






Hyperuniform Point Sets on the Sphere: Deterministic Aspects

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Abstract The notion of hyperuniformity originally introduced as a measure of regularity of infinite point sets in Euclidean space is generalized and extended to sequences of finite point sets on the sphere. It is shown that hyperuniformity implies uniform distribution. Furthermore, it is shown that Quasi-Monte Carlo design sequences with strength at least $\frac{d+1}{2}$ and especially sequences of spherical designs of optimal growth order are hyperuniform.

Keywords Hyperuniformity · Uniform distribution · QMC designs · Discrepancy

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1 Introduction

Hyperuniformity was introduced by Torquato and Stillinger [27] (cf. [21]) to describe idealized *infinite* point configurations, which exhibit properties between order and disorder. Such configurations X occur as jammed packings, in colloidal suspensions, and as quasi-crystals. The main feature of hyperuniformity is the fact that local density fluctuations are of smaller order than for a random (“Poissonian”) point configuration. Alternatively, hyperuniformity can be characterized in terms of the structure factor

$$S(\mathbf{k}) = \lim_{B \rightarrow \mathbb{R}^d} \frac{1}{\#(B \cap X)} \sum_{\mathbf{x}, \mathbf{y} \in B \cap X} e^{i(\mathbf{k}, \mathbf{x} - \mathbf{y})} \quad (\text{thermodynamic limit})$$

by $\lim_{\mathbf{k} \rightarrow \mathbf{0}} S(\mathbf{k}) = 0$. This *thermodynamic limit* is understood in the sense that the volume B (for instance a ball of radius R) tends to the whole space \mathbb{R}^d while $\lim_{B \rightarrow \mathbb{R}^d} \frac{\#(B \cap X)}{\text{vol}(B)} = \rho$, the density.

For a long time in the physics literature it has been observed that there are large (ideally infinite) particle systems that exhibit structural behavior between crystalline order and total disorder. Very prominent examples are given by quasi-crystals and jammed sphere packings. The discovery of such physical materials that lie between crystalline order and disordered materials has initiated research in physics as well as in mathematics. We just mention de Bruijn’s Fourier analytic explanation for the diffraction pattern of quasi-crystals [10] and the extensive collection of articles on quasi-crystals [2].

Since the introduction of hyperuniformity in [27] as a concept to measure the occurrence of “intermediate” order as for quasi-crystals or jammed packings, the notion has developed tremendously. Hyperuniformity has found applications far beyond physics: color receptors in bird eyes exhibit hyperuniform structure [13], as do the keratin nanostructures in bird feathers [17], as do energy minimizing point configurations, and of course quasi-crystals [20].

The basic framework is as follows. Let X be a countable discrete subset of \mathbb{R}^d and $\Omega \subset \mathbb{R}^d$ be a test set (“window”), in most cases the unit ball. Then $N_{\mathbf{x} + t\Omega} = \#((\mathbf{x} + t\Omega) \cap X)$ counts the number of points in the translated and dilated copy of Ω . As a general assumption, we take that X has a density ρ , meaning that

$$N_{\mathbf{x} + t\Omega} \sim \rho t^d \text{vol}(\Omega)$$

for $t \rightarrow \infty$, independent of \mathbf{x} . Based on this assumption, the thermodynamic limit can be taken to define the expectation of $N_{\mathbf{x} + t\Omega}$ as

$$\langle N_{t\Omega} \rangle = \lim_{R \rightarrow \infty} \frac{1}{\text{vol}(B(\mathbf{0}, R))} \int_{B(\mathbf{0}, R)} N_{\mathbf{x} + t\Omega} \, d\mathbf{x},$$

where $B(\mathbf{0}, R)$ denotes the ball of radius R around $\mathbf{0}$. For a random (“Poissonian”) point pattern, the variance satisfies $\langle N_{t\Omega}^2 \rangle - \langle N_{t\Omega} \rangle^2 = \langle N_{t\Omega} \rangle = \rho t^d \text{vol}(\Omega)$. For point

sets like quasi-crystals or jammed packings, the behavior is different: the variance has smaller order of magnitude as $t \rightarrow \infty$, ideally

$$\langle N_{t\Omega}^2 \rangle - \langle N_{t\Omega} \rangle^2 = \mathcal{O}(t^{d-1}) \asymp \text{surface}(t\Omega). \tag{1}$$

Here and throughout, we use the notation $f(t) \asymp g(t)$ for $f(t) = \mathcal{O}(g(t))$ and $g(t) = \mathcal{O}(f(t))$ for the indicated range of x .

Such behavior is clearly displayed by lattices and randomly distorted lattices, and some quasi-crystals (depending on Diophantine properties of their construction parameters) [20]. There is numerical evidence that jammed sphere packings [14,28] also exhibit such behavior. More generally, a point set is called hyperuniform if

$$\langle N_{t\Omega}^2 \rangle - \langle N_{t\Omega} \rangle^2 = o(t^d);$$

it is called strongly hyperuniform if (1) holds. It has been shown in [27] that (1) is the best possible order that can occur.

2 Hyperuniformity on the Sphere

Complementing the extensive study of the notion of hyperuniformity in the infinite setting, we are interested in studying an analogous property of sequences of point sets in compact spaces. For convenience, we study the d -dimensional sphere \mathbb{S}^d . Our ideas immediately generalize to homogeneous spaces; further generalizations might be more elaborate, since we rely heavily on harmonic analysis and specific properties of special functions. Throughout this paper, $\sigma = \sigma_d$ will denote the normalized surface area measure on \mathbb{S}^d . We suppress the dependence on d in this notation.

