Point distributions on the sphere: energy minimization, discrepancy, and more.

Dmitriy Bilyk
University of Minnesota

ICERM Semester Program on
"Point Configurations in Geometry, Physics and Computer Science"

Workshop "Optimal and Random Point Configurations"

Providence, RI

February 27, 2018

Discrepancy

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)

Discrepancy

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)
- $\mathcal{A}$ - a collection of subsets of U ("test sets", e.g., balls, cubes, convex sets, spherical caps)

Discrepancy

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)
- $\mathcal{A}$ - a collection of subsets of U ("test sets", e.g., balls, cubes, convex sets, spherical caps)
- Let $Z = \{z_1, \ldots, z_N\} \subset U$ be an N-point set.

Discrepancy

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)
- $\mathcal{A}$ - a collection of subsets of U ("test sets", e.g., balls, cubes, convex sets, spherical caps)
- Let $Z = \{z_1, \dots, z_N\} \subset U$ be an N-point set.
- Discrepancy of Z with respect to $\mathcal{A}$:

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

Discrepancy

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)
- $\mathcal{A}$ - a collection of subsets of U ("test sets", e.g., balls, cubes, convex sets, spherical caps)
- Let $Z = \{z_1, \dots, z_N\} \subset U$ be an N-point set.
- Discrepancy of Z with respect to $\mathcal{A}$:

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

- Optimal discrepancy wrt $\mathcal{A}$:

$$D_N(\mathcal{A}) = \inf_{\#Z = N} D_{\mathcal{A}}(Z).$$

- U: a set with a natural probability measure μ (e.g., $[0,1]^d$, $\mathbb{T}^d$, $\mathbb{S}^d$, etc.)
- $\mathcal{A}$ - a collection of subsets of U ("test sets", e.g., balls, cubes, convex sets, spherical caps)
- Let $Z = \{z_1, \dots, z_N\} \subset U$ be an N-point set.
- Discrepancy of Z with respect to $\mathcal{A}$:

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

- Optimal discrepancy wrt $\mathcal{A}$:

$$D_N(\mathcal{A}) = \inf_{\#Z = N} D_{\mathcal{A}}(Z).$$

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

Disk (ball) disrepancy on $\mathbb{T}^d$

Theorem (Montgomery; Beck; 80's)

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2 \simeq [0,1)^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

$$\left| \frac{\#\{1 \le i \le N : z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

Disk (ball) disrepancy on $\mathbb{T}^d$

Theorem (Montgomery; Beck; 80's)

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2 \simeq [0,1)^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

$$\left| \frac{\#\{1 \le i \le N : z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

- Higher-dimensional version for $Z \subset \mathbb{T}^d$ holds with $N^{-\frac{1}{2} - \frac{1}{2d}}$.

Disk (ball) disrepancy on $\mathbb{T}^d$

Theorem (Montgomery; Beck; 80's)

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2 \simeq [0,1)^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

$$\left| \frac{\#\{1 \le i \le N : z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

- Higher-dimensional version for $Z \subset \mathbb{T}^d$ holds with $N^{-\frac{1}{2}-\frac{1}{2d}}$.
- Is one radius enough? Still an open question!

Disk (ball) disrepancy on $\mathbb{T}^d$

Theorem (Montgomery; Beck; 80's)

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2 \simeq [0,1)^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

$$\left| \frac{\#\{1 \le i \le N : z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

- Higher-dimensional version for $Z \subset \mathbb{T}^d$ holds with $N^{-\frac{1}{2}-\frac{1}{2d}}$.
- Is one radius enough? Still an open question!
- Sharp up to logarithms: jittered sampling.

Disk (ball) disrepancy on $\mathbb{T}^d$

Theorem (Montgomery; Beck; 80's)

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2 \simeq [0,1)^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

$$\left| \frac{\#\{1 \le i \le N : z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

- Higher-dimensional version for $Z \subset \mathbb{T}^d$ holds with $N^{-\frac{1}{2}-\frac{1}{2d}}$.
- Is one radius enough? Still an open question!
- Sharp up to logarithms: jittered sampling.
- Sharp in L^2 sense: lattice.

