

Discrepancy and energy optimization on the sphere

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“Optimal point configurations and orthogonal polynomials”

CIEM, Castro Urdiales, Cantabria, Spain
April 2017

April 19, 2017

Good point distributions

- Lattices
- Energy minimization
- Monte-Carlo
- Other random point processes (jittered sampling, determinantal point process)
- Covering/packing problems
- Low-discrepancy sets
- Cubature formulas, numerical integration
- Uniform tessellation, almost isometric embeddings

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- Choose an N -point set in $Z \subset U$
- Discrepancy of Z with respect to \mathcal{A} :

$$D_{\mathcal{A}}(Z) = \sup_{A \in \mathcal{A}} \left| \frac{\#(Z \cap A)}{N} - \mu(A) \right|.$$

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- $\sup \rightarrow L^2$ -average: L^2 discrepancy.

Spherical cap discrepancy

For $x \in \mathbb{S}^d$, $t \in [-1, 1]$ define spherical caps:

$$C(x, t) = \{y \in \mathbb{S}^d : \langle x, y \rangle \geq t\}.$$

For a finite set $Z = \{z_1, z_2, \dots, z_N\} \subset \mathbb{S}^d$ define

$$D_{cap}(Z) = \sup_{x \in \mathbb{S}^d, t \in [-1, 1]} \left| \frac{\#(Z \cap C(x, t))}{N} - \sigma(C(x, t)) \right|.$$

Theorem (Beck, '84)

There exists constants $c_d, C_d > 0$ such that

$$c_d N^{-\frac{1}{2} - \frac{1}{2d}} \leq \inf_{\#Z=N} D_{cap}(Z) \leq C_d N^{-\frac{1}{2} - \frac{1}{2d}} \sqrt{\log N}.$$

Spherical caps: L^2 Stolarsky Principle

Define the spherical cap L^2 discrepancy

$$D_{cap,L^2}(Z) = \left(\int_{\mathbb{S}^d} \int_{-1}^1 \left| \frac{\#(Z \cap C(x,t))}{N} - \sigma(C(x,t)) \right|^2 dt d\sigma(x) \right)^{\frac{1}{2}}.$$

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Theorem (Stolarsky invariance principle)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

$$\begin{aligned} \frac{1}{N^2} \sum_{i,j=1}^N \|z_i - z_j\| + c_d \left[D_{L^2, cap} \right]^2 &= \text{const} \\ &= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y). \end{aligned}$$

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- Stolarsky '73, Brauchart, Dick '12, DB, Dai, Matzke '16.

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- Define the spherical cap discrepancy of fixed height t :

$$D_{L^2, \text{cap}}^{(t)}(Z) := \left(\int_{\mathbb{S}^d} \left| \frac{1}{N} \sum_{j=1}^N \mathbf{1}_{C(x,t)}(z_j) - \sigma(C(x,t)) \right|^2 d\sigma(x) \right)^{1/2}$$

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$$\int_{-1}^1 (\sigma(C(p, t)))^2 dt = 1 - C_d \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\| d\sigma(x) d\sigma(y).$$

Hemisphere discrepancy

- L^2 discrepancy for spherical cap discrepancy of fixed height t satisfies:

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- Taking $t = 0$ (i.e. hemispheres):

$C(z_i, t) \cap C(z_j, t) = \frac{1}{2}(1 - d(x, y))$, where d is the normalized geodesic distance $d(x, y) = \frac{1}{\pi} \cos^{-1}(x \cdot y)$.

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Theorem (Stolarsky for hemispheres, DB '16, Skriyanov '16)

$$\begin{aligned} [D_{L^2, \text{hem}}(Z)]^2 &= [D_{L^2, \text{cap}}^{(0)}(Z)]^2 \\ &= \frac{1}{2} \left(\int_{\mathbb{S}^d} \int_{\mathbb{S}^d} d(x, y) d\sigma(x) d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^N d(z_i, z_j) \right). \end{aligned}$$

Hemisphere Stolarsky: simple corollaries

$$[D_{L^2, \text{hem}}(Z)]^2 = \frac{1}{2} \left(\frac{1}{2} - \frac{1}{N^2} \sum_{i,j=1}^N d(z_i, z_j) \right).$$

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- For any $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

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- For even N :

$$\frac{1}{N^2} \sum_{i,j=1}^N d(z_i, z_j) = \frac{1}{2} \iff Z \text{ - symmetric.}$$

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- Fejes-Toth '59: $d = 1$ and conjectured for $d \geq 2$.
- Sperling, '60 ($d = 2$, even N)
- Larcher, '61 ($d = 2$, odd N)

