Discrepancy and energy minimization on the sphere

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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 $Z = \{z_1, z_2, ..., z_N\} \subset \mathbb{S}^d$ define

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

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 discrepancy

Define the spherical cap L^2 discrepancy

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

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Spherical cap discrepancy: refinement of lower bound

Theorem (Beck, '84)

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

$$D_{cap}(Z) \gtrsim N^{-\frac{1}{2}-\frac{1}{2d}}.$$

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Theorem (DB, Dai, Steinerberger, '18)

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

$$D_{cap}(Z) \gtrsim N^{-\frac{1}{2}-\frac{1}{2d}} \left(\frac{1}{N} \sum_{i,j=1}^{N} \frac{1}{(1 + N^{1/d}\|z_i - z_j\|)^{d+1}} \right)^{1/2}.$$

Discrete energy

Let $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$ and let $F : [-1, 1] \to \mathbb{R}$.

Discrete energy:

$$E_F(Z) = \frac{1}{N^2} \sum_{i,j=1}^{N} F(z_i \cdot z_j)$$

Questions:

- What are the minimizing configurations?
- Almost minimizers?
- Lower bounds?

Energy integral

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

Energy integral

$$I_F(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} F(x \cdot y)\, d\mu(x) d\mu(y).$$

i.e. $E_F(Z) = I_F\left(\frac{1}{N} \sum \delta_{z_i}\right)$

Questions:

- What are the minimizers?
- Is σ a minimizer?
- Is it unique?

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 $\mathbb{S}^d$, i.e. for any set of points $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$, the matrix $\big[F(z_i \cdot z_j)\big]_{i,j=1}^N$ is positive semidefinite*
- ii *Gegenbauer coefficients of F are non-negative, i.e.*

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

- 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*

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

Positive definite functions and energy minimization

Lemma

Let $F \in C[-1,1]$.

- *The energy* $I_F(\mu)$ *is minimized by* σ
  if and only if
  $\widehat{F}(n,\lambda) \geq 0$ *for all* $n \geq 1$,
  i.e. F is positive definite up to a constant term.

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- *The energy* $I_F(\mu)$ *is uniquely minimized by* σ
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Spherical cap L^2 discrepancy

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

Discrepancy + energy: Stolarsky Invariance Principle

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Theorem (Stolarsky invariance principle)

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

$$c_d D^2_{cap,L^2}(Z) = \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} \|x-y\| \, d\sigma(x) d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^{N} \|z_i - z_j\|.$$

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Proofs:

- Stolarsky '73, Brauchart, Dick '12, DB, Dai, Matzke '18.

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

Generalized Stolarsky principle

Define the L^2 discrepancy of a Borel probability measure μ w.r.t. the function $f : [-1,1] \to \mathbb{R}$ as

$$D^2_{L^2,f}(\mu) = \int\limits_{\mathbb{S}^d} \left| \int\limits_{\mathbb{S}^d} f(x \cdot y) d\mu(y) - \int\limits_{\mathbb{S}^d} f(x \cdot y) d\sigma(y) \right|^2 d\sigma(x).$$

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Let F be positive definite and f as in (iv), *then*

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- Important ingredient: $I_F(\mu) - I_F(\sigma) = I_F(\mu - \sigma)$.

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- Arbitrary compact metric spaces (DB, O. Vlasiuk '18)

Discrepancy/energy bounds

Theorem (DB, F. Dai, '17)

Assume that F is positive definite and f as in (iv)*.*

Let $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$ *and* $\mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i}$.

- `Upper bound:`

$$\inf_{\#Z=N} D^2_{L^2,f}(\mu) \lesssim \frac{1}{N} \max_{0\le\theta\lesssim N^{-\frac{1}{d}}} \big(F(1) - F(\cos\theta)\big).$$

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- Lower bound:

$$\inf_{\#Z=N} D^2_{L^2,f}(\mu) \gtrsim \min_{1\le k\lesssim N^{1/d}} \widehat{F}(k,\lambda).$$

Stolarsky principle for hemispheres

Theorem (DB, Dai, Matzke '18, Skriganov '18)

$$D^2_{L^2,\text{hemisphere}}(Z) \quad = \frac{1}{2\pi}\left(\int\limits_{\mathbb{S}^d}\int\limits_{\mathbb{S}^d} d(x,y)\, d\sigma(x)\, d\sigma(y) - \frac{1}{N^2}\sum_{i,j=1}^{N} d(z_i,z_j) \right),$$

where $d(x,y) = \arccos(x\cdot y)$ *is the geodesic distance.*

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Corollary (DB, Dai, Matzke '18)

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

$$\frac{1}{N^2}\sum_{i,j=1}^{N} d(z_i, z_j) \leq \frac{\pi}{2}$$

with equality if and only if Z *is symmetric.*

`(This solves a 1959 conjecture of Fejes Tóth.)`

Another conjecture of Fejes Tóth

Conjecture (Sum of acute angles)

Let $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$ *and define*

$$F(x \cdot y) = \min \Big\{ \arccos(x \cdot y), \, \pi - \arccos(x \cdot y) \Big\} = \arccos |x \cdot y|,$$

i.e. the acute angle between the lines through x, $y \in \mathbb{S}^d$.

