HYPERUNIFORM POINT SETS ON THE SPHERE: PROBABILISTIC ASPECTS

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Abstract. The concept of hyperuniformity has been introduced by Torquato and Stillinger in 2003 as a notion to detect structural behaviour intermediate between crystalline order and amorphous disorder. The present paper studies a generalisation of this concept to the unit sphere. It is shown that several well studied determinantal point processes are hyperuniform.

1. Introduction

It has been observed for a long time in the physics literature that large (ideally infinite) particle systems can exhibit structural behaviour between crystalline order and total disorder. Very prominent examples are given by quasi-crystals and jammed sphere packings. Research in mathematics and physics has been inspired by the discovery of such materials which lie between crystalline order and amorphous disorder. We just mention de Bruijn's Fourier analytic explanation for the diffraction pattern of quasi-crystals [7] and the extensive collection of articles on quasi-crystals [3].

Hyperuniformity was introduced in [19] as a concept to measure the occurrence of "intermediate" order. Such configurations X occur in jammed packings, in colloids, as well as in quasi-crystals. The main feature of hyperuniformity is the fact that local density fluctuations ("number variance") are of smaller order than for an i.i.d. random ("Poissonian") point configuration.

The point of view taken in [19] was probabilistic based on point processes. It has since been observed that determinantal point processes

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exhibit less disordered behaviour in comparison to i.i.d. points due to the built in mutual repulsion of particles (see [9]). The prototypical example of such a point process is given by the distribution of fermionic particles, whose joint wave function is given as a determinant expressed in terms of the individual wave functions.

An infinite discrete point set $X \subset \mathbb{R}^d$ is then defined to be hyperuniform if the variance of the random variable ("number variance") $\#((\mathbf{x}+t\Omega)\cap X)$ behaves like $o(t^d)$ as $t \to \infty$. Here, Ω is a fixed compact test set ("window"); in most of the cases Ω is chosen as a Euclidean ball. Notice that the number variance for i.i.d. point sets is of exact order t^d. Thus, hyperuniformity is characterised by a smaller order of magnitude of the variance. It was shown in [19] that the best possible order for the variance is t^{d-1}.

In [6] a notion of hyperuniformity for sequences of finite point sets on the sphere was introduced. In that paper three regimes of hyperuniformity were identified and studied, and several deterministically given point sets such as designs, QMC-designs, and certain energy minimising point sets were shown to exhibit hyperuniform behaviour. We also refer the reader to related recent work [14, 16].

It is the aim of the present paper to study hyperuniformity on the sphere for samples of point processes on the sphere. Especially, we study the spherical ensemble (see [9, 10]) on $\mathbb{S}^2$ (Section 5), the harmonic ensemble introduced in [4] (Section 6), and the jittered sampling process (Section 7). We observe that the jittered sampling process can be seen as a determinantal point process. All processes turn out to be hyperuniform in all three regimes. The harmonic ensemble has slightly weaker behaviour in the threshold order regime.

2. Point Processes

We consider a point process $\mathscr{X}_N$ sampling N points given by the *joint densities* $(X_1, \dots, X_N) \sim \rho^{(N)}$, which describe the distribution of N points. We will assume throughout this paper that the number of points N is fixed and that the process is simple, which means that the probability of sampling a point more than once is zero. In some of the studied examples the number of points will depend on a parameter L; in these cases we write N_L for this number. Furthermore, we always assume that the particles are exchangeable; i.e., the joint densities are invariant under permutation of the entries

$$\rho^{(N)}(\mathbf{x}_{\tau(1)}, \dots, \mathbf{x}_{\tau(N)}) = \rho^{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \text{ for all } \mathbf{x}_i \in \mathbb{S}^d,\ \tau \in \mathrm{S}_N. \tag{1}$$

The *reduced densities*

$$\rho_k^{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_k) := \int_{(\mathbb{S}^d)^{N-k}} \rho^{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \, \mathrm{d}\sigma(\mathbf{x}_{k+1}) \cdots \mathrm{d}\sigma(\mathbf{x}_N),$$

$1 \leq k \leq N$, describe how k of N points are distributed. Note that in the literature (e.g., [9]) the process is often given in terms of its *joint intensities* which are given by $\frac{N!}{(N-k)!}\rho_k^{(N)}$. We use joint densities in this paper since they make the asymptotic dependence on N more transparent. The number of points that are put into a test set $B \subseteq \mathbb{S}^d$ by the process is the random variable $\mathscr{X}_N(B) := \sum_{i=1}^N \mathbb{1}_B(X_i)$, or with other words N times the empirical measure of B. As usual, $\mathbb{1}_B$ denotes the indicator function of the set B.

For most of our study, we restrict ourselves to processes that are invariant under isometries of the sphere

$$\rho^{(N)}(A\mathbf{x}_1, \dots, A\mathbf{x}_N) = \rho^{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \qquad \text{for all } \mathbf{x}_i \in \mathbb{S}^d, \; A \in \mathrm{SO}(d+1). \tag{2}$$

By summation over permutations and integration over isometries, joint densities satisfying (1) and (2) do exist. In this case we obtain

$$\mathbb{E}\mathscr{X}(B) = N\sigma(B), \tag{3}$$

$$\begin{aligned} \mathbb{V}\mathscr{X}(B) &= \mathbb{E}(\mathscr{X}(B)^2) - (\mathbb{E}\mathscr{X}(B))^2 \\ &= N\sigma(B)(1-\sigma(B)) \\ &\quad + N(N-1) \iint_{B\times B} \left(\rho_2^{(N)}(\mathbf{x}_1, \mathbf{x}_2) - 1\right) \mathrm{d}\sigma(\mathbf{x}_1) \, \mathrm{d}\sigma(\mathbf{x}_2). \end{aligned} \tag{4}$$

The variance is independent of the position and orientation of the test set B. So for a spherical cap the number variance only depends on the radius of the cap.

