Hyperuniformity in compact spaces

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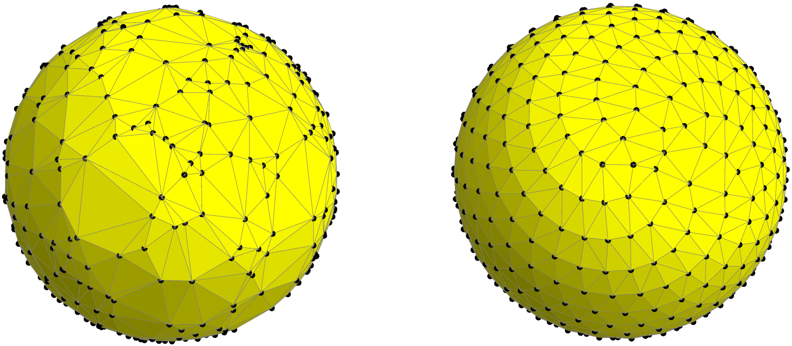
Two point distributions



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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

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

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- dispersion

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

- separation

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

Analytic measures

- error in numerical integration

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

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

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

L^2-discrepancy and energy

- L^2-discrepancy:

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

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- (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.

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where g denotes a positive definite function.

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

Discrepancy

Discrepancy is the most classical measure for the difference of two distributions

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It is rather difficult to compute explicitly, even for moderate values of N.

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Irregularities

On the other hand the theory of irregularities of distributions developed by K. F. Roth, W. Schmidt, J. Beck, W. Chen, . . . gives a lower bound

$$D_N(X_N) \geq C N^{-\frac{1}{2}-\frac{1}{2d}}.$$

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The proof of this result uses Fourier-analytic techniques. The caps contributing to the lower bound have the property

$$\lim_{N\to\infty} \sigma(C_N) = 0 \text{ and } \lim_{N\to\infty} N\sigma(C_N) = \infty.$$

(for later reference)

Irregularities

Beck's lower bound

$$D_N(X_N) \geq CN^{-\frac{1}{2}-\frac{1}{2d}}.$$

is essentially best possible. Namely, for every N there exists a point set X_N such that

$$DN(X_N) \leq CN^{-\frac{1}{2}-\frac{1}{2d}} \log N.$$

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The construction of this point set is probabilistic.
No explicit construction is known.

A new measure

The aim of this talk is to introduce a new measure for the quality of point distributions on compact spaces, especially the sphere and the torus.

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The ideas can be extended to compact homogeneous spaces.

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(b) invariant under Euclidean motion (for $V \nearrow \mathbb{R}^d$)

Hence, a single particle is distributed with density

$$\int_{V^{N-1}} \rho_V^{(N)}(r_1, \ldots, r_N)\, \mathrm{d}r_2 \cdots \mathrm{d}r_N = \frac{1}{|V|}$$

Assume $\frac{N}{|V|} \to \rho$ (*thermodynamic limit*).
$\Rightarrow$ distribution is asymptotically uniform with density ρ.

Hyperuniformity in $\mathbb{R}^d$

Heuristic

Hyperuniformity = asymptotically uniform + extra order

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

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

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

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

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

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  $\Rightarrow$ R^{d-1}-term cannot vanish.
- Hyperuniformity is a long-scale property.

Hyperuniformity in compact spaces

Compact sets have finite volume
$\Rightarrow$ the thermodynamical limit doesn't make sense!

Therefore consider distributions $(\rho^{(N)})_{N\in\mathbb{N}}$ on $M = \mathbb{T}^d$ or $\mathbb{S}^d$ satisfying

(a) $\rho^{(N)}(x_{\sigma 1}, \ldots, x_{\sigma N}) = \rho^{(n)}(x_1, \ldots, x_N)$ for all $x_i \in M,\ \sigma \in \mathsf{S}_N$.