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int\limits_{\mathbb{T}^d} \left| \frac{\#\left\{Z \cap B_r(x)\right\}}{N} - |B_r| \right|^2 dx$$

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int\limits_{\mathbb{T}^d} \left| \frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| \right|^2 dx$$

Let $L_M = \left\{ \left(\frac{r_1}{M}, \ldots, \frac{r_d}{M} \right) : \, r_i = 0, 1, \ldots, M-1 \right\} \subset \mathbb{T}^d$

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int_{\mathbb{T}^d} \left| \frac{\#\left\{Z \cap B_r(x)\right\}}{N} - |B_r| \right|^2 dx$$

Let $L_M = \left\{ \left(\frac{r_1}{M}, \dots, \frac{r_d}{M} \right) : r_i = 0, 1, \dots, M-1 \right\} \subset \mathbb{T}^d$ and set

$D_{\text{lattice}}(M) = D_{L^2}\big(L_M\big)$ and $D_{\text{jittered}}(M) = \mathbb{E}\, D_{L^2}\big(L_M^{\text{jittered}}\big)$.

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int_{\mathbb{T}^d} \left| \frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| \right|^2 dx$$

Let $L_M = \left\{ \left(\frac{r_1}{M}, \dots, \frac{r_d}{M} \right) : r_i = 0, 1, \dots, M-1 \right\} \subset \mathbb{T}^d$ and set

$$D_{\text{lattice}}(M) = D_{L^2}\big(L_M\big) \quad \text{and} \quad D_{\text{jittered}}(M) = \mathbb{E}\, D_{L^2}\big(L_M^{\text{jittered}}\big).$$

Theorem (Chen, Travaglini, '08)

- *For $d = 1$ or 2, $D_{\text{lattice}}(M) < D_{\text{jittered}}(M)$.*

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int\limits_{\mathbb{T}^d} \left| \frac{\#\left\{Z \cap B_r(x)\right\}}{N} - |B_r| \right|^2 dx$$

Let $L_M = \left\{ \left(\frac{r_1}{M}, \dots, \frac{r_d}{M} \right) : r_i = 0, 1, \dots, M-1 \right\} \subset \mathbb{T}^d$ and set

$$D_{\text{lattice}}(M) = D_{L^2}\big(L_M\big) \qquad \text{and} \qquad D_{\text{jittered}}(M) = \mathbb{E}\, D_{L^2}\big(L_M^{\text{jittered}}\big).$$

Theorem (Chen, Travaglini, '08)

- *For* $d = 1$ *or* 2, $D_{\text{lattice}}(M) < D_{\text{jittered}}(M)$.
- *For large* d, $D_{\text{lattice}}(M) > D_{\text{jittered}}(M)$.

L^2 discrepancy: lattice vs jittered sampling

Denote

$$D^2_{L^2}(Z) = \int\limits_{\mathbb{T}^d} \left| \frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| \right|^2 dx$$

Let $L_M = \left\{ \left(\frac{r_1}{M}, \dots, \frac{r_d}{M} \right) : r_i = 0, 1, \dots, M-1 \right\} \subset \mathbb{T}^d$ and set

$D_{\text{lattice}}(M) = D_{L^2}\big(L_M\big)$ and $D_{\text{jittered}}(M) = \mathbb{E}\, D_{L^2}\big(L_M^{\text{jittered}}\big)$.

Theorem (Chen, Travaglini, '08)

- *For* $d = 1$ *or* 2, $D_{\text{lattice}}(M) < D_{\text{jittered}}(M)$.
- *For large* d, $D_{\text{lattice}}(M) > D_{\text{jittered}}(M)$.

`unless` $d \equiv 1$ `mod` 4 `and` $d > 1$.

