the sequel, to avoid cumbersome computational details, we may adopt $\bar{\theta}$ for the MLE of μ and write $\theta_i \equiv \theta_i - \bar{\theta}$. Some likelihood functions which can be useful for computations are listed below. Observe that initial estimates for r and ρ may be obtained from the marginal distribution of Θ. These may be substituted in the joint likelihood to get an initial estimate of β. These may then be used as an initial set of estimates in the joint likelihood to obtain the final MLEs of the parameter vector (β, ρ, r) by some optimization sub-routine, e.g., *constrOptim* function in R package (R Core Team 2017).

1. For computation of initial value of ρ given particular r, we use marginal likelihood of ρ,

$$l(\rho) = \ln L(\rho | r, \boldsymbol{\theta}) = K_1 + \sum\nolimits_{i=1}^{k} r n_i \ln y_i - N \ln D,$$

   where $\boldsymbol{\theta} = (\theta_1, \theta_2, \cdots, \theta_k)'$, K_1 is a constant, $N = n_1 + \cdots + n_k$ is total frequency, n_i is the frequency of the $i-$th class with mid-point θ_i, and $y_i = 1 + \rho \cos\theta_i$. Denote for brevity,

$$D = \int_0^{2\pi} [1 + \rho \cos\theta]^r d\theta \equiv C_r(\rho)^{-1}.$$

2. For simultaneous computation of initial values of both r and ρ, we use the likelihood $l(r, \rho)$ which has the identical functional form as $l(\rho)$ above, but now r is also treated as an unknown parameter in it.

3. For computation of initial value of β, we may take both r and ρ as the initial values obtained in Item 2 above, and then obtain β by maximizing the joint likelihood,

$$l_1(\beta) = \ln L(\beta | r, \rho, \boldsymbol{\theta}) = K_2 - \beta S_1 + T \ln \beta - S_2,$$

where K_2 is a constant,

$$S_1 = \sum_{i=1}^{k} n_i y_i, \; S_2 = N \ln P(X \geq x_0) \text{ and } T = \sum_{i=1}^{k} \sum_{j=1}^{n_i} x_{ij}.$$

4. For simultaneous computation of MLEs of (r, ρ, β), we maximize the joint likelihood

$$\begin{aligned} l_2(r, \rho, \beta) &= \ln L(r, \rho, \beta | \boldsymbol{\theta}, x_{ij}, \forall (i, j)) \\ &= K_3 - \beta S_1 + T \ln \beta - S_2 + S_3 + S_4 - N \ln D, \end{aligned}$$

where K_3 is a constant, $S_3 = \sum_{i=1}^{k} \sum_{j=1}^{n_i} x_{ij} \ln y_i$ and $S_4 = \sum_{i=1}^{k} r n_i \ln y_i$.

5. The initial value of parameter vector needed for the above numerical optimization using, e.g., method of *constrOptim* sub-routine in R for box constraints (R Core Team 2017) can be taken as the estimated set from Item 3 above.
6. Item 3 encompasses a special setup where the observations on X are censored at $x_0 - 1$. $x_0 = 0$ when there is no truncation. Since the truncated marginal distribution is derived from the original joint distribution (1), no new distribution is warranted for this special setup. For the example in Sect. 7, $x_0 = 10$ and $k = 8$.

6 Characterizations and Tests for Independence

We now present two interesting and useful results below. First, it is shown that the model admits of a single parameter, e.g., ρ, whose nullity is equivalent to the nullity of the linear-circular correlation coefficient η^2. Next, it is shown that this parameter is indeed the dependency parameter, i.e., its nullity is equivalent to the independence of X and Θ. This independence yields a special member of the power cardioid family, e.g., the circular uniform distribution. It maybe worthwhile to recall that similar situations arise with distributions on torus too, i.e., independence can hold only under a special member of the marginal family and not for all its members. For example, for bivariate circular normal (von Mises) distribution, independence occurs with circular normal marginals, which is a special case of the general family of marginals under the general (dependent) joint pdf.

Result 3. $\eta^2(X, \Theta) = 0$ iff $\rho = 0$.

Proof Recall from Sect. 4.1 that for our model, $\eta^2(X, \Theta)$ reduces to ρ_{xc}^2 by virtue of the symmetry of the joint pdf in terms of Θ. Next,

$$E_{X,\Theta}(X\cos\Theta) = \beta C_r(\rho)\int_0^{2\pi} y((y-1)/\rho)y^r d\theta = (\beta/\rho)[E_\Theta(Y^2) - E_\Theta(Y)],$$
$$E_X(X) = \beta E_\Theta(Y) \text{ and } E_\Theta(\cos\Theta) = (1/\rho)[E_\Theta(Y) - 1].$$

Thus,

$$\mathrm{Cov}(X, \cos\Theta) = (\beta/\rho)\mathrm{Var}_\Theta(Y) = (\beta\rho)\mathrm{Var}_\Theta(\cos(\Theta - \mu)),$$

which can be 0 iff $\rho = 0$.

Theorem 2 *X and Θ are independent iff $\rho = 0$ and hence, iff $\eta^2(X, \Theta) = 0$.*

Proof The result follows directly from the form of the joint pdf and Result 3. The necessity part is immediate. For the sufficiency part, note that the joint pdf in (1) can be written as

$$f(\theta, x) = u(x)v(\theta)w(x, \theta),$$

where $w(x, \theta)$ is the only function involving x and θ and is given by

$$w(x, \theta) = (1 + \rho\ \cos\theta)^x.$$

Note that x is an integer and so $w(.) > 0$ is a polynomial of degree x in $\cos\theta$. Thus, we can have the representation $w(x, \theta) = a_1(x)b_1(\theta)\ \forall(x, \theta)$ iff both $a_1(x)$ and $b_1(\theta)$ are constant functions, i.e., iff $\rho = 0$.

Note 3. Some remarks regarding identifiability may be interesting. For the marginal circular pdf, the power cardioid distribution reduces to the circular uniform density for $\rho = 0$ or $r = 0$ or both. This may create identifiability problems, unless either ρ or r is assumed to be non-zero. But the interesting fact is, for the joint likelihood independence occurs only when $\rho = 0$; r has no role.

Theorem 3 *The dependency parameter ρ characterizes the test for independence of Θ and X as the test for $H_0 : \rho = 0$ vs $H_1 : \rho \neq 0$.*

Proof The theorem follows by combining Result 3 and Theorem 2 above.

We can construct the LRT easily since the MLEs are available. Under H_0, substantial simplification results in the joint pdf and there is only one unknown parameter β, and then $\hat{\beta}_0 = \bar{X}$. So, the estimated log-likelihood function under H_0, L_0 is given by,

$$\hat{l}_0 \equiv \ln\hat{L}_0 = -\bar{X} + \sum_{ij}[(\ln\bar{X})(x_{ij}) - \ln(x_{ij}!)] - N\ln(2\pi).$$

Under the unconstrained parameter space, the MLEs of the parameters need to be obtained numerically. Then, denoting the estimated likelihood function by $\hat{L}$, and writing $\ln\hat{L} = \hat{l}$, we have

Theorem 4 *The LR test statistic for testing independence of X and Θ is given by*

$$-2ln\lambda = -2[\hat{l}_0 - \hat{l}].$$

Under H_0, the asymptotic distribution of the LR statistic $-2ln\lambda$ is χ^2_3.

7 Application to a Real-Life Data Set

Considered below, as an example, is a data set (adapted from the portal www.ncrb.gov.in) on number of yearly traffic accidents in 3-hour time periods of a day over 8 years, 2011–2017 (excluding 2012, for which data were not available) in Amritsar, a fast growing industrial city in north India. The interest being on incidence of significant number of accidents, we censored the data set for single-digit accidents, i.e., we took the threshold as 10 (=x_0 in the notation of Sect. 2.3, Item 4) and noted the records for 10 or more yearly accidents. This yielded the corresponding weighted or truncated distribution for $X \geq 10$. There were several years having single-digit number of accidents over certain 3 h time periods and thus these observations got dropped. 3 h time periods were recorded as 0–3, 3–6, …, 21–24. Mapping 24 h to 360°, we have 1 h = 15°, which defines our circular random variable, $\theta \in [0, 360°)$. For example, the mid-point of the first time period is 1.5 h which transforms to 22.5°. These 3 h time periods were mapped to 8 mutually exclusive and exhaustive groups or classes of 45° width each, thus retaining the quantitative nature of the original data. There will be of course the usual unavoidable loss of precision due to this grouping. For simplicity and also since it is not the focus of this paper, we have not invoked the grouping corrections here. The final data set is exhibited below in Table 1. The estimation of the parameters were done following essentially the steps mentioned in Sect. 5. Under unrestricted parameter space, the resulting MLEs were $\hat{\mu} = 3.7317$, $\hat{r} = 1.2793$, $\hat{\rho} = 0.2849$, $\hat{\beta} = 18.5536$. Under $H_0 : \rho = 0$, MLE of the only one unknown parameter is $\hat{\beta}_0 = \sum_{i,j} x_{ij}/N = 19.7907$. Then, $-2 \ln \lambda = 24.3554$ with the p-value of 2.1056e-05, implying that the hypothesis of independence of X and Θ is very strongly rejected. This means, among others, that in Amritsar the incidence of accidents is not isotropic, but rather the time of the day has a significant bearing on the number of occurrences of traffic accidents. These information may be used by the Traffic Department for monitoring and taking preventive/abatement measures in specific time periods to mitigate/compromise the incidence of large number of accidents in those periods (Table 1).

Table 1 Yearly Accidents over 3 h daily time periods

θ_i	No. of accidents (x_{ij})	Frequency (n_i)
22.5	10 11	2
67.5	16 14 15	3
112.5	18 18 19 21 24	5
157.5	16 18 11 16 22 24 28 22	8
202.5	12 15 18 19 30 30 20	7
247.5	16 18 18 24 31 26	6
292.5	15 30 28 36 36 23	6
337.5	13 14 14 11 11 20	6
	Total frequency	$N = 43$

8 Concluding Remarks

This is a maiden contribution to mixed linear—circular distribution. We have enhanced a flexible family of distributions and indicated its appealing generalizations. The family is amenable to ML estimation of its parameters. A significant result obtained is the characterization of independence of X and Θ through the nullity of a linear-circular correlation coefficient, which in turn is characterized by the nullity of a scalar dependency parameter. Such a result is not commonly available in directional distributions. This facilitates the application of LRT for independence. Many practical situations with linear-circular data warrant truncated distributions and we analyze such a data set as on number—time of incidents of traffic accidents. This work exposes the need of generalizations to real-life situations where both the count as well as the circular variable may exhibit distributions which differ in shapes from the ones considered in this paper. An important use of our proposed model lies in the errors-in-variables regression modeling. We intend to pursue some of these topics in our future research.

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Tests of Fit for Wrapped Stable Distributions Based on the Characteristic Function

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Abstract We consider composite goodness-of-fit tests for wrapped stable distributions on the circle with unknown parameters, based on the empirical characteristic function. The tests are implemented in particular for testing goodness of fit of the symmetric stable family against general alternatives. An extensive Monte Carlo study is carried out by using the parametric bootstrap in order to compare the new tests with other existing omnibus tests for goodness of fit, which demonstrates that the tests proposed here perform better against a large variety of alternatives. We then illustrate our methods by applying the tests to a real data set.

Keywords Goodness of fit · Circular distributions · Wrapped stable family · Empirical characteristic function · Parametric bootstrap

1 Introduction

The family of wrapped stable distributions (WSDs) is one of the most flexible models for circular data. Specifically, this four-parameter family of distributions includes symmetric as well as asymmetric members, with varying tail features ranging from the medium-tailed wrapped normal distribution to the wrapped Cauchy distribution with heavier tails, and beyond.

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The most convenient way to introduce the WSD is by means of its characteristic function (CF) which is given by

$$C_{\boldsymbol{\varphi}}(r) = e^{i\mu r - \tau^\gamma |r|^\gamma \{1 - i\delta \mathrm{sgn}(r) \tan(\pi\gamma/2)\}}, \ \gamma \neq 1, \tag{1}$$

$$= e^{i\mu r - \tau |r| \{1 + i\delta \frac{2}{\pi} \mathrm{sgn}(r) \log |r|\}}, \quad \gamma = 1,$$

where (μ, τ) are location and scale parameters, and (γ, δ) are shape and skewness parameters, respectively. We will write $\boldsymbol{\varphi} = (\gamma, \delta, \tau, \mu)$ for the entire vector of parameters, with the parameter space specified by $(\mu, \tau) \in [0, 2\pi) \times (0, \infty)$ and $(\gamma, \delta) \in (0, 2] \times [-1, 1]$. The parameter γ is often called the characteristic exponent and regulates tail behavior. Specifically, smaller values of γ progressively lead from lighter to heavier tails. On the other hand, δ is a skewness parameter, with $\delta = 0$ corresponding to a distribution that is symmetric, while with increasing $|\delta|$, and as δ approaches $+1$ (resp. -1), the density becomes asymmetric to the right (resp. to the left). In this connection, note that as $\gamma \to 2$, the parameter δ loses its significance with $\gamma = 2$ since it leads to the wrapped Normal distribution. The other well-known member of the class of wrapped stable (WS) laws is the wrapped Cauchy distribution for $(\gamma, \delta) = (1, 0)$ which admits a closed-form density, with all other WSDs admitting only series representations for densities. See Jammalamadaka and SenGupta 2001, pp. 44–48 for a brief discussion of these distributions for modeling circular data.

In this article, we suggest a class of goodness-of-fit tests for the family of WSDs which utilizes the CF of these distributions. Specifically, let X be an arbitrary circular random variable. Then on the basis of independent and identically distributed (i.i.d.) copies $X_1, ..., X_n$ of X, we are interested in testing the (goodness-of-fit) composite null hypothesis,

$$\mathcal{H}_0 : X \text{ follows } \mathcal{S}_{\boldsymbol{\varphi}}, \text{ for some } \boldsymbol{\varphi} \in \Phi, \tag{2}$$

against general alternatives, where $\mathcal{S}_{\boldsymbol{\varphi}} = \{S(\cdot; \boldsymbol{\varphi}), \boldsymbol{\varphi} \in \Phi\}$ denotes the family of WSDs with distribution function $S(\cdot; \boldsymbol{\varphi})$, and $\Phi = (0, 2) \times (-1, 1) \times [0, 2\pi) \times (0, \infty)$.

We note that the CF of an arbitrary linear random variable at a given integer argument $r = 1, 2, ...$ is equal to the trigonometric moment of order r of the corresponding distribution wrapped around the unit circle (see, e.g., Proposition 2.1 in Jammalamadaka and SenGupta 2001). Although this connection of the CF with circular distributions has been noticed early on by Epps (1993), its use for performing statistical inference in the circular context has been hitherto mostly confined to the case of testing for uniformity or symmetry. The reader is referred to the early work of Beran (1969), and to the more recent contributions of Pycke (2010) and Meintanis and Verdebout (2019), and references therein. This is despite the fact that for conventional stable distributions on the real line, CF-based methods have proved to be more convenient to apply and have been shown to compete well with other methods; see Csörgő (1987), Koutrouvelis and Meintanis (1999), Matsui and Takemura (2008), Meintanis (2005), and Meintanis et al. (2015).

The article is organized as follows. In Sect. 2, we introduce the new test procedure for goodness of fit for wrapped stable distributions, while in Sect. 3, we focus on testing for the symmetric WSD against general alternatives and study it in detail. In Sect. 4, finite-sample properties and comparisons with some existing procedures are elaborated using an appropriate resampling version of the test and by means of a Monte Carlo study. In Sect. 5, we consider a practical application, and finally end in Sect. 6 with a brief discussion and conclusions.

2 Tests Based on the Characteristic Function

In order to test the null hypothesis $\mathcal{H}_0$ specified in (2), we propose to use a distance between the CF of the WS law given in (1) and the empirical CF based on the data, defined for integers r, by

$$C_n(r) = \frac{1}{n}\sum_{j=1}^{n} e^{\mathrm{i}rX_j} := \alpha_n(r) + \mathrm{i}\beta_n(r), \mathrm{i} = \sqrt{-1}, \tag{3}$$

where

$$\alpha_n(r) = \frac{1}{n}\sum_{j=1}^{n}\cos(rX_j), \quad \beta_n(r) = \frac{1}{n}\sum_{j=1}^{n}\sin(rX_j) \tag{4}$$

are the Cartesian coordinates of the empirical CF. $\alpha_n(r)$ and $\beta_n(r)$ are also called the empirical trigonometric moments.

We now take into consideration two important facts, namely (i) for circular distributions, the CF needs to be evaluated only at the integers (see, e.g., Jammalamadaka and SenGupta 2001, Sect. 2.2) and (ii) the CF as well as the empirical CF enjoy certain symmetry, namely that their value evaluated at arbitrary integers r and $-r$ are a pair of complex conjugates. In view of this, our test statistic can be formulated to compare just the non-negative theoretical and empirical trigonometric moments. Specifically, we suggest rejecting the null hypothesis $\mathcal{H}_0$ for large values of the test statistic

$$T_{n,f} = n\sum_{r\geq 0}\left|C_n(r) - C_{\widehat{\boldsymbol{\varphi}}}(r)\right|^2 f(r), \tag{5}$$

where $\widehat{\boldsymbol{\varphi}}$ is a suitable estimator of the parameter $\boldsymbol{\varphi}$, and $f(\cdot)$ denotes a "weight function" which we may take to be a probability function over the non-negative integers.

