Hyperuniformity on the Sphere

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Workshop on “Computation and Optimization of Energy, Packing, and Covering”
April 11, 2018

Two point distributions

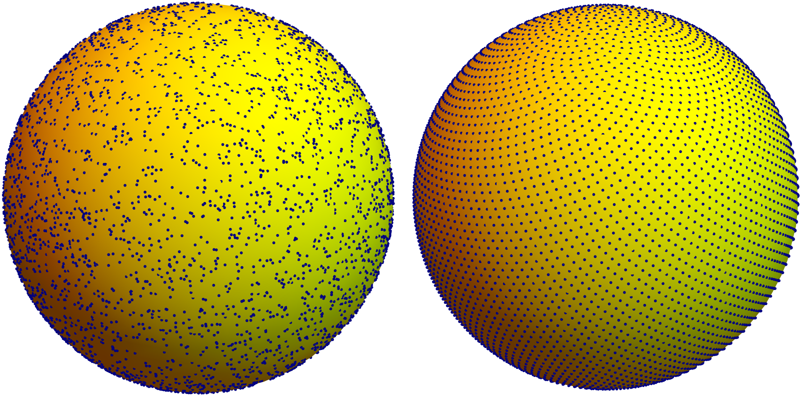

Figure: 6765 i.i.d. random points/ Fibonacci points

Uniform distribution

Definition

A sequence of point sets $(X_N)_{N\in\mathbb{N}}$ ($X_N \subset \mathbb{S}^d$) is called uniformly distributed, if

$$\lim_{N\to\infty} \frac{\#\left(X_N \cap C\right)}{N} = \sigma_d(C),$$

for all spherical caps C.

Throughout, $\sigma = \sigma_d$ will denote the normalised surface area measure on $\mathbb{S}^d$.
This is equivalent to

$$\lim_{N\to\infty} \frac{1}{N} \sum_{\mathbf{x}\in X_N} f(\mathbf{x}) = \int_{\mathbb{S}^d} f(\mathbf{x})\, d\sigma_d(\mathbf{x})$$

for all continuous (or even Riemann-integrable) functions f.

Uniform distribution

By the density of spherical harmonics in the continuous functions

$$\lim_{N\to\infty} \frac{1}{N^2} \sum_{\mathbf{x},\mathbf{y}\in X_N} P_n^{(d)}(\langle \mathbf{x}, \mathbf{y} \rangle) = 0$$

for all $n \geq 1$ is equivalent to uniform distribution.
We denote by $P_n^{(d)}$ the Legendre-polynomials for $\mathbb{S}^d$ normalised by $P_n^{(d)}(1) = 1$. These are Gegenbauer-polynomials for parameter $\lambda = \frac{d-1}{2}$ up to a scaling factor.

Quantify evenness

For every point set $X_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ of *distinct* points, we assign several qualitative measures that describe aspects of even distribution.

Then we can try to minimise or maximise these measures for given N.

Combinatorial measures

- discrepancy

$$D_N(X_N) = \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(\mathbf{x}_n) - \sigma(C) \right|$$

- covering radius

$$\delta(X_N) = \sup_{\mathbf{x}\in\mathbb{S}^d} \min_k |\mathbf{x} - \mathbf{x}_k|$$

- separation

$$\rho(X_N) = \min_{i\neq j} |\mathbf{x}_i - \mathbf{x}_j|$$

Analytic measures

- error in numerical integration

$$I_N(f, X_N) = \left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) - \int_{\mathbb{S}^d} f(\mathbf{x})\, d\sigma_d(\mathbf{x}) \right|$$

- Worst-case error for integration in a normed space H:

$$\mathrm{wce}(X_N, H) = \sup_{\substack{f \in H \\ \|f\|=1}} I_N(f, X_N)),$$

L^2-discrepancy and energy

- L^2-discrepancy:

$$\int_0^\pi \int_{\mathbb{S}^d} \left| \frac{1}{N} \sum_{n=1}^{N} \chi_{C(\mathbf{x},t)}(\mathbf{x}_n) - \sigma_d(C(\mathbf{x},t)) \right|^2 d\sigma_d(\mathbf{x})\, dt$$

- (generalised) energy:

$$E_g(X_N) = \sum_{\substack{i,j=1\\ i\neq j}}^{N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = \sum_{\substack{i,j=1\\ i\neq j}}^{N} \tilde{g}(\|\mathbf{x}_i - \mathbf{x}_j\|),$$

  where g denotes a positive definite function.

L^2-discrepancy and the worst case error (for many function spaces) turn out to be generalised energies of the underlying point configuration.

Hyperuniformity in $\mathbb{R}^d$

The concept of hyperuniformity was introduced by Torquato and Stillinger to describe idealised *infinite* point configurations, which exhibit properties between order and disorder.

Such configurations X occur as jammed packings, in colloidal suspensions, as well as quasi-crystals. The main feature of hyperuniformity is the fact that local density fluctuations are of smaller order than for an i. i. d. random ("Poissonian") point configuration.