Hemisphere Stolarsky for general measures

Let μ be a probability measure on \mathbb{S}^d . Define the geodesic distance energy integral

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Let $H(x) = C(x, 0)$ denote the hemisphere with center at x . Then the following version of the Stolarsky principle holds:

$$\int_{\mathbb{S}^d} \left(\mu(H(x)) - \frac{1}{2} \right)^2 d\sigma(x) = \frac{1}{2} \cdot \left(\frac{1}{2} - I_g(\mu) \right).$$

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- $I_g(\mu) = \frac{1}{2}$ (i.e. μ is a maximizer) **iff**
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 $\mu(H(x)) = \frac{1}{2}$ for σ -a.e. $x \in \mathbb{S}^d$ **iff**
 μ is symmetric, i.e. $\mu(E) = \mu(-E)$.

Distance energy integrals

Let μ be a Borel probability measure on \mathbb{S}^d .

Then

$$I_E(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} |x - y| d\mu(x) d\mu(y)$$

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However,

$$I_g(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} d(x, y) d\mu(x) d\mu(y)$$

is maximized by any symmetric measure μ .

Euclidean distance energy integrals

Let μ be a Borel probability measure on the sphere \mathbb{S}^d . For $\lambda > 0$ define the energy integral

$$I_\lambda = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} |x - y|^\lambda d\mu(x) d\mu(y)$$

Maximizers (Bjorck '56):

- $0 < \lambda < 2$: unique maximizer is surface measure σ ,
- $\lambda = 2$: any measure with center of mass at 0,
- $\lambda > 2$: mass $\frac{1}{2}$ at two opposite poles.

Riesz energy

- $-d < \lambda \leq 0$: unique minimizer is surface measure σ

Geodesic distance energy integrals

Let μ be a Borel probability measure on the sphere \mathbb{S}^d . For $\lambda > 0$ define the energy integral

$$I_\lambda = \int \int_{\mathbb{S}^d \mathbb{S}^d} (d(x, y))^\lambda d\mu(x) d\mu(y)$$

Maximizers (DB, Dai, Matzke '16):

- $-d < \lambda \leq 0$: unique minimizer is σ
- $0 < \lambda < 1$: unique maximizer is σ ,
- $\lambda = 1$: any symmetric measure,
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$d = 1$: Brauchart, Hardin, Saff, '12

Positive definite functions on the sphere

Consider the energy integral

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A function $F \in C[-1, 1]$ is called *positive definite* on the sphere \mathbb{S}^d if for any set of points $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$, the matrix $[F(z_i \cdot z_j)]_{i,j=1}^N$ is positive semidefinite, i.e.

$$\sum_{i,j} F(z_i \cdot z_j) c_i c_j \geq 0 \quad \text{for all } c_i \in \mathbb{R}.$$

Positive definite functions on the sphere

Lemma

For a function $F \in C[-1, 1]$ the following are equivalent:

- (i) F is positive definite on \mathbb{S}^d .
- (ii) Gegenbauer coefficients of F are non-negative, i.e.

$$\widehat{F}(n, \lambda) \geq 0 \text{ for all } n \geq 0.$$

- (iii) For any signed measure $\mu \in \mathcal{B}$ the energy integral is non-negative: $I_F(\mu) \geq 0$.
- (iv) There exists a function $f \in L^2_{w_\lambda}[-1, 1]$ such that

$$F(x \cdot y) = \int_{\mathbb{S}^d} f(x \cdot z) f(z \cdot y) d\sigma(z), \quad x, y \in \mathbb{S}^d,$$

i.e. F is the spherical convolution of f with itself.

$$\widehat{f}(n, \lambda)^2 = \widehat{F}(n, \lambda)$$

Theorem (DB, F. Dai, '16)

- *Generalized Stolarsky principle:*

$$I_F(\mu) - I_F(\sigma) = D_{L^2, f}^2(\mu).$$

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- *Generalized Stolarsky principle:*

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- *Estimates for optimal N -point discrepancy:*

$$\min_{1 \leq k \lesssim N^{1/d}} \widehat{F}(k, \lambda) \lesssim \mathcal{D}_{L^2, f, N}^2 \lesssim \frac{1}{N} \max_{0 \leq \theta \lesssim N^{-\frac{1}{d}}} (F(1) - F(\cos \theta))$$

Asymptotics of optimal discrete geodesic energy

Let

$$\mathcal{E}_{d,\delta} = \inf_{Z_N} \sum_{1 \leq i < j \leq N} (d(z_i, z_j))^\delta,$$

$$I_{d,\delta}(\sigma) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} (d(x, y))^\delta d\sigma(x) d\sigma(y).$$