Remark 1 We note that in some of these definitions and quantities, there is no loss in omitting the term $r = 0$ and considering the index r running over $r = 1, 2, \ldots$. However, this is not the case in every subsequent equation so we decided to consider $r \geq 0$ throughout.

Remark 2 If the parameter φ is fixed (known), the test statistic proposed above is equivalent to the test statistics which measure the squared length between the uniform distribution function and the empirical distribution function; see Beran (1969). This is not the case, however, for distributions with estimated parameters since then such tests cannot be reduced to testing uniformity even asymptotically; see Jammalamadaka et al. (2019) for a detailed analysis.

By straightforward algebra, (5) may be re-written as

$$T_{n,f} = n \sum_{r\geq 0} \left\{ |C_n(r)|^2 + \left|C_{\widehat{\boldsymbol{\varphi}}}(r)\right|^2 - 2\left(\alpha_n(r)\alpha_{\widehat{\boldsymbol{\varphi}}}(r) + \beta_n(r)\beta_{\widehat{\boldsymbol{\varphi}}}(r)\right)\right\} f(r), \quad (6)$$

where $\alpha_{\boldsymbol{\varphi}}(r)$ and $\beta_{\boldsymbol{\varphi}}(r)$ denote the population trigonometric moments of the WS law, and $|z|^2$ stands for the modulus of a complex number z.

3 Tests for the Symmetric WSD

Although the test as proposed in (5) is for the general case, the analytics for the case of testing *symmetric* wrapped stable (SWS) distributions happen to be considerably simpler, and we focus on this particular subclass and develop it in detail, in this section.

3.1 The Test Statistic and Consistency for SWS Family

By a proper location shift, we can simplify the problem to testing the null hypothesis that $\mathcal{H}_0^{(\mathrm{s})} : C \equiv C_{\gamma,\tau}$ where $C_X(r) = \mathbb{E}(e^{\mathrm{i}rX})$ is the CF of X and $C_{\gamma,\tau}(\cdot)$ denotes the CF of the zero-location SWS law that results from (1) by replacing $\boldsymbol{\varphi}$ by $(\gamma, 0, \tau, 0)$. In fact, since the population resultant length ϱ is equivalent to $\exp\{-\tau^\gamma\}$, the test statistic figuring in (5) may conveniently be reparameterized as

$$T_{n,f} = n \sum_{r\geq 0} \left| \widehat{C}_n(r) - \widehat{\varrho}^{\,r^{\widehat{\gamma}}} \right|^2 f(r) := n\Delta_{n,f}, \quad (7)$$

where $\widehat{C}_n(r)$ is the empirical CF resulting from (3) by replacing X_j by

$$Y_j = X_j - \widehat{\mu}, \;\; j = 1, ..., n, \quad (8)$$

and where $\widehat{\gamma}$, $\widehat{\mu}$, and $\widehat{\varrho}$ denote consistent estimators of the parameters γ, μ, and ϱ, respectively (discussed later in Sect. 3.3).

Before going any further, we will investigate the consistency of the test based on $T_{n,f}$ against all fixed alternative circular distributions. To this end, we assume

that (i) the estimator $\widehat{\boldsymbol{\varphi}}^{(\mathrm{s})} := (\widehat{\gamma}, \widehat{\varrho}, \widehat{\mu})$ attains a strong probability limit, say $\boldsymbol{\varphi}_{\mathrm{A}}^{(\mathrm{s})} := (\gamma_{\mathrm{a}}, \varrho_{\mathrm{a}}, \mu_{\mathrm{a}})$, even under alternatives, and (ii) $f(r) > 0$. Then we have the following functional Law of Large Numbers.

Theorem 1 *Let $\{X_1, \ldots, X_n\}$ be i.i.d. copies of an arbitrary circular random variable X with CF $C_X(\cdot)$. Then under assumptions (i) and (ii), we have*

$$\frac{T_{n,f}}{n} \longrightarrow \sum_{r \geq 0} \left| e^{-\mathrm{i}\mu_{\mathrm{a}} r} C_X(r) - {\varrho_{\mathrm{a}}}^{r^{\gamma_{\mathrm{a}}}} \right|^2 f(r) := \Delta_f, \text{ a.s. as } n \to \infty, \tag{9}$$

which implies the strong consistency of the test which rejects the null hypothesis $\mathcal{H}_0^{(\mathrm{s})}$ for large values of $T_{n,f}$.

Proof Clearly, $\left| \widehat{C}_n(r) - {\widehat{\varrho}}^{r^{\widehat{\gamma}}} \right|^2 \leq 4$. Also by means of the strong pointwise consistency of the empirical CF (see Feuerverger and Mureika 1977), we have $C_n(r) \to C_X(r)$, $r \geq 0$, a.s. as $n \to \infty$. Then (9) follows by invoking Lebesgue's dominated convergence theorem.

To proceed further, recall the definition of the parameter ϱ and thus replace ${\varrho_{\mathrm{a}}}^{r^{\gamma_{\mathrm{a}}}}$ by $C_{\gamma_{\mathrm{a}}, \tau_{\mathrm{a}}}(r) = e^{-(\tau_{\mathrm{a}} r)^{\gamma_{\mathrm{a}}}}$, where $\tau_{\mathrm{a}} = (-\log \varrho_{\mathrm{a}})^{1/\gamma_{\mathrm{a}}}$. Then clearly the quantity Δ_f figuring in (9) is positive, unless $C_X(r) = e^{\mathrm{i}\mu_{\mathrm{a}} r - (\tau_{\mathrm{a}} r)^{\gamma_{\mathrm{a}}}}$, identically in r, which by the uniqueness of the CF would imply that X follows a SWS law indexed by $\boldsymbol{\varphi}_{\mathrm{A}}^{(\mathrm{s})}$, and the proof is complete.

3.2 Computational Details

Let us return to Eq. (6). Recall from the previous section that under the null hypothesis $\mathcal{H}_0^{(\mathrm{s})}$, we have that $\beta_{\boldsymbol{\varphi}}(\cdot) \equiv 0$, and hence the test statistic figuring in (6) reduces to

$$T_{n,f} = \Sigma_1 + \Sigma_2 - 2\Sigma_3, \tag{10}$$

with

$$\Sigma_1 = \frac{1}{n} \sum_{j,k=1}^{n} \mathcal{E}_1(Y_j - Y_k), \tag{11}$$

$$\Sigma_2 = n\mathcal{E}_2(\widehat{\gamma}, \widehat{\tau}), \tag{12}$$

and

$$\Sigma_3 = \sum_{j=1}^{n} \mathcal{E}_3(Y_j; \widehat{\gamma}, \widehat{\tau}), \tag{13}$$

where the series figuring in (11)–(13) are defined by

$$\mathcal{E}_1(x) = \sum_{r\geq 0} \cos(xr) f(r), \tag{14}$$

$$\mathcal{E}_2(\gamma, \tau) = \sum_{r\geq 0} e^{-2\tau^\gamma r^\gamma} f(r), \tag{15}$$

and

$$\mathcal{E}_3(x; \gamma, \tau) = \sum_{r\geq 0} \cos(xr) e^{-\tau^\gamma r^\gamma} f(r). \tag{16}$$

Now recall that $f(r),\ r \geq 0$, is a probability function and therefore $\mathcal{E}_k,\ k = 1, 2, 3$, may be viewed as expectations of corresponding quantities taken with respect to the law $f(r)$. Then after some extra manipulations, it follows that these three series may be written as

$$\mathcal{E}_1(x) = \mathbb{E}_r[\cos(xr)], \tag{17}$$

$$\mathcal{E}_2(\gamma, \tau) = \mathbb{E}_r \mathbb{E}_X[\cos(2^{1/\gamma} Xr)], \tag{18}$$

and

$$\mathcal{E}_3(x; \gamma, \tau) = \frac{1}{2}\big\{\mathbb{E}_r \mathbb{E}_X[\cos((X - x)r)] + \mathbb{E}_r \mathbb{E}_X[\cos((X + x)r)]\big\}, \tag{19}$$

where $\mathbb{E}_r[\cdot]$ and $\mathbb{E}_X[\cdot]$ are meant as expectations taken with respect to the law $f(r)$ and with respect to the SWS distribution with parameter $\boldsymbol{\varphi} = (\gamma, 0, \tau, 0)$, respectively.

While the expectations shown in (17)–(19) are generally not easy to compute analytically, they nevertheless allow for some simplification if the law $f(r)$ corresponding to the weights is properly chosen. Specifically, letting $f(r)$ be a Poisson distribution with mean λ, we have

$$\mathcal{E}_1(x) = \cos(\lambda \sin x) e^{\lambda(\cos x - 1)}. \tag{20}$$

Moreover, since $\mathcal{E}_k,\ k = 2, 3$, are absolutely convergent, by application of Fubini's theorem we have $\mathbb{E}_r \mathbb{E}_X(\cdot) = \mathbb{E}_X \mathbb{E}_r(\cdot)$, so that the expectations in (18)–(19) may be Monte-Carlo-approximated by the quantities

$$\mathcal{E}_{2,M}(\gamma, \tau) = \frac{1}{M} \sum_{m=1}^{M} \mathcal{E}_1(2^{1/\gamma} x_m), \tag{21}$$

and

$$\mathcal{E}_{3,M}(x; \gamma, \tau) = \frac{1}{2} \frac{1}{M} \sum_{m=1}^{M} \left(\mathcal{E}_1(x_m - x) + \mathcal{E}_1(x_m + x)\right), \tag{22}$$

respectively, where M is a large positive integer, and x_m, $m = 1, ..., M$, denote i.i.d. observations from the SWS distribution with parameter $\boldsymbol{\varphi} = (\gamma, 0, \tau, 0)$.

Alternatively, since we have rapid convergence at least for $\gamma \geq 1$, one can compute the test statistic $T_{n,f}$ given in (7) by means of direct numerical computation of only the first few terms of the series defined in $\mathcal{E}_2$ and $\mathcal{E}_3$.

3.3 Estimation of Parameters

From Eq. (7), it is clear that the test statistic requires consistent estimators of the stable law parameters. As estimators of the parameters (γ, ϱ, μ) of a SWS law, we suggest the moment estimators given by the following equations (see Sect. 4.6 of Jammalamadaka and SenGupta 2001):

$$\widehat{\mu} = \tan^{-1}\left(\frac{\beta_n(1)}{\alpha_n(1)}\right), \tag{23}$$

$$\widehat{\varrho} = \sqrt{\alpha_n^2(1) + \beta_n^2(1)}, \tag{24}$$

$$\widehat{\gamma} = \frac{1}{\log 2} \log\left(\frac{\log(\sqrt{\alpha_n^2(2) + \beta_n^2(2)})}{\log(\sqrt{\alpha_n^2(1) + \beta_n^2(1)})}\right), \tag{25}$$

where $\alpha_n(\cdot)$, $\beta_n(\cdot)$ are the trigonometric moments defined in (4), and $\tan^{-1}(\cdot)$ denotes the principal inverse of $\tan(\cdot)$.

We note that moment estimation of parameters yields an interesting limit for the test statistic $T_{n,f}$ figuring in (7). To this end, notice that $C_n(0) = C(0) = 1$, and hence the first term in $T_{n,f}$ (resulting from (7) for $r = 0$) vanishes regardless of the distribution being tested and for any function $f(r)$ used as a probability function. In addition, the second term involves the quantity $|\widehat{C}_n(1) - \widehat{\varrho}|$ which also vanishes on account of (23) and (24), and because $\widehat{\beta}_n(1) = 0$. Then write $T_{n,\lambda}$ for the statistic in (7) with $f(r)$ being the Poisson probability function with mean λ, so that

$$T_{n,\lambda} = n\, e^{-\lambda}\left(\left|\widehat{C}_n(2) - \widehat{\varrho}^{2^{\hat{\gamma}}}\right|^2 \frac{\lambda^2}{2} + o(\lambda^2)\right), \ \lambda \to 0, \tag{26}$$

which leads to

$$\lim_{\lambda \to 0} \frac{2T_{n,\lambda}}{n\lambda^2} = \left|\widehat{C}_n(2) - \widehat{\varrho}^{2^{\hat{\gamma}}}\right|^2 := T_{n,0}. \tag{27}$$

Clearly, the limit statistic $T_{n,0}$ simply compares the trigonometric moment computed from the sample with the trigonometric moment of the SWS law, both of order $r = 2$. (In this connection, note that $T_{n,0}$ vanishes as $n \to \infty$ under the null hypothesis). On the other hand, the test statistic $T_{n,\lambda}$ employs an infinite weighted sum in which the

empirical trigonometric moments of all integer orders $r \geq 0$ are accounted for, and with the probability function $f(r)$ playing the role of a weight function. Consequently if this function is decreasing with r (which is typically the case at least for large r), $f(r)$ down-weights higher order trigonometric moments that are more prone to periodic behavior (see, e.g., Epps 1993).

4 Finite-Sample Comparisons with Competing Tests

This section summarizes the results of a simulation study designed to evaluate the performance of the proposed test and compare it with other existing tests. As competitors, we include the Kuiper test (K) and the Watson test (W) for which there exist computationally convenient formulae (Jammalamadaka and SenGupta 2001, Sect. 7.2.1).

Specifically recall the notation $S(\cdot; \boldsymbol{\varphi})$ for the distribution function of the WSD, let $U_j = S(X_j; \widehat{\boldsymbol{\varphi}})$, and write $U_{(j)}$, $j = 1, ..., n$, for the corresponding order statistics. Then we have

$$\mathrm{K} = \max_{1 \leq j \leq n} \left\{ U_{(j)} - \frac{j-1}{n} \right\} + \max_{1 \leq j \leq n} \left\{ \frac{j}{n} - U_{(j)} \right\}, \tag{28}$$

$$\mathrm{W} = \frac{1}{12n} + \sum_{j=1}^{n} \left(\left(U_{(j)} - \frac{2j-1}{2n} \right) - \left(\overline{U} - \frac{1}{2} \right) \right)^2, \tag{29}$$

where $\overline{U} = n^{-1} \sum_{j=1}^{n} U_j$.

The asymptotic properties of test statistics such as $T_{n,f}$ have been recently studied in a general context by Jammalamadaka et al. (2019). As shown in that article, the limit null distribution of $T_{n,f}$ (as well as that of the statistics K and W) is complicated and depends on several unknown quantities. Therefore, all tests are implemented based on parametric bootstrap resampling which, as also shown in Jammalamadaka et al. (2019), is under weak conditions an asymptotically valid method.

We now outline the steps involved in the parametric bootstrap procedure in a fairly general setting of testing the null hypothesis $\mathcal{H}_0$ in (2) by means of an arbitrary statistic $T := T(X_1, \ldots, X_n)$. More specifically, write $\widehat{T} := T(X_1, \ldots, X_n; \widehat{\boldsymbol{\varphi}})$ for this test statistic involving the original observations as well as the resulting parameter estimate $\widehat{\boldsymbol{\varphi}} := \widehat{\boldsymbol{\varphi}}(X_1, ..., X_n)$. Then parametric bootstrap critical points are computed as follows:

1. Generate i.i.d. observations, $\{X_j^*, 1 \leq j \leq n\}$ from $S(\cdot; \widehat{\boldsymbol{\varphi}})$.
2. Using these observations, obtain the bootstrap estimate $\widehat{\boldsymbol{\varphi}}^* := \widehat{\boldsymbol{\varphi}}(X_1^*, ..., X_n^*)$ of $\boldsymbol{\varphi}$.
3. Calculate the bootstrap test statistic, say $T^* := T(X_1^*, ..., X_n^*; \widehat{\boldsymbol{\varphi}}^*)$.
4. Repeat Steps 1–3 a number of times, say B, and obtain $\{T_b^*\}_{b=1}^{\mathrm{B}}$.

Table 1 Null and Alternative hypotheses used for data simulation

Hypothesis	Distribution
Null 1	SWS$(2, 0.5, \pi)$
Null 2	SWS$(1, 0.5, \pi)$
Null 3	SWS$(1, 1, \pi)$
Null 4	SWS$(1.9, 1, \pi)$
Null 5	SWS$(1.75, 1, \pi)$
Null 6	SWS$(1.5, 1, \pi)$
Alternative 1	$0.8\text{vM}(\pi, 5) + 0.2\text{vM}(\pi/2, 5)$
Alternative 2	$0.65\text{vM}(\pi, 5) + 0.35\text{vM}(\pi/2, 5)$
Alternative 3	$0.5\text{vM}(\pi, 5) + 0.5\text{vM}(\pi/2, 5)$
Alternative 4	$(1/3)\text{vM}(\pi, 8) + (2/3)\text{vM}(\pi, 0.1)$
Alternative 5	$\text{vM}(\pi/2, 2)$
Alternative 6	AWS$(1.2, -1, 0.5, \pi)$
Alternative 7	$0.5\text{SWS}(2, 0.75, 0) + 0.5\text{AWS}(1.5, -1, 0.5, \pi)$
Alternative 8	GvM$(\pi, 3\pi/4, 1, 5)$

5. Calculate the critical point of a test of size α as the order $(1-\alpha)$ empirical quantile $T^*_{1-\alpha}$ of $T^*_{(b)}$, $(b = 1, ..., \text{B})$, where $T^*_{(1)} \leq T^*_{(2)} \leq \ldots \leq T^*_{(\text{B})}$ are the corresponding order statistics.
6. Reject the null hypothesis if $\widehat{T} > T^*_{1-\alpha}$.