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- *The discrete energy* $E_F(Z) = \dfrac{1}{N^2} \sum_{i,j=1}^{N} F(z_i \cdot z_j)$ *is maximized by the set* $Z = \{z_1, ..., z_N\} \subset \mathbb{S}^d$ *with* $z_i = e_{i \bmod (d+1)}$.

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- $\max I_F(\mu) = I_F(\nu_{ONB}) = \frac{\pi}{2} \cdot \frac{d}{d+1}$, *where*

$$\nu_{ONB} = \frac{1}{d+1} \sum_{i=1}^{d+1} \delta_{e_i}$$

Acute angles: known results

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$$I_F(\mu) \leq \frac{\pi}{2} - \frac{69}{150} = 1.110796... < \frac{3\pi}{8} = 1.178097.... $$

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- Conjectured maximum in $d = 2$ is $\frac{\pi}{3} = 1.047198...$.

Frame energy

- $Z = \{z_1, \ldots, z_N\} \subset \mathbb{S}^d$ is a tight frame iff there exists $A > 0$ such that for any $x \in \mathbb{R}^{d+1}$

$$\sum_k |\langle x, z_k \rangle|^2 = A\|x\|^2,$$

or, equivalently,

$$x = \frac{1}{A} \sum \langle x, z_k \rangle \, z_k.$$

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Theorem (Benedetto, Fickus, '03)

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

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

Frame energy

Let $F(t) = |t|^2$. Then for each Borel probability measure μ on $\mathbb{S}^d$

$$I_F(\mu) = \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} |x \cdot y|^2 \, d\mu(x) d\mu(y) \geq \frac{1}{d+1},$$

and the equality is achieved iff μ is an isotropic measure, i.e. $\int_{\mathbb{S}^d} x_i x_j d\mu(x) = c\delta_{i,j}$.

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Thus global minimizers include, in particular:

- discrete tight frames of any cardinality,
- including orthonormal bases or regular simplex,
- normalized surface measure σ.

p-Frame energy

Let $F(t) = |t|^p$ with $p > 0$. Consider the p-frame energy:

$$I_p(\mu) = \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} |x \cdot y|^p d\mu_x d\mu_y$$

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- $p > 2$, $p = 2k$ even integer (Ehler, Okoudjo)
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  - discrete "spherical designs"

Spherical designs

A set $\{p_1, \dots p_N\} \subset \mathbb{S}^d$ is called a spherical design of strength t iff

$$\frac{1}{N}\sum_{i=1}^{N} f(p_i) = \int_{\mathbb{S}^d} f(x)d\sigma(x)$$

for any polynomial f of degree at most t.

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Bondarenko, Radchenko, Viazovska, '11 (settling the conjecture of Korevaar and Meyers):

For any $N \geq c_d t^d$, there exists a spherical t-design with N points.

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- $0 < p < 2$: ONB (but **not** σ or other frames)
- $p > 2$, $p = 2k$ even integer:
  - σ (but **not** ONB)
  - discrete "spherical designs"
- $p > 2$, but $p \neq 2k$: **???** (**not** σ, **not** ONB)

“Tight” designs

Following Cohn–Kumar and Cohn-Kumar–Minton, we say that a symmetric set $\{z_1, \dots z_N\} \subset \mathbb{S}^d$ is a *tight design* if

- it is a $(2m-1)$-design
- inner products between points $z_i \cdot z_j$ take $m+1$ values,

i.e. a design of *high* degree with *few* distances.

Some known tight designs

n	N	M	$m+1$	configuration
n	n	3	3	cross polytope
2	$N \geq 2$	$N-1$	$\lfloor \frac{N}{2} \rfloor + 1$	regular polygon
3	12	5	4	icosahedron
8	240	7	5	E_8 root system
24	$196,560$	11	7	Leech Lattice minimal vectors

... and some others...

$n = d + 1$ is the ambient dimension
M is the strength of the design

Main result

Theorem (DB, A. Glazyrin, R. Matzke, J. Park, O. Vlasiuk, 2018)

If $\{z_1, ..., z_N\}$ *is tight design with parameter* m*, then the measure*

$$\mu = \frac{1}{N} \sum \delta_{z_i}$$

is a global minimizer of the p-frame energy for every $p \in (2m-4, 2m-2)$.

Moreover, any other minimizer is a discrete measure with the same distribution of absolute values of inner products.

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- a maximal ETF (equiangular tight frame), whenever it exists, is minimizer of $I_p(\mu)$ for $p \in (2,4)$.
- etc.

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