During a semester program on "Minimal Energy Point Sets, Lattices, and Designs" in fall 2014 at the Erwin Schrödinger Institute in Vienna Salvatore Torquato asked, whether a notion of hyperuniformity could be defined for point sets (or point processes) on the sphere.

Heuristic

Hyperuniformity = asymptotically uniform + extra order

Counting points in test sets, e.g. balls B_R

$$N_R := \sum_{i=1}^{N} \mathbb{1}_{B_R}(X_i)\ , \quad \text{where } (X_1, \ldots, X_N) \sim \rho_V^{(N)}$$

The **expected** number of points in B_R is

$$\mathbb{E}\left[N_R\right] \overset{th.}{\to} \rho |B_R|$$

Hyperuniformity in $\mathbb{R}^d$

The **variance** measures the rate of convergence.

Example: $(X_i)_i$ i.i.d. $\Rightarrow \ \mathbb{V}[N_R] \stackrel{th.}{\to} \rho|B_R|$.

Definition

$(\rho^{(N)})_{N\in\mathbb{N}}$ hyperuniform $\Longleftrightarrow \lim_{th.} \mathbb{V}[N_R] \sim |\partial B_R|$ for large R

Remarks:

- If $(\rho^{(N)})_{N\in\mathbb{N}}$ hyperuniform, i.e. R^d-term of $\lim_{th.} \mathbb{V}\left[N_R\right]$ vanishes
  $\Rightarrow \ R^{d-1}$-term cannot vanish.
- Hyperuniformity is a long-scale property.

Hyperuniformity on the sphere

Definition (Hyperuniformity)

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

$$V(X_N, \phi) = \mathbb{V}_{\mathbf{x}} \# \left(X_N \cap C(\mathbf{x}, \phi)\right). \tag{1}$$

A sequence is called

- **hyperuniform for large caps** if

$$V(X_N, \phi) = o\left(N\right) \quad \text{as } N \to \infty \tag{2}$$

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

Hyperuniformity on the sphere (continued)

Definition (continued)

- **hyperuniform for small caps** if

$$V(X_N, \phi_N) = o\left(N\sigma(C(\cdot, \phi_N))\right) \quad \text{as } N \to \infty \tag{3}$$

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

  1. $\lim_{N\to\infty} \phi_N = 0$
  2. $\lim_{N\to\infty} N\sigma(C(\cdot, \phi_N)) = \infty$.

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

$$\limsup_{N\to\infty} V(X_N, tN^{-\frac{1}{d}}) = \mathcal{O}(t^{d-1}) \quad \text{as } t \to \infty. \tag{4}$$

Large caps

If $(X_N)_{N\in\mathbb{N}}$ is hyperuniform for large caps, then

$$\lim_{N\to\infty}\frac{1}{N}\sum_{\mathbf{x},\mathbf{y}\in X_N} P_n^{(d)}(\langle\mathbf{x},\mathbf{y}\rangle)=0$$

for all $n\geq 1$. This implies uniform distribution of $(X_N)_{N\in\mathbb{N}}$. Furthermore, it is not enough to require the defining relation for hyperuniformity for only one value of ϕ.

Small caps

If $(X_N)_{N\in\mathbb{N}}$ is hyperuniform for small caps, then

$$\limsup_{N\to\infty} \frac{1}{N} \sum_{\mathbf{x},\mathbf{y}\in X_N} P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle) < \infty$$

for all $n \geq 1$. This again implies uniform distribution of $(X_N)_{N\in\mathbb{N}}$.

Threshold order

If $(X_N)_{N\in\mathbb{N}}$ is hyperuniform at threshold order, then

$$\lim_{N\to\infty} \frac{1}{N^2} \sum_{\mathbf{x},\mathbf{y}\in X_N} P_n^{(d)}(\langle \mathbf{x}, \mathbf{y}\rangle) = 0$$

for all $n \geq 1$, which again gives uniform distribution of $(X_N)_{N\in\mathbb{N}}$. In the cases of small caps and caps of threshold order the conclusion of uniform distribution is not immediately obvious, since the range of caps for testing the distribution is quite restricted.

Relations to irregularities of distribution

In the development of the theory of uniform distribution it has been observed that the discrepancy of point sets has a general lower bound of larger order than the obvious $1/N$.
The theory of irregularities of distribution has been developed by J. Beck, W. Chen, K. F. Roth, W. Schmidt, and many others.
For the spherical cap discrepancy it gives the lower bound

$$D_N(X_N) \gg N^{-\frac{1}{2}-\frac{1}{2d}}$$

valid for all point sets X_N.
The lower bound is derived by considering the deviation for "small caps" in the sense introduced above.
There is a new proof of this lower bound by Bilyk and Dai, which is based on a very general version of Stolarsky's invariance principle.