Montgomery's lower bound

- Let $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| = (\mathbf{1}_{B_r} * \mathcal{D}_Z)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
-
$$D^2_{L^2}(Z) = \sum_{\mathbf{n}\in\mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}}\cos(t - 3\pi/4) + O(t^{-3/2})$

Montgomery's lower bound

- Let $Z = \{z_1, \ldots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| = \left(\mathbf{1}_{B_r} * \mathcal{D}_Z\right)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
-
$$D^2_{L^2}(Z) = \sum_{\mathbf{n}\in\mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}}\cos(t - 3\pi/4) + O(t^{-3/2})$

Montgomery's lower bound

- Let $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| = \left(\mathbf{1}_{B_r} * \mathcal{D}_Z\right)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
-
$$D^2_{L^2}(Z) = \sum_{\mathbf{n} \in \mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}} \cos(t - 3\pi/4) + O(t^{-3/2})$

Montgomery's lower bound

- Let $Z = \{z_1, \ldots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| = (\mathbf{1}_{B_r} * \mathcal{D}_Z)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
-
$$D^2_{L^2}(Z) = \sum_{\mathbf{n}\in\mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}} \cos(t - 3\pi/4) + O(t^{-3/2})$

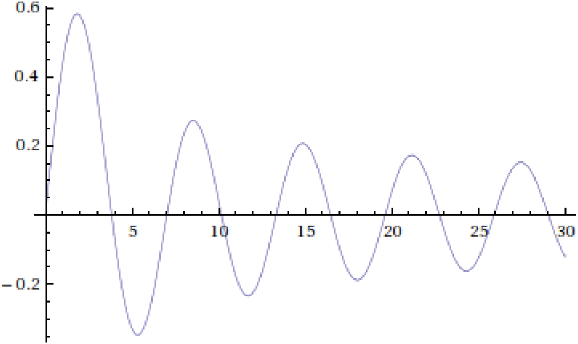
Montgomery's lower bound

- Let $Z = \{z_1, \ldots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\left\{Z \cap B_r(x)\right\}}{N} - |B_r| = \left(\mathbf{1}_{B_r} * \mathcal{D}_Z\right)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
-
$$D_{L^2}^2(Z) = \sum_{\mathbf{n}\in\mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}}\cos(t - 3\pi/4) + O(t^{-3/2})$

Montgomery's lower bound

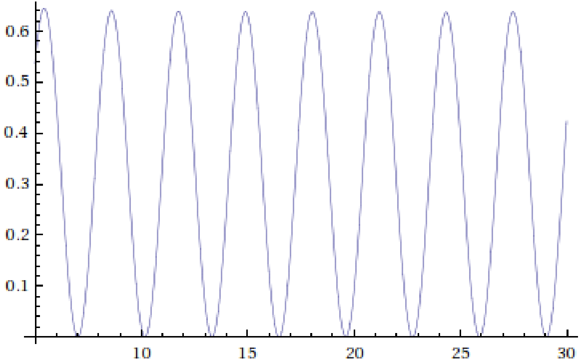
- Let $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2$.
- Then
$$\frac{\#\{Z \cap B_r(x)\}}{N} - |B_r| = (\mathbf{1}_{B_r} * \mathcal{D}_Z)(x),$$
- where $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
- $$D_{L^2}^2(Z) = \sum_{\mathbf{n} \in \mathbb{Z}^2} |\widehat{\mathbf{1}}_{B_r}(\mathbf{n})|^2 \cdot |\widehat{\mathcal{D}_Z}(\mathbf{n})|^2$$
- $\widehat{\mathbf{1}}_{B_r}(\mathbf{n}) = \frac{r}{|\mathbf{n}|} J_1(2\pi|\mathbf{n}|r)$ - Bessel function of the first kind
- $J_1(t) = \sqrt{\frac{2}{\pi t}} \cos(t - 3\pi/4) + O(t^{-3/2})$