In order to adapt to the compact setting, we replace the infinite set X studied in the classical notion of hyperuniformity by a sequence of finite point sets $(X_N)_{N \in A}$, where we assume that $\#X_N = N$. By using an infinite set $A \subseteq \mathbb{N}$ as index set, we always allow for subsequences. Furthermore, the set $X_N = \{\mathbf{x}_1^{(N)}, \dots, \mathbf{x}_N^{(N)}\}$ consists of points depending on N ; for the ease of notation, we omit this dependence throughout the paper. We propose the Definition 3 below, which we study in further detail in this paper.

Throughout the paper, we use the notation

$$C(\mathbf{x}, \phi) = \{\mathbf{y} \in \mathbb{S}^d \mid \langle \mathbf{x}, \mathbf{y} \rangle > \cos \phi\}$$

for the spherical cap of opening angle ϕ with center \mathbf{x} . The normalized surface area of the cap is given by

$$\sigma(C(\mathbf{x}, \phi)) = \gamma_d \int_0^\phi \sin(\theta)^{d-1} d\theta \asymp \phi^d \quad \text{as } \phi \rightarrow 0, \tag{2}$$

where

$$\gamma_d = \left(\int_0^\pi \sin(\theta)^{d-1} d\theta \right)^{-1} = \frac{\Gamma(d)}{2^{d-1} \Gamma(d/2)^2}.$$

Notice that $\gamma_d = \frac{\omega_{d-1}}{\omega_d}$, where ω_d is the surface area of \mathbb{S}^d .

For the reader’s convenience and for later reference, we first recapitulate the definition of uniform distribution of a sequence $(X_N)_{N \in A}$ of point sets on the sphere \mathbb{S}^d (see [11, 16] as general references on the theory of uniform distribution).

Definition 1 (Uniform distribution) A sequence of point sets $(X_N)_{N \in A}$ is called uniformly distributed on \mathbb{S}^d if for all caps $C(\mathbf{x}, \phi)$ ($\mathbf{x} \in \mathbb{S}^d$ and $\phi \in [0, \pi]$), the relation

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{C(\mathbf{x}, \phi)}(\mathbf{x}_i) = \sigma(C(\mathbf{x}, \phi)) \tag{3}$$

holds. Here $\mathbb{1}_C$ denotes the indicator function of the set C .

It is known from the general theory of uniform distribution (see [16]) that (3) is equivalent to

$$\lim_{N \rightarrow \infty} \frac{1}{N^2} \sum_{i, j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0 \quad \text{for } n \geq 1, \tag{4}$$

where $P_n^{(d)}$ is the n th (generalized) Legendre polynomial normalized by $P_n^{(d)}(1) = 1$. These functions are the zonal spherical harmonics on \mathbb{S}^d (see [19]). Notice that

$$Z(d, n) P_n^{(d)}(x) = \frac{n + \lambda}{\lambda} C_n^\lambda(x),$$

where C_n^λ is the n th Gegenbauer polynomial with index $\lambda = \frac{d-1}{2}$ (see [18]). We write $Z(d, n) = \frac{2n+d-1}{d-1} \binom{n+d-2}{d-2}$ for the dimension of the space of spherical harmonics of degree n on \mathbb{S}^d .

The spherical cap discrepancy

$$D_N^\infty(X_N) = \sup_{\mathbf{x}, \phi} \left| \sum_{n=1}^N \mathbb{1}_{C(\mathbf{x}, \phi)}(\mathbf{x}_n) - N\sigma(C(\cdot, \phi)) \right|$$

provides a well studied quantitative measure of uniform distribution (see [4, 16]). Uniform distribution of $(X_N)_{N \in A}$ is equivalent to

$$\lim_{N \rightarrow \infty} \frac{1}{N} D_N^\infty(X_N) = 0.$$

In this paper, we will study the *number variance*.

Definition 2 (Number variance) Let $(X_N)_{N \in \mathbb{N}}$ be a sequence of point sets on the sphere \mathbb{S}^d . The *number variance* of the sequence for caps of opening angle ϕ is given by

$$\begin{aligned}
 V(X_N, \phi) &:= \mathbb{V}_{\mathbf{x}\#}(X_N \cap C(\mathbf{x}, \phi)) \\
 &= \int_{\mathbb{S}^d} \left(\sum_{n=1}^N \mathbb{1}_{C(\mathbf{x}, \phi)}(\mathbf{x}_n) - N\sigma(C(\cdot, \phi)) \right)^2 d\sigma(\mathbf{x}).
 \end{aligned}$$

This quantity appears in the classical measure of uniform distribution given by the L^2 -discrepancy

$$D_N^2(X_N) = \left(\int_0^\pi V(X_N, \phi) \sin(\phi) d\phi \right)^{\frac{1}{2}}, \tag{5}$$

where uniform distribution of $(X_N)_{N \in \mathbb{A}}$ is also equivalent to

$$\lim_{N \rightarrow \infty} \frac{1}{N} D_N^2(X_N) = 0.$$

As in the Euclidean case, we define hyperuniformity by a comparison between the behavior of the number variance of a sequence of point sets and the i.i.d case. For i.i.d points, the variance is $N\sigma(C(\cdot, \phi))(1 - \sigma(C(\cdot, \phi)))$, which has order of magnitude N , $N\sigma(C(\cdot, \phi_N))$, and t^d , respectively, in the three cases (6), (7), and (8) listed below.