Known upper bounds

It was also shown by Beck that there exists a point set with N points with

$$D_N(X_N) \ll N^{-\frac{1}{2}-\frac{1}{2d}}\sqrt{\log N}.$$

This proof is probabilistic and does not give a construction for this point set.
The best known construction is due to Aistleitner, Brauchart, and Dick, projecting the so called Fibonacci point set to the sphere. This gives

$$D_N \ll N^{-\frac{1}{2}}.$$

Deterministic hyperuniform point sets

- t-designs of minimal order
- point sets maximising

$$\sum_{\mathbf{x},\mathbf{y}\in X} \|\mathbf{x}-\mathbf{y}\|$$

- sequences of QMC-designs
- many candidates like Fibonacci-points or spiral points, but no proofs…

Probabilistic aspects

The original setting of hyperuniformity comes from statistical physics. The points are assumed to be sampled from a point process. The number variance is then the variance with respect to the process.
In this context the i.i.d. random case is referred to as the “Poissonian point process”. This process is – of course – not hyperuniform.

Determinantal point processes

A point process is determinantal on M with kernel $K : M \times M \to \mathbb{R}$, if its joint densities are given by

$$\rho_N(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{N!} \det \left(K(\mathbf{x}_i, \mathbf{x}_j)_{i,j=1}^N \right).$$

This notion was originally developed in physics, where the joint wave function of N fermionic particles can be expressed as a determinant of the above form.
The fact that the determinant vanishes, if $\mathbf{x}_i = \mathbf{x}_j$ for some $i \neq j$, implies a mutual repulsion of the sample points ("particles").

Determinantal point processes

The eigenvalues of random matrices, as well as the roots of random polynomials can also be modelled by determinantal point processes.
One special case is especially important and easy to understand:Let $H \subset L^2(M)$ be a finite dimensional space and K_H be the orthogonal projection to this space. If $N = \dim H$, then the DPP given by the kernel K_H samples exactly N points.

The spherical ensemble on $\mathbb{S}^2$

The kernel

$$\tilde{K}^{(N)}(x,y) = \frac{N(1+x\bar{y})^{N-1}}{4\pi(1+|x|^2)^{N+1}(1+|y|^2)^{N+1}}$$

on $\mathbb{C}^2$ describes the distribution of the eigenvalues of AB^{-1} for two $N \times N$ matrices A, B with i.i.d. complex Gaussian entries. Stereographically projecting the eigenvalues to the sphere $\mathbb{S}^2$ gives a point process; the spherical ensemble. Its joint densities are given by

$$C_N \prod_{1 \le i < j \le N} \|\mathbf{x}_i - \mathbf{x}_j\|^2$$

with a normalising constant C_N.
It has been shown by Alishahi and Zamani that samples of the spherical ensemble are hyperuniform for small caps.

Sample of spherical ensemble

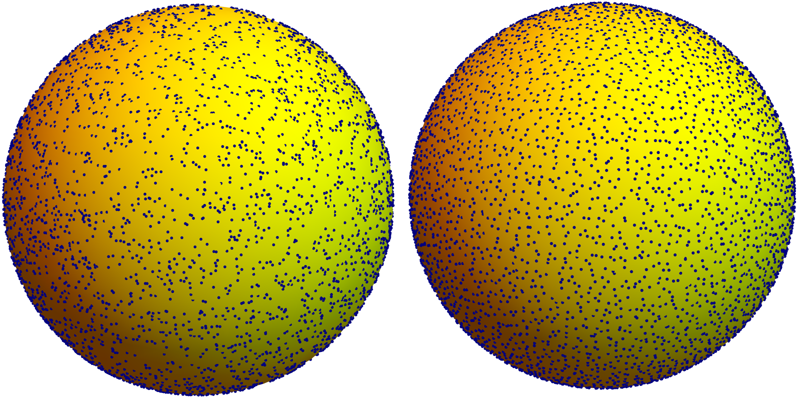

Figure: 6765 sampled points from an i.i.d. process and a DPP, resp.

The harmonic ensemble on $\mathbb{S}^d$

Let H_L be the span of all spherical harmonics of degree $\leq L$ on $\mathbb{S}^d$. Then the corresponding projection kernel defines a determinantal point process sampling $\dim H \sim L^d$ points. This process was introduced and studied by Beltrán, Marzo, and Ortega-Cerdá.

They proved *inter alia* that samples of this process are hyperuniform for small caps.

Jittered sampling

Let A_i ($i = 1, \ldots, N$) be an area regular partition of $\mathbb{S}^d$ with $\mathrm{diam}(A_i) \leq CN^{-\frac{1}{d}}$ and $\sigma(A_i) = \frac{1}{N}$. Such partitions exist by work of Kuijlaars and Saff and Gigante and Leopardi.
Then define point process by taking N points idependently uniformly from the sets A_i (one point per set). This process is the determinantal process given by the projection to the space of functions measurable with respect to the finite σ-algebra generated by $(A_i)_{i=1}^{N}$.
Jittered sampling points are hyperuniform in all three regimes.

Open questions

- Find relations with other measures of uniformity: discrepancy, error of integration, energy...
- Find more explicit deterministic constructions for hyperuniform point sets for any N.
- Find explicit deterministic constructions for point sets achieving the best possible discrepancy bound (or even a bound better than $N^{-\frac{1}{2}}$)