Bessel functions



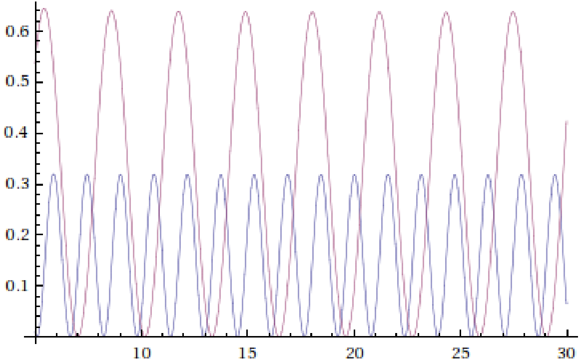
$J_1(t)$

Bessel functions



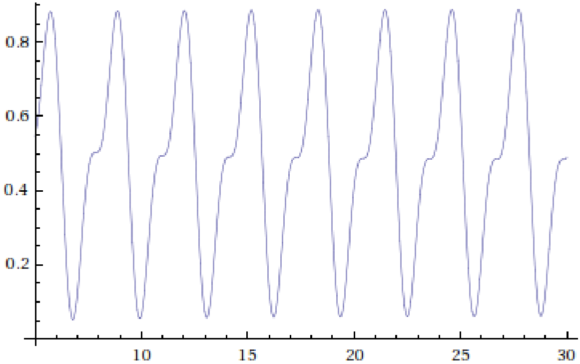
$$t \cdot J_1^2(t)$$

Bessel functions



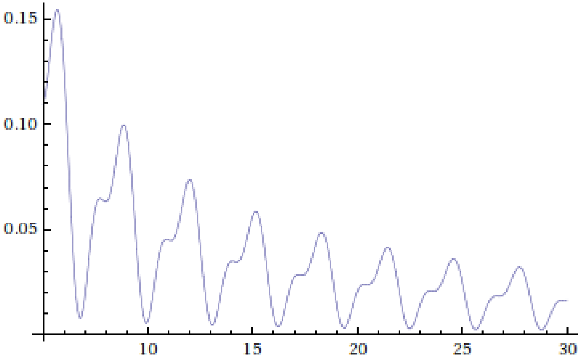
$t \cdot J_1^2(t)$ and $t \cdot J_1^2(2t)$

Bessel functions



$$t \cdot (J_1^2(t) + J_1^2(2t))$$

Bessel functions



$$J_1^2(t) + J_1^2(2t) \gtrsim \frac{1}{t}$$

Thus $|\widehat{\mathbf{1}}_{B_{1/4}}(\mathbf{n})|^2 + |\widehat{\mathbf{1}}_{B_{1/2}}(\mathbf{n})|^2 \gtrsim \frac{1}{|\mathbf{n}|^3}$

Exponential sums

- $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`

- For $\mathbf{n} \neq 0$, $\widehat{\mathcal{D}_Z}(\mathbf{n}) = \frac{1}{N}\sum_{i=1}^{N} e^{-2\pi i\,\mathbf{n}\cdot z_i}$.

- Montgomery's esimate:

$$\sum_{\|\mathbf{n}\|\leq X} \left|\sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i}\right|^2 \gtrsim X^2 N$$

  and taking $X \approx N^{1/2}$ leads to the discrepancy bound.

- Refinement (Steinerberger, '17):

$$\sum_{\|\mathbf{n}\|\leq X} \left|\sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i}\right|^2 \gtrsim \sum_{i,j=1}^{N} \frac{X^2}{1 + X^4 \|z_i - z^j\|^4}$$

Exponential sums

- $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`

- For $\mathbf{n} \neq 0$, $\widehat{\mathcal{D}_Z}(\mathbf{n}) = \frac{1}{N}\sum_{i=1}^{N} e^{-2\pi i\, \mathbf{n}\cdot z_i}$.

- Montgomery's esimate:

$$\sum_{\|\mathbf{n}\|\leq X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i} \right|^2 \gtrsim X^2 N$$

  and taking $X \approx N^{1/2}$ leads to the discrepancy bound.