Since the parametric bootstrap is somewhat time-consuming, we employ instead its warp-speed version. In order to produce replications, this method capitalizes on the inherent repetition of every Monte Carlo simulation, rather than relying on a separate "bootstrap loop". Specifically with the warp-speed bootstrap, conditionally on the $m-$th Monte Carlo sample, we compute the corresponding parameter estimate $\widehat{\boldsymbol{\varphi}}_m$, and draw a single bootstrap resample $X^*_{1,m}, ..., X^*_{n,m}$ from $S(\cdot; \widehat{\boldsymbol{\varphi}}_m)$. Having calculated the bootstrap parameter estimate $\widehat{\boldsymbol{\varphi}}^*_m := \widehat{\boldsymbol{\varphi}}(X^*_{1,m}, ..., X^*_{n,m})$, we compute the value of the test statistic for this resample, $T^*_m := T(X^*_{1,m}, ..., X^*_{n,m}; \widehat{\boldsymbol{\varphi}}^*_m)$. Then the critical point is computed as in Step 5 above from T^*_m, $(m = 1, ..., \text{MC})$, where MC denotes the number of Monte Carlo samples drawn; for more details, the reader is referred to Giacomini et al. (2013).

In this simulation study, we chose six distributions from the family of SWS distributions (under the null hypothesis) and eight distributions from alternative hypotheses, including

- von Mises (vM) distributions.
- 2-component mixtures of vM distributions.
- Asymmetric WS (AWS) distributions.
- 2-component mixtures of an SWS distribution with an AWS distribution.
- Generalized von Mises (GvM) distributions (discussed in Gatto and Jammalamadaka 2007).

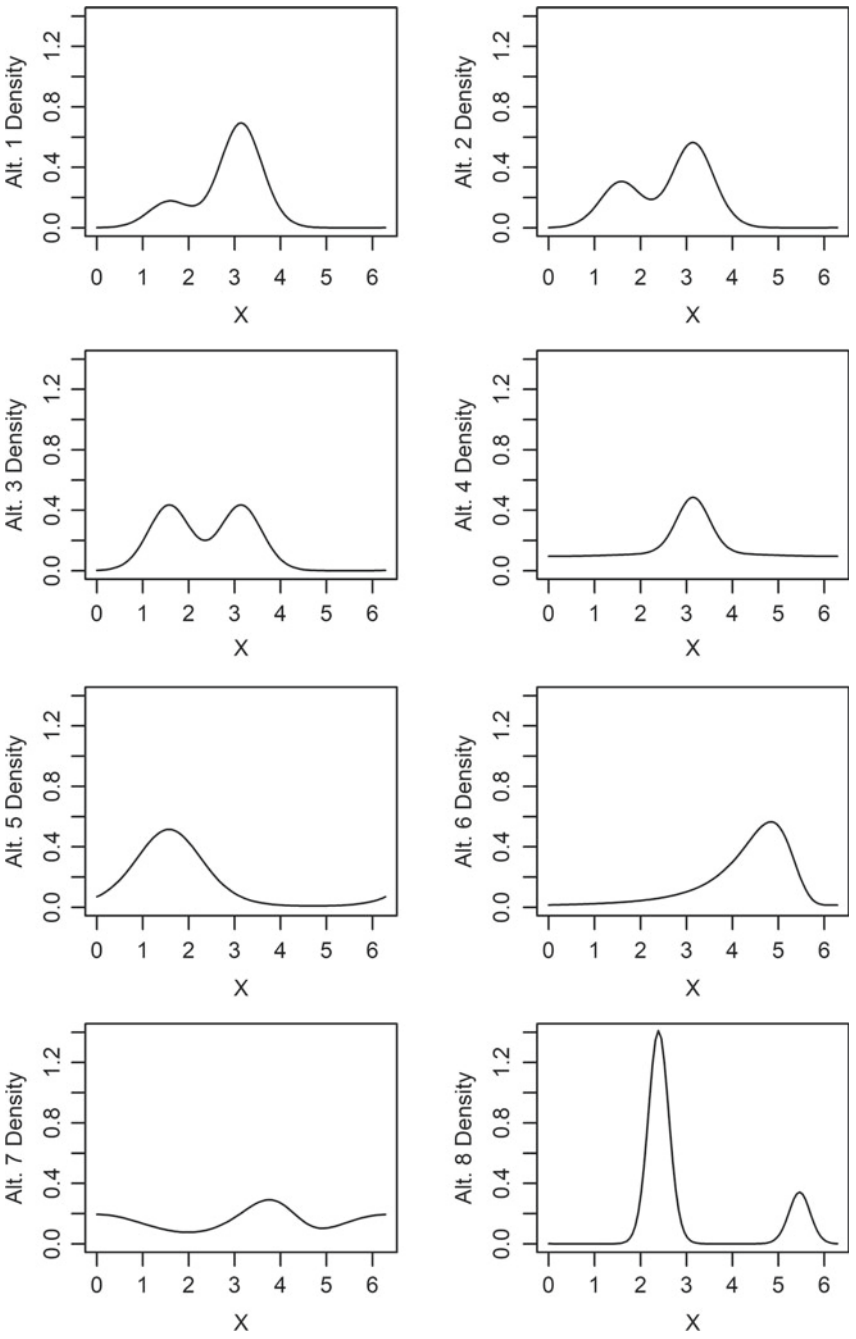

Fig. 1 Alternative densities considered

Parameter configurations of simulated distributions (both under the null and alternatives) are shown in Table 1. The densities of the simulated alternatives are depicted in Fig. 1.

The computations were carried out in `R`, utilizing `CircStats` package to generate random samples for WS and vM distributions. We choose $\lambda = 0.3, 0.5, 0.7, 0.9$, with $f(r)$ being the Poisson probability function with mean λ, and write T_λ for our test statistic. The proportion of rejections of the null hypothesis under each null and alternative distribution is computed by applying the tests to MC $= 5{,}000$ iterations, with the critical points estimated using the warp-speed method (similar results were obtained when we used MC $= 10{,}000$ iterations and we report the former). The results for samples of size $n = 100$, 50, and 30 are summarized in Tables 3, 4, and 5, respectively, given in Appendix, at nominal levels $\alpha = 0.05$ and $\alpha = 0.10$. On the basis of these extensive simulation results, we make the following observations:

1. The empirical level of our test is close to the nominal level for Null 1 (which is at the boundary of the parameter space), and Null 2, 3, and 6, while it is slightly higher than the actual α for Null 4 and 5. (This type of inaccuracy was also noticed in the Monte Carlo results of Koutrouvelis and Meintanis 1999).
2. The empirical power of our test is high for Alt. 1, 2, 3, 6, and 8, while it is very low (almost indistinguishable from the level of the test) for Alt. 4 and Alt. 5. This may be explained by the fact that distributions Alt. 4 and Alt. 5 are unimodal and symmetrical, and thus they can be approximated sufficiently well by a SWS distribution.
3. Compared with our test, both the Kuiper and the Watson tests exhibit a lower percentage of rejection both under the null as well as under alternatives, except for Null 1. Generally, these tests perform much worse, and certainly no better than our test in most cases, with rare exceptions like Null 4 with $n = 100$ and Alt. 3 with $n = 30$. In particular, for Alt. 8, both tests have almost no power while our test attains higher power when the sample size is large.
4. The test statistic T_λ is robust with respect to the choice of λ and thus the value of λ does not significantly affect the empirical level/power of our test. In other testing situations though, finding a good value for λ turns out to be important; see, for instance, Allison and Santana (2015) for more details on this issue.

5 Real Data Applications

This section shows the application of our proposed test on a couple of real data sets. Taylor and Burns (2016) collected data sets for the radial distributions of mistletoes and epiphytes from 5 different species, and discovered that they are highly directional and related to the availability of light and humidity. We consider two of their data sets: Data Set 1 consists of $n = 67$ observations on *peraxilla colensoi* and Data Set 2 consists of $n = 65$ observations on *asplenium flaccidum*. Figure 2 shows the histograms of two data sets. The corresponding fitted SWS density functions are

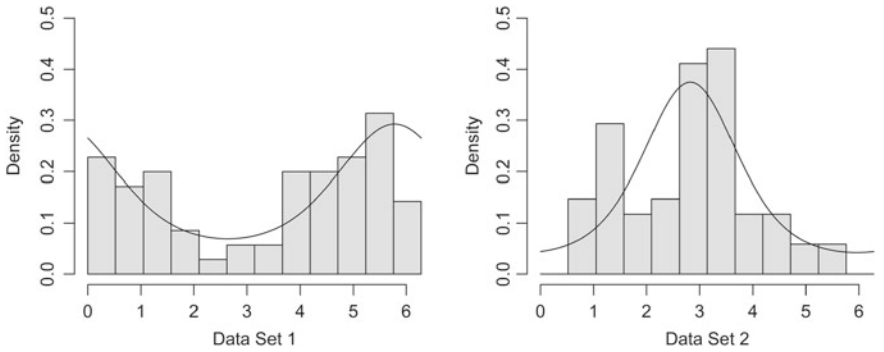

Fig. 2 Histograms of real data sets together with the fitted SWS density functions

Table 2 Parameter estimates and p-values of the tests for Data Sets 1 and 2

Data set	Estimated parameters	K	W	$T_{0.3}$	$T_{0.5}$	$T_{0.7}$	$T_{0.9}$	T_1
1	$\widehat{\gamma} = 1.32, \widehat{\tau} = 1.06, \widehat{\mu} = 5.78$	0.502	0.586	0.316	0.344	0.370	0.412	0.434
2	$\widehat{\gamma} = 1.40, \widehat{\tau} = 0.79, \widehat{\mu} = 2.82$	0.036	0.012	0.028	0.020	0.014	0.008	0.006

shown in black lines. Table 2 gives the estimated parameters and p-values of the tests for Data Sets 1 and 2. At $\alpha = 0.05$, all tests fail to reject the null hypothesis for Data Set 1 and reject the null hypothesis for Data Set 2.

6 Discussion

We propose a goodness-of-fit test for the family of symmetric wrapped stable distributions with unknown parameters. The proposed test statistic is based on the characteristic function of this family, which unlike its density may be written in a closed form. Furthermore, the estimation of the stable law parameters also utilizes the characteristic function, and thus avoids numerically complicated likelihood-based procedures. The suggested test statistic, which is expressed as a weighted L^2-type distance between empirical trigonometric moments and the corresponding theoretical quantities, is shown to be consistent against general alternatives. The findings of a Monte Carlo study show that the proposed test statistic competes well and indeed does better than some of the existing procedures for the same problem. Finally, a couple of real data examples further illustrate the applicability of the new procedures.

Appendix

See Tables 3, 4, and 5.

Table 3 Observed proportion of rejection at nominal level α for 5000 Monte Carlo samples of size $n = 100$

Law	α	K	W	$T_{0.3}$	$T_{0.5}$	$T_{0.7}$	$T_{0.9}$	T_1
Null 1	0.05	0.049	0.049	0.054	0.055	0.059	0.059	0.060
	0.10	0.098	0.107	0.108	0.108	0.107	0.108	0.108
Null 2	0.05	0.010	0.014	0.047	0.047	0.045	0.045	0.042
	0.10	0.038	0.043	0.096	0.096	0.094	0.092	0.092
Null 3	0.05	0.008	0.014	0.033	0.033	0.031	0.031	0.031
	0.10	0.034	0.041	0.073	0.071	0.071	0.067	0.067
Null 4	0.05	0.044	0.059	0.101	0.101	0.098	0.098	0.097
	0.10	0.092	0.117	0.183	0.180	0.175	0.172	0.169
Null 5	0.05	0.031	0.047	0.093	0.089	0.087	0.083	0.084
	0.10	0.074	0.102	0.158	0.156	0.152	0.148	0.145
Null 6	0.05	0.022	0.031	0.063	0.062	0.061	0.058	0.056
	0.10	0.062	0.071	0.112	0.112	0.111	0.110	0.108
Alt. 1	0.05	0.729	0.907	0.984	0.986	0.987	0.986	0.986
	0.10	0.861	0.959	0.995	0.995	0.995	0.994	0.995
Alt. 2	0.05	0.933	0.987	0.982	0.986	0.989	0.990	0.990
	0.10	0.972	0.994	0.994	0.995	0.996	0.996	0.996
Alt. 3	0.05	0.910	0.978	0.955	0.966	0.970	0.976	0.976
	0.10	0.960	0.992	0.983	0.987	0.989	0.990	0.991
Alt. 4	0.05	0.000	0.000	0.038	0.036	0.033	0.033	0.032
	0.10	0.003	0.008	0.090	0.086	0.082	0.079	0.077
Alt. 5	0.05	0.039	0.042	0.047	0.048	0.046	0.047	0.045
	0.10	0.091	0.089	0.095	0.095	0.094	0.095	0.095
Alt. 6	0.05	0.294	0.317	0.696	0.715	0.725	0.730	0.731
	0.10	0.526	0.579	0.816	0.834	0.842	0.844	0.844
Alt. 7	0.05	0.003	0.038	0.518	0.496	0.474	0.448	0.437
	0.10	0.015	0.110	0.637	0.615	0.600	0.583	0.572
Alt. 8	0.05	0.000	0.000	0.947	0.933	0.910	0.872	0.848
	0.10	0.000	0.001	0.982	0.975	0.967	0.952	0.943

Table 4 Observed proportion of rejection at nominal level α for 5000 Monte Carlo samples of size $n = 50$

Law	α	K	W	$T_{0.3}$	$T_{0.5}$	$T_{0.7}$	$T_{0.9}$	T_1
Null 1	0.05	0.049	0.053	0.051	0.048	0.048	0.049	0.049
	0.10	0.093	0.097	0.099	0.104	0.107	0.108	0.107
Null 2	0.05	0.005	0.011	0.035	0.036	0.036	0.034	0.034
	0.10	0.031	0.038	0.078	0.076	0.074	0.078	0.076
Null 3	0.05	0.003	0.008	0.031	0.031	0.029	0.028	0.027
	0.10	0.018	0.027	0.071	0.068	0.065	0.064	0.064
Null 4	0.05	0.015	0.035	0.110	0.109	0.106	0.102	0.103
	0.10	0.049	0.080	0.190	0.185	0.181	0.175	0.174
Null 5	0.05	0.015	0.029	0.085	0.084	0.080	0.077	0.076
	0.10	0.046	0.075	0.152	0.153	0.152	0.149	0.148
Null 6	0.05	0.009	0.017	0.063	0.064	0.063	0.060	0.058
	0.10	0.036	0.046	0.128	0.125	0.119	0.116	0.114
Alt. 1	0.05	0.298	0.506	0.788	0.786	0.786	0.779	0.776
	0.10	0.470	0.667	0.876	0.875	0.877	0.873	0.867
Alt. 2	0.05	0.588	0.778	0.770	0.796	0.813	0.828	0.831
	0.10	0.729	0.865	0.889	0.901	0.909	0.910	0.911
Alt. 3	0.05	0.586	0.763	0.657	0.704	0.732	0.752	0.764
	0.10	0.725	0.871	0.817	0.841	0.859	0.873	0.876
Alt. 4	0.05	0.001	0.003	0.049	0.049	0.045	0.044	0.042
	0.10	0.010	0.016	0.092	0.090	0.087	0.084	0.083
Alt. 5	0.05	0.037	0.034	0.043	0.042	0.042	0.038	0.039
	0.10	0.083	0.082	0.088	0.084	0.086	0.084	0.084
Alt. 6	0.05	0.038	0.035	0.327	0.342	0.343	0.346	0.348
	0.10	0.145	0.136	0.498	0.508	0.510	0.518	0.521
Alt. 7	0.05	0.004	0.012	0.252	0.241	0.224	0.213	0.205
	0.10	0.019	0.062	0.396	0.382	0.367	0.352	0.342
Alt. 8	0.05	0.000	0.001	0.658	0.595	0.538	0.467	0.423
	0.10	0.000	0.005	0.794	0.754	0.705	0.656	0.620

Table 5 Observed proportion of rejection at nominal level α for 5000 Monte Carlo samples of size $n = 30$

Law	α	K	W	$T_{0.3}$	$T_{0.5}$	$T_{0.7}$	$T_{0.9}$	T_1
Null 1	0.05	0.041	0.049	0.043	0.047	0.050	0.050	0.051
	0.10	0.093	0.091	0.106	0.106	0.104	0.104	0.102
Null 2	0.05	0.004	0.006	0.033	0.033	0.030	0.028	0.029
	0.10	0.023	0.031	0.081	0.080	0.081	0.076	0.076
Null 3	0.05	0.003	0.007	0.032	0.033	0.032	0.031	0.029
	0.10	0.021	0.027	0.082	0.081	0.078	0.072	0.072
Null 4	0.05	0.005	0.014	0.084	0.082	0.077	0.075	0.074
	0.10	0.035	0.052	0.150	0.148	0.147	0.143	0.140
Null 5	0.05	0.008	0.016	0.081	0.079	0.077	0.076	0.075
	0.10	0.033	0.053	0.146	0.147	0.141	0.137	0.137
Null 6	0.05	0.005	0.011	0.061	0.059	0.056	0.053	0.052
	0.10	0.025	0.039	0.112	0.110	0.105	0.104	0.105
Alt. 1	0.05	0.081	0.157	0.500	0.512	0.509	0.504	0.499
	0.10	0.231	0.357	0.634	0.640	0.638	0.627	0.624
Alt. 2	0.05	0.262	0.430	0.522	0.540	0.559	0.566	0.572
	0.10	0.437	0.610	0.695	0.715	0.727	0.729	0.729
Alt. 3	0.05	0.292	0.447	0.387	0.435	0.482	0.509	0.516
	0.10	0.470	0.623	0.598	0.623	0.642	0.655	0.661
Alt. 4	0.05	0.003	0.005	0.056	0.055	0.052	0.050	0.047
	0.10	0.013	0.022	0.108	0.105	0.101	0.099	0.098
Alt. 5	0.05	0.020	0.018	0.041	0.040	0.040	0.039	0.040
	0.10	0.066	0.059	0.091	0.092	0.089	0.087	0.087
Alt. 6	0.05	0.015	0.016	0.177	0.183	0.183	0.183	0.184
	0.10	0.070	0.066	0.314	0.315	0.319	0.322	0.321
Alt. 7	0.05	0.004	0.009	0.163	0.154	0.145	0.136	0.129
	0.10	0.022	0.043	0.261	0.258	0.250	0.239	0.232
Alt. 8	0.05	0.000	0.002	0.408	0.377	0.343	0.276	0.251
	0.10	0.000	0.006	0.565	0.536	0.478	0.427	0.405

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Applications

Partial Differential Equation Models and Riemann–Stieltjes Integrals in Measuring Sustainability

Arni S. R. Srinivasa Rao and Sireesh Saride

Abstract Abstract understanding sustainability through modeling involves one of the complex and interdisciplinary activities where mathematics plays a key role. We provide arguments favoring the need for developing global models for measuring the status of sustainability. A global model (applicable in broader perspective) and global sustainability indices are proposed which can be used with real-world data. The solutions of the proposed Partial Differential Equations (PDEs) are blended with the weight functions of Riemann–Stieltjes integrals to capture the differential importance of sustainability associated factors. The ideas, methods, and models are new and are prepared for handling multidimensional and multivariate data. A practically adaptable formula for measuring the sustainability index is developed with few key variables. We provide a real-world example arising in civil engineering applications with a numerical example to demonstrate our models.