Theorem (DB, Dai '16)

- If $-d < \delta < 1$ and $\delta \neq 0$, then

$$I_{d,\delta}(\sigma) - \frac{2}{N^2} \mathcal{E}_{d,\delta}(N) \sim N^{-1-\frac{\delta}{d}}$$

- In the logarithmic case, $\delta = 0$,

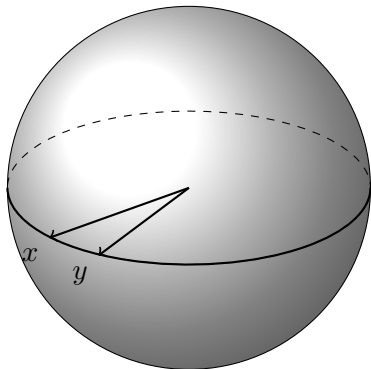
$$I_{d,0}(\sigma) - \frac{2}{N^2} \mathcal{E}_{d,0}(N) \sim N^{-1} \log N.$$

In the Euclidean case: Wagner, Saff–Kuijlaars, Brauchart

Tessellations of spheres (joint work with Michael Lacey)

Let $x, y \in \mathbb{S}^d$

choose a random hyperplane $z^\perp, z \in \mathbb{S}^d$.



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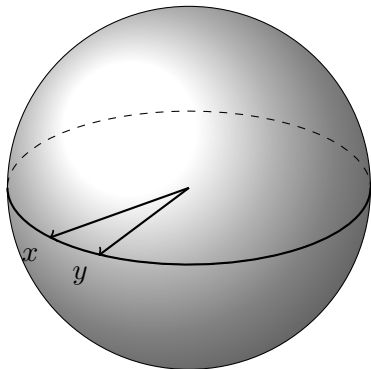
choose a random hyperplane z^\perp , $z \in \mathbb{S}^d$.

Then

$$\begin{aligned}\mathbb{P}(z^\perp \text{ separates } x \text{ and } y) \\ &= \mathbb{P}(\text{sign}\langle z, x \rangle \neq \text{sign}\langle z, y \rangle) \\ &= d(x, y),\end{aligned}$$

where d is the normalized geodesic distance on the sphere, i.e.

$$d(x, y) = \frac{\cos^{-1}\langle x, y \rangle}{\pi}.$$



Hamming distance

Consider a set of vectors $Z = \{z_1, z_2, \dots, z_N\}$ on the sphere \mathbb{S}^d . Define the Hamming distance as

$$d_H(x, y) := \frac{\#\{z_k \in Z : \text{sign}(x \cdot z_k) \neq \text{sign}(y \cdot z_k)\}}{N},$$

i.e. the proportion of hyperplanes z_k^\perp that *separate* x and y .

Define

$$\Delta_Z(x, y) := d_H(x, y) - d(x, y).$$

The main question

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$$\sup_{x, y \in K} |\Delta_Z(x, y)| \leq \delta.$$

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Equivalently, the *sign-linear* map

$$\phi_Z(x) = \{\text{sign}(x \cdot z_k)\}_{k=1}^N = \text{sign}(Zx)$$

is a δ -isometry from K into the Hamming cube $\mathcal{H}^N = \{-1, 1\}^N$.

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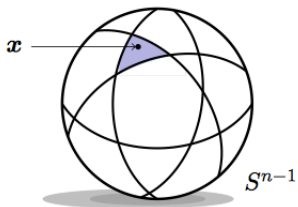
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Prior results:

Plan, Vershynin, '13: $N = C\delta^{-6}\omega(K)^2$ random points yield a δ -uniform tessellation of K with high probability.

Cells with small diameter

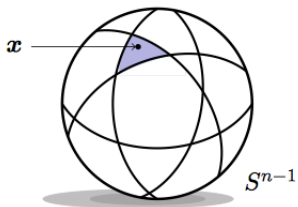


Lemma

Every cell of a δ -uniform tessellation of K by hyperplanes has diameter at most δ .