Definition 3 (Hyperuniformity) Let $(X_N)_{N \in \mathbb{N}}$ be a sequence of point sets on the sphere \mathbb{S}^d . A sequence is called

- **hyperuniform for large caps** if

$$V(X_N, \phi) = o(N) \quad \text{as } N \rightarrow \infty \tag{6}$$

for all $\phi \in (0, \frac{\pi}{2})$;

- **hyperuniform for small caps** if

$$V(X_N, \phi_N) = o(N\sigma(C(\cdot, \phi_N))) \quad \text{as } N \rightarrow \infty \tag{7}$$

and all sequences $(\phi_N)_{N \in \mathbb{N}}$ such that

- (1) $\lim_{N \rightarrow \infty} \phi_N = 0$
- (2) $\lim_{N \rightarrow \infty} N\sigma(C(\cdot, \phi_N)) = \infty$, which is equivalent to $\phi_N N^{\frac{1}{d}} \rightarrow \infty$.

- **hyperuniform for caps at threshold order** if

$$\limsup_{N \rightarrow \infty} V(X_N, tN^{-\frac{1}{d}}) = \mathcal{O}(t^{d-1}) \quad \text{as } t \rightarrow \infty. \tag{8}$$

Remark 1 The case analogous to the Euclidean definition is the third case: hyperuniform for caps at threshold order. The limit $N \rightarrow \infty$ is the analogue of the thermodynamic limit by rescaling to a sphere of radius $N^{\frac{1}{d}}$.

In order to determine further properties of hyperuniform sequences of sets, we derive an alternative expression for the number variance $V(X_N, \phi_N)$. We refer to [19] as a general reference for spherical harmonics in arbitrary dimension and to [1, 18] as

references for the various formulas and relations between special functions, especially orthogonal polynomials.

Recall the Laplace series for the indicator function of the spherical cap $C(\mathbf{x}, \phi)$:

$$\mathbb{1}_{C(\mathbf{x}, \phi)}(\mathbf{y}) = \sigma(C(\cdot, \phi)) + \sum_{n=1}^{\infty} a_n(\phi) Z(d, n) P_n^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle),$$

where the Laplace coefficients for $n \geq 1$ are given by

$$a_n(\phi) = \gamma_d \int_0^\phi P_n^{(d)}(\cos(\theta)) \sin(\theta)^{d-1} d\theta = \frac{\gamma_d}{d} \sin(\phi)^d P_{n-1}^{(d+2)}(\cos(\phi)). \tag{9}$$

The variance $V(X_N, \phi)$ can be expressed formally as

$$\begin{aligned} V(X_N, \phi) &= \int_{\mathbb{S}^d} \left(\sum_{i=1}^N \mathbb{1}_{C(\mathbf{x}_i, \phi)}(\mathbf{x}) - N\sigma(C(\cdot, \phi)) \right)^2 d\sigma(\mathbf{x}) \\ &= \sum_{i,j=1}^N \sum_{n=1}^{\infty} a_n(\phi)^2 Z(d, n) P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \end{aligned} \tag{10}$$

by interpreting the integral as a (spherical) convolution. This follows from the Funk–Hecke formula

$$\int_{\mathbb{S}^d} P_m^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) P_n^{(d)}(\langle \mathbf{y}, \mathbf{z} \rangle) d\sigma(\mathbf{y}) = \delta_{m,n} P_n^{(d)}(\langle \mathbf{x}, \mathbf{z} \rangle).$$

We also remark here that

$$\sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \geq 0 \tag{11}$$

by the positive definiteness of $P_n^{(d)}$ (see [22]).

Notice that the function

$$g_\phi(x) = \sum_{n=1}^{\infty} a_n(\phi)^2 Z(d, n) P_n^{(d)}(x), \quad -1 \leq x \leq 1, \tag{12}$$

is positive definite in the sense of Schoenberg [22]. Furthermore, the estimate

$$\left| P_n^{(d)}(\cos(\phi)) \right| \leq \min \left(1, \frac{c_d}{(n \sin(\phi))^{\frac{d-1}{2}}} \right) \tag{13}$$

holds for a constant c_d depending only on the dimension d (see [15, 26]). This gives the estimate

$$a_n(\phi)^2 = \mathcal{O} \left(\frac{\sin(\phi)^{d-1}}{n^{d+1}} \right),$$

which holds uniformly for $\phi \in [0, \pi]$. This together with $Z(d, n) = \mathcal{O}(n^{d-1})$ shows absolute and uniform convergence of the series (12) and thus (10).

2.1 Hyperuniformity for Large Caps

Theorem 1 *Let $(X_N)_{N \in \mathbb{N}}$ be a sequence of point sets that is hyperuniform for large caps. Then for all $n \geq 1$,*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0. \tag{14}$$

As a consequence, sequences that are hyperuniform for large caps are uniformly distributed.

