

Geodesic Riesz Energy on Spheres and Projective Spaces

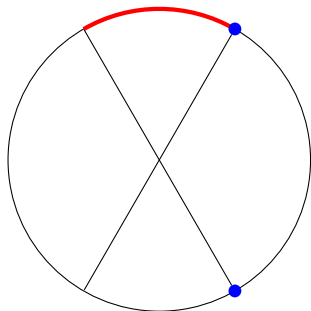
Ryan W. Matzke

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June 5, 2024

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Sum of Angles Between Lines



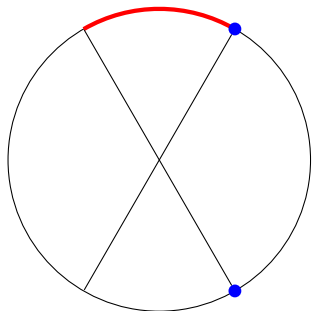
Fejes Tóth Sum of Acute Angles Problem '59

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

$$\begin{aligned}\phi(x, y) &= \arccos(|\langle x, y \rangle|) \\ &= \min\{\arccos(\langle x, y \rangle), \pi - \arccos(\langle x, y \rangle)\}\end{aligned}$$

Which N -point (multi)sets $\{x_1, \dots, x_N\} \subset \mathbb{S}^d$ maximize the sum $\sum_{i,j=1}^N \phi(x_i, x_j)$?

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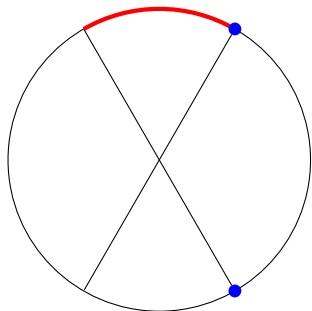
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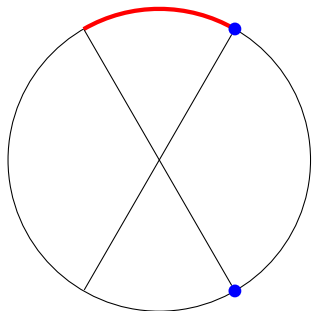
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- Conjecture is true on \mathbb{S}^1 (Fodor, Vígh, Zarnócz '16) and true for \mathbb{S}^2 for $N \leq 6$ (Fejes Tóth '59).
- Several partial results suggesting the conjecture is likely correct.

Discrete Energy

Let (Ω, ρ) be a (compact) metric space. Given a lower semi-continuous, symmetric (potential) function $K : \Omega \times \Omega \rightarrow (-\infty, \infty]$ the **(discrete) energy** of a configuration (multiset) $\omega_N = \{z_1, \dots, z_N\} \subset \Omega$ is

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- Also interesting: Dynamics, systems at nonzero temperatures, systems with external fields.

Frame Energy

A set of points $\omega_N = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$ is a **tight frame** iff for any $x \in \mathbb{R}^{d+1}$

$$\sum_{k=1}^N |\langle x, z_k \rangle|^2 = \frac{N}{d+1} \|x\|^2,$$

or, equivalently,

$$x = \frac{d+1}{N} \sum_{k=1}^N \langle x, z_k \rangle z_k.$$

Theorem (Benedetto, Fickus '03)

*A set $\omega_N = \{z_1, \dots, z_N\} \subset \mathbb{S}^d$, $N \geq d+1$, is a tight frame in \mathbb{R}^{d+1} if and only if ω_N is a local/global minimizer of the **frame energy**:*

$$E_{\text{Frame}}(\omega_N) = \frac{1}{N^2} \sum_{i,j=1}^N |\langle z_i, z_j \rangle|^2.$$

Riesz s -kernels

For $s \in \mathbb{R}$, we define the Riesz kernel as

$$R_s(x, y) = \begin{cases} \frac{1}{s} \|x - y\|^{-s} & s \neq 0 \\ -\log(\|x - y\|) & s = 0 \end{cases}.$$

- $s = -1$ (sum of distances): Minimizers also minimize quadratic spherical cap discrepancy (Stolarsky '73) and worst-case error for a numeric integration in a certain Sobolev space (Brauchart, Dick '13).

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- $s \rightarrow \infty$: Minimizers of $E_{R,s}$ become best-packings on the sphere.

Electrostatics: Thomson Problem

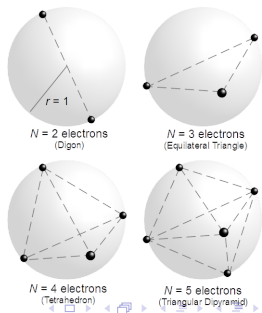
Thomson problem (1904)

Find the minimal energy configuration of N electrons interacting according to Coulomb's Law and constrained to the sphere \mathbb{S}^2 , i.e. minimize the energy

$$E_{R,1}(\omega_N) = \frac{1}{N^2} \sum_{i \neq j} \frac{1}{\|z_i - z_j\|}.$$

- Answer is known for $N = 2, 3, 4, 5, 6$ and $N = 12$
- 5 points: triangular bi-pyramid (R.E. Schwartz, 2013, computer-assisted proof)

Solutions of the Thomson Problem



Continuous Energy

Let (Ω, ρ) be a (compact) metric space. Given a lower semi-continuous, symmetric (potential) function $K : \Omega