- Refinement (Steinerberger, '17):

$$\sum_{\|\mathbf{n}\|\leq X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i} \right|^2 \gtrsim \sum_{i,j=1}^{N} \frac{X^2}{1 + X^4 \|z_i - z^j\|^4}$$

Exponential sums

- $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N}\delta_{z_i} - \lambda_2$ (discrepancy measure).
- For $\mathbf{n} \neq 0$, $\widehat{\mathcal{D}_Z}(\mathbf{n}) = \frac{1}{N}\sum_{i=1}^{N} e^{-2\pi i\, \mathbf{n}\cdot z_i}$.
- Montgomery's esimate:

$$\sum_{\|\mathbf{n}\|\leq X}\left|\sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i}\right|^2 \gtrsim X^2 N$$

and taking $X \approx N^{1/2}$ leads to the discrepancy bound.

- Refinement (Steinerberger, '17):

$$\sum_{\|\mathbf{n}\|\leq X}\left|\sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i}\right|^2 \gtrsim \sum_{i,j=1}^{N}\frac{X^2}{1+X^4\|z_i - z^j\|^4}$$

Exponential sums

- $\mathcal{D}_Z = \frac{1}{N} \sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
- For $\mathbf{n} \neq 0$, $\widehat{\mathcal{D}_Z}(\mathbf{n}) = \frac{1}{N} \sum_{i=1}^{N} e^{-2\pi i\, \mathbf{n} \cdot z_i}$.
- Montgomery's esimate:

$$\sum_{\|\mathbf{n}\| \leq X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n} \cdot z_i} \right|^2 \gtrsim X^2 N$$

and taking $X \approx N^{1/2}$ leads to the discrepancy bound.

- Refinement (Steinerberger, '17):

$$\sum_{\|\mathbf{n}\| \leq X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n} \cdot z_i} \right|^2 \gtrsim \sum_{i,j=1}^{N} \frac{X^2}{1 + X^4 \|z_i - z^j\|^4}$$

Exponential sums

- $\mathcal{D}_Z = \frac{1}{N}\sum_{i=1}^{N} \delta_{z_i} - \lambda_2$ `(discrepancy measure).`
- For $\mathbf{n} \neq 0$, $\widehat{\mathcal{D}_Z}(\mathbf{n}) = \frac{1}{N}\sum_{i=1}^{N} e^{-2\pi i\,\mathbf{n}\cdot z_i}$.
- Montgomery's esimate:

$$\sum_{\|\mathbf{n}\|\le X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i} \right|^2 \gtrsim X^2 N$$

  and taking $X \approx N^{1/2}$ leads to the discrepancy bound.
- Refinement (Steinerberger, '17):

$$\sum_{\|\mathbf{n}\|\le X} \left| \sum_{i=1}^{N} e^{-2\pi i \mathbf{n}\cdot z_i} \right|^2 \gtrsim \sum_{i,j=1}^{N} \frac{X^2}{1 + X^4 \|z_i - z^j\|^4}$$

Refined discrepancy estimate

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

Refined discrepancy estimate

For any N-point set $Z = \{z_1, \dots, z_N\} \subset \mathbb{T}^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius 1/4 or 1/2 such that

- Montgomery, '89:

$$\left| \frac{\#\{z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

Refined discrepancy estimate

For any N-point set $Z = \{z_1, \ldots, z_N\} \subset \mathbb{T}^2$ there exists a disk $D \subset \mathbb{T}^2$ of radius $1/4$ or $1/2$ such that

- Montgomery, '89:

$$\left| \frac{\#\{z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{3}{4}}.$$

- Steinerberger, '17:

$$\left| \frac{\#\{z_i \in D\}}{N} - |D| \right| \gtrsim N^{-\frac{7}{4}} \left(\sum_{i,j=1}^{N} \frac{N}{1 + N^2 \|z_i - z^j\|^4} \right)^{\frac{1}{2}}.$$

Spherical cap discrepancy

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

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

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

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

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 exist 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 cap discrepancy: refinement of lower bound

Theorem (Beck, '84)

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

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

Spherical cap discrepancy: refinement of lower bound

Theorem (Beck, '84)

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

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

Theorem (DB, Dai, Steinerberger, '17)

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

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

Discrepancy and energy: Stolarsky Principle

Define the spherical cap L^2 discrepancy

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

Discrepancy and energy: Stolarsky Principle

Define the spherical cap L^2 discrepancy

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

Theorem (Stolarsky invariance principle)