Proof Assume that $(X_N)_{N \in \mathbb{N}}$ is hyperuniform for large caps. Then inserting the definition into (10) gives

$$0 = \lim_{N \rightarrow \infty} \frac{V(X_N, \phi)}{N} \geq Z(d, n) a_n(\phi)^2 \limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle)$$

for every n and every $\phi \in (0, \frac{\pi}{2})$, which implies (14) by the positive definiteness of Legendre polynomials (11), positivity of the Laplace coefficients of the series, and uniform convergence. □

Remark 2 Of course, the uniform distribution of hyperuniform point sets is no surprise, since the uniform density of points was built into the computation of variance. Furthermore, all caps of a fixed size are used in the definition of this regime of hyperuniformity, similarly to the definition of uniform distribution. The extra convergence order in (14) is the key observation in Theorem 1. Similar phenomena will occur in Sect. 3, where the notion of a Quasi-Monte Carlo (QMC) design as defined in [9] is exploited further and hyperuniformity of QMC designs of sufficient “strength” is shown.

Remark 3 Notice that it does not suffice to assume that (6) holds for only one value of $\phi \in (0, \frac{\pi}{2})$. For values of ϕ for which one of the coefficients $a_{n_0}(\phi)$ vanishes, nothing can be said about the limit (14) for $n = n_0$. There are of course only countably many such values of ϕ . Furthermore, it has been conjectured by T. J. Stieltjes [3] that the (classical) Legendre polynomials $P_{2n}(x)$ and $P_{2n+1}(x)/x$ are irreducible over \mathbb{Q} . An extension of this still unproved conjecture to higher dimensional Legendre polynomials would imply that at most one coefficient $a_n(\phi)$ could vanish for a given value of $\phi \in (0, \frac{\pi}{2})$.

Proof We construct point sets such that (14) holds for all $n \neq n_0$ and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j=1}^N P_{n_0}^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = \infty. \tag{15}$$

Take a nonzero real spherical harmonic function f of order n_0 that has all values less than 1 in modulus. Then $d\mu(\mathbf{x}) = (1 + f(\mathbf{x})) d\sigma(\mathbf{x})$ is a positive measure on \mathbb{S}^d . Then by a result of Seymour and Zaslavsky [23], for every t there exists an $N(t)$ such that for every $N \geq N(t)$ there is a point set X_N such that

$$\frac{1}{N} \sum_{i=1}^N p(\mathbf{x}_i) = \int_{\mathbb{S}^d} p(\mathbf{x}) d\mu(\mathbf{x}) = \langle 1 + f, p \rangle_{L^2(\mathbb{S}^d)}$$

for all spherical harmonics p of degree $\leq t$. Now let $p(\mathbf{x}) = P_n^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle)$ for fixed $\mathbf{y} \in \mathbb{S}^d$. For all $n \neq n_0$ and $1 \leq n \leq t$, we have

$$\frac{1}{N} \sum_{i=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{y} \rangle) = 0 \quad \text{for every } \mathbf{y} \in \mathbb{S}^d,$$

from which we conclude

$$\frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0.$$

This gives the desired limit relation.

For $n = n_0$ and $t \geq n_0$, we have

$$\frac{1}{N} \sum_{i=1}^N P_{n_0}^{(d)}(\langle \mathbf{x}_i, \mathbf{y} \rangle) = \int_{\mathbb{S}^d} f(\mathbf{x}) P_{n_0}^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) d\sigma(\mathbf{x}) \quad \text{for every } \mathbf{y} \in \mathbb{S}^d.$$

Taking $\mathbf{y} = \mathbf{x}_j$ and summing again yields

$$\begin{aligned} \frac{1}{N^2} \sum_{i,j=1}^N P_{n_0}^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) &= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} f(\mathbf{x}) P_{n_0}^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) f(\mathbf{y}) d\sigma(\mathbf{x}) d\sigma(\mathbf{y}) \\ &= \frac{\|f\|_{L^2(\mathbb{S}^d)}^2}{Z(d, n_0)} \neq 0, \end{aligned}$$

which implies (15). □

2.2 Hyperuniformity for Small Caps

Using the definition of hyperuniformity together with (10), we have

$$\frac{V(X_N, \phi_N)}{N\sigma(C(\cdot, \phi_N))} = \sum_{n=1}^{\infty} Z(d, n) \frac{a_n(\phi_N)^2}{\sigma(C(\cdot, \phi_N))} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \rightarrow 0. \quad (16)$$

By (9) the n th Laplace coefficient of (16) behaves like

$$\frac{a_n(\phi_N)^2}{\sigma(C(\cdot, \phi_N))} = \left(\frac{\gamma_d}{d} P_{n-1}^{(d+2)}(\cos \phi_N)\right)^2 \frac{\sin(\phi_N)^{2d}}{\sigma(C(\cdot, \phi_N))} \asymp \phi_N^d$$

for $\phi_N \rightarrow 0$ as assumed. Since ϕ_N is allowed to tend to 0 arbitrarily slowly and all coefficients in (16) are positive, this implies that

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) < \infty$$

for all $n \geq 1$.

Using the fact that (4) is equivalent to uniform distribution of $(X_N)_{N \in \mathbb{A}}$, we have proved:

Theorem 2 *Let $(X_N)_{N \in \mathbb{N}}$ be a sequence of point sets on the sphere that is hyperuniform for small caps. Then $(X_N)_{N \in \mathbb{N}}$ is asymptotically uniformly distributed.*

Motivated by the analogous definition in the Euclidean case, we call the function

$$s(n) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle)$$

the *spherical structure factor* if the limit exists for all $n \geq 1$. Notice that by a diagonal argument, we can always achieve that all such limits exist along some subsequence.