Determinantal Point Processes. Following [9], we introduce determinantal point processes. As pointed out before, we formulate the description in terms of joint densities, rather than joint intensities.

Definition 1. A simple point process (on a locally compact Polish space M) is called determinantal with kernel K if its joint densities (with respect to the background measure μ) are given by

$$\rho_k^{(N)}(x_1, \dots, x_k) = \frac{(N-k)!}{N!} \det\left(K(x_i, x_j)\right)_{i,j=1}^k, \qquad 1 \leq k \leq N. \tag{5}$$

From the definition, permutations of the variables do not change the process. Furthermore, if $x_i = x_j$ for some $i \neq j$, then the density is zero.

In [9] it is shown that a process $\mathscr{X}_N$ samples exactly N points if and only if it is associated with the projection of L^2 to an N-dimensional subspace H. Let $\psi_1, \dots, \psi_N$ be an orthonormal basis of H, then the kernel is given by

$$K_H(x,y) = \sum_{i=1}^{N} \psi_i(x)\overline{\psi_i(y)}. \tag{6}$$

3. 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 unit sphere $\mathbb{S}^d$. Our ideas immediately generalise to homogeneous spaces; further generalisations 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 normalised 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, $(X_N)_{N\in\mathcal{J}}$, where we assume that the cardinality $\#X_N$ is N. By using an infinite set $\mathcal{J} \subseteq \mathbb{N}$ as index set, we always allow for subsequences.

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 with center $\mathbf{x}$ and opening angle ϕ. The normalised surface area of the cap is given by

$$\sigma\left(C(\mathbf{x},\phi)\right) = \gamma_d \int_0^{\phi} \sin(\theta)^{d-1}\mathrm{d}\theta \asymp \phi^d \quad \text{as } \phi \to 0, \tag{7}$$

where

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

Notice that $\gamma_d = \frac{\omega_{d-1}}{\omega_d}$, where ω_d is the surface area of $\mathbb{S}^d$. Here and throughout the paper, we shall use $f(x) \asymp g(x)$ as $x \to x_0$ to mean that there exist positive constants c and C such that $c\,g(x) \le f(x) \le C\,g(x)$ for x sufficiently close to x_0.

In this paper we shall study the *number variance.*

Definition 2 (Number variance)**.** Let $\mathscr{X}_N$ be a point process on the sphere $\mathbb{S}^d$ sampling N points. The *number variance* of $\mathscr{X}_N$ for caps of opening angle ϕ is given by
(8)

$$V(\mathscr{X}_N, \phi) := \mathbb{V}\mathscr{X}_N(C(\cdot, \phi)) := \mathbb{E}\left(\mathscr{X}_N(C(\cdot, \phi))^2\right) - \left(\mathbb{E}\mathscr{X}_N(C(\cdot, \phi))\right)^2 .$$

If the process $\mathscr{X}_N$ is rotation invariant, the implicit integration with respect to the center of the cap $C(\cdot, \phi)$ can be omitted.

Throughout the paper, we write $\sigma(C(\phi))$ for the normalised surface area of the cap $C(\cdot, \phi)$.

As in the Euclidean case we define hyperuniformity by a comparison between the behaviour of the number variance of a sequence of point sets and of the i.i.d. case. For i.i.d. random points, the variance is $N\sigma(C(\phi))(1 - \sigma(C(\phi)))$ (see (4)), which has order of magnitude N, $N\sigma(C(\phi_N))$, and t^d, respectively, in the three cases (9), (10), and (11) listed below.

Definition 3 (Hyperuniformity)**.** Let $\mathscr{X}_N$ be a point process on the sphere $\mathbb{S}^d$ sampling N points. The process $(\mathscr{X}_N)$ is called

- **hyperuniform for large caps** if

$$V(\mathscr{X}_N, \phi) = o\,(N) \quad \text{as } N \to \infty \tag{9}$$

  for all $\phi \in (0, \frac{\pi}{2})$;
- **hyperuniform for small caps** if

$$V(\mathscr{X}_N, \phi_N) = o\,(N\sigma(C(\phi_N))) \quad \text{as } N \to \infty \tag{10}$$

  and all sequences $(\phi_N)_{N\in\mathbb{N}}$ such that
  (1) $\lim_{N\to\infty} \phi_N = 0$
  (2) $\lim_{N\to\infty} N\sigma(C(\phi_N)) = \infty$, which is equivalent to $\phi_N N^{\frac{1}{d}} \to \infty$ as $N \to \infty$.
- **hyperuniform for caps at threshold order** if

$$\limsup_{N\to\infty} V(\mathscr{X}_N, tN^{-\frac{1}{d}}) = \mathcal{O}(t^{d-1}) \quad \text{as } t \to \infty. \tag{11}$$

  The $\mathcal{O}(t^{d-1})$ in (11) could be replaced by the less strict $o(t^d)$ in a more general setting.

4. Intersection Volume of Spherical Caps

In this section we collect some formulas and properties of the intersection volume of two spherical caps that will be needed in the discussion later on. Besides a possibly new formula for the volume of the intersection of two caps of equal size we provide sharp inequalities and asymptotic expansions, which enable us to obtain precise results on the number variance.