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

$$\frac{1}{N^2} \sum_{i,j=1}^{N} \|z_i - z_j\| + c_d \Big[D_{L^2,cap}\Big]^2 = \text{const}$$

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

Discrepancy and energy: Stolarsky Principle

Define the spherical cap L^2 discrepancy

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

Theorem (Stolarsky invariance principle)

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

$$c_d \Big[D_{cap,L^2}(Z) \Big]^2 =$$

$$= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\|\, d\sigma(x) d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^{N} \|z_i - z_j\|.$$

Discrepancy and energy: Stolarsky Principle

Define the spherical cap L^2 discrepancy

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

Theorem (Stolarsky invariance principle)

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

$$c_d \Big[D_{cap,L^2}(Z) \Big]^2 =$$

$$= \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} \|x - y\|\, d\sigma(x) d\sigma(y) - \frac{1}{N^2} \sum_{i,j=1}^{N} \|z_i - z_j\|.$$

- Stolarsky '73, Brauchart, Dick '12, DB, Dai, Matzke '17

Spherical caps: L^2 Stolarsky Principle

- Define the spherical cap discrepancy of fixed height t:

$$\left[D^{(t)}_{L^2,\text{cap}}(Z)\right]^2 := \int\limits_{\mathbb{S}^d} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbf{1}_{C(x,t)}(z_j) - \sigma\big(C(x,t)\big) \right|^2 d\sigma(x)$$

Spherical caps: L^2 Stolarsky Principle

- Define the spherical cap discrepancy of fixed height t:

$$\Big[D^{(t)}_{L^2,\text{cap}}(Z)\Big]^2 := \int\limits_{\mathbb{S}^d} \left| \frac{1}{N}\sum_{j=1}^{N} \mathbf{1}_{C(x,t)}(z_j) - \sigma\big(C(x,t)\big)\right|^2 d\sigma(x)$$

- $$\Big[D^{(t)}_{L^2,\text{cap}}(Z)\Big]^2 = \frac{1}{N^2}\sum_{i,j=1}^{N} \sigma\big(C(z_i,t)\cap C(z_j,t)\big) - \big(\sigma\big(C(p,t)\big)\big)^2 .$$

Spherical caps: L^2 Stolarsky Principle

- Define the spherical cap discrepancy of fixed height t:

$$\left[D^{(t)}_{L^2,\mathrm{cap}}(Z)\right]^2 := \int\limits_{\mathbb{S}^d} \left| \frac{1}{N}\sum_{j=1}^{N} \mathbf{1}_{C(x,t)}(z_j) - \sigma\big(C(x,t)\big) \right|^2 d\sigma(x)$$

- $$\left[D^{(t)}_{L^2,\mathrm{cap}}(Z)\right]^2 = \frac{1}{N^2}\sum_{i,j=1}^{N} \sigma\big(C(z_i,t)\cap C(z_j,t)\big) - \Big(\sigma\big(C(p,t)\big)\Big)^2 .$$

- Averaging over $t \in [-1,1]$

$$\int_{-1}^{1} \sigma\big(C(x,t)\cap C(y,t)\big)\, dt \quad = \quad 1 - C_d\|x-y\|$$

Spherical caps: L^2 Stolarsky Principle

- Define the spherical cap discrepancy of fixed height t:

$$\left[D^{(t)}_{L^2,\text{cap}}(Z)\right]^2 := \int\limits_{\mathbb{S}^d} \left| \frac{1}{N} \sum_{j=1}^{N} \mathbf{1}_{C(x,t)}(z_j) - \sigma\big(C(x,t)\big) \right|^2 d\sigma(x)$$

-

$$\left[D^{(t)}_{L^2,\text{cap}}(Z)\right]^2 = \frac{1}{N^2} \sum_{i,j=1}^{N} \sigma\big(C(z_i,t) \cap C(z_j,t)\big) - \Big(\sigma\big(C(p,t)\big)\Big)^2 .$$

- Averaging over $t \in [-1,1]$

$$\int_{-1}^{1} \sigma\big(C(x,t) \cap C(y,t)\big)\, dt \quad = \quad 1 - C_d \|x-y\|$$

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

$$\sigma\big(C(x,0) \cap C(y,0)\big) = \frac{1}{2}\big(1 - d(x,y)\big),$$

where $d(x,y) = \frac{\arccos(x \cdot y)}{\pi}$ (normalized geodesic distance).