Remark 4 As opposed to the case of hyperuniformity for large caps discussed in Remark 2, in the case of small caps, the conclusion of uniform distribution is not directly obvious, because only “small” caps in the sense of (7) are tested for the definition of uniform distribution.

2.3 Hyperuniformity for Caps of Threshold Order

Theorem 3 *Let $(X_N)_{N \in \mathbb{N}}$ be a sequence of point sets on the sphere that is hyperuniform for caps of threshold order. Then $(X_N)_{N \in \mathbb{N}}$ is asymptotically uniformly distributed.*

Proof We insert the definition of hyperuniformity for caps of threshold order into (10) to obtain

$$V(X_N, tN^{-\frac{1}{d}}) \geq a_n \left(tN^{-\frac{1}{d}}\right)^2 Z(d, n) \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle).$$

Then (9) and the fact that the Legendre polynomials assume value 1 at 1 yield

$$a_n \left(tN^{-\frac{1}{d}}\right)^2 \sim \left(\frac{\gamma_d}{d}\right)^2 t^{2d} N^{-2}$$

for fixed $n \geq 1$ and fixed $t > 0$ and $N \rightarrow \infty$. Now by definition (8), we have

$$\begin{aligned} & \left(\frac{\gamma_d}{d}\right)^2 t^{2d} Z(d, n) \limsup_{N \rightarrow \infty} \frac{1}{N^2} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \\ & \leq \limsup_{N \rightarrow \infty} V(X_N, tN^{-\frac{1}{d}}) = \mathcal{O}(t^{d-1}). \end{aligned}$$

This relation can only hold if

$$\limsup_{N \rightarrow \infty} \frac{1}{N^2} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0$$

for all $n \geq 1$, which implies uniform distribution of the sequence $(X_N)_{N \in \mathbb{N}}$. □

Remark 5 Similarly to the case of hyperuniformity for small caps, the conclusion of uniform distribution of sequences of hyperuniform points sets for caps at threshold order is not obvious.

3 Hyperuniformity of QMC Design Sequences

A QMC method is an equal weight numerical integration formula that, in contrast to Monte Carlo methods, approximates the exact integral $I(f)$ of a given continuous real function f on \mathbb{S}^d using a *deterministic* node set $X_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^d$:

$$I(f) := \int_{\mathbb{S}^d} f(\mathbf{x}) d\sigma_d(\mathbf{x}) \approx \frac{1}{N} \sum_{k=1}^N f(\mathbf{x}_k) =: Q[X_N](f).$$

The node set X_N is chosen in a sensible way so as to guarantee “small” worst-case error of numerical integration,

$$\text{wce}(Q[X_N]; \mathbb{H}^s(\mathbb{S}^d)) := \sup \left\{ \left| Q[X_N](f) - I(f) \right| \mid f \in \mathbb{H}^s(\mathbb{S}^d), \|f\|_{\mathbb{H}^s} \leq 1 \right\}$$

with respect to a Sobolev space $\mathbb{H}^s(\mathbb{S}^d)$ over \mathbb{S}^d with smoothness index $s > \frac{d}{2}$.

Motivated by certain estimates for the worst-case error, the concept of QMC design sequences was introduced in [9]. In the following, we assume that A is an infinite subset of \mathbb{N} . Then a QMC design sequence $(X_N)_{N \in A}$ for $\mathbb{H}^s(\mathbb{S}^d)$, $s > \frac{d}{2}$, is characterized by

$$|Q[X_N](f) - I(f)| \leq \frac{c_{s,d}}{N^{\frac{s}{d}}} \|f\|_{\mathbb{H}^s} \quad \text{for all } f \in \mathbb{H}^s(\mathbb{S}^d). \tag{17}$$

We note that the order of N cannot be improved [9, Thm. 3]. It is shown in [9, Thm. 4] that a QMC design sequence for $\mathbb{H}^s(\mathbb{S}^d)$, $s > \frac{d}{2}$, is also a QMC design sequence for

$\mathbb{H}^{s'}(\mathbb{S}^d)$ for all $\frac{d}{2} < s' < s$. A fundamental unresolved problem is to determine the supremum s^* (called the strength of the sequence) of those s for which (17) holds. We prove the following result.

Theorem 4 *A QMC design sequence for $\mathbb{H}^s(\mathbb{S}^d)$ with $s \geq \frac{d+1}{2}$ is hyperuniform for large caps, small caps, and caps at threshold order.*