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(b) $\rho^{(n)}(\tau x_1, \dots, \tau x_N) = \rho^{(N)}(x_1, \dots, x_N)$ for all $x_i \in M,\ \tau \in \mathbb{T}^d$ or $\mathrm{SO}(d+1)$, resp. *"isometry invariance"*

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Averaging over permutations and isometries
$\Rightarrow$ joint densities with (a) and (b) exist.

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Test sets B_R are balls or spherical caps, resp. and the **point counting function** is

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

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The **reduced density** is

$$\rho_k^{(N)}(r_1, \ldots, r_k) := \int_{M^{N-k}} \rho^{(N)}(r_1, \ldots, r_N)\, \mathrm{d}r_{k+1} \cdots \mathrm{d}r_N$$

where we integrate with respect to the normalized Lebesgue measure.

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where we integrate with respect to the normalized Lebesgue measure.The **expectation** remains N-dependent

$$\mathbb{E}\,[N_R] = \sum_{i=1}^{N} \mathbb{E}[\mathbb{1}_{B_R}(X_i)] = N \int_{B_R} \rho_1^{(N)}(r) \, \mathrm{d}r = N|B_R|.$$

Hyperuniformity in compact spaces

The **variance** depends on n and the pair correlation $\rho_2^{(n)}$

$$\mathbb{V}\left[N_R\right] = N|B_R|(1-|B_R|) + N(N-1)\int_{B_R^2} (\rho_2^{(n)}(x,y)-1)\,\mathrm{d}x\,\mathrm{d}y$$

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Example: $(X_i)_i$ i.i.d. (i.e. $\rho^{(N)}=1$)
$\Rightarrow\ \mathbb{E}\left[N_R\right] = N|B_R|$ and $\mathbb{V}\left[N_R\right] = N|B_R|(1-|B_R|)$.

Remark:

- From (a) and (b) $\Rightarrow\ \rho_2^{(N)}(x,y) = \rho_2^{(N)}(x-y)$.

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Remark:

- From (a) and (b) $\Rightarrow\ \rho_2^{(N)}(x,y) = \rho_2^{(N)}(x-y)$.
- For $M = \mathbb{S}^d$: $\int_0^\pi \mathbb{V}\left[N_R\right]\mathrm{d}R = L^2$-discrepancy.

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Hyperuniformity in compact spaces

Heuristic

Hyperuniformity *in the compact setting*

$$\Longleftrightarrow$$

For $|B_R| \to 0$ *and* $N \to \infty$ *such that* $N|B_R| = \mathbb{E}\left[N_R\right] \to \infty$*:*
$\mathbb{V}\left[N_R\right]$ *is of smaller order than in the i.i.d. case.*

Two examples to make this more precise…

Lattice on the torus $\mathbb{T}^2$

$(X_1, \dots, X_N) \sim \rho^{(N)}$,
where $A_N := \{a_1, \dots, a_N\} \subseteq \mathbb{T}^2$ **square lattice** (N a square for simplicity) and

$$\rho^{(N)}(x_1, \dots, x_N) = \frac{1}{N!} \sum_{\sigma \in \mathsf{S}_n} \int_{\mathbb{T}^2} \prod_{i=1}^{N} \delta(x_{\sigma_i} - a_i - t)\, \mathrm{d}t$$

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Therefore

$$\mathbb{V}\left[N_R\right] = N^2 |B_R| \left(\frac{1}{N} \sum_{i=1}^{N} \alpha_R(a_i) - \int_{\mathbb{T}^2} \alpha_R(r)\, \mathrm{d}r \right),$$

where $\alpha_R(r) := \mathrm{vol}(B_R(0) \cap B_R(r))$.