Stolarsky principle for hemispheres

Theorem (DB, Dai, Matzke '17, Skriganov '17)

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

Stolarsky principle for hemispheres

Theorem (DB, Dai, Matzke '17, Skriganov '17)

$$[D_{L^2,\mathrm{hem}}(Z)]^2 = [D^{(0)}_{L^2,\mathrm{cap}}(Z)]^2 = \frac{1}{2}\left(\frac{1}{2} - \frac{1}{N^2}\sum_{i,j=1}^{N} d(z_i, z_j)\right).$$

Stolarsky principle for hemispheres

Theorem (DB, Dai, Matzke '17, Skriganov '17)

$$[D_{L^2,\mathrm{hem}}(Z)]^2 = [D^{(0)}_{L^2,\mathrm{cap}}(Z)]^2 = \frac{1}{2}\left(\frac{1}{2} - \frac{1}{N^2}\sum_{i,j=1}^{N} d(z_i, z_j)\right).$$

Corollary (DB, Dai, Matzke '17)

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

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

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

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

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?

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

Energy integral

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

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?

Spherical harmonics and energy minimization

Gegenbauer polynomials form an orthogonal basis on the space $L^2([-1,1], w_\lambda)$ with weight $w_\lambda(t) = (1-t^2)^{\lambda - \frac{1}{2}}$:

$$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \frac{n+\lambda}{\lambda} C_n^\lambda(t)$$

Spherical harmonics and energy minimization

Gegenbauer polynomials form an orthogonal basis on the space $L^2([-1,1], w_\lambda)$ with weight $w_\lambda(t) = (1-t^2)^{\lambda-\frac{1}{2}}$:

$$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \frac{n+\lambda}{\lambda} C_n^\lambda(t)$$

$$I_F(\mu) = \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \frac{n+\lambda}{\lambda} \int\limits_{\mathbb{S}^d} \int\limits_{\mathbb{S}^d} C_n^\lambda(x \cdot y) d\mu(x) d\mu(y)$$

Spherical harmonics and energy minimization

Gegenbauer polynomials form an orthogonal basis on the space $L^2([-1,1], w_\lambda)$ with weight $w_\lambda(t) = (1-t^2)^{\lambda-\frac{1}{2}}$:

$$F(t) \sim \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \frac{n+\lambda}{\lambda} C_n^\lambda(t)$$

$$\begin{aligned} I_F(\mu) &= \sum_{n=0}^{\infty} \widehat{F}(n;\lambda) \frac{n+\lambda}{\lambda} \int_{\mathbb{S}^d} \int_{\mathbb{S}^d} C_n^\lambda(x\cdot y)\, d\mu(x)\, d\mu(y) \\ &= \widehat{F}(0;\lambda) + \sum_{n=1}^{\infty} \widehat{F}(n;\lambda) b_{n,\mu}, \qquad \text{where} \quad b_{n,\mu} \geq 0, \end{aligned}$$

Spherical harmonics and energy minimization

Gegenbauer polynomials form an orthogonal basis on the space $L^2([-1,1],w_\lambda)$ with weight $w_\lambda(t)=(1-t^2)^{\lambda-\frac{1}{2}}$:

$$F(t)\sim\sum_{n=0}^{\infty}\widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}C_n^\lambda(t)$$

$$\begin{aligned}I_F(\mu)&=\sum_{n=0}^{\infty}\widehat{F}(n;\lambda)\frac{n+\lambda}{\lambda}\int_{\mathbb{S}^d}\int_{\mathbb{S}^d}C_n^\lambda(x\cdot y)d\mu(x)d\mu(y)\\&=\widehat{F}(0;\lambda)+\sum_{n=1}^{\infty}\widehat{F}(n;\lambda)b_{n,\mu},\quad\text{where}\quad b_{n,\mu}\geq 0,\\&\geq\widehat{F}(0;\lambda)=I_F(\sigma),\quad\text{if}\quad\widehat{F}(n;\lambda)\geq 0.\end{aligned}$$

Positive definite functions on the sphere

Lemma

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

- $I_F(\mu)$ *is minimized by* σ *iff* $\widehat{F}(n,\lambda) \geq 0$ *for all* $n \geq 1$.