It is known [9, Thm. 14] that points that maximize their sum of mutual generalized Euclidean distances, $\sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k|^{2\tau-d}$, form a QMC design sequence $(X_{N,\tau}^*)_{N \in \mathbb{N}}$ for $\mathbb{H}^\tau(\mathbb{S}^d)$ if $\tau \in (\frac{d}{2}, \frac{d}{2} + 1)$; i.e.,

$$|Q[X_{N,\tau}^*](f) - I(f)| \leq \frac{c_{s,d}}{N^{\frac{s}{d}}} \|f\|_{\mathbb{H}^s} \quad \text{for all } f \in \mathbb{H}^s(\mathbb{S}^d) \text{ and all } \frac{d}{2} < s \leq \tau,$$

whereas a sequence $(Z_{N_t})_{t \in \mathbb{N}}$ of spherical t -designs with exactly the optimal order of points, $N_t \asymp t^d$, has the remarkable property [9, Thm. 6] that

$$|Q[Z_{N_t}](f) - I(f)| \leq \frac{c_{s,d}}{N_t^{\frac{s}{d}}} \|f\|_{\mathbb{H}^s} \quad \text{for all } f \in \mathbb{H}^s(\mathbb{S}^d) \text{ and all } s > \frac{d}{2},$$

and, therefore, $(Z_{N_t})_{t \in \mathbb{N}}$ is a QMC design sequence for $\mathbb{H}^s(\mathbb{S}^d)$ for every $s > \frac{d}{2}$. As corollaries to Theorem 4, we obtain:

Corollary 1 *Let $\tau \in (\frac{d+1}{2}, \frac{d}{2} + 1)$. A sequence $(X_{N,\tau}^*)_{N \in \mathbb{N}}$ of N -point sets that maximize the sum $\sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k|^{2\tau-d}$ is hyperuniform for large caps, small caps, and caps at threshold order.*

Corollary 2 *A sequence $(X_N)_{N \in A}$ of spherical $t(N)$ -designs with $t(N) \geq c_d N^{\frac{1}{d}}$, $N \in A$, for some $c_d > 0$ is hyperuniform for large caps, small caps, and caps at threshold order.*

The Sobolev space $\mathbb{H}^s(\mathbb{S}^d)$ consists of L_2 -functions on \mathbb{S}^d with finite Sobolev norm

$$\|f\|_{\mathbb{H}^s} := \sqrt{\langle f, f \rangle_{\mathbb{H}^s(\mathbb{S}^d)}} = \sqrt{\sum_{n=0}^{\infty} \frac{\|Y_n[f]\|_{L^2(\mathbb{S}^d)}^2}{b_n(s)}},$$

where $Y_n[f]$, $n \in \mathbb{N}$, are the projections

$$Y_n[f](\mathbf{x}) := \int_{\mathbb{S}^d} Z(d, n) P_n^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) f(\mathbf{y}) \, d\sigma(\mathbf{y}), \quad \mathbf{x} \in \mathbb{S}^d,$$

and $(b_n(s))_{n \in \mathbb{N}}$ can be any fixed sequence of positive real numbers satisfying

$$b_n(s) \asymp (1 + n)^{-2s}. \tag{18}$$

Since the point-evaluation functional is a bounded operator on $\mathbb{H}^s(\mathbb{S}^d)$ whenever $s > \frac{d}{2}$, the Riesz representation theorem assures the existence of a reproducing kernel for $\mathbb{H}^s(\mathbb{S}^d)$. It can be readily verified that the zonal kernel

$$K^{(s)}(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{\infty} b_n(s) Z(d, n) P_n^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle)$$

has the reproducing kernel properties

$$K^{(s)}(\cdot, \mathbf{x}) \in \mathbb{H}^s(\mathbb{S}^d), \quad \mathbf{x} \in \mathbb{S}^d, \\ \langle f, K^{(s)}(\cdot, \mathbf{x}) \rangle_{\mathbb{H}^s(\mathbb{S}^d)} = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{S}^d, f \in \mathbb{H}^s(\mathbb{S}^d).$$

Thus, reproducing kernel Hilbert space techniques (see [12] for the case of the unit cube) provide the means to compute the worst-case error. Standard arguments (see [9]) yield

$$\left[\text{wce}(\mathbb{Q}[X_N]; \mathbb{H}^s(\mathbb{S}^d)) \right]^2 = \frac{1}{N^2} \sum_{i,j=1}^N \sum_{n=1}^{\infty} b_n(s) Z(d, n) P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle). \quad (19)$$

We exploit the flexibility in the choice of the sequence $(b_n(s))_{n \in \mathbb{N}}$ defining reproducing kernel, Sobolev norm, and worst-case error to connect the Laplace–Fourier expansion of the number variance given in (10) with an appropriately chosen worst-case error.

Lemma 1 *The number variance satisfies*

$$V(X_N, \phi) \ll (\sin \phi)^{d-1} N^2 \left[\text{wce}(\mathbb{Q}[X_N]; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)) \right]^2 \quad (20)$$

for any N -point set $X_N \subset \mathbb{S}^d$ and opening angle $\phi \in (0, \frac{\pi}{2})$.

Proof Using the estimate (13), the coefficients in (10) satisfy the relation

$$a_n(\phi)^2 \ll \frac{(\sin \phi)^{d-1}}{n^{d+1}} \asymp \frac{(\sin \phi)^{d-1}}{(1+n)^{d+1}}.$$

The positive definiteness of the kernel function (12) yields

$$V(X_N, \phi) \ll (\sin \phi)^{d-1} \sum_{i,j=1}^N \sum_{n=1}^{\infty} (1+n)^{-(d+1)} Z(d, n) P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle).$$