Lattice on the torus $\mathbb{T}^2$

The Fourier series of ball intersection volume is

$$\alpha_R(r) = \sum_{k\in\mathbb{Z}^2} b_k e^{2\pi i\langle k,r\rangle}, \quad b_k := \frac{1}{4\pi^2}\int_{\mathbb{T}^2} \alpha_R(|x|)e^{2\pi i\langle k,x\rangle}\,\mathrm{d}x$$

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For the variance this gives

$$\begin{aligned}\mathbb{V}\left[N_R\right] &= N^2|B_R|\left(\frac{1}{N}\sum_{i=1}^{N}\alpha_R(a_i) - \int_{\mathbb{T}^2}\alpha_R(r)\,\mathrm{d}r\right)\\ &= N^2|B_R|\sum_{k\in\mathbb{Z}^2\setminus\{0\}} b_{\sqrt{N}k}\end{aligned}$$

Lattice on the torus $\mathbb{T}^2$

Ball intersection volume $=$ convolution of indicator functions
$\Rightarrow$ Fourier coefficients b_k $=$ product of Bessel functions.

Lattice on the torus $\mathbb{T}^2$

Ball intersection volume = convolution of indicator functions
$\Rightarrow$ Fourier coefficients b_k = product of Bessel functions.

Asymptotic: $|b_k| \leq \frac{c}{|k|^3 R}$, for $|k|R \geq 0,\ c = const. > 0$.
Therefore for small $|B_R|$:

$$\mathbb{V}_\rho\left[N_R\right] \leq N^2 |B_R| \frac{c}{RN^{3/2}} \sum_{k \in \mathbb{Z}^2 \setminus \{0\}} \frac{1}{\|k\|^3}$$
$$= \tilde{c}\sqrt{N}\ |\partial B_R|$$

Compare to

$$\mathbb{V}_{i.i.d.}\left[N_R\right] = N|B_R|.$$

Remark: This method works for lattices in $\mathbb{T}^d$, $d \geq 3$.

Determinantal point process in $\mathbb{S}^2$

Definition

A point process on M with joint densities $(\rho^{(N)})_{N\in\mathbb{N}}$ is called **determinantal with kernel** $K^{(n)}$, if

$$\rho^{(N)}(x_1,\dots,x_n) = \det(K^{(N)}(x_i,x_j))_{i,j=1}^{N}, \quad \text{for all } N\in\mathbb{N},\ x_i\in M.$$

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Let $\tilde{K}^{(N)}(x,y) = \frac{N(1+x\bar{y})^{N-1}}{4\pi(1+|x|^2)^{(N+1)/2}(1+|y|^2)^{(N+1)/2}}$ on $\mathbb{C}^2$ with resp. to the Lebesgue measure λ on $\mathbb{C}$. Then

$$\tilde{\rho}^{(N)}(x_1,\dots,x_N) = \det(\tilde{K}^{(N)}(x_i,x_j))_{i,j=1}^N$$
$$= const. \prod_{i<j} \frac{|x_i-x_j|^2}{(1+|x_i|)(1+|x_j|)} \prod_{k=1}^N \frac{1}{(1+|x_k|^2)^2}$$

Determinantal point process in $\mathbb{S}^2$

Using stereographic projection $g : \mathbb{C} \times \mathbb{R} \to \mathbb{C},\ (z, x) \mapsto \frac{z}{1-x}$:

$$\rho^{(N)}(p_1, \ldots, p_N) := g^* \tilde{\rho}^{(N)}(p_1, \ldots, p_N)$$
$$= const. \prod_{i<j} \|p_i - p_j\|^2_{\mathbb{R}^3},$$

with resp. to the normalized Lebesgue measure σ on $\mathbb{S}^2$.

Remark: Configurations, where points are close together have low weight $\Rightarrow$ repulsion!

Determinantal point process in $\mathbb{S}^2$

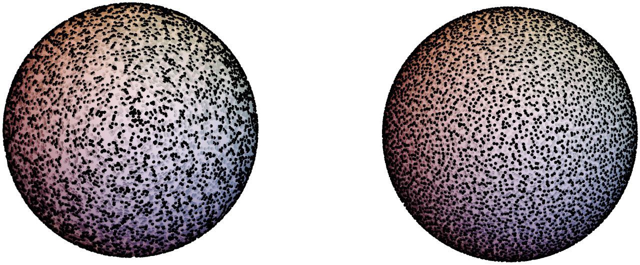

Figure: 10000 sampled points from an i.i.d. process and a DPP, resp.