We will briefly introduce some basic facts and notation regarding spherical harmonics. Let $\mathcal{H}_\ell$ denote the vector space of spherical harmonics of degree $\ell \in \mathbb{N}$. Its dimension is

$$Z(d,\ell) = \frac{2\ell + d - 1}{d-1}\binom{\ell + d - 2}{d-2}.$$

With respect to the $L^2(\mathbb{S}^d, \sigma)$ inner product, $\mathcal{H}_\ell$ has a real orthonormal basis $\{Y_{\ell,k}\}_{k=1}^{Z(d,\ell)}$. The addition theorem for spherical harmonics (cf. [18]) gives

$$\sum_{k=1}^{Z(d,\ell)} Y_{\ell,k}(\mathbf{x}) Y_{\ell,k}(\mathbf{y}) = Z(d,\ell) P_\ell^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle), \quad \mathbf{x}, \mathbf{y} \in \mathbb{S}^d,$$

where $P_\ell^{(d)}$, $\ell \geq 0$, are the Legendre polynomials for the sphere $\mathbb{S}^d$ normalised by $P_\ell^{(d)}(1) = 1$. Notice that for $d \geq 2$ these are Gegenbauer polynomials for the parameter $\frac{d-1}{2}$:

$$Z(d,\ell) P_\ell^{(d)}(x) = \frac{2\ell + d - 1}{d-1} C_\ell^{\frac{d-1}{2}}(x). \tag{12}$$

It is well-known that the Laplace series for the indicator function of the spherical cap $C(\mathbf{x}, \phi)$ is given by

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

where the Laplace coefficients are given by

$$a_n(\phi) = \gamma_d \int_0^\phi P_n^{(d)}(\cos(\theta)) \sin(\theta)^{d-1} \,\mathrm{d}\theta = \frac{\gamma_d}{d} \sin(\phi)^d P_{n-1}^{(d+2)}(\cos(\phi)) \tag{13}$$

for $n \geq 1$. The intersection volume is then obtained as the spherical convolution of the indicator function with itself. This gives

$$\begin{aligned} g_\phi(\langle \mathbf{x}, \mathbf{y}\rangle) &:= \sigma(C(\mathbf{x}, \phi) \cap C(\mathbf{y}, \phi)) - \sigma(C(\phi))^2 \\ &= \sum_{n=1}^{\infty} a_n(\phi)^2 Z(d,n) P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle). \end{aligned} \tag{14}$$

In [12] formulas for the volume of the intersection of two spherical caps have been derived. In our special case of the intersection of two caps of equal size, we get

$$\sigma(C(\mathbf{x},\phi)\cap C(\mathbf{y},\phi))=\frac{d-1}{\pi}\int_{\frac{\psi}{2}}^{\phi}\sin(t)^{d-1}\int_0^{\arccos(\frac{\tan(\frac{\psi}{2})}{\tan(t)})}\sin(u)^{d-2}\,\mathrm{d}u\,\mathrm{d}t,$$

where $\langle\mathbf{x},\mathbf{y}\rangle=\cos\psi$ and $\psi\le 2\phi$.

The change of variables

$$\tan(v)=\tan(t)\cos(u),$$
$$\sin(w)=\sin(t)\sin(u)$$

transforms the double integral into

$$\frac{1}{\pi}\int_{\frac{\psi}{2}}^{\phi}\frac{(\sin^2\phi-\sin^2 v)^{\frac{d-1}{2}}}{\cos(v)^{d-1}}\,\mathrm{d}v.$$

This gives

(15)

$$g_\phi(1)-g_\phi(\cos\psi)=\sigma(C(\mathbf{x},\phi)\setminus C(\mathbf{y},\phi))=\frac{1}{\pi}\int_0^{\frac{\psi}{2}}\frac{\left(\sin^2\phi-\sin^2 v\right)_+^{\frac{d-1}{2}}}{\cos(v)^{d-1}}\,\mathrm{d}v$$

for all $0<\psi<\pi$; here we define $(a)_+:=\max(0,a)$.

From this we obtain the following lemma.

Lemma 1. *There exists a positive constant A such that for all (ϕ,ψ) with $0\le\psi\le 2\phi\le\pi$ the inequalities*

(16)

$$\frac{1}{2\pi}\psi(\sin\phi)^{d-1}-A\psi^3\sin(\phi)^{d-3}\le\sigma(C(\mathbf{x},\phi)\setminus C(\mathbf{y},\phi))\le\frac{1}{2\pi}\psi(\sin\phi)^{d-1}$$

hold. Here, $\cos\psi=\langle\mathbf{x},\mathbf{y}\rangle$. For $d\le 3$, these inequalities hold for $(\phi,\psi)\in[0,\frac{\pi}{2}]\times[0,\pi]$.

Proof. Consider the function

$$\frac{g_\phi(1)-g_\phi(\cos\psi)-\frac{1}{2\pi}\psi\sin(\phi)^{d-1}}{\sin(\phi)^{d-3}\psi^3}.$$

This function is continuous on $0<\psi\le 2\phi\le\pi$. The limit for $\psi\to 0+$ exists for every $\phi\in(0,\frac{\pi}{2}]$ and depends continously on ϕ. Therefore, the function has a continuous extension to $0\le\psi\le 2\phi\le\pi$; the constant A is obtained from its minimum. The upper bound is obtained by estimating the integral in (15) trivially. $\square$

For $d = 2$, we get

$$\sigma\left(C(\mathbf{x},\phi)\setminus C(\mathbf{y},\phi)\right) = \begin{cases} \frac{1}{\pi}\left(\arcsin\left(\frac{\sin\frac{\psi}{2}}{\sin\phi}\right) - \arcsin\left(\frac{\tan\frac{\psi}{2}}{\tan\phi}\right)\cos\phi\right) & \text{for } \psi \leq 2\phi \\ \sin^2\frac{\phi}{2} & \text{for } \psi > 2\phi, \end{cases}$$

where $\cos\psi = \langle \mathbf{x}, \mathbf{y}\rangle$.

