Hyperuniformity on the Sphere

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Two point distributions
For every point set \( X_N = \{x_1, \ldots, x_N\} \) 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

\[ D_N(X_N) = \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(x_n) - \sigma(C) \right| \]

- dispersion

\[ \delta_N(X_N) = \sup_{x \in S^d} \min_k \min_{x \in S^d} |x - x_k| \]

- separation

\[ \Delta_N(X_N) = \min_{i \neq j} |x_i - x_j| \]
error in numerical integration

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

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

\[ I_N(X_N, H) = \sup_{f \in H, \|f\| = 1} I_N(f, X_N) \]
\( L^2 \)-discrepancy and energy

- \( L^2 \)-discrepancy:

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

- (generalised) energy:

\[
E_g(X_N) = \sum_{i,j=1 \atop i \neq j}^{N} g(\langle x_i, x_j \rangle) = \sum_{i,j=1 \atop i \neq j}^{N} \tilde{g}(\|x_i - x_j\|),
\]

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

\[ D_N(X_N) = \sup_C \left| \frac{1}{N} \sum_{n=1}^{N} \chi_C(x_n) - \sigma(C) \right|. \]

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

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

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)
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

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

The construction of this point set is probabilistic. No explicit construction is known. The best known deterministic construction by Aistleitner, Brauchart, and Dick gives a discrepancy bound of order \( O(N^{-\frac{1}{2}}) \).
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. The ideas can be extended to compact homogeneous spaces.
Remember Salvatore Torquato’s talks yesterday 
Distribute $N$ particles in a volume $V \subseteq \mathbb{R}^d$ according to a point process with **joint density** $\rho^{(N)}_V$ being 

(a) invariant under permutation of the particles 
(b) invariant under Euclidean motion (for $V \nearrow \mathbb{R}^d$) 

Hence, a single particle is distributed with density 

$$ \int_{V^{N-1}} \rho^{(N)}_V(r_1, \ldots, r_N) \, dr_2 \cdots dr_N = \frac{1}{|V|} $$ 

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

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Hyperuniformity in $\mathbb{R}^d$

**Heuristic**

*Hyperuniformity = asymptotically uniform + extra order*

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

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

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

$$\mathbb{E} [N_R] \xrightarrow{th} \rho |B_R|$$
The **variance** measures the rate of convergence.

**Example:** \((X_i)_i\) i.i.d. \(\Rightarrow \nabla[N_R] \xrightarrow{th.} \rho |B_R|.

**Definition**

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

**Remarks:**

- If \((\rho^{(N)})_{N \in \mathbb{N}} \text{ hyperuniform}, \text{i.e. } R^d\text{-term of } \lim_{th.} \nabla[N_R]
  \text{ vanishes}
  \Rightarrow R^{d-1}\text{-term cannot vanish.}

- Hyperuniformity is a long-scale property.
Compact sets have finite volume
⇒ the thermodynamical limit doesn’t make sense!

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

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

“particles are exchangeable”

(b) \( \rho^{(N)}(\tau x_1, \ldots, \tau x_N) = \rho^{(N)}(x_1, \ldots, x_N) \) for all \( x_i \in M, \tau \in \mathbb{T}^d \) or \( \text{SO}(d + 1) \), resp.

“isometry invariance”

Averaging over permutations and isometries
⇒ joint densities with (a) and (b) exist.
Hyperuniformity in compact spaces

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

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

The reduced density is

$$\rho^{(N)}_k(r_1, \ldots, r_k) := \int_{M^{N-k}} \rho^{(N)}(r_1, \ldots, r_N) \, dr_{k+1} \cdots dr_N$$

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

$$\mathbb{E}[N_R] = \sum_{i=1}^{N} \mathbb{E}[1_{B_R}(X_i)] = N \int_{B_R} \rho^{(N)}_1(r) \, dr = N|B_R|.$$
Hyperuniformity in compact spaces

The variance depends on \( N \) and the pair correlation \( \rho_2^{(N)} \)

\[
\mathbb{V}[N_R] = N|B_R|(1 - |B_R|) + N(N - 1) \int_{B_R^2} (\rho_2^{(N)}(x, y) - 1) \, dx \, dy
\]

**Example:** \((X_i)_i \) i.i.d. (i.e. \( \rho^{(N)} = 1 \))

\[
\Rightarrow \mathbb{E}[N_R] = N|B_R| \text{ and } \mathbb{V}[N_R] = N|B_R|(1 - |B_R|).
\]