Keywords Key words · Modeling · Partial differential equations · Riemann weight functions.

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1 Introduction

According to the United States Environmental Protection Agency (USEPA 2021), "Sustainability creates and maintains the conditions under which humans and nature can exist in productive harmony, that permit fulfilling the social, economic, and other requirements of present and future generations" and according to Oxford English Dictionary (OXD 2020), sustainable means—"able to be maintained at a certain rate or level". Sustainability is a highly complex and very broad-meaning word amalgamated from several cross-disciplinary subjects and also influenced by political and governmental involvement. Specific to Civil Engineering, American Society of Civil Engineers (ASCE) defines sustainability as" a set of economic, Environmental, and social conditions in which all of society has the capacity and opportunity to maintain and improve its quality of life indefinitely, without degrading the quantity, quality, or the availability of natural, economic, and social resources (Ref: https://www.asce.org/advocacy/energy). It is within and beyond the subject of academic collaboration. There are discussions on achieving sustainability at academic and government levels (see for example, May 2002) and there is a need to address sustainability from a common platform (Ostrom 2009). When we speak of the mathematics of sustainability, the first question which comes to me as a mathematical modeler is, can we build a global comprehensive mathematical model to explain the status of sustainability? And secondly, can we use it for predicting whether the system under investigation is sustainable or not**?** Supposing we can able to build one such model, then how does the mathematical modeler (or mathematical community) present itto people with a non-mathematical background such that people who are responsible for policy, government administrators, and all other responsible individuals understand the importance and implications of sustainability and can foresee the predictions of a sustainability model? (It is, of course, possible that people with a mathematical background occupy government, political, and other responsible professions). Mathematical ideas cannot be adopted for the overall development of mankind and for the betterment of species surrounded by mankind unless they can be appreciated and encouraged by non-mathematicians.

A mathematician might develop an excellent model to solve/explain certain practical issues, however, there are often ''gulfs" between 'the people handling practical issues related to sustainability' and 'the mathematicians who are building and analyzing models'. These gulfs maybe both ideological and conceptual. Ideological gulfs can be broadly classified as undermining the applicability of mathematical ideas and models for practical use in general, whereas conceptual gulfs can be broadly classified as a lack of sufficient background in mathematical sciences. Unless these concepts are accessible to non-mathematicians, the fruits of mathematical reasoning would not benefit mankind (and also surrounding species). But who will cross the gap? Whether it is non-mathematicians who will cross the bridge to reach mathematical thinkers or mathematicians who take their concepts across the bridge could be a topic of consideration. One argument could be that, since mathematicians produce mathematical models (methods), they need to take them to other people and

make them use models (like a salesman sells his/her product). How often do mathematicians take things in this direction? There are occasions when cross-disciplinary teams including mathematicians build models for real-world solutions in science and engineering. Although there may be an overlap in techniques, modeling global sustainability is different from the modeling to explain a particular phenomenon of science (or engineering), which is usually conducted by a group of people with science (or engineering) and mathematical backgrounds. There were several collaborative attempts with mathematicians at building models for health policies that were conceived by people responsible for policy formulation and successfully implemented at the country level (for example, see Rao et al. 2012 and Rao et al. 2009).

Sustainability is a broader term than health policy formulation. For example, if we have to formulate a mathematical model based policy for controlling an epidemic and suppose we have the following information: (i) health professionals who are handling population-level treatment of this particular epidemic are aware of the transmission dynamics of associated disease, (ii) time-series data on incidence and prevalence, (iii) basic socio-demographic data for the population of concern, (iv) intervention strategies by the government for controlling the epidemic, (v) vaccine availability and distribution if at all there exists a vaccination, and (vi) any other relevant factors those are essential in controlling the given epidemic. When a team of medical and public health professionals with the above information approaches a mathematician, the job of a mathematician is to understand the transmission dynamics and develop a model for the same with all the variables and parameters of interest. In case parameters are not readily available, one has to use statistical procedures for estimation before model building. It is also necessary to involve health professionals at every stage of the model building for maximum flexibility and accuracy of the model. Once a model is built and successfully tested for its performance by taking inputs from health professionals in the team, one can adapt the model for predicting the epidemic spread with and without interventions. We can also measure the impact of certain policies through such modeling. Understanding the sustainability status of the population is not about to health alone. As mentioned previously, it involves obtaining accurate information in all aspects of population well-being, ranging from health, climate, food, agriculture resources, science and technology to economic situation. Each category of this information across various fields is required to use independently and dependently in the models for sustainability status. Modeling sustainability needs a cross-disciplinary team with an understanding of cross-disciplinary data. See Figure schematic structure of the process model building through the teamwork of cross-disciplinary scientists, government agencies, politicians, etc. (Fig. 1).

For measuring the status of sustainability, we need global models with all-round global data, however, such a global model could have components of sub-models (or local models) quantifying sustainability status at various geographic regions on our planet. These computationally intense models should be able to update global and local sustainability status periodically such that time-dependent action-oriented policies can be skimmed from these efforts. Existing models for sustainability involved variables from one or two categories and these models are well constructed (Ostrom 2009; Gunderson 2006; Pretty et al. 2002; Ravindranath et al. 2006). Our models

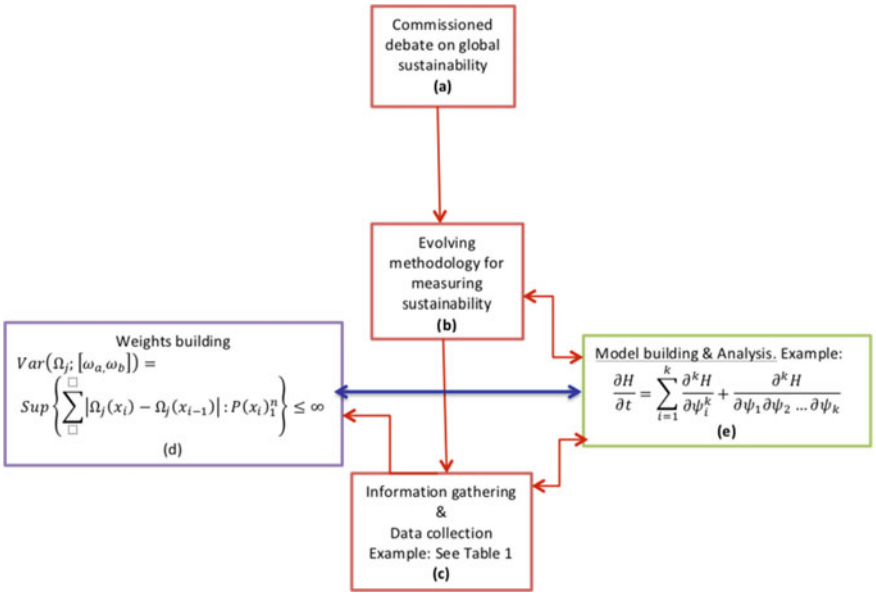

Fig. 1 Schematic diagram of bridging between various sustainability stake holders. **a** Commissioned debate on global sustainability: Team of scientists, politicians, government and non-government agencies will debate on the status of sustainability, required further information, direction of research needed for better understanding the status; **b** Evolving methodology for measuring sustainability: Scientists who are working on sustainability issues and organizations and individuals who are working in practical implementation of maintaining sustainable environment (see, for example, see www.epa.gov), statisticians and mathematicians discuss as a team on the method of measuring sustainability status; **c** Information gathering & data collection: Required information as decided in **b** will be collected which will eventually help to arrive at Table 1; **d** Weights building: With the help of **c** weight functions will be formed and ordering of the weights by relative importance in-terms of their contribution to the sustainability status is decided; **e** Model building and analysis: Models will be developed since completion of **b.** The ideas generated in **b, c** and using the values obtained at **d**, model based output will generated. There will be back-and-forth activities between **b–d** and **e**

proposed are new in terms of structure and conceptualization and methods involve are different from the general sustainability modeling framework proposed, see for example, Phillips (2010), Todorov and Marinova (2011). We have proposed to use the weight functions of Riemann–Stieltjes for giving differential importance to various factors involved in sustainability measures. Since the length of the partitions in Riemann-Stieltjes could be dynamically arranged, the corresponding weight functions proposed in the work are flexible to capture variation in the sustainability data of road transportation. In the next section, we propose sustainability indices and models and show that these indices are solutions to proposed models.

2 Global Sustainability Models

A general global model using a Partial Differential Equation (PDE) for studying a measure of sustainability (say, sustainability index, H at time t), involving components $\psi_1, \psi_2, ..., \psi_k$ (i.e., independent variables) that determine sustainability and partial derivatives of H can be conceptualized as one or more of the following equations:

$$S\left(t, \psi_1, \psi_2, ..., \psi_k, H, H_t, H_{\psi_1}, H_{\psi_2}, \cdots, H_{\psi_k}\right) = 0 \tag{1}$$

$$S\left(\begin{array}{c} t, \psi_1, \psi_2, ..., \psi_k, H, H_t, H_{\psi_1}, H_{\psi_2}, \cdots, \\ H_{\psi_k}, H_{\psi_1\psi_2}, H_{\psi_1\psi_3}, H_{\psi_2\psi_3}, \cdots, H_{\psi_1\psi_k}, H_{\psi_2\psi_k}, \cdots \end{array}\right) = 0$$

$$\vdots \qquad\qquad \vdots \tag{2}$$

$$S\left(\begin{array}{c} t, \psi_1, \psi_2, ..., \psi_k, H, H_t, H_{\psi_1}, H_{\psi_2}, \cdots, \\ H_{\psi_k}, H_{\psi_1\psi_2}, H_{\psi_1\psi_3}, \cdots, H_{\psi_2\psi_{3,\cdots,\psi_k}} \end{array}\right) = 0 \tag{3}$$

where $H_{\psi_1}, H_{\psi_2}, ...H_{\psi_k}$ are partial derivatives and $H_{\psi_1\psi_2}, H_{\psi_1\psi_3}, H_{\psi_2\psi_3}, \cdots, H_{\psi_1\psi_k}, H_{\psi_2\psi_k}, \cdots, H_{\psi_2\psi_{3,\cdots,\psi_k}}$ are mixed partial derivatives. For example,

$$H_{\psi_i} = \frac{\partial H}{\partial \psi_i},$$

$$H_{\psi_1\psi_2\cdots\psi_k} = \frac{\partial^k H}{\partial \psi_1\psi_2\cdots\psi_k},$$

$$H_{\psi_k\psi_k\cdots\psi_k} = \frac{\partial^k H}{\partial \psi_k^k},$$

and for $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_k$ where α_i is a non-negative integer, the mixed partial derivative, $H_{\psi_k\psi_k\cdots\psi_k}$, means,

$$H_{\psi_1(\alpha_1 \text{ times})\psi_k(\alpha_2 \text{ times})\cdots\psi_k(\alpha_k \text{ times})} = \frac{\partial^k H}{\partial \psi_1^{\alpha_1}\psi_2^{\alpha_2}\cdots\psi_k^{\alpha_k}}.$$

Here, $H : U \to \mathbb{R}$, where U is an open subset in $\mathbb{R}^k$ and $\psi_i \in U$. (1) is first order, (2) is second order, and (3) is kth-order PDE. In general,

$$S\left(t, \psi_1, \psi_2, ..., \psi_k, H, DH, D^2H, \cdots, D^{k-1}H, D^kH\right) = 0 \tag{4}$$

for $(t, \psi_1, \psi_2, ..., \psi_k \in U)$, is called a k^{th}order PDE, where $S : \mathbb{R}^k \times \mathbb{R}^{k-1} \times \cdots \times \mathbb{R} \to \mathbb{R}$ and $D^i H$ is the set of all partial derivatives of order i for $i = 1, 2, \cdots, k$. The PDE (4) could be linear or non-linear. It is linear, by using $D^\alpha H$, and using two functions, $f_\alpha\,(t, \psi_1, \psi_2, ..., \psi_k)$ and $f\,(t, \psi_1, \psi_2, ..., \psi_k)$, if we can write in the form (5), else, we can say it is not linear.

$$\sum_{|\alpha| \le k} f_\alpha\,(t, \psi_1, \psi_2, ..., \psi_k)\, D^\alpha H = f\,(t, \psi_1, \psi_2, ..., \psi_k) \tag{5}$$

The degree and combination of number of independent variables in $\Psi = (\psi_1, \psi_2, ..., \psi_k)$ and construction of H using Ψ needs inputs from the global community who are working on sustainability issues. The impact of each of $\psi_1, \psi_2, ..., \psi_k$ could be different in quantifying H and hence, we might have to introduce global weight functions $\boldsymbol{\Omega} = (\Omega_1, \Omega_2, \cdots, \Omega_k)$ corresponding to each independent variable. We associate Ω with a Riemann-Stieltjes integrable function F such that $F, \boldsymbol{\Omega} : [\omega_a, \omega_b] \to \mathbb{R}$ are bounded functions on a compact interval $[\omega_a, \omega_b]$. A range of weights depending upon the fluctuations in independent variables, for example, economic depression, shortage of resources like food, energy, etc. have to be assessed with cross-disciplinary data such that a tagged partition function P of $[\omega_a, \omega_b]$ is obtained. Since F is Riemann–Stieltjes integrable, we will have,

$$\left| \Sigma\,(F, \Omega, P) - \int_{\omega_a}^{\omega_b} F d\Omega \right| < \eta \tag{6}$$

for every $\eta > 0$. Here,

$$\Sigma\,(F, \Omega, P) = \Sigma_{i=1}^{g} F(t_i) \left[\Omega(x_i) - \Omega(x_{i-1})\right] \tag{7}$$

is the Riemann–Stieltjes sum of F with respect to global sustainability weight function Ω for $P = \left\{\left(\left[x_{i-1}, x_i\right], t_i\right)\right\}_{i=1}^{g}$, where $g$is the size of partitions. For definitions, properties and general description of Riemann–Stieltjes integrals, refer to Tao (2009), Nielsen (1997). Similarly, a general PDE for a specific geographic regional model can be written in similar construction as that of model (3). The regional specific independent variables and regional specific weights depending upon the regional sustainability indicators satisfying the following Riemann–Stieltjes set up at the hth region are

$$\left| \Sigma\,(F_h, \Omega_h, P_h) - \int_{\omega_a}^{\omega_b} F_h d\Omega_h \right| < \eta \tag{8}$$

$$\Sigma\left(F_h, \Omega_h, P_h\right) = \Sigma_{i=1}^{g_1} F_h(t_i)\left[\Omega_h(x_i) - \Omega_h(x_{i-1})\right] \tag{9}$$

$$P_h = \left\{\left(\left[x_{i-1}, x_i\right], t_i\right)\right\}_{i=1}^{g_1} \tag{10}$$

where g_1 is the size of partitions at the hth region. Global models need to run simultaneously with regional models over the time to obtain global sustainability measures. Measurement of sustainability requires understanding influences of more than one factor or variable and mutual inter-dependencies within these variables. In fact, there will be several factors or variables (see Table 1) that influence the population sustainability over time period. Depending upon the situation one may consider two factors or more factors together that influence the overall status of sustainability. In Table 1, a list of variables provided for a general guidance. This is a probable list and an effective list of sustainability influencing could be emerged by splitting or combining variables from this list.