5. The Spherical Ensemble

The spherical ensemble of N points is obtained by stereographically projecting the eigenvalues of $A^{-1}B$ to the sphere, where A and B are $N \times N$ matrices with i.i.d. random complex Gaussian entries (see [9, 10]).

These eigenvalues form a determinantal point process $\mathscr{X}_N^S$ with kernel

$$\widetilde{K}_N(z,w) := (1 + z\overline{w})^{N-1}$$

with respect to the measure

$$\mathrm{d}\mu_N(z) := \frac{N}{\pi(1+|z|^2)^{N+1}}\,\mathrm{d}\lambda_2(z),$$

where λ_2 denotes the Lebesgue measure on $\mathbb{C}$. The corresponding function space is the space of square integrable entire functions

$$\mathscr{P}_N := L^2(\mathbb{C}, \mathrm{d}\mu_N) \cap H(\mathbb{C}),$$

which consists exactly of the polynomials of degree $\leq N-1$. The kernel $\widetilde{K}_N$ is the reproducing kernel of this Hilbert space.

Applying the stereographic projection to the kernel $\widetilde{K}_N$ and the space $\mathscr{P}_N$, we obtain

$$K_N(\mathbf{x},\mathbf{y}) = \frac{N}{2^{N-1}}\Big(\frac{1 + \langle\mathbf{x},\mathbf{y}\rangle - x_3 - y_3 + i(x_2y_1 - x_1y_2)}{\sqrt{(1-x_3)(1-y_3)}}\Big)^{N-1}$$

and the space of functions on $\mathbb{S}^2$ is spanned by

$$(x_1 + ix_2)^\ell (1-x_3)^{\frac{N-1}{2}-\ell}, \quad \ell = 0, \dots, N-1.$$

These functions are orthogonal with respect to σ.

In order to compute the expectation of a general energy sum with respect to the process generated by K_N, we compute the determinant

$$\begin{aligned} N(N-1)\rho_2^{(N)}(\mathbf{x},\mathbf{y}) &= K_N(\mathbf{x},\mathbf{x})K_N(\mathbf{y},\mathbf{y}) - |K_N(\mathbf{x},\mathbf{y})|^2 \\ &= N^2\left(1 - \left(\frac{1+\langle\mathbf{x},\mathbf{y}\rangle}{2}\right)^{N-1}\right). \end{aligned}$$

Now let $g : [-1,1] \to \mathbb{R}$ be a function with $\int_{-1}^{1} g(x)\,\mathrm{d}x = 0$. Then

$$\begin{aligned}(17)\quad E_g(N) &:= \mathbb{E}\sum_{i,j=1}^{N} g\left(\langle \mathbf{x}_i, \mathbf{x}_j\rangle\right) \\ &= Ng(1) + N^2 \iint_{\mathbb{S}^2\times\mathbb{S}^2} g\left(\langle \mathbf{x}, \mathbf{y}\rangle\right)\left(1 - \left(\frac{1+\langle \mathbf{x}, \mathbf{y}\rangle}{2}\right)^{N-1}\right)\mathrm{d}\sigma(\mathbf{x})\,\mathrm{d}\sigma(\mathbf{y}) \\ &= \frac{N^2}{2}\int_{-1}^{1}\left(g(1)-g(x)\right)\left(\frac{1+x}{2}\right)^{N-1}\mathrm{d}x.\end{aligned}$$

We apply (17) to the function g_ϕ given by (14). Putting everything together, we obtain

$$\begin{aligned}V(\mathscr{X}_N^S, \phi) &= E_{g_\phi}(N) \\ &= \frac{N^2}{4\pi}\sin\phi \int_{-1}^{1}\arccos(x)\left(\frac{1+x}{2}\right)^{N-1}\mathrm{d}x \\ (18)\qquad &\quad + \mathcal{O}\left(\frac{N^2}{\sin\phi}\int_{-1}^{1}\arccos(x)^3\left(\frac{1+x}{2}\right)^{N-1}\mathrm{d}x\right) \\ &= \frac{\sin\phi}{2\sqrt{\pi}}\,\frac{\Gamma(N+\frac{1}{2})}{\Gamma(N)} + \mathcal{O}\Big(\frac{1}{N^{1/2}\sin\phi}\Big) \\ (19)\qquad &= \frac{\sqrt{\sigma(C(\phi))(1-\sigma(C(\phi)))}}{\sqrt{\pi}}N^{1/2} + \mathcal{O}\Big(\frac{1}{N^{1/2}\sin\phi}\Big)\end{aligned}$$

valid for $\phi \in (0, \frac{\pi}{2})$. Thus, we have proved the following lemma. We remark that (19) was obtained in [2, Lemma 2.1] with the restriction that $\sigma(C(\phi))^{-1} = o(N)$ and with a weaker error term.