Comparison with (19) while taking into account (18) gives the result. □

Remark 6 It is interesting that the Sobolev space $\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)$ plays such a special role: When endowed with the reproducing kernel $1 - \frac{\gamma_d}{d} |\mathbf{x} - \mathbf{y}|$ for $\mathbf{x}, \mathbf{y} \in \mathbb{S}^d$, the worst-case

error satisfies the following invariance principle [7] (see [5,6,8,24] for generalizations):

$$\frac{1}{N^2} \sum_{j,k=1}^N |\mathbf{x}_j - \mathbf{x}_k| + \frac{d}{\gamma_d} \left[\text{wce}(\mathbb{Q}[X_N]; \mathbb{H}^s(\mathbb{S}^d)) \right]^2 = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} |\mathbf{x} - \mathbf{y}| \, d\sigma(\mathbf{x}) \, d\sigma(\mathbf{y}),$$

which is equivalent [7] with Stolarsky’s invariance principle [25], where the place of the worst-case error is taken by the L^2 -discrepancy given in (5). Hence, an N -point system with maximal sum of all mutual Euclidean distances is both a node set for a QMC method that minimizes the worst-case error in the above setting and a point set with smallest possible L^2 -discrepancy among all N -point sets on \mathbb{S}^d . A sequence of such maximal sum-of-distance N -point sets as $N \rightarrow \infty$ is a QMC design sequence for at least $\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)$ with yet unknown strength s^* and thus is hyperuniform for large caps, small caps, and caps at threshold order (Corollary 1). For the Weyl sums, we get (cf. Remark 7) for every fixed $n \in \mathbb{N}$ the limit relation

$$\lim_{N \rightarrow \infty} N^{-1+\frac{1}{d}-\varepsilon} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0 \quad \text{for all sufficiently small } \varepsilon > 0.$$

We are ready to prove Theorem 4.

Proof of Theorem 4 Let $(X_N)_{N \in \mathbb{A}}$ be a QMC design sequence for $\mathbb{H}^s(\mathbb{S}^d)$ with $s \geq \frac{d+1}{2}$. Then, by [9, Theorem 4], it is also a QMC design sequence for $\mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)$; i.e.,

$$\left[\text{wce}(\mathbb{Q}[X_N]; \mathbb{H}^{\frac{d+1}{2}}(\mathbb{S}^d)) \right]^2 \leq c N^{-\frac{d+1}{d}}$$

for some constant $c > 0$. By Lemma 1,

$$V(X_N, \phi) \ll (\sin \phi)^{d-1} N^2 N^{-\frac{d+1}{d}} = (\sin \phi)^{d-1} N^{1-\frac{1}{d}} \tag{21}$$

for the X_N of the QMC design sequence $(X_N)_{N \in \mathbb{A}}$ and any opening angle $\phi \in (0, \frac{\pi}{2})$.

(i) Large cap regime Let $\phi \in (0, \frac{\pi}{2})$. Then, by (21),

$$\frac{1}{N} V(X_N, \phi) \ll (\sin \phi)^{d-1} N^{-\frac{1}{d}} \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Consequently, for all $\phi \in (0, \frac{\pi}{2})$,

$$V(X_N, \phi) = o(N) \quad \text{as } N \rightarrow \infty,$$

and $(X_N)_{N \in \mathbb{A}}$ is hyperuniform for large caps.

(ii) Small cap regime Let $(\phi_N)_{N \in A}$ be a sequence of radii satisfying $\phi_N \rightarrow 0$ and $N\sigma(C(\cdot, \phi_N)) \rightarrow \infty$ as $N \rightarrow \infty$. Then, by (21) and (2),

$$\frac{V(X_N, \phi_N)}{N\sigma(C(\cdot, \phi_N))} \ll \frac{(N(\sin \phi_N)^d)^{\frac{d-1}{d}}}{N(\sin \phi_N)^d} \ll \left(N\sigma(C(\cdot, \phi_N))\right)^{-\frac{1}{d}} \rightarrow 0 \quad \text{as } N \rightarrow \infty;$$

thus, $(X_N)_{N \in A}$ is hyperuniform for small caps.

(iii) Threshold regime Suppose $(\phi_N)_{N \in A}$, $\phi_N \in (0, \frac{\pi}{2})$ such that $\phi_N = t N^{-\frac{1}{d}}$, $t > 0$. By (21),

$$\begin{aligned} V(X_N, \phi_N) &\ll \left(\frac{\sin \phi_N}{\phi_N}\right)^{d-1} (\phi_N)^{d-1} N^{1-\frac{1}{d}} \\ &= \left(t N^{-\frac{1}{d}}\right)^{d-1} N^{1-\frac{1}{d}} \\ &= t^{d-1} \quad \text{as } N \rightarrow \infty. \end{aligned}$$

The implied constant does not depend on t . Since $t > 0$ was arbitrary,

$$\limsup_{\substack{N \rightarrow \infty \\ N \in A}} V\left(X_N, t N^{-\frac{1}{d}}\right) = \mathcal{O}(t^{d-1}) \quad \text{as } t \rightarrow \infty$$

and $(X_N)_{N \in A}$ is hyperuniform for caps at threshold order. \square

Remark 7 Any QMC design sequence $(X_N)_{N \in A}$ for $\mathbb{H}^s(\mathbb{S}^d)$, $s \geq \frac{d+1}{2}$, is hyperuniform for large caps and thus, by Theorem 1, satisfies the property

$$\lim_{\substack{N \rightarrow \infty \\ N \in A}} \frac{1}{N} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0 \quad \text{for every } n \in \mathbb{N}.$$