Determinantal point process in $\mathbb{S}^2$

For following set

$$C = C(\mathbf{x}, \phi) = \{\mathbf{y} \in \mathbb{S}^2 \mid \langle \mathbf{x}, \mathbf{y} \rangle \geq \cos(\phi)\}$$

for the cap with angle ϕ around $\mathbf{x}$.

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$$C = C(\mathbf{x},\phi) = \{\mathbf{y} \in \mathbb{S}^2 \mid \langle \mathbf{x},\mathbf{y}\rangle \geq \cos(\phi)\}$$

for the cap with angle ϕ around $\mathbf{x}$.
Reduction of $\rho^{(N)}$:

$$\rho_k^{(N)}(p_1,\dots,p_k) = \frac{(N-k)!}{N!}\det(K(p_i,p_j))_{i,j=1}^k$$

In particular: $\rho_2^{(N)}(p,q) = \frac{N}{N-1}[1-(1-\|p-q\|^2/4)^{N-1}]$.
Therefore

$$\mathbb{V}\left[\#(X_N \cap C)\right] = N\left[\sigma(C) - N\int_{C^2}(1-\|p-q\|^2/2)^{N-1}(\mathrm{d}\sigma)^2(p,q)\right]$$
$$= \dots$$

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Lemma (Alishahi, Zamani '15)

If $N\sigma(C) \to \infty$*, when* $N \to \infty$ *and* $\phi \to 0$*. Then for all* $\epsilon > 0$*:*

$$\mathbb{V}\left[\#(X_N \cap C)\right] = \sqrt{N\sigma(C)} + o(\log(N\sigma(C))^{1/2+\epsilon}).$$

Higher dimensional spheres

The approach given before is principally restricted to the sphere $\mathbb{S}^2$. In a recent paper by C. Beltrán, J. Marzo and J. Ortega-Cerdà for certain values of n determinantal point processes on $\mathbb{S}^d$ are constructed, which exhibit a similar behaviour as for the process on $\mathbb{S}^2$.

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Deterministic point of view

The definition of hyperuniformity was based on an underlying probabilistic model producing the points. We would like to apply a similar concept to define hyperuniformity of a deterministic sequence of point sets $(X_N)_N$.

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Definition

A sequence $(X_N)_N$ of point sets on $\mathbb{S}^d$ is called hyperuniformly distributed, if

$$\int_{\mathbb{S}^d} \left(\sum_{n=1}^{N} \chi_{C(\mathbf{x},\phi_N)}(\mathbf{x}_n) - N\sigma_d(C_{\mathbf{x},\phi_N}) \right)^2 d\sigma_d(\mathbf{x}) = o(N\sigma_d(C(\cdot,\phi_N)))$$

for all $(\phi_N)_N$ such that

$$\lim_{N\to\infty} \sigma_d(C(\cdot,\phi_N)) = 0 \text{ and } \lim_{N\to\infty} N\sigma_d(C(\cdot,\phi_N)) = \infty.$$

Concluding remarks

The results on determinantal point processes show that hyperuniformly distributed point sequences exist.

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The quantity

$$\int_{\mathbb{S}^d} \left(\sum_{n=1}^{N} \chi_{C(\mathbf{x},\phi_N)}(\mathbf{x}_n) - N\sigma_d(C_{\mathbf{x},\phi_N}) \right)^2 \, d\sigma_d(\mathbf{x})$$

is a localised version of the L^2-discrepancy.

Concluding remarks

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Together with

$$\mathbb{V}(\#(X_N \cap C_{\mathbf{x},\phi_N})) = o(N\sigma_d(C_{\mathbf{x},\phi_N}))$$

this implies uniform distribution of the sequence of point sets $(X_N)_N$.