Lemma 2. *The number variance of the spherical ensemble satisfies for* $\phi \in (0, \pi)$

$$(20)\qquad V(\mathscr{X}_N^S, \phi) = \frac{\sqrt{\sigma(C(\phi))(1-\sigma(C(\phi)))}}{\sqrt{\pi}}N^{1/2} + \mathcal{O}\Big(\frac{1}{N^{1/2}\sin\phi}\Big)$$

with an absolute implied constant; especially,

$$(21)\qquad \lim_{N\to\infty} V(\mathscr{X}_N^S, tN^{-\frac{1}{2}}) = \frac{t}{2\sqrt{\pi}} + \mathcal{O}(t^{-1}).$$

Remark 1. Inserting (15) directly into (17) gives the closed formula

$$E_{g_\phi}(N) = \frac{N\sin^2\phi}{\pi}\int_{0}^{1}\left(1-v^2\right)^{\frac{1}{2}}\left(1-v^2\,\sin^2\phi\right)^{N-1}\mathrm{d}v,$$

which could be used for an alternative yet slightly more elaborate proof of Lemma 2.

From this lemma we immediately obtain the following theorem.

Theorem 1. *The spherical ensemble is hyperuniform in all three regimes.*

Proof. For the large cap case, we obtain $V(\mathscr{X}_N^S,\phi)=\mathcal{O}(N^{1/2})$; for the small cap case, we obtain $V(\mathscr{X}_N^S,\phi_N)=\mathcal{O}((N\phi_N)^{1/2})=o(N\phi_N)$. In the threshold order case, we use (21). □

Remark 2. The error term in (20) has the correct order with respect to N and ϕ. This shows that taking $\phi_N=o(N^{-\frac{1}{2}})$ does not make sense, because then the error term would become the dominant term that tends to ∞.

6. The Harmonic Ensemble

The function space of spherical harmonics of degree $\leq L$ and the projection kernel to this space of dimension $Z(d+1,L)=\frac{2L+d}{d}\binom{L+d-1}{d-1}$ was used in [4] to define a determinantal point process $\mathscr{X}_L^H$, the *harmonic ensemble*. This process samples $N:=N_L:=Z(d+1,L)\asymp L^d$ points. We will study this process with respect to hyperuniformity in this section.

The projection kernel to this space is given by

$$K_L(\langle\mathbf{x},\mathbf{y}\rangle):=\sum_{\ell=0}^{L}Z(d,\ell)P_\ell^{(d)}(\langle\mathbf{x},\mathbf{y}\rangle)=\frac{Z(d+1,L)}{\binom{L+d/2}{L}}\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\langle\mathbf{x},\mathbf{y}\rangle)$$

for $\mathbf{x},\mathbf{y}\in\mathbb{S}^d$, where $\mathcal{P}_L^{(\alpha,\beta)}$, $L\geq 0$, are the usual Jacobi polynomials.

Theorem 2. *The harmonic ensemble is hyperuniform for large and small caps. In the threshold order regime the weaker property*

$$\limsup_{L\to\infty}V(\mathscr{X}_L^H,tN_L^{-\frac{1}{d}})=\mathcal{O}(t^{d-1}\log t)=o(t^d) \tag{22}$$

holds.

Proof. The number variance $V(\mathscr{X}_L^H,\phi)$ can be expressed as (cf. similar computations that lead to (17))

$$\int_0^\pi(g_\phi(1)-g_\phi(\cos\theta))K_L(\cos\theta)^2(\sin\theta)^{d-1}\,\mathrm{d}\theta,$$

where g_ϕ is given by (14). Using Lemma 1 we obtain

$$
\begin{aligned}
&V(\mathscr{X}_L^H,\phi)\\
&=\left(\frac{Z(d+1,L)}{\binom{L+\frac{d}{2}}{L}}\right)^2(2\sin\phi)^{d-1}\int_0^{2\phi}\left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2\left(\sin\frac{\theta}{2}\right)^d\left(\cos\frac{\theta}{2}\right)^{d-1}\mathrm{d}\theta\\
&+\mathcal{O}\left(L^d(\sin\phi)^{d-3}\int_0^{2\phi}\left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2\left(\sin\frac{\theta}{2}\right)^{d+2}\left(\cos\frac{\theta}{2}\right)^{d-1}\mathrm{d}\theta\right)\\
&+\left(\frac{Z(d+1,L)}{\binom{L+\frac{d}{2}}{L}}\right)^2\sigma(C(\phi))\int_{2\phi}^{\pi}\left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2(\sin\theta)^{d-1}\,\mathrm{d}\theta.
\end{aligned}
$$

The case of large and small caps was studied in [4]; we summarise the computations given there for completeness. The case of caps at threshold order is new and will be given in more detail. We make use of known asymptotic expansions for the Jacobi polynomials (cf. [15, 5.2.3 and 5.2.4])

$$
\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)=\frac{\cos\left(\left(L+\frac{d}{2}\right)\theta-\frac{\pi}{4}(d+1)\right)}{\sqrt{\pi L}\left(\sin\frac{\theta}{2}\right)^{\frac{d+1}{2}}\left(\cos\frac{\theta}{2}\right)^{\frac{d-1}{2}}}+\mathcal{O}(L^{-\frac{3}{2}}) \tag{23}
$$

$$
\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}\left(\cos\frac{\tau}{L}\right)=L^{\frac{d}{2}}\left(\frac{2}{\tau}\right)^{\frac{d}{2}}J_{\frac{d}{2}}(\tau)+\mathcal{O}(L^{\frac{d}{2}-1}), \tag{24}
$$

where $J_{\frac{d}{2}}$ denotes the Bessel function of the first kind of index $\frac{d}{2}$. Given a constant $C>0$, the asymptotic relation (23) is used for $\theta>\frac{C}{L}$, whereas the relation (24) is used for $\theta=\frac{\tau}{L}\leq\frac{C}{L}$.