Picture from Baraniuk, Foucart, Needell, Plan,
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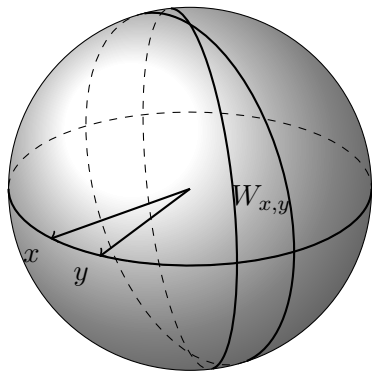
Proof:

if x and y are in the same cell then

$$d(x, y) = |d(x, y) - \underbrace{d_H(x, y)}_{=0}| \leq \delta.$$

- **Small cells:** If $N \gtrsim \delta^{-1} \log N(K, c\delta)$, then w.h.p. N random vectors induce a tessellation with δ -small cells.
- **Uniform tessellation:** If $N \gtrsim \delta^{-2} H(K)^2$, then there exists a δ -isometry $\phi : \mathbb{S}^d \rightarrow \mathcal{H}^N$.
- **Sparse case:** Let K_s be the set of s -sparse vectors in \mathbb{S}^d . If $N \gtrsim \delta^{-2} s \log_+ \frac{d}{s}$, then for a random set Z of m points in \mathbb{S}^d w.h.p. the *sign-linear map* is a δ -isometry from K_s to \mathcal{H}^N .
- **One-bit Johnson-Lindenstrauss lemma:** If K is finite and $m \gtrsim \delta^{-2} \log(\#K)$, then there exists a δ -isometry between $K \subset \mathbb{S}^d$ and the Hamming cube \mathcal{H}^m .

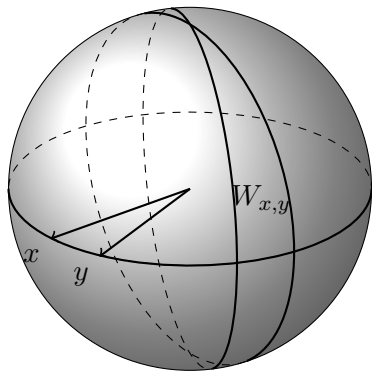
Tessellations and discrepancy



$$H_x = \{z : \langle z, x \rangle > 0\}$$

$$\begin{aligned} W_{xy} &= H_x \Delta H_y \\ &= \{z \in \mathbb{S}^d : \text{sign}\langle z, x \rangle \neq \text{sign}\langle z, y \rangle\} \end{aligned}$$

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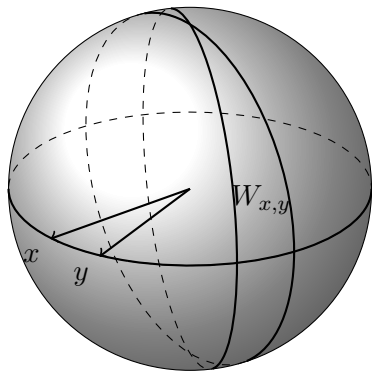


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$$\Delta_Z(x, y) = d_H(x, y) - d(x, y) = \frac{\#(Z \cap W_{xy})}{N} - \sigma(W_{xy})$$

$$D_{\text{wedge}}(Z) = \|\Delta_Z(x, y)\|_\infty = \sup_{x, y \in \mathbb{S}^d} \left| \frac{\#(Z \cap W_{xy})}{N} - \sigma(W_{xy}) \right|.$$

- There exist constants c_d, C_d , such that the following discrepancy bounds hold:

$$c_d N^{-\frac{1}{2} - \frac{1}{2d}} \leq \inf_{Z \subset \mathbb{S}^d: \#Z=N} D_{\text{wedge}}(Z) \leq C_d N^{-\frac{1}{2} - \frac{1}{2d}} \sqrt{\log N}.$$

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- Inverting this we find that the optimal value of N satisfies

$$\delta^{-2 + \frac{2}{d+1}} \lesssim N \lesssim \delta^{-2 + \frac{2}{d+1}} \left(\log \frac{1}{\delta} \right)^{\frac{d}{d+1}}.$$

Define the L^2 discrepancy for wedges

$$[D_{L^2, \text{wedge}}(Z)]^2 = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \left(\frac{1}{N} \sum_{k=1}^N \mathbf{1}_{W_{xy}}(z_k) - \sigma(W_{xy}) \right)^2 d\sigma(x) d\sigma(y)$$

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Theorem (Stolarsky for wedges, DB, Lacey, '15)

For any finite set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$

$$[D_{L^2, \text{wedge}}(Z)]^2 = \frac{1}{N^2} \sum_{i,j=1}^N \left(\frac{1}{2} - d(z_i, z_j) \right)^2 - \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \left(\frac{1}{2} - d(x, y) \right)^2 d\sigma(x) d\sigma(y).$$

Frame potential

- $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$ is a frame in \mathbb{R}^d iff there exist $c, C > 0$ such that for any $x \in \mathbb{R}^{d+1}$

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Theorem (Benedetto, Fickus)

A set $Z = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$ is a tight frame in \mathbb{R}^{d+1} if and only if Z is a local minimizer of the frame potential:

$$F(Z) = \sum_{i,j=1}^N |\langle z_i, z_j \rangle|^2.$$