We propose two types of PDE models for H, one without the mixed partial derivatives and second with the mixed partial derivatives. First model (11) is a simple starting point, because second-order PDEs are known to have wider applications in science and engineering (for example, see Krantz 1992; Strauss 2008). This model is good when each dependent variable is considered in the dynamics of sustainability status. When we need to incorporate interaction (or influence) of more variables then model (12) will be suitable. In this model we have considered the term $\frac{\partial^k H}{\partial\psi_1\cdots\partial\psi_k}$ for demonstration of our analysis. One can consider other mixed partial derivatives such as $\frac{\partial^k H}{\partial\psi_\Lambda\partial\psi_\Theta\partial\psi_\Delta\cdots\partial\psi_k}$ or other combination or order of the partial derivatives. For demonstration of the solution in this paper, we use the model (12), and similar approach can be adapted for all other models with different mixed partial derivatives, for example see (12) and (12).

$$\frac{\partial H}{\partial t} = \Sigma_{i=1}^{k} \frac{\partial^2 H}{\partial\psi_i^2} \quad (k > 1) \tag{11}$$

$$\frac{\partial H}{\partial t} = \Sigma_{i=1}^{k} \frac{\partial^k H}{\partial\psi_i^k} + \frac{\partial^k H}{\partial\psi_1\cdots\partial\psi_k} \quad (k > 1) \tag{12}$$

If we ignore mixed partial derivatives in Model (12) and fix $k = 2$, then model (12) becomes model (11). Other PDE model by varying mixed partial derivatives as described above are,

$$\frac{\partial H}{\partial t} = \Sigma_{i=1}^{k} \frac{\partial^k H}{\partial \psi_i^k} + \frac{\partial^k H}{\partial \psi_3 \partial \psi_2 \partial \psi_1 \cdots \partial \psi_k} \quad (k > 1) \tag{13}$$

$$\frac{\partial H}{\partial t} = \Sigma_{i=1}^{k} \frac{\partial^k H}{\partial \psi_i^k} + \frac{\partial^k H}{\partial \psi_1 \cdots \partial \psi_k} + \frac{\partial^{k-1} H}{\partial \psi_1 \cdots \partial \psi_{k-1}} + \quad (k > 1)$$
$$\frac{\partial^{k-2} H}{\partial \psi_3 \partial \psi_2 \partial \psi_1 \cdots \partial \psi_{k-2}} + \cdots + \frac{\partial H}{\partial \psi_k} \tag{14}$$

Actual function form of a PDE model with a suitable order and degree are usually decided by the experts working in the field and in this case the team of cross-disciplinary scientists after sufficient debate. We confine to the model (12) for obtaining a sustainability index to be used by groups or individuals working on practical modeling.

Theorem 1 *For the Model (11), (i)* $H = kt + \frac{1}{2}\Sigma_{i=1}^{k} \psi_i^2$ *and (ii)* $H = (2k)t + \Sigma_{i=1}^{k} \psi_i^2$ *are solutions.*

Proof (i) For $k = 1$, the model (11) is a heat equation and the solution is $H = t + \frac{1}{2}\psi_1^2$. For $H = kt + \frac{1}{2}\Sigma_{i=1}^{k} \psi_i^2$, we have $\frac{\partial H}{\partial t} = k = \Sigma_{i=1}^{k} \frac{\partial^2 H}{\partial \psi_i^2}$.

(ii) For $H = (2k)t + \Sigma_{i=1}^{k} \psi_i^2$ we have $\frac{\partial H}{\partial t} = 2k = \Sigma_{i=1}^{k} \frac{\partial^2 H}{\partial \psi_i^2}$. Hence the theorem is proved.

Theorem 2 *For the Model (12), (i)* $H = (k+1)t + \frac{1}{k!}\Sigma_{i=1}^{k} \psi_i^k + \Pi_{i=1}^{k} \psi_i$ *and (ii)* $H = ((k!k) + 1)\, t + \Sigma_{i=1}^{k} \psi_i^k + \Pi_{i=1}^{k} \psi_i$ *are solutions.*

Proof (i) Let $H = (k+1)t + \frac{1}{k!}\Sigma_{i=1}^{k} \psi_i^k + \Pi_{i=1}^{k} \psi_i$. We have $\frac{\partial H}{\partial \psi_i} = \frac{k}{k!}\psi_i^{k-1} + \psi_1 \cdots \psi_{i-1}\psi_{i+1} \cdots \psi_k$ and $\frac{\partial^k H}{\partial^k \psi_i} = 1$. We have,

$$\begin{aligned} \frac{\partial^k H}{\partial \psi_1 \cdots \partial \psi_k} &= \frac{\partial^{k-1}}{\partial \psi_1 \cdots \partial \psi_{k-1}} \left(\frac{\partial H}{\partial \psi_k} \right) \\ &= \frac{\partial^{k-1}}{\partial \psi_1 \cdots \partial \psi_{k-1}} \left(\frac{k}{k!} \psi_k^{k-1} + \Pi_{i=1}^{k-1} \psi_i \right) \\ &= \frac{\partial^{k-2}}{\partial \psi_1 \cdots \partial \psi_{k-2}} \left(\Pi_{i=1}^{k-2} \psi_i \right) = 1 \end{aligned}$$

Therefore,
$\frac{\partial H}{\partial t} = k + 1 = \Sigma_{i=1}^{k} \frac{\partial^k H}{\partial \psi_i^k} + \frac{\partial^k H}{\partial \psi_1 \cdots \partial \psi_k}$ $(k > 1)$, which confirms that given H is a solution.

(ii) Let $H = ((k!k) + 1)\, t + \Sigma_{i=1}^{k} \psi_i^k + \Pi_{i=1}^{k} \psi_i$. We have $\frac{\partial H}{\partial \psi_i} = k\psi_i^{k-1} + \psi_1 \cdots \psi_{i-1}\psi_{i+1} \cdots \psi_k$ and $\frac{\partial^k H}{\partial^k \psi_i} = k!$. We have,

$$\begin{aligned}\frac{\partial^k H}{\partial\psi_1\cdots\partial\psi_k} &= \frac{\partial^{k-1}}{\partial\psi_1\cdots\partial\psi_{k-1}}\left(\frac{\partial H}{\partial\psi_k}\right)\\ &= \frac{\partial^{k-1}}{\partial\psi_1\cdots\partial\psi_{k-1}}\left(k\psi_k^{k-1}+\Pi_{i=1}^{k-1}\psi_i\right)\\ &= \frac{\partial^{k-2}}{\partial\psi_1\cdots\partial\psi_{k-2}}\left(\Pi_{i=1}^{k-2}\psi_i\right)=1\end{aligned}$$

Therefore,
$\frac{\partial H}{\partial t} = k!k+1 = \Sigma_{i=1}^{k}\frac{\partial^k H}{\partial\psi_i^k} + \frac{\partial^k H}{\partial\psi_1\cdots\partial\psi_k}$ $(k>1)$, which confirms that given H is a solution.

Corollary 1 *Suppose $\alpha>0$ and $\beta>0$ are two parameters, then the function, $H(t,\psi_1,\cdots,\psi_k;\alpha,\beta) = (k\alpha k!+\beta)\,t + \frac{1}{k!}\Sigma_{i=1}^{k}\psi_i^k + \Pi_{i=1}^{k}\psi_i$ is also a solution of the model (12).*

These two theorems provide basic general idea of solutions for the models in (11) and (12). These solutions are two proposed candidates for sustainability indices without weights. In the next theorem we provide a solution for above models (we will call weighted sustainability index, $H(\Omega)$), which has weight functions described in this section.

Theorem 3 *The weighted sustainability index*
$H(\Omega) = \left(k!\Sigma_{i=1}^{k}\Omega_i + \prod_{i=1}^{k}\Omega_i\right)t + \Sigma_{i=1}^{k}\Omega_i\psi_i^k + \prod_{i=1}^{k}\Omega_i\psi_i$ *is a solution for the sustainability model (12) with mixed partial derivatives.*

Proof We have, $\frac{\partial H(\Omega)}{\partial\psi_i} = \Omega_i k\psi_i^{k-1} + \Omega_1\psi_1\cdots\Omega_{i-1}\psi_{i-1}\Omega_i\Omega_{i+1}\psi_{i+1}\cdots\Omega_k\psi_k$ and $\frac{\partial^k H(\Omega)}{\partial^k\psi_i} = \Omega_i k!$. The mixed partial derivative terms in the model (12) can be obtained for the given index as,

$$\begin{aligned}\frac{\partial^k H(\Omega)}{\partial\psi_1\cdots\partial\psi_k} &= \frac{\partial^{k-1}}{\partial\psi_1\cdots\partial\psi_{k-1}}\left(\frac{\partial H(\Omega)}{\partial\psi_k}\right)\\ &= \frac{\partial^{k-1}}{\partial\psi_1\cdots\partial\psi_{k-1}}\left(\Omega_k k\psi_k^{k-1}+\Omega_k\Pi_{i=1}^{k-1}\psi_i\right)\\ &= \frac{\partial^{k-2}}{\partial\psi_1\cdots\partial\psi_{k-2}}\left(\Omega_k\Omega_{k-1}\Pi_{i=1}^{k-2}\psi_i\right)\\ &= \prod_{i=1}^{k}\Omega_i\end{aligned}$$

Therefore,

$$\frac{\partial H(\Omega)}{\partial t} = k!\Sigma_{i=1}^{k}\Omega_i\psi_i + \prod_{i=1}^{k}\Omega_i = \Sigma_{i=1}^{k}\frac{\partial^k H}{\partial\psi_i^k} + \frac{\partial^k H}{\partial\psi_1\cdots\partial\psi_k}\ (k>1)$$

Hence, the weighted function proposed is a solution of the model (12).

Corollary 2 *From theorem (3), we can see that*
$H(\Omega) = \left(\Sigma_{i=1}^{k}\Omega_i + \prod_{i=1}^{k}\Omega_i\right)t + \frac{1}{k!}\Sigma_{i=1}^{k}\Omega_i\psi_i^k + \prod_{i=1}^{k}\Omega_i\psi_i$ is also a solution for the model (12).

Corollary 3 *Suppose* $\alpha > 0$ *and* $\beta > 0$ *are two parameters, then the function,*

$$H(t, \psi_1, \cdots, \psi_k, \Omega_1, \cdots, \Omega_k; \alpha, \beta) = \left(\alpha k!\Sigma_{i=1}^{k}\Omega_i + \beta\prod_{i=1}^{k}\Omega_i\right)t + \alpha\Sigma_{i=1}^{k}\Omega_i\psi_i^k + \beta\prod_{i=1}^{k}\Omega_i\psi_i$$

is also a solution of the model (12).

We shortlist seven key independent variables based on May (2002) and also using self-intuition in measuring sustainability.Seven variables are, food and agriculture (ψ_1), climate and environment (ψ_2), population and economics (ψ_3), political situation(ψ_4), medical technology (ψ_5), energy (ψ_6), and science and technology (ψ_7). These variables reduce the models (11) and (12) with a lesser number of realistic variables. Models with reduced variables are to be run along with regional level sub-models with regional specific weight functions and regional specific combinations of key variables listed. A hypothetical description of these seven variables and expected data at a country or a concerned region is given in Table 1.Some of these variables can be split into two or more variables if there is enough evidence from the data. For smaller regions, one can have a larger number of variables because the data needed for obtaining an index would be relatively easier to collect. For larger countries, the more the number of variables more will be the potential variation in the index. We suggest $H(\Omega_7)$ and $H(\Omega_7; \alpha, \beta)$ as two candidates for the sustainability index using the **seven** variables.

The seven variable sustainability index based on Corollary 2 is,

$$H(\Omega_7) = \left(\Sigma_{i=1}^{7}\Omega_i + \prod_{i=1}^{7}\Omega_i\right)t + \frac{1}{7!}\Sigma_{i=1}^{7}\Omega_i\psi_i^7 + \prod_{i=1}^{7}\Omega_i\psi_i \tag{15}$$

and the seven variable sustainability index based on Corollary 3 is,

Table 1 Seven variables required for the sustainability index

Variable	Description	Symbol
Food and agriculture	Proportion of yield of food production to the arable land	ψ_1
Climate and environment	tproportion of people who are living under the clean air, Clearn water facilities and normal climatic conditions	ψ_2
Population and economics	Proportion of people who are above he poverty levels Prescribed by the multidimensional poverty index and proportion of skilled population required for economic growth	ψ_3
Political situation	Duration of the time period where the population Concerned or a region or a country is living under Stable political situation as per global perspective	ψ_4
Medical technology	Proportion of people who are living Within the reach of best medical treatment and health facilities	ψ_5
energy	Proportion of industrial sector, transportation sector and agricultural sector, general population infrastructure Which are availaling sufficient electricity for Optimum productivity	ψ_6
Science and technology	Level of research in basic sciences and Overall technological advancements or Availability of technology to support the needs of concerned population or a region or a country	ψ_7

$$H(\Omega_7;\alpha,\beta) = \left(\alpha 6!\Sigma_{i=1}^{7}\Omega_i + \beta\prod_{i=1}^{7}\Omega_i\right)t + \alpha\Sigma_{i=1}^{6}\Omega_i\psi_i^7 + \beta\prod_{i=1}^{7}\Omega_i\psi_i \tag{16}$$

Once we have data for the variables in Table 1 are collected and weights are computed, the index given in (16) or similar index with different mixed partial derivatives can be constructed. We have two more parameters, α and β in (16) which can be fitted using a least square method or suitable method depending upon the dimension of the data. Weight computation is needed to be done with the help of experts in the respective field. The relative importance of various weights can be decided by the entire team to capture the differential influences of variables in global sustainability status.

3 Properties of $H(\Omega)$

We investigate properties of the sustainability index proposed in Sect. 2. For measuring $H(\Omega_j)$ we need practical weight functions which is possible by assuming

$$\Sigma_{i=1}^{n} \left|\Omega_j(x_i) - \Omega_j(x_{i-1})\right| \leq M \in \mathbb{R} \text{ for each } j = 1, 2, \cdots, k \tag{17}$$

for all partitions of $[\omega_a, \omega_b]$. In this case, Ω_j is an increasing function. Since $\Omega_j : [\omega_a, \omega_b] \to \mathbb{R}$, the variation of Ω_j over $[\omega_a, \omega_b]$ is

$$Var\left(\Omega_j; [\omega_a, \omega_b]\right) = \sup\left\{\Sigma_{i=1}^{n} \left|\Omega_j(x_i) - \Omega_j(x_{i-1})\right| : P\right\} \leq \infty$$

This implies, Ω_j has bounded variation (BV) on $[\omega_a, \omega_b]$ and written as, $\Omega_j \in BV([\omega_a, \omega_b])$ and Ω_j is bounded on $[\omega_a, \omega_b]$. Each of the Ω_j is constructed from the $\Omega_j(h)$, which is a weight function for $h^{th}-$region.

Theorem 4 *For an Ω_j satisfying (17),*

$$\sup\left\{\Sigma_{i=1}^{n} \left|\Omega_j(x_i) - \Omega_j(x_{i-1})\right| : P\right\} \geq \frac{\left|\int_{\omega_a}^{\omega_b} F d\Omega_j\right|}{\left[\sup_{t\in[\omega_a,\omega_b]} |F(t)|\right]}.$$

Proof From the existence theorem for the Riemann–Stieltjes integral (see for example, Nielsen 1997), we have,

$$\left|\int_{\omega_a}^{\omega_b} F d\Omega_j\right| \leq \left[\sup_{t\in[\omega_a,\omega_b]} |F(t)|\right] \times Var\left(\Omega_j; [\omega_a, \omega_b]\right)$$

$$\implies \left|\int_{\omega_a}^{\omega_b} F d\Omega_j\right| \leq \left[\sup_{t\in[\omega_a,\omega_b]} |F(t)|\right] \times \sup\left\{\Sigma_{i=1}^{n} \left|\Omega_j(x_i) - \Omega_j(x_{i-1})\right| : P\right\}$$

(for all partitions P of $[\omega_a, \omega_b]$)

$$\implies \sup\left\{\Sigma_{i=1}^{n} \left|\Omega_j(x_i) - \Omega_j(x_{i-1})\right| : P\right\} \geq \frac{\left|\int_{\omega_a}^{\omega_b} F d\Omega_j\right|}{\left[\sup_{t\in[\omega_a,\omega_b]} |F(t)|\right]}$$

Remark 1 Suppose $\Omega_j(\omega_a) = A_{j1}$ and $\Omega_j(\omega_b) = A_{j2}$, and assuming Ω_j is an $1-1$ function for all $j = 1, 2, \cdots, k$, then using Theorem 3 and Corollary 2, we have, $\frac{\partial H(\Omega_j)}{\partial t} = \left(\Sigma_{j=1}^{k}\left[A_{j1}, A_{j2}\right] + \prod_{j=1}^{k}\left[A_{j1}, A_{j2}\right]\right)$.

4 Real World Situations: Recycling in Pavement Construction

The availability of high-quality aggregates for the construction of highways is scarce across the world; hence the cost of construction has become prohibitively high due to increased lead distance to mobilize suitable quality materials. A simple calculation shows that approx. Twelve thousand tons of Natural Aggregates are required per lane kilometer to build an express highway. If locally available marginal or recycled aggregates can be used after a proper stabilization process can solve the issue. Besides, recycling the existing distressed pavements and reusing them back in the construction of new and rehabilitated pavements has become a viable alternative to natural aggregates. Recycling can address some of the sustainability issues such as the conservation of natural resources and fossil fuels, preservation of the environment, and retention of the existing highway geometrics (Taha et al. 2002). Reusing the construction and demolition waste generated from the construction industry can reduce the burden on the landfills, thus reducing the impact on the environment; otherwise, the waste would have been ended up in landfills. The sustainable cycle of the construction industry can be seen in Fig. 2.