This gives

$$
\begin{aligned}
&\int_0^{\frac{C}{L}}\left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2\left(\sin\frac{\theta}{2}\right)^d\left(\cos\frac{\theta}{2}\right)^{d-1}\mathrm{d}\theta\\
&\qquad=\frac{1}{L}\int_0^{C}J_{\frac{d}{2}}(\theta)^2\,\mathrm{d}\theta+\mathcal{O}(L^{-2})
\end{aligned} \tag{25}
$$

for the integral over the "small" values of θ,

$$
\begin{aligned}
&\int_{\frac{C}{L}}^{\alpha}\left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2\left(\sin\frac{\theta}{2}\right)^d\left(\cos\frac{\theta}{2}\right)^{d-1}\mathrm{d}\theta\\
&\qquad=\frac{1}{\pi L}\int_{\frac{C}{L}}^{\alpha}\frac{\cos\left(\left(L+\frac{d}{2}\right)\theta-\frac{\pi}{4}(d+1)\right)^2}{\sin(\frac{\theta}{2})}\mathrm{d}\theta+\mathcal{O}(L^{-2})
\end{aligned} \tag{26}
$$

for the integral over the "large" values of θ,

$$\int_{\alpha}^{\pi} \left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2 (\sin\theta)^{d-1}\,\mathrm{d}\theta \tag{27}$$
$$= \frac{1}{\pi L}\int_{\alpha}^{\pi} \frac{\cos\left(\left(L+\frac{d}{2}\right)\theta - \frac{\pi}{4}(d+1)\right)^2}{\sin(\frac{\theta}{2})^2}\,\mathrm{d}\theta + \mathcal{O}(L^{-2}) = \mathcal{O}((L\alpha)^{-1})$$

and

$$\int_{0}^{\alpha} \left(\mathcal{P}_L^{(\frac{d}{2},\frac{d}{2}-1)}(\cos\theta)\right)^2 \left(\sin\frac{\theta}{2}\right)^{d+2} \left(\cos\frac{\theta}{2}\right)^{d-1}\,\mathrm{d}t \tag{28}$$
$$= \frac{1}{\pi L}\int_{0}^{\alpha} \cos\left(\left(L+\frac{d}{2}\right)\theta - \frac{\pi}{4}(d+1)\right)^2 \sin\left(\frac{\theta}{2}\right)\mathrm{d}\theta + \mathcal{O}(L^{-2}) = \mathcal{O}(L^{-1})$$

for the integral in the error term.

In the case of large caps ($0 < \phi < \frac{\pi}{2}$ fixed), the number variance computes as

$$\begin{aligned} V(\mathscr{X}_L^H,\phi) &= \left(\frac{Z(d+1,L)}{\binom{L+\frac{d}{2}}{L}}\right)^2 \frac{(2\sin\phi)^{d-1}}{L}\left(\int_0^C J_{\frac{d}{2}}(\theta)^2\,\mathrm{d}\theta \right.\\ &\quad \left. + \frac{1}{\pi}\int_{\frac{C}{L}}^{2\phi} \frac{\cos\left(\left(L+\frac{d}{2}\right)\theta - \frac{\pi}{4}(d+1)\right)^2}{\sin(\frac{\theta}{2})}\,\mathrm{d}\theta + \mathcal{O}(L^{-1}) + \mathcal{O}(\phi^{-1})\right) \\ &= \mathcal{O}((\sin\phi)^{d-1}L^{d-1}\log L), \end{aligned}$$

where we have used $\left(Z(d+1,L)/\binom{L+\frac{d}{2}}{L}\right)^2 \asymp L^d$ and the logarithmic term comes from the second summand. This is the true asymptotic order and due to $N_L \asymp L^d$ we have $V(\mathscr{X}_L^H,\phi) = o\left(N_L\right)$ as $L\to\infty$ for all $\phi\in(0,\frac{\pi}{2})$.

In the case of small caps, a similar computation gives

$$\begin{aligned} V(\mathscr{X}_L^H,\phi_L) &= \mathcal{O}((\sin\phi_L)^{d-1}L^{d-1}\log L) \\ &= o((L\sin\phi_L)^d) = o(N_L\,\sigma(C(\phi_L))). \end{aligned}$$

For caps at threshold order, we compute

$$\begin{aligned} &V(\mathscr{X}_L^H, tL^{-1}) \\ &\quad = \left(\frac{Z(d+1,L)}{\binom{L+\frac{d}{2}}{L}}\right)^2 \frac{(2\sin tL^{-1})^{d-1}}{L}\left(\int_0^t J_{\frac{d}{2}}(\theta)^2\,\mathrm{d}\theta + \mathcal{O}(L^{-1})\right). \end{aligned}$$

We use the asymptotic behaviour of the Bessel function for $\theta \to \infty$ (cf. [15, 3.14.1]):

$$J_{\frac{d}{2}}(\theta) = \frac{\cos\left(\theta - \frac{\pi(d+1)}{4}\right)}{\sqrt{\frac{\pi\theta}{2}}} + \mathcal{O}(\theta^{-\frac{3}{2}}).$$

This gives

$$\int_0^t J_{\frac{d}{2}}(\theta)^2 \,\mathrm{d}\theta = \frac{1}{\pi}\log t + \mathcal{O}(1),$$

which yields

$$V(\mathscr{X}_L^H, tL^{-1}) = \mathcal{O}(t^{d-1}\log t)$$

and concludes our proof. □

7. Jittered Sampling

In [8] it is shown that on arbitrary Ahlfors regular metric measure spaces there exist area-regular partitions $\mathcal{A} = \{A_1, \ldots, A_N\}$ with $\bigcup_{i=1}^N A_i = \mathbb{S}^d$, $\sigma(A_i) = \frac{1}{N}$, and $i \neq j \Rightarrow A_i \cap A_j = \emptyset$ satisfying

$$\operatorname{diam}(A_i) \leq C_d N^{-1/d}, \qquad i = 1, \ldots, N, \tag{29}$$

with a constant depending only on d (see also [1,5,11,13,17]).