As QMC design sequences are characterized by a bound on the worst-case error, we can use such bounds to quantify the convergence of Weyl sums along the sequence. More generally, let $(X_N)_{N \in A}$ be a sequence of N -point sets on \mathbb{S}^d with finite strength $s^* > \frac{d}{2}$; i.e.,

$$|\mathcal{Q}[X_N](f) - \mathbf{I}(f)| \leq \frac{c_{s,d}}{N^{\frac{s}{d}}} \|f\|_{\mathbb{H}^s} \quad \text{for all } f \in \mathbb{H}^s(\mathbb{S}^d) \text{ and all } \frac{d}{2} < s < s^*, \quad (22)$$

and this relation fails if $s > s^*$. Then for every fixed $n \in \mathbb{N}$, we get the limit relation

$$\lim_{\substack{N \rightarrow \infty \\ N \in A}} N^{-1 + \frac{2s^* - d(1+\varepsilon)}{d}} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = 0 \quad (23)$$

for all sufficiently small $\varepsilon > 0$.

This follows from the estimate combining (19) and (22): for $s = s^* - \frac{d}{4} \varepsilon$,

$$0 \leq \sum_{n=1}^{\infty} b_n(s) Z(d, n) N^{\frac{2s^*}{d}-2-\varepsilon} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \leq \frac{c_{s,d}^2}{N^{\frac{\varepsilon}{2}}}$$

holds for all sufficiently small but fixed $\varepsilon > 0$. Thus, the critical exponent

$$-1 + \frac{2s^* - d}{d}$$

of a given sequence of N -point sets is limited by its strength. The connection between number variance and worst-case error given in Lemma 1 indicates that sequences with strength $s^* \geq \frac{d+1}{2}$, where the critical exponent satisfies

$$-1 + \frac{2s^* - d}{d} \geq -1 + \frac{1}{d},$$

are of particular interest.

We conclude this remark by considering the case when n in (23) is not fixed. Assume $n \leq c N^{\frac{\alpha}{d}} \Psi(N)$, $N \in A$, for some $c_d > 0$, $\alpha \in \mathbb{R}$, and Ψ such that $\Psi(N) \rightarrow 0$ and $N^{\frac{\alpha}{d}} \Psi(N) \rightarrow \infty$ as $N \rightarrow \infty$. Then, by (18) and $Z(d, n) \asymp n^{d-1}$, we get for $\frac{d}{2} < s < s^*$,

$$\begin{aligned} b_n(s) Z(d, n) N^{\frac{2s}{d}-2} &\asymp n^{-(2s-d+1)} N^{-1+\frac{2s-d}{d}} \\ &\gg N^{-1-\frac{1}{d}+\frac{1-\alpha}{d}(2s-d+1)} (\Psi(N))^{-(2s-d+1)} \end{aligned}$$

and thus

$$N^{-1-\frac{1}{d}+\frac{1-\alpha}{d}(2s-d+1)} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = O((\Psi(N))^{2s-d+1}) \tag{24}$$

uniformly in $n \leq c N^{\frac{\alpha}{d}} \Psi(N)$, $N \in A$. (The implied constant is independent of n and N .) The function $\Psi(N)$ may tend to zero arbitrarily slowly as $N \rightarrow \infty$. The value of α in the power $N^{\frac{\alpha}{d}}$ determines three regimes of growth of the bound of n . If the bound for n does not grow too fast (i.e., $\alpha \in (0, 1)$), the parameter s effectively enlarges the exponent of N . A sequence of higher strength s^* allows for larger powers of N . The effective exponent is then strictly larger than $-1 - \frac{\alpha}{d}$. For the critical value $\alpha = 1$, the exponent of N does not depend on s at all. It is always $-1 - \frac{1}{d}$. If the bound for n grows too fast (i.e., $\alpha > 1$), then the effective exponent of N is strictly smaller than $-1 - \frac{\alpha}{d}$.

Remark 8 A sequence $(Z_N)_{N \in A}$ with infinite strength has the property

$$\lim_{\substack{N \rightarrow \infty \\ N \in A}} N^{-1+\beta} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{z}_i, \mathbf{z}_j \rangle) = 0 \quad \text{for every fixed } \beta > 0 \text{ and fixed } n \in \mathbb{N},$$

while relation (24), in particular, implies that

$$\lim_{\substack{N \rightarrow \infty \\ N \in A}} N^{-1+\beta} \sum_{i,j=1}^N P_n^{(d)}(\langle \mathbf{z}_i, \mathbf{z}_j \rangle) = 0 \quad \text{for every fixed } \beta > 0$$

uniformly in $n \leq c N^{\frac{\alpha}{d}} \Psi(N)$, $N \in A$, if $0 < \alpha < 1$ and under the assumptions $\Psi(N) = o(1)$ and $N^{\frac{\alpha}{d}} \Psi(N) \rightarrow \infty$ as $N \rightarrow \infty$.

So far (see [9]), the only example of such sequences are sequences of spherical $t(N)$ -designs with $t(N) \asymp N^{\frac{1}{d}}$.

Remark 9 As indicated in Sect. 2, we restricted this study to the sphere for ease of computation. Most of the results would extend *mutatis mutandis* to other homogeneous spaces like the torus or the projective plane. We expect that the definition of hyperuniformity would carry over to compact Riemannian manifolds with considerably more effort and technicalities in the harmonic analysis.

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