There are different types of recycled and/or reclaimed materials generated across the world from different processes, include but not limited to construction and demolition waste (C&D), crushed bricks (CB), recycled concrete aggregate (RCA), reclaimed asphalt pavement (RAP), quarry waste, (QA), recycled glass (RG), roofing shingles (RS), etc. Among these recycled materials, the RAP, RAC, and C&D are generated in substantial quantities. The Federal Highway Administration (FHWA) has estimated that close to 100 million tons of RAP material is produced by milling HMA

Fig. 2 Sustainable life cycle of a construction materials—When the civil structures are demolished and recycles at the end of their design life, can be recycled and prepare for reuse them as a resource materials in a new and rehabilitation works. When we reuse the reclaimed materials, the demand on the natural materials can be reduced. This cycle continues to reduce the use of natural resources and increases the sustainability index

(Hot mix asphalt) each year (MO Asphalt Pavement Association 2007). According to United States Geological Survey (USGS), the use of recycled crushed concrete aggregates is still constituted by only about 0.5% of the total aggregates consumed in the US (Gnanendran and Woodburn 2003). As high as 41 million tons of quarry by-products are generated per annum in the United Kingdom (Manning 2004).

However, these recycled aggregates 'as is' can't meet the structural and strength characteristics required for various civil engineering applications, including pavement construction due to their inferior characteristics. Several researchers have pointed that stabilizing RAP and natural virgin aggregate (VA) mixes with conventional cementitious materials like cement and lime have yielded superior strength and stiffness properties (Taha et al. 2002; Puppala et al. 2009). However, they could not promote the high replacement of VA with RAP. In the US, state transportation agencies allowed only up to 20% RAP due to a lack of understanding of their behavior. Nevertheless, the production of Portland cement is associated with a substantial amount of energy depletion (5,000 MJ/ton cement), non-renewable resources (1.5-ton limestone and clay/ton cement) as well as CO_2 emissions (0.95 ton CO_2/ton cement) which leads to climate change and ecological imbalance (Higgins 2007; Yi et al. 2013). Hence, there is a necessity to ascertain more environmentally friendly and green materials that can match at least the performance of the traditional materials (cement and lime) under similar circumstances. Thus the utilization of potential industrial by-products is envisioned to replace either in the partial or full amount of conventional stabilizers.

With the substantial availability of industrial by-products such as fly ash and ground granulated blast furnace slag (GGBS), stabilizing RAP:VA blends with these materials could reduce not only the cost of construction but also protect the environment (Saride et al. 2015; Arulrajah et al. 2017; Saride snd Jallu 2020). Besides, Agarwal et al. (2019) have demonstrated the geotechnical characteristics of recycled aggregates, including C&D waste, and reported that these aggregates possess considerable engineering properties, which can further be improved by stabilization.

Besides, Saride and Jallu (2020) have shown that about 60% of RAP can be used in base layers stabilized with low calcium fly ash geopolymer through a series of laboratory studies and field test sections. Geopolymer is an inorganic alumina-silicate polymer material synthesized using alkaline activation of alumina-silicate source materials (Davidovits 1991). Several researchers have reported that the geopolymer stabilized materials possess higher compressive strength and durability characteristics (Song et al. 2005; Fernandez-Jimenez et al. 2007). Nevertheless, if the reactive silica content is low in the source material (fly ash), in addition to the alkali hydroxides, an external supplement of silica is suggested to improve the formation of geopolymer structures. In general, sodium silicate (Na_2SiO_3) or potassium silicate (K_2SiO_3) are supplemented for this purpose.

It was reported that the stabilization of RAP with fly ash geopolymer would not produce a unique product as it depends on the quality of fly ash and the RAP (Saride snd Jallu 2020). They have also demonstrated that the layer coefficients used in the design of flexible pavements by the American Association of State Highway and Transportation Officials (AASHTO) method produce either conservative or unsafe

base course thicknesses when fly ash geopolymers are used. They have proposed a new set of layer coefficients for FRG stabilized RAP bases.

4.1 Design of a Flexible Pavement Using Reclaimed Material

Based on the recently developed novel approaches to accommodate secondary/alternative materials in pavement construction, a full-scale study was undertaken to evaluate the performance of fly ash stabilized RAP as a base course for a flexible pavement (Saride et al. 2018). As part of the study, extensive laboratory and field studies were undertaken.

The key features of the study are outlined below:

- As high as eighty percent of virgin aggregate was successfully replaced with RAP aggregate. About 20–30% of low calcium fly ash was utilized by activating the fly ash with alkali activators. About 350 metric tons of fly ash were consumed per lane kilometer of national highway construction, which amounts to 1400 tons of fly ash required for 4-lane express highways.
- Most of the pavement design guidelines across the world limit the amount of RAP in the base course up to 30% by weight of the virgin aggregates (VA), due to the presence of aged bitumen coating on the RAP aggregates. It was demonstrated that at least 60% of the VA could be replaced while meeting all design requirements.
- The critical design parameters, including the Unconfined Compressive Strength (UCS) and Resilient Modulus (Mr) characteristics of the FA geopolymer stabilized RAP: VA blends were found to meet the threshold values proposed by various design codes.
- Besides, exposure of these mixes to the severe moisture and temperature variations may alter the cementation. The permanency of the stabilizer was also verified through rigorous wet-dry durability and leachate studies. The UCS tests, durability tests, and resilient modulus test (Mr) result indicated that the strength loss of RAP: VA mixes were very minimal and were found suitable for the base course applications.
- Based on the laboratory performance of the product, the performance of the design mix was studied under actual traffic conditions for three years by laying a trial road stretch (200 m) as part of a state highway (SH 207) near Vijayawada in Andhra Pradesh.
- Overall, based on the experimental and field data, a reduction in pavement base course thickness by about 30% and cost of construction by about 20% was achieved with a similar or better performance of the pavement.

4.2 Variables Influence the Sustainability of Pavements

To establish the sustainability index for pavements, a typical cross-section of flexible pavement is shown in Fig. 3 is proposed to build on a weak sub-grade with a resilient modulus of 30 MPa. The pavement is designed according to Indian Roads Congress (2018) for the traffic of 20 million standard axles (msa). The description of the variables used and the range are presented in Table 2. According to Indian Roads Congress (2018), the standard base layer thickness, when virgin aggregate (VA) is used, is found to be 275 mm with an 80 mm thick asphalt layer and 200 mm sub-base layer (See Table 3). Based on the above discussion, if the base layer is chosen to be replaced with a recycled aggregate base (RAP), the thickness of the base layer may be reduced, as suggested in Table 3. As discussed above, since VA is replaced with RAP, stabilization is inevitable to meet the structural strength and stiffness criteria of the base layer. Further, to enhance sustainability in the construction, fly ash was adopted against the conventional stabilizer such as cement. To quantify the effectiveness of the method, the sustainability indicator for the proposed approach may be evaluated to choose an appropriate design mix for the pavement design. To calculate sustainability, several design mixes were considered ranging from replacing

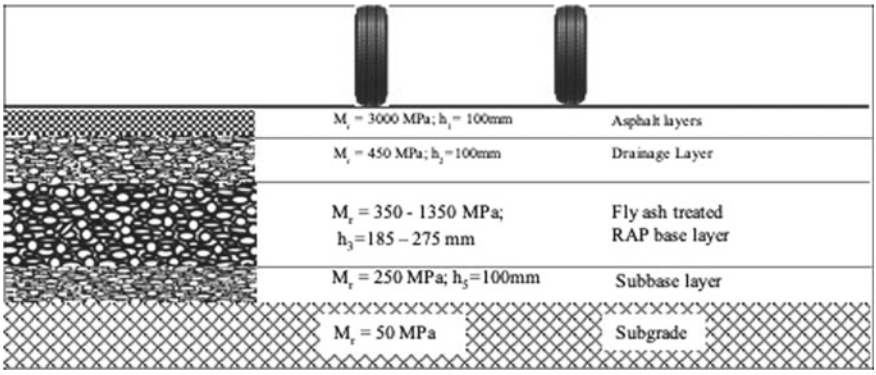

Fig. 3 A typical cross-section of a flexible pavement with recycled base material

Table 2 Description and range of variables used in the pavement design

Sr. No.	Variables	Description	Range of values
1	RAP	Reclaimed asphalt pavement material, obtained from the milling of distressed pavements	50, 60, 80
2	VA	Natural aggregates used for road construction	50, 40, 20
3	FA	Fly ash, obtained from coal combustion in power plants	20, 30
4	Mr	Resilient modulus, a stiffness parameter used in the design of pavement layer thickness	350 to 1350

Table 3 Design of a flexible pavement with recycled materials in the base layer. Note: *The pavement is designed using IRC 37:2018 guidelines for the design traffic of 20 million standard axles (msa) and subgrade modulus of 50 MPa. **Remarks:** Subgrade: Mr = 50 MPa, Sub-base Layer: Mr = 250 MPa, Drainage Layer: Mr =450 MPa, AC Layer: Mr =3000 MPa

Sr. No.	Mix combination	AC	Drainage	Sub-base	Base	Total Thickness	Base Mr (MPa) considered	Reference
1	0R:100VA	80	NA	200	275	555	350	IRC:37 (2018)
2	50R:50V+20F	70	100	100	185	455	1344	–
3	60R:40V+20F	70	100	100	195	465	1191	Saride et al. (2015)
4	80R:20V+20F	70	100	100	205	475	988	Avirneni et al. (2016)
5	100R:0VA+20F	70	100	100	240	510	565	Arulrajah et al. (2017)
6	50R:50V+30F	70	100	100	195	465	1156	–
7	60R:40V+30F	70	100	100	205	475	968	Saride snd Jallu (2020)
8	80R:20V+30F	70	100	100	215	485	824	Saride et al. (2018)

50% VA with 50% RAP stabilized with fly ash. The variation in the combination of RAP:VA blends are presented in Table 3. The suitability of each design mix was established by conducting the strength in terms of unconfined compressive strength (UCS) and resilient modulus (Mr) (Arulrajah et al. 2017; Saride snd Jallu 2020; Avirneni et al. 2016). The Mr values corresponding to each design mix (See Table 3) are used to obtain the design thickness of the base layer for each combination. It is very clear from the Table 3 that if the VA is replaced by 100% RAP, the overall thickness of the pavement has reduced from 555 mm to 510 mm (8% reduction) if it is 50% the reduction is 18% and 14.5% for 60% replacement for the similar performance of the pavement. However, if the overall performance in terms of safety and cost is considered, a 60% replacement of VA is more sustainable. We have plotted Figs. 4 and 5 based on the data collected in this section. The scenario presented in Tables 2 and 3 is evaluated using the proposed sustainability model (11) by analyzing the density functions as explained in Figs. 4 and 5. Figure 4 depicts that when the range is increased from 1 to 9, the relative influence of the variables is reducing, indicating that when the proportion of RAP and VA are the same. Figure 5 is plotted by considering the RAP and VA proportion as 60% and 40%, respectively. Now the influence of RAP on VA is skewed when the range increases. A similar analysis is suggested to perform by considering all the variables in the given scenario to estimate the sustainability index.

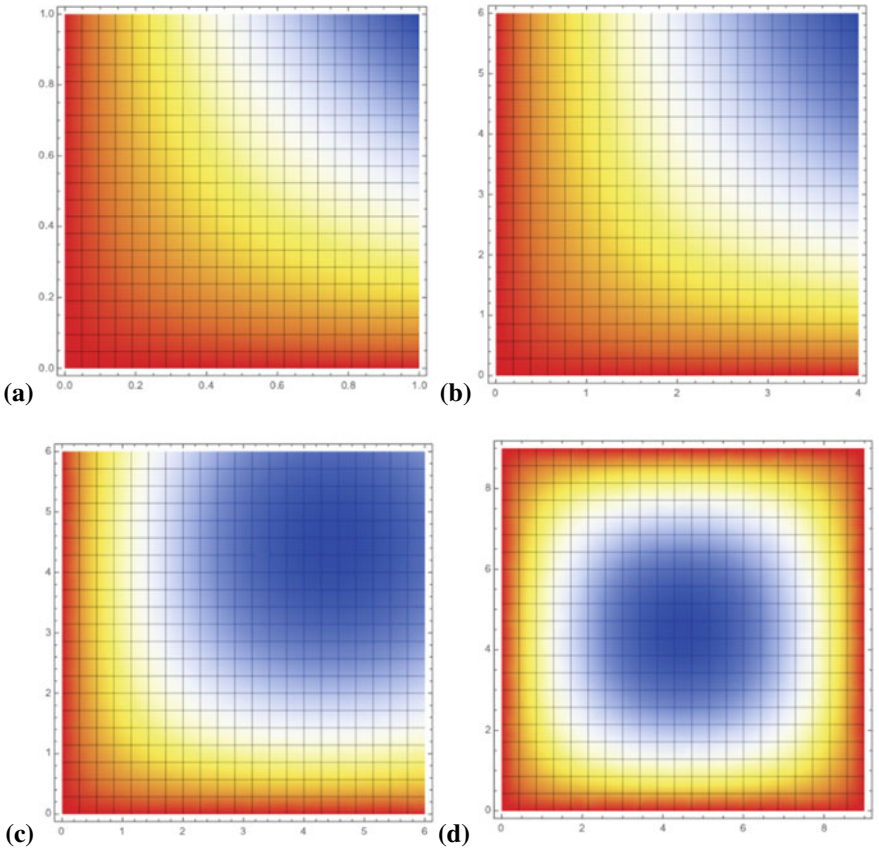

Fig. 4 Plotting of the model for $k = 2$ based on two variables RAP and VA in the Table 2. **a** $\psi_1 \to [0, 1]$ and $\psi_2 \to [0, 1]$, **b** $\psi_1 \to [0, 3]$ and $\psi_2 \to [0, 3]$, **c** $\psi_1 \to [0, 6]$ and $\psi_2 \to [0, 6]$, **d** $\psi_1 \to [0, 9]$ and $\psi_2 \to [0, 9]$. We have used the initial and boundary conditions as follows: $H(\psi_1, \psi_2, 0) = 0$, $H(0, \psi_2, t) = st$, $H(9, \psi_2, t) = st$, $H(\psi_1, 0, t) = st$, $H(\psi_1, 9, t) = st$ and $s = 10, t \in [0, 1000]$

5 Conclusions

There is a great need for collaborative efforts to build mathematical models for measuring and understanding sustainability based on the perception of the people who work on sustainability and who work for sustainability. The models (11) and (12) are very flexible, can accommodate a variety of options to measure sustainability that could arise from the cross-discipliners team of scientists. Using these models, one can measure the overall sustainability of human life in a country or a region as a result of several variables by treating each factor independently (model (11)) or resultant measure of sustainability as a result of various overlapping variables (model (12)). When there are not enough evidence on the dependencies of variables for a par-

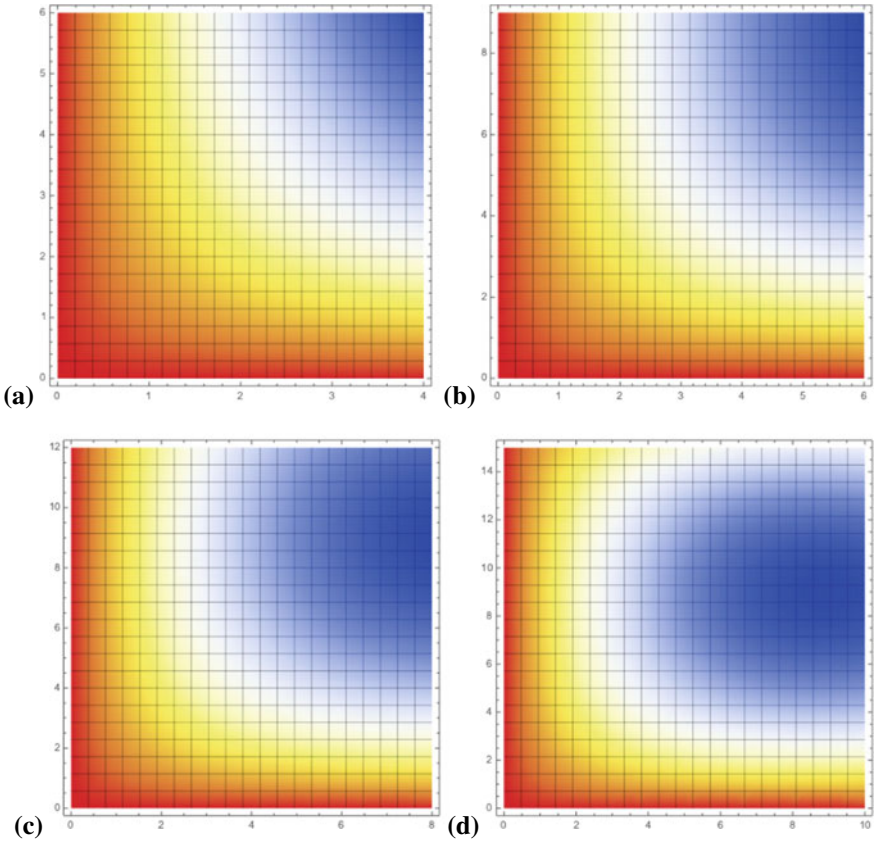

Fig. 5 Plotting of the model for $k = 2$ based on two variables RAP and VA in the Table 2. **a** $\psi_1 \to [0, 4]$ and $\psi_2 \to [0, 6]$, **b** $\psi_1 \to [0, 6]$ and $\psi_2 \to [0, 9]$, **c** $\psi_1 \to [0, 8]$ and $\psi_2 \to [0, 12]$, **d** $\psi_1 \to [0, 10]$ and $\psi_2 \to [0, 15]$. We have used the initial and boundary conditions as follows: $H(\psi_1, \psi_2, 0) = 0$, $H(0, \psi_2, t) = st$, $H(18, \psi_2, t) = st$, $H(\psi_1, 0, t) = st$, $H(\psi_1, 18, t) = st$ and $s = 10, t \in [0, 1000]$

ticular population concerned to study sustainability, we can start the analysis using the model (11). In fact, the model (11) is a subset of the model (12) under certain situations. Usually, second-order PDEs arise in most of the natural and engineering sciences situations. However, higher order PDEs are also prevalent in handling questions related to mechanics and elasticity. The degree and size of information to be used at a country or regional level could be data-dependent, hence, we have proposed flexible models. Mathematical models might help to understand factors and features of sustainability, however, for practical solutions, these models must reach mainstream developmental activities. Obtaining relevant data from the seven variables mentioned might not be an easy exercise and could involve time-consuming efforts

by people involved in sustainability research and other key people in political and government circles.