Positive definite functions on the sphere

Lemma

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

- $I_F(\mu)$ *is minimized by* σ *iff* $\widehat{F}(n,\lambda) \geq 0$ *for all* $n \geq 1$.
- σ *is the unique minimizer of* $I_F(\mu)$ *iff* $\widehat{F}(n,\lambda) > 0$ *for all* $n \geq 1$.

Positive definite functions on the sphere

Lemma

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

- $I_F(\mu)$ *is minimized by* σ *iff* $\widehat{F}(n,\lambda) \geq 0$ *for all* $n \geq 1$.
- σ *is the unique minimizer of* $I_F(\mu)$ *iff* $\widehat{F}(n,\lambda) > 0$ *for all* $n \geq 1$.

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

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.*

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

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.*

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

- iii *For any signed measure* $\mu \in \mathcal{B}$ *the energy integral is non-negative:* $I_F(\mu) \geq 0$.

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.*

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

- 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*

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

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

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

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

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

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

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

Theorem (DB, R. Matzke, F. Dai, '17)

Generalized Stolarsky principle:

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

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

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

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

Theorem (DB, R. Matzke, F. Dai, '17)

Generalized Stolarsky principle:

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

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

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

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:`

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

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:`

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

- `Lower bound:`

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

Refined lower bounds (DB, Dai, Steinerberger, '17)

- Montgomery-type lemma:

$$\sum_{n=0}^{L}\sum_{k=1}^{d_n}\left|\sum_{j=1}^{N} Y_{n,k}(x_j)\right|^2 \gtrsim L^d \sum_{i,j=1}^{N} \frac{\log(2+L\|z_i-z_j\|)}{(1+L\|z_i-z_j\|)^{d+1}}.$$

Refined lower bounds (DB, Dai, Steinerberger, '17)

- Montgomery-type lemma:

$$\sum_{n=0}^{L}\sum_{k=1}^{d_n}\left|\sum_{j=1}^{N} Y_{n,k}(x_j)\right|^2 \gtrsim L^d \sum_{i,j=1}^{N} \frac{\log(2+L\|z_i-z_j\|)}{(1+L\|z_i-z_j\|)^{d+1}}.$$

- Discrepancy bound:

$$D^2_{L^2,f}(Z) \gtrsim \frac{1}{N}\cdot \min_{1\le k\lesssim N^{1/d}} \widehat{F}(n,\lambda)\cdot \sum_{i,j=1}^{N} \frac{\log(2+N^{1/d}\|z_i-z_j\|)}{(1+N^{1/d}\|z_i-z_j\|)^{d+1}}$$

Refined lower bounds (DB, Dai, Steinerberger, '17)

- Montgomery-type lemma:

$$\sum_{n=0}^{L}\sum_{k=1}^{d_n}\left|\sum_{j=1}^{N} Y_{n,k}(x_j)\right|^2 \gtrsim L^d \sum_{i,j=1}^{N} \frac{\log(2+L\|z_i-z_j\|)}{(1+L\|z_i-z_j\|)^{d+1}}.$$

- Discrepancy bound:

$$D^2_{L^2,f}(Z) \gtrsim \frac{1}{N}\cdot \min_{1\leq k\lesssim N^{1/d}} \widehat{F}(n,\lambda)\cdot \sum_{i,j=1}^{N} \frac{\log(2+N^{1/d}\|z_i-z_j\|)}{(1+N^{1/d}\|z_i-z_j\|)^{d+1}}$$

- Spherical caps:

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