**Remark:**

- From (a) and (b) \( \Rightarrow \rho_2^{(N)}(x, y) = \rho_2^{(N)}(x - y) \).
- For \( M = S^d \):
  \[
  \int_0^\pi \mathbb{V}[N_R] \, dR = L^2\text{-discrepancy}.
  \]
Hyperuniformity in the compact setting

\[ \iff \]

For \( |B_R| \to 0 \) and \( N \to \infty \) such that \( N|B_R| = \mathbb{E}[N_R] \to \infty \):

\( \forall [N_R] \text{ is of smaller order than in the i.i.d. case.} \)

Two examples to make this more precise...
Lattice on the torus $\mathbb{T}^2$

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

$$\rho^{(N)}(x_1, \ldots, x_N) = \frac{1}{N!} \sum_{\sigma \in S_n} \int_{\mathbb{T}^2} \prod_{i=1}^N \delta(x_{\sigma_i} - a_i - t) \, dt$$

Therefore

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

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

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

The Fourier series of ball intersection volume is

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

$\alpha_R$ can be written as a convolutional square, which implies $b_k \geq 0$.

For the variance this gives

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

$$= N^2 |B_R| \sum_{k \in \mathbb{Z}^2 \setminus \{0\}} b_{\sqrt{N}k} \sqrt{N}k$$
Lattice on the torus $\mathbb{T}^2$

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

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

$$\nabla_\rho [N_R] \leq N^2|B_R| \frac{c}{RN^{3/2}} \sum_{k \in \mathbb{Z}^2 \setminus \{0\}} \frac{1}{\|k\|^3}$$

$$= \tilde{c} \sqrt{N} |\partial B_R|$$

Compare to

$$\nabla_{i.i.d.} [N_R] = N|B_R|.$$  

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

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

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

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 $\lambda$ on $\mathbb{C}$. Then

$$\tilde{\rho}^{(N)}(x_1, \ldots, x_N) = \det(\tilde{K}^{(N)}(x_i, x_j))_{i,j=1}^N$$

$$= \text{const.} \prod_{i<j} \frac{|x_i - x_j|^2}{(1 + |x_i|)(1 + |x_j|)} \prod_{k=1}^N \frac{1}{(1 + |x_k|^2)^2}$$
Determinantal point process in $S^2$

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

$$\rho^{(N)}(p_1, \ldots, p_N) := g^* \tilde{\rho}^{(N)}(p_1, \ldots, p_N) = \text{const.} \prod_{i<j} \| p_i - p_j \|_2^2,$$

with resp. to the normalized Lebesgue measure $\sigma$ on $S^2$.

**Remark:** Configurations, where points are close together have low weight $\Rightarrow$ repulsion!
Figure: 10000 sampled points from an i.i.d. process and a DPP, resp.
Determinantal point process in $S^2$

For following set

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

for the cap with angle $\phi$ around $x$.

Reduction of $\rho^{(N)}$:

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

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

$$\forall \left[ \#(X_N \cap C) \right] = N \left[ \sigma(C) - N \int_{C^2} (1 - \|p - q\|^2 / 4)^{N-1} (d\sigma)^2(p, q) \right]$$

$$= \ldots$$
Lemma (Alishahi, Zamani '15)

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

\[
\nabla \left[ \#(X_N \cap C) \right] = \sqrt{N\sigma(C)} + o(\log(N\sigma(C))^{1/2+\epsilon}).
\]
Higher dimensional spheres

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

- discrepancy
- Riesz energy
- separation

of the sample points.
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 $(X_N)_N$.

**Definition**

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

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

for all $(\phi_N)_N$ such that

$$\lim_{N \to \infty} \sigma_d(C(\cdot,\phi_N)) = 0 \text{ and } \lim_{N \to \infty} N\sigma_d(C(\cdot,\phi_N)) = \infty.$$
The results on determinantal point processes show that hyperuniformly distributed point sequences exist.

The definition uses exactly those spherical caps for assessing the quality of the point distribution, which attain Beck’s lower bound for the discrepancy.

The quantity

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

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

- Prove (or disprove) that hyperuniformity implies uniform distribution.
- Find relations with other measures of uniformity: discrepancy, error of integration, energy...
- Find 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 $N^{-\frac{1}{2}}$)