The data from atmosphere, oceans, vegetation, food, wetlands, species, and several environmental parameters could generate multiple sources of errors and bias. Hence, there is a requirement for the estimation of variability. As pointed out in Levin et al. (2013) there is good scope for statistical thinking as well. There are documented arguments on how collective efforts by social, political, government setup could form a network that could help to maintain adaptability and transformability in ecological dynamics (Gunderson 2006) and sustainable agriculture and energy and impact of climate in developing countries (Pretty et al. 2002; Ravindranath et al. 2006). There are several advances in computational techniques, and facilities to conduct global level high intense computational experiments of complex mathematical models so that the global community can easily come together for sustainable development.

Our approach of modeling the phenomena is also computationally challenging, in terms of numerical approximation and numerical solutions to the proposed PDEs. There is no unified approach for computing Riemann–Stieltjes weights when they are used in PDEs. Even the decision of using an appropriate partition of the intervals $[\omega_a, \omega_b]$ needs construction of complex algorithms because we have mixed weights with the PDEs. In fact, this kind of modeling initiation and developing global indices will help to strengthen the data collection and information gathering activities. Governments and non-government agencies like the UN, the World Bank, MacArthur Foundation, Gates Foundation, etc., needs to encourage cross-disciplinary modeling research teams and data collection programs. There is an urgent need to bring al the activities into a common platform and need for standardization of the sustainability control activities across the globe. Countries should take efforts to bring transparency in the data collection methods and definitions of variables for the global health of the human population. There is a need to start providing annual sustainability indices for the country, region (formed by a group of countries), continent, and World.

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Extreme Point Methodology in Power Calculations—The Case of Hardy–Weinberg Equilibrium

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Abstract As a prelude to genetic analysis, one needs to check whether a specific bi-allelic Single Nucleotide Polymorphism (SNP) is in Hardy–Weinberg Equilibrium. Several tests are available to check equilibrium based on data collected on genotypes at the location of interest. Comparing the powers of these tests, especially for small sample sizes, is fraught with difficulties. Typically, comparisons are made based on extensive simulations. In this note, we propose extreme point methodology, which will facilitate exact computation of the power of a test at a specific alternative and thus paving the way for power comparisons.

1 Introduction

Let A and a be the alleles of a SNP and AA, Aa, aa the associated genotypes. The distribution P of the genotypes in the population is reported in the form of a Punnett table, which is symmetric (Table 1).

The genotypes are AA, Aa, and aa with probabilities P_{AA}, $2P_{Aa}$, and P_{aa}, respectively. The allele probabilities of A and a are p and $1-p$, respectively, obeying the requirements $P_{AA}+P_{Aa}=p$ and $P_{Aa}+P_{aa}=1-p$. The SNP is in Hardy–Weinberg equilibrium if $P_{AA}=p^2$. The concept has profound implications. If the SNP is in equilibrium, it will be in equilibrium, under random mating, in every subsequent generation. See Gondro (2015), Zheng et al. (2012), Foulkes (2009), Weir (1996), Wigginton et al. (2005), Lange (2002).

The null hypothesis to test is $H_0: P_{AA}=p^2$ for some $0<p<1$. The alternative is $H_1: P_{AA}\neq p^2$ for any p. Both hypotheses are composite. The data consists of

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Table 1 Joint Distribution of Genotypes

	Allels		
Allels	A	a	*Allele Probability*
A	P_{AA}	P_{Aa}	p
a	P_{Aa}	P_{aa}	$1-p$
Allele Probability	p	$1-p$	1

genotype frequencies n_1, n_2, and n_3 compiled on a random sample of n subjects, where n_1 is the number of subjects in the sample with genotype AA, n_2 with genotype Aa, and n_3 with genotype aa. Theoretically, the vector (n_1, n_2, n_3) has a multinomial distribution $(n, P_{AA}, 2P_{Aa}, P_{aa})$. A plethora of tests is available in the literature. The Exact Test is natural when we have small samples. The chi-squared test is the standard staple for testing. The chi-squared test with continuity correction $(cc) = 0.5$ is implemented in many a software. See Yates (1934). The variation with $cc = 0.25$ was considered by Emigh (1980). See also Grizzle (1967) and Mantel and Greenhouse (1968). The conditional chi-squared test was proposed by Li (1955) and the tests with $cc = 0.5$ or $cc = 0.25$ were discussed by Emigh (1980). Several variations were discussed and analyzed in papers by Emigh (1980), Elston and Forthofer (1977), Freeman and Tukey (1950), Mantel and Li (1974). A comparison of these tests through extensive simulations was carried out in Emigh (1980). Our line of enquiry in this paper whether it is feasible to compare the performance of these tests theoretically. We will demonstrate that it is doable, and we introduce extreme point methodology in this connection. We will discuss the performance of three tests in this connection along with our innovation to provide a contrast. A comprehensive comparison of tests a la Emigh (1980) would be a laudable goal and this will be our future project. Tests T_2, T_3, and T_4 presented below (Table 2) are, basically, modifications of T_1 with their avowed cc. All tests are at 5% level of significance.

The work carried out in the paper is useful when testing Hardy–Weinberg equilibrium for small sample sizes. The choice of a test should be carefully weighed in before making a judgement on the equilibrium. It is also useful when some genotype frequencies are small, which will certainly arise when a particular allele frequency is very small. One thousand genome project with rare variants is a prime example.

2 Extreme Point Methodology

Let $0 < p < 1$ be fixed. Assume $p \leq \frac{1}{2}$, without loss of generality. Let $\Omega(p)$ be the collection of all 2×2 symmetric matrices P with non-negative entries and row sums equal to p and $1 - p$. Note that $\Omega(p)$ is a compact convex set. Each entry in $\Omega(p)$ is a prototype of the joint distribution of the genotypes. It has two extreme points P_1

Table 2 Description of Tests

Tests	*Description*
T_1	Traditional Chi-Squared Test, Reject H_0 if $n(\frac{(n_2^2-4n_1n_2)^2}{(2n_1+n_2)^2(n_2+2n_3)^2}) > 3.8416$
T_2	Yates' Test with $cc = 0.5$, Reject H_0 if $\frac{(\left\|n_1-\frac{(2n_1+n_2)^2}{4n}\right\|-0.5)^2}{\frac{(2n_1+n_2)^2}{4n}} + \frac{(\left\|n_2-\frac{(2n_1+n_2)(n_2+2n_3)}{2n}\right\|-0.5)^2}{\frac{(2n_1+n_2)(n_2+2n_3)}{2n}} + \frac{(\left\|n_3-\frac{(n_2+2n_3)^2}{4n}\right\|-0.5)^2}{\frac{(n_2+2n_3)^2}{4n}} > 3.8416$
T_3	Emigh's Test with $cc = 0.25$, Reject H_0 if $\frac{(\left\|n_1-\frac{(2n_1+n_2)^2}{4n}\right\|-0.25)^2}{\frac{(2n_1+n_2)^2}{4n}} + \frac{(\left\|n_2-\frac{(2n_1+n_2)(n_2+2n_3)}{2n}\right\|-0.25)^2}{\frac{(2n_1+n_2)(n_2+2n_3)}{2n}} + \frac{(\left\|n_3-\frac{(n_2+2n_3)^2}{4n}\right\|-0.25)^2}{\frac{(n_2+2n_3)^2}{4n}} > 3.8416$
T_4	New Test with $cc = 0.35$, Reject H_0 if $\frac{(\left\|n_1-\frac{(2n_1+n_2)^2}{4n}\right\|-0.35)^2}{\frac{(2n_1+n_2)^2}{4n}} + \frac{(\left\|n_2-\frac{(2n_1+n_2)(n_2+2n_3)}{2n}\right\|-0.35)^2}{\frac{(2n_1+n_2)(n_2+2n_3)}{2n}} + \frac{(\left\|n_3-\frac{(n_2+2n_3)^2}{4n}\right\|-0.35)^2}{\frac{(n_2+2n_3)^2}{4n}} > 3.8416$

and P_2 given by

$$P_1 = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix} \; and \; P_2 = \begin{pmatrix} 0 & p \\ p & 1-2p \end{pmatrix} \tag{1}$$

Every matrix P in $\Omega(p)$ is a convex combination of P_1 and P_2, i.e.,

$$P = \gamma P_1 + (1-\gamma)P_2, where \, \gamma = \frac{p_{AA}}{p}$$

Using the structure of P, we give a representation theorem below for the power function of any test of Hardy–Weinberg equilibrium. Let T^* be a test proposed for testing the null hypothesis at a given level of significance $0 < \alpha < 1$. Let $T = T(n_{11}, n_{12}, n_{22})$ be the underlying test statistic and c the critical value. Structurally, the test T^* is spelled out as follows:

$$Reject \; the \; null \; hypothesis \; if \; and \; only \; if \; T \geq c \; (c = 3.8416 \; for \; \alpha = 0.05).$$

The test statistic T has a chi-squared distribution under the null hypothesis based on the asymptotic theory. The power function of T^* is a function of the genotype distribution P. The distribution P is uniquely determined by the specification of any two entities from $\{p, p_{AA}, p_{Aa}, p_{aa}\}$. We will stick to p and p_{AA}. Thus, the power function of T^* is defined by, $P_0(T; p_{AA}, p) = Pr(T \geq c \mid p, p_{AA})$. For the computation of the probability involved, we need the distribution of T when the genotype probabilities are p_{AA}, $2p_{Aa}$, and p_{aa}. In order to compare the performance of two tests, T^* and T^{**}, with their underlying test statistics T_1 an T_2, we need to compare,

$$P_0(T_1;\, p,\, p_{AA})\ and\ P_0(T_2;\, p,\, p_{AA})\ for\ every\ 0 < p \leq \frac{1}{2}\ and\ 0 \leq p_{AA} \leq p.$$

In order to facilitate such a comparison, we have the following representation theorem for the power function. Let $0 < p \leq \frac{1}{2}$ and $0 \leq p_{AA} \leq p$ be given. Let P_1 and P_2 be the extreme points spelled out in (1). Let the individuals sampled be denoted by $I_1, I_2, \ldots, I_n$. Let $\Psi_i = Pr(T \geq c | I_1, I_2, \ldots, I_i$ have genotype distribution P_1 and $I_{i+1}, I_{i+2}, \ldots, I_n$ have distribution $P_2)$, $i = 0, 1, 2, \ldots, n$. Note that Ψ_i is a function of p and n only. The following result gives an expression for the power function of T.

2.1 Theorem

$$P_0(T;\, p,\, p_{AA}) = \sum_{i=0}^{n} \binom{n}{i} \gamma^i\ (1-\gamma)^{n-i} \Psi_i,\ where\ \gamma = \frac{p_{AA}}{p} \tag{2}$$

2.2 Proof

The individuals $I_1, I_2, ..., I_n$ have independent and identically distributed genotype distribution P given by,

$$P = \begin{pmatrix} P_{AA} & P_{Aa} \\ P_{Aa} & P_{aa} \end{pmatrix}$$

with marginal row sums p and $1 - p$. The joint genotype distribution of the individuals is given by the product probability measure $P^n = P \times P \times \cdots \times P$. Since $P = \gamma P_1 + (1-\gamma) P_2$, the product probability measure is given by

$$P^n = (\gamma\, P_1 + (1-\gamma)\, P_2)^n = \sum_{i=0}^{n} \binom{n}{i} \gamma^i\ P_1^i (1-\gamma)^{n-i}\ P_2^{n-i}$$

Consequently,

$$\begin{aligned} P_0(T;\, p,\, p_{11}) &= Pr(T \geq c \,|\, I_1, I_2, \ldots, I_n\ have\ joint\ genotype\ distribution\ P^n) \\ &= \sum_{i=0}^{n} \binom{n}{i} \gamma^i\ (1-\gamma)^{n-i} \Psi_i. \end{aligned}$$

3 Comments

1. The power function is a convex combination of $\Psi_0, \Psi_1, \Psi_2, \ldots, \Psi_n$, each of which is a function of p and n only.
2. The entity $\gamma = \frac{p_{AA}}{p}$ depends on both p and p_{AA}.
3. The above representation theorem helps us in comparing the power functions of any two tests T_1^* and T_2^* of the same sample size at any vector (p, p_{AA}) of arguments for all $0 < p_{AA} \leq p$. Let T_1 and T_2 be the corresponding test statistics and c_1 and c_2 their respective critical values at level α. There is no need to compute $Pr(T_1 \geq c_1 \mid p, p_{AA})$ and $Pr(T_2 \geq c_2 \mid p, p_{AA})$ afresh for every choice of p and p_{AA}. Let $\Psi_i = Pr(T_1 \geq c_1 | I_1, I_2, \ldots, I_i$ have genotype distribution P_1 and $I_{i+1}, I_{i+2}, \ldots, I_n$ have distribution $P_2)$ and $\Psi_i^{'} = Pr(T_2 \geq c_2 | I_1, I_2, \ldots, I_i$ have allele distribution P_1 and $I_{i+1}, I_{i+2}, \ldots, I_n$ have distribution $P_2)$, $i = 0, 1, 2, \ldots, n$. The quantities Ψ_i and $\Psi_i^{'}$ can be used to calculate the powers of the test T_1^* and T_2^*. If $\Psi_i \geq \Psi_i^{'}$ for all i, then $P_0(T_1 \ ; \ p, p_{AA}) \geq P_0(T_2 \ ; \ p, p_{AA})$ for all $0 < p_{AA} \leq p$. This means that the test T_1^* is superior to T_2^* in the sense it has higher powers.
4. The power function formula works in practice as follows. Let n be given. Let T^* be a given test at level α with the underlying statistic T. Let $0 < p \leq \frac{1}{2}$ and $0 < p_{AA} \leq p$ be given. This will determine the joint distribution of the genotypes. Compute $\Psi_0, \Psi_1, \Psi_2, \ldots, \Psi_n$. These entities need only p and n. If $p_{AA} = p^2$, the joint distribution falls under the spell of the null hypothesis. Then the power (2) gives the exact level of the test. If $p_{AA} \neq p^2$, the genotype distribution P comes under the purview of the alternative hypothesis. In that case, the power (2) gives the exact power of the test at P.
5. If one wants to compare the power functions of two tests, compare their respective fundamental probabilities Ψ_is.

4 Computation of Fundamental Probabilities

Let $0 < p \leq \frac{1}{2}$ and n be given. Let T^* be the test under scrutiny and T the underlying test statistic built on the data n_1, n_2, n_3 (sum = n). The fundamental probability $\Psi_i (i = 0, 1, 2, \ldots, n)$ is given by $\Psi_i = \Psi_i(p, n) = Pr(T(n_1, n_2, n_3) \geq c \mid I_1, I_2, \ldots, I_i \sim P_1$ and $I_{i+1}, I_{i+2}, \ldots, I_n \sim P_2)$. We need to enumerate all possible (n_1, n_2, n_3) with corresponding probabilities under the conditions spelled out. If $I_1, I_2, \ldots, I_i \sim P_1$, then $(n_1, n_2, n_3) \sim Multinomial(i, p, 0, 1 - p)$, which means $n_1 \sim Binomial(i, p)$, $n_2 = 0$, and $n_3 = i - n_1$. If $I_{i+1}, I_{i+2}, \ldots, I_n \sim P_2$, then $(n_1, n_2, n_3) \sim Multinomial(n - i, 0, 2p, 1 - 2p)$, which means $n_1 = 0, n_2 \sim Binomial(n - i, 2p)$ and $n_3 = (n - i) - n_2$. Every realization of (n_1, n_2, n_3) is the sum of realizations (n_1, n_2, n_3) under P_1 and of (n_1, n_2, n_3) under P_2 with the corresponding probabilities multiplied. For example, suppose $i = 4$, and $n = 10$.

$I_1, I_2, I_3, I_4 \sim P_1$. This means $n_1 \sim Binomial(4, p)$, $n_2 = 0$, and $n_3 = 4 - n_1$. Then $(1, 0, 3)$ is a possible realization of (n_1, n_2, n_3) with probability $\binom{4}{1} p\,(1-p)^3$.