Such partitions allow us to consider the average behaviour of *jittered sampling*; the point process $\mathscr{X}_N^{\mathcal{A}}$ constructed by sampling the sphere with the condition that each of the N points lies in a distinct region of the partition.

The jittered sampling variance integral is written as:

$$\begin{aligned} &V(\mathscr{X}_N^{\mathcal{A}}, \phi) \\ =&\int_{\mathbb{S}^d}\int_{A_1}\cdots\int_{A_N}\left(\sum_{i=1}^N \mathbb{1}_{C(\mathbf{x},\phi)}(\mathbf{y}_i) - N\sigma(C(\phi))\right)^2 \mathrm{d}\sigma_1(\mathbf{y}_1)\cdots\mathrm{d}\sigma_N(\mathbf{y}_N)\,\mathrm{d}\sigma(\mathbf{x}),\end{aligned}$$

where $\sigma_i(\cdot) := N\sigma(\cdot \cap A_i)$ is the uniform probability measure on A_i. The integral can be split into off-diagonal and diagonal terms

$$
\begin{aligned}
V(\mathscr{X}_N^{\mathcal{A}}, \phi) = &\sum_{\substack{i,j=1\\ i\neq j}}^{N} \int\limits_{A_i} \int\limits_{A_j} \sigma(C(\mathbf{y}_i,\phi) \cap C(\mathbf{y}_j,\phi)) \, \mathrm{d}\sigma_i(\mathbf{y}_i) \, \mathrm{d}\sigma_j(\mathbf{y}_j) \\
&+ N\sigma(C(\phi)) - N^2 \sigma(C(\phi))^2 \\
=& N \sum_{i=1}^{N} \int\limits_{A_i} \Bigg(\int\limits_{\mathbb{S}^d} \sigma(C(\mathbf{y}_i,\phi) \cap C(\mathbf{y},\phi)) \, \mathrm{d}\sigma(\mathbf{y}) \\
&- \int\limits_{A_i} \sigma(C(\mathbf{y}_i,\phi) \cap C(\mathbf{y},\phi)) \, \mathrm{d}\sigma(\mathbf{y}) \Bigg) \mathrm{d}\sigma_i(\mathbf{y}_i) + N\sigma(C(\phi)) - N^2 \sigma(C(\phi))^2 \\
=& N^2 \Bigg(\int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \sigma(C(\mathbf{x},\phi) \cap C(\mathbf{y},\phi)) \, \mathrm{d}\sigma(\mathbf{x}) \, \mathrm{d}\sigma(\mathbf{y}) - \sigma(C(\phi))^2 \Bigg) \\
&+ \sum_{i=1}^{N} \int\limits_{A_i} \int\limits_{A_i} \Big(\sigma(C(\mathbf{x}_i,\phi)) - \sigma(C(\mathbf{x}_i,\phi) \cap C(\mathbf{y}_i,\phi)) \Big) \, \mathrm{d}\sigma_i(\mathbf{x}_i) \, \mathrm{d}\sigma_i(\mathbf{y}_i) \\
=& \frac{1}{2} \sum_{i=1}^{N} \int\limits_{A_i} \int\limits_{A_i} \sigma(C(\mathbf{x}_i,\phi) \triangle C(\mathbf{y}_i,\phi)) \, \mathrm{d}\sigma_i(\mathbf{x}_i) \, \mathrm{d}\sigma_i(\mathbf{y}_i),
\end{aligned}
$$

where $\triangle$ denotes the symmetric difference operator of two sets. For the last equality, we have used

$$
\begin{aligned}
&\int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \sigma(C(\mathbf{x},\phi) \cap C(\mathbf{y},\phi)) \, \mathrm{d}\sigma(\mathbf{x}) \, \mathrm{d}\sigma(\mathbf{y}) \\
&= \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \mathbb{1}_{C(\mathbf{x},\phi)}(\mathbf{z}) \mathbb{1}_{C(\mathbf{y},\phi)}(\mathbf{z}) \, \mathrm{d}\sigma(\mathbf{z}) \, \mathrm{d}\sigma(\mathbf{x}) \, \mathrm{d}\sigma(\mathbf{y}) \\
&= \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \mathbb{1}_{C(\mathbf{z},\phi)}(\mathbf{x}) \mathbb{1}_{C(\mathbf{z},\phi)}(\mathbf{y}) \, \mathrm{d}\sigma(\mathbf{x}) \, \mathrm{d}\sigma(\mathbf{y}) \, \mathrm{d}\sigma(\mathbf{z}) = \sigma(C(\phi))^2.
\end{aligned}
$$

So in fact the variance of the jittered sampling process reduces to the diagonal terms. The measure of the symmetric difference can be bounded

$$
\sigma(C(\mathbf{x}_i,\phi) \triangle C(\mathbf{y}_i,\phi)) \leq \arccos(\langle \mathbf{x}_i, \mathbf{y}_i \rangle) \, \mathrm{surface}(\partial C(\mathbf{x}_i,\phi)).
$$

From the diameter bounds coming from our choice of equipartition, every summand can be bounded by $\mathcal{O}(\phi^{d-1}N^{-\frac{1}{d}})$, which gives

$$V(\mathscr{X}_N^{\mathcal{A}},\phi)=\mathcal{O}\left(\phi^{d-1}N^{\frac{d-1}{d}}\right); \tag{30}$$

the implied constant depends only on the dimension and the constants in (29).