$I_5, I_6, I_7, I_8, I_9, I_{10} \sim P_2$. This means $n_1 = 0, n_2 \sim Binomial(6, 2p)$, and $n_3 = n_1 - n_2$. One possible realization is $(0, 2, 4)$ with probability $\binom{6}{2} (2p)^2(1-2p)^4$. Then $(1, 0, 3) + (0, 2, 4) = (1, 2, 7)$ is a possible realization of (n_1, n_2, n_3) with probability $\binom{4}{1} p\,(1-p)^3 \times \binom{6}{2} (2p)^2(1-2p)^4$.

5 Comparison of 4 Tests

We have calculated the fundamental probabilities Ψ_i, $i = 0, 1, 2, \ldots, n$ when $n = 10$ and $p = 0.1, 0.2, 0.25, 0.3, 0.4$, for four tests, Chi-squared, Yates' test with $cc = 0.5$, Emigh's test with $cc = 0.25$, and our interjection with $cc = 0.35$. The computations are executed with Python and the code is available on request. The actual probabilities are reported in Table 3 for $p = 0.25$. The other probabilities are reported in a graphical format (Fig. 1).

5.1 Comments on the Graphs

1. The fundamental probabilities are indistinguistable for the chi-squared test and Emigh's for all p under consideration.
2. When $p = 0.1$, our interjection out-performs all other tests.
3. When $p = 0.2$, then there is no clear-cut winner.
4. When $p = 0.25, 0.3$ and 0.4, chi-squared test out-performs all other tests.

Table 3 Fundamental Probabilities Ψ_I for $n = 10$ and $p = 0.25$

i	*Tests*			
	Chi-Squared	Emigh's	Yates'	New
0	0.05468749	0.01074218	0.0205078	0.0205078
1	0.01562499	0.0024414	0.01513671	0.01562499
2	0.00610351	0.0036621	0.01782226	0.0192871
3	0.01306152	0.01306152	0.02429199	0.02844238
4	0.03521729	0.03521729	0.03411866	0.04510499
5	0.08120728	0.08120728	0.05099488	0.07708741
6	0.16789246	0.16789246	0.08296205	0.13822938
7	0.31645966	0.31645966	0.14539338	0.24969483
8	0.54142378	0.54142378	0.26308058	0.43556593
9	0.81223488	0.81223488	0.46523857	0.69899178
10	0.94368553	0.94368553	0.7559452	0.94368553

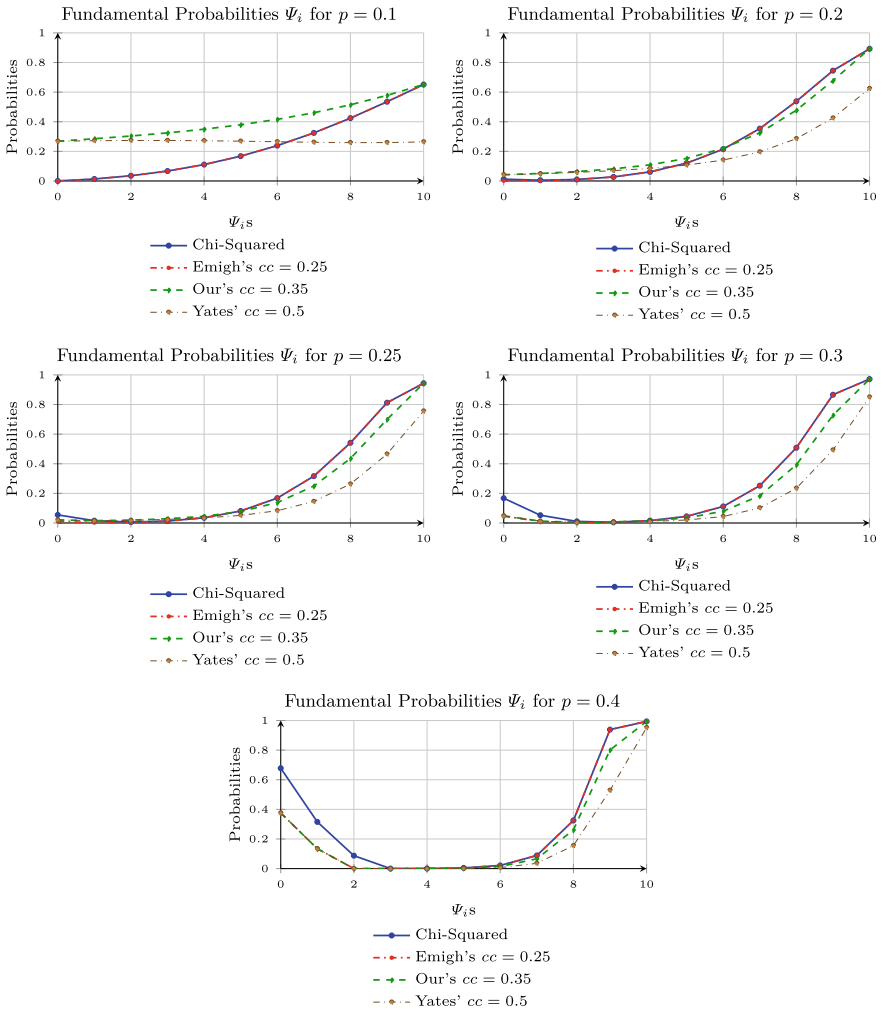

Fig. 1 Fundamental Probabilities of four tests for $p = 0.10, 0.20, 0.25, 0.30$ and 0.40

6 Conclusion

We have utilized extreme point methodology in order to derive a formula for the power function of any test of Hardy–Weinberg equilibrium in the context of bi-allelic markers. We compared the performance of three tests of equilibrium, namely, the traditional chi-squared test, Yates' test, and Emigh's test with a sample size of $n = 10$ and allele frequencies of $p = 0.1, 0.2, 0.25, 0.3, 0.4$. We proposed a new test and examined its power function vis-á-vis the other three tests. A close inspection of

the fundamental probabilities reveals that at a lower allele frequency ($p = 0.1$), our improvisation $cc = 0.35$ outperforms all other tests considered. This has implication in testing HW equilibrium in the environment of rare variants. In Genome Wide Association Studies (GWAS), HW equilibrium is tested at thousands of SNPs, in which one sees substantial variation in the allele frequency p. The study on Restless Leg Syndrome conducted by Stefansson et al. (2007) is a prime example. In other cases of common variants, the classical chi-squared test is as good as other tests considered.

This is just a beginning of our research demonstrating the potentiality of extreme point analysis for power comparisons. Future work will consist of comparing power functions of some more tests for a variety of sample sizes and for $0 < p \leq 0.5$.

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All knowledge is, in final analysis, history.
All sciences are, in the abstract, mathematics.
All judgements are, in their rationale, statistics C.R. Rao.

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General

On the Association of Professor C. R. Rao with the Poznań School of Mathematical Statistics and Biometry

Tadeusz Caliński

Abstract The long-standing association of C. R. Rao with Polish mathematicians and statisticians started in 1954 when he visited Berkeley, at the invitation of Jerzy Neyman. His first visit to Poland (to Warsaw) was in 1956, at the invitation of Oscar Lange. C. R. Rao's next visit to Warsaw was in 1964, under the exchange scheme between the Indian Statistical Institute and the Polish Academy of Sciences. His third visit to Poland was in 1975, in connection with the Session of the International Statistical Institute in Warsaw. At this occasion, we invited Professor C. R. Rao to Poznań, to give a talk at our weekly seminar. In that way, a closer contact between him and our school started. In 1991, Professor C. R. Rao received from the Adam Mickiewicz University in Poznań the highest academic distinction, Honoris Causa Doctoris. This was then followed by active research collaboration and personal contacts with him. There were some exchanges of visits and joint publications.

Keywords Biometric research · Design and analysis of experiments · Gauss–Markov model · Linear statistical inference · Modern mathematical statistics

1 Foreword

The Poznań school of mathematical statistics and biometry has been developed under a predominant influence of the works of Professor C. Radhakrishna Rao, whose two classical books, on statistical methods in biometric research (Rao 1952) and on linear statistical inference (Rao 1973), have been used as the main textbooks of statistical knowledge. These and other works of the prominent Author have stirred interest in statistical methodology among students, scientists, and research workers of the various academical and research institutes in Poznań and its region. Theoretical and applied results of C. R. Rao have been presented and discussed at the weekly joint

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statistical seminars conducted in Poznań since 1965. These results, thoroughly studied, have inspired research undertaken by mathematicians and biometricians from Adam Mickiewicz University, Academy of Agriculture and from other educational and research organizations of Poznań. Many young statisticians have obtained their doctoral degrees after presenting theses influenced in various ways by C. R. Rao's published works. Now influences of C. R. Rao's works can easily be traced in the majority of results published by statisticians and biometricians from Poznań.

2 Memoirs

It may be interesting to recall the longstanding association of Professor Calyampudi Radhakrishna Rao with Polish mathematicians and statisticians. It started in 1954 when he, for the first time, visited the University of California, invited by Professor Jerzy Neyman, a distinguished Polish statistician, who was from 1938 on living and working in the USA, as director of the famous Statistical Laboratory in Berkeley. Professor Rao considered Neyman to be a scientist who essentially influenced the character of research in mathematical statistics. According to C. R. Rao, Jerzy Neyman was generous in giving his time and ideas to young mathematicians and statisticians working under his guidance. It should also be noted that Jerzy Neyman, before that visit, took interest in some results of C. R. Rao on estimation of parameters, and named one of Rao's results as the "Cramér-Rao inequality."

The next contact, of C. Radhakrishna Rao with Polish scientists, was with the Polish econometrician Professor Oscar Lange, who in the mid-50s visited the Indian Statistical Institute, where C. R. Rao was working as the head of the Division of Theoretical Research and Training. Oscar Lange was invited by Professor P. C. Mahalanobis, the director of that Institute, to participate in the discussion on 5-year economic plans for India. On that occasion, Oscar Lange gave lectures on some problems in econometrics.

The first visit of C. Radhakrishna Rao to Poland was in 1956. He was returning from a conference in the Soviet Union and stopped in Warsaw for a few days, as a guest of the Polish Academy of Sciences, at the invitation of Oscar Lange. That was an occasion for Rao to establish contact with several well-known Polish mathematicians and other scientists. That visit also gave him an opportunity to see the massive reconstruction work being undertaken in the capital of Poland which had been so much damaged during the Second World War.

The next visit of C. Radhakrishna Rao to Warsaw was in 1964 to attend a special seminar held in honor of Jerzy Neyman on his seventieth birthday. That visit was arranged under the exchange scheme of scholars between the Indian Statistical Institute and the Polish Academy of Sciences.

In 1972, a Polish delegation visited India to participate in the Mahalanobis Memorial Conference. This was another occasion to strengthen the contacts between Indian and Polish scholars. Since then, several researchers from India visited Poland to work with Polish mathematicians and statisticians.

The third visit of C. Radhakrishna Rao to Poland was in 1975, in connection with the Session of the International Statistical Institute held in Warsaw. That was an excellent occasion to have a visit of Professor C. R. Rao to Poznań. An invitation from the Department of Mathematical and Statistical Methods at the Academy of Agriculture in Poznań (now the Poznań University of Life Sciences) was sent to him. C. R. Rao was invited to give a talk at our weekly seminar on mathematical statistics and its applications, attended not only by people from our department but also by colleagues from Adam Mickiewicz University in Poznań and from other institutes. This invitation was kindly accepted and we had the privilege of having such an excellent speaker at our seminar. This seminar was attended also by Parachuri R. Krishnaiah from Ohio in the USA, who also kindly accepted our invitation. A picture of this seminar can be seen in the journal Statistical Science, Vol. 30, No. 3 (August 2015) on p. 437. After the seminar, we had a very friendly meeting with our guests.

This visit of Professor Rao in Poznań paved the way for very active collaboration between statisticians in Poznań and the scientists connected with the Indian Statistical Institute. Several exchanges of visits started, often leading to joint publications.

From the Poznań side, the individual most active in this fruitful cooperation was Jerzy K. Baksalary. The main results of this joint work have been published in the following papers. Those by Baksalary and Mathew (1986), Baksalary and Mathew (1988) concern some applications of the general Gauss–Markov model. Next, three by Baksalary and Puri (1987, 1988, 1990) are devoted to some conditions for block designs. In addition, that by Baksalary and Mitra (1991) is devoted to the problem of matrix ordering. Of particular interest are two other papers. That by Baksalary et al. (1992) concerning some estimation problems in the singular Gauss–Markov model, and the paper by Baksalary et al. (1995) related to the problem of admissibility of linear estimation in the general Gauss–Markov model.

Most of the research on which these last two papers are based, was carried when Jerzy K. Baksalary was a frequent visitor at the Center for Multivariate Analysis at Pennsylvania State University. It is to be noted that from 1988 C. Radhakrishna Rao was the director of that Center. This made it possible for Rao and Baksalary to work together. The third co-author of these two papers, Augustyn Markiewicz, was involved in this research by correspondence from our department in Poznań.

The next visit of Professor Rao to Poznań was connected with a special event. On 29 November 1989 the Senate of the Adam Mickiewicz University in Poznań conferred an honorary doctoral degree (Honoris Causa Doctoris) on Professor Calyampudi Radhakrishna Rao, to express the highest recognition of his achievements in building modern mathematical statistics. This decision of the University Senate was undertaken due to the initiative of the Institute of Mathematics of this University and the application of scientists from the Poznań school of mathematical statistics and biometry.

The great official ceremony of conferring on Professor C. R. Rao, in person, the highest academic distinction took place in Poznań on 14 January 1991. In orations of the Rector of the Adam Mickiewicz University, the Dean of the Faculty of Mathematics and Physics, and particularly in the speech of the Promotor, Professor Mirosław Krzyśko, attention was drawn to the great scientific results of C. Radhakrishna Rao,

particularly in the development of mathematical statistics and its applications. But also, on this occasion, the Dean of the Faculty of Mathematics and Physics recalled the Indian invention of the decimal system and the introduction of the zero symbol. Professor Rao in his speech, given in response to the award of Honoris Causa Doctoris, recalled in a very interesting form his long standing association with Polish mathematicians and statisticians. Particularly, he cordially described his first visit to Poznań in 1975.

After the official ceremony in the Adam Mickiewicz University we had the pleasure of spending together with C. Radhakrishna Rao some time in Poznań, on that and the next day. In the afternoon of the first day (Monday, 14 January), I took him for a walk to show him interesting places in the town, particularly those of historical importance. He was very interested in places connected with the battle of Poznań in January/February 1945. In the evening after the walk we had, together with several colleagues, a friendly dinner at the Old Market of Poznań. On the next day (Tuesday, 15 January) we had a special seminar at the Academy of Agriculture in Poznań (now the Poznań University of Life Sciences) organized by our department. The first speaker was C. R. Rao, with a talk on "Robust inference in linear models: a review and some problems." The next speakers were Jerzy K. Baksalary, Tadeusz Caliński, and Mirosław Krzyśko. There was much interesting discussion during this seminar.

After returning to his home in Pennsylvania, Professor Rao sent me a very cordial letter (dated 16 January 1991), in which he wrote (in particular): "Thanks for all that you have done—an excellent guided tour of Poznań, delightful dinner, and the fruitful one day seminar."

This interesting contact with C. Radhakrishna Rao was followed by further active scientific collaboration. As already mentioned, two joint papers with C. R. Rao were published, in 1992 and 1995. We had also the pleasure of meeting him at various international conferences. In fact, before the meeting in Poznań, some of us already had the privilege of attending the International Workshop on Linear Models, Experimental Designs, and Related Matrix Theory held on 6–8 August 1990 at the University of Tampere in Finland, at which the two main lectures were given by C. Radhakrishna Rao.

The next such occasion, after the celebration in Poznań, was at ProbaStat'94, i.e., at the International Conference on Mathematical Statistics, held on May 30–June 3, 1994, at Smolenice in Slovakia. The Opening Ceremony started with the lecture of C. Radhakrishna Rao on "Recent contributions to statistical inference in censored regression models." This conference was attended by many Polish statisticians. It was really a pleasure to meet Professor Rao and his wife there.

Another important occasion to meet Professor C. R. Rao was at SCRA 2006, i.e., at the Interdisciplinary Mathematical and Statistical Techniques—Thirteenth International Conference of the Forum for Interdisciplinary Mathematics, held on 1–4 September 2006 at the Polytechnic Institute of Tomar in Portugal. This conference was organized in connection with another honorary distinction of Professor C. Radhakrishna Rao. In the year 2006, the New University of Lisbon conferred the Honoris Causa degree on him. The Honoris Causa Ceremony for Professor C. R. Rao was held on the first day of the Conference. It was followed by the Keynote Session

with the lecture of C. R. Rao entitled "Statistics: Reflections on the past and visions for the future." On the second day, at the first Plenary Session, I had the pleasure to give a talk with the title "On some results of C. Radhakrishna Rao applicable to the analysis of multi-environment variety trials." In this presentation, published in the following year (Caliński 2007), references have been made to 10 publications of C. R. Rao, from the years 1947–1999. His results have been very useful in analyzing agricultural experiments, not only crop variety trials.

I recall this conference in Tomar with a great pleasure. It was very well organized, both from the scientific and the social point of view. Personally it gave me many opportunities to meet famous people from various countries. Particularly I had many private contacts with C. R. Rao, including friendly walks to interesting places.

Let me consider these contacts with Professor C. Radhakrishna Rao as a completeness of my memoirs.

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