Theorem 3. *The jittered sampling point process is hyperuniform in all three regimes.*

Proof. From (30) it is now immediate that $V(\mathscr{X}_N^{\mathcal{A}},\phi)=o(N)$ for all $\phi\in(0,\frac{\pi}{2})$, which proves hyperuniformity for large caps.

Again from (30) we obtain

$$V(X_N,\phi_N)=\mathcal{O}\Big((\phi_N N^{\frac{1}{d}})^{d-1}\Big)=o\Big((\phi_N N^{\frac{1}{d}})^{d}\Big)=o\big(\phi_N^d N\big)$$

under the assumptions on $(\phi_N)_{N\in\mathbb{N}}$ in Definition 3, which proves hyperuniformity for small caps.

Inserting $\phi_N=tN^{-\frac{1}{d}}$ into (30) yields

$$V(\mathscr{X}_N^{\mathcal{A}},tN^{-\frac{1}{d}})=\mathcal{O}\big(t^{d-1}\big)\qquad\text{as } t\to\infty,$$

which implies hyperuniformity at threshold order. □

Jittered Sampling is Determinantal. Consider an area-regular partition $\mathcal{A}=\{A_1,\dots,A_N\}$ of the space Λ into pairwise disjoint measurable sets; i.e.,

$$\begin{aligned} A_i\cap A_j&=\emptyset, &\quad i\neq j,\\ \mu\Big(\bigcup_{i=1}^N A_i\Big)&=1,\\ \mu(A_i)&=\frac{1}{N}, &\quad i=1,\dots,N. \end{aligned}$$

Define the projection operator

$$p_{\mathcal{A}}(f)(x):=\sum_{i=1}^N\frac{\mathbb{1}_{A_i}(x)}{\mu(A_i)}\int_{A_i}f(y)\,\mathrm{d}\mu(y)=\int_\Lambda K_{\mathcal{A}}(x,y)f(y)\,\mathrm{d}\mu(y)$$

to the space of functions measurable with respect to the finite σ-algebra generated by $\mathcal{A}$. The kernel of this operator is given by

$$K_{\mathcal{A}}(x,y):=\sum_{i=1}^N\frac{\mathbb{1}_{A_i}(x)\mathbb{1}_{A_i}(y)}{\mu(A_i)}.$$

The determinantal point process $\mathscr{X}_N^{\mathcal{A}}$ defined by the projection kernel $K_{\mathcal{A}}$ is then equal to the jittered sampling process associated to the partition $\mathcal{A}$, which can be seen by computing

$$\mathbb{E}\mathscr{X}_N^{\mathcal{A}}(A_1)\cdots\mathscr{X}_N^{\mathcal{A}}(A_N) \\ = \int_{A_1}\cdots\int_{A_N}\det\left(K_{\mathcal{A}}(x_i,x_j)_{i,j=1}^N\right)\,\mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_N).$$

Expanding the determinant gives

$$\mathbb{E}\mathscr{X}_N^{\mathcal{A}}(A_1)\cdots\mathscr{X}_N^{\mathcal{A}}(A_N) \\ = \sum_{\pi}\operatorname{sgn}(\pi)\int_{A_1}\cdots\int_{A_N}\prod_{i=1}^N K_{\mathcal{A}}(x_i,x_{\pi(i)})\,\mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_N).$$

Now we notice that $K_{\mathcal{A}}(x_i,x_j)=0$ if $i\neq j$ and $x_i\in A_i$ and $x_j\in A_j$. Thus, the integrand in the sum vanishes for all $\pi\neq\mathrm{id}$, which gives

$$\mathbb{E}\mathscr{X}_N^{\mathcal{A}}(A_1)\cdots\mathscr{X}_N^{\mathcal{A}}(A_N) = \prod_{i=1}^N\int_{A_i}K_{\mathcal{A}}(x_i,x_i)\,\mathrm{d}\mu(x_i)=1. \tag{31}$$

The process $\mathscr{X}_N^{\mathcal{A}}$ samples N points almost surely by [9]; thus the product of random variables $\mathscr{X}_N^{\mathcal{A}}(A_1)\cdots\mathscr{X}_N^{\mathcal{A}}(A_N)$ is either 0 or 1 (a.s.) and thus equal to 1 (a.s.) by (31). This implies that the process samples exactly one point per set of the partition $\mathcal{A}$. Furthermore, we have

$$\mathbb{E}\mathscr{X}_N^{\mathcal{A}}(D) = \int_D K(x,x)\,\mathrm{d}\mu(x) = \sum_{i=1}^N\int_D\frac{\mathbb{1}_{A_i}(x)^2}{\mu(A_i)}\,\mathrm{d}\mu(x) \\ = \sum_{i=1}^N\frac{\mu(A_i\cap D)}{\mu(A_i)} = N\mu(D),$$

and, for $D\subseteq A_i$, this implies $\mathbb{E}\mathscr{X}_N^{\mathcal{A}}(D)=\mu(D)/\mu(A_i)$; the sample point chosen from A_i is distributed with measure μ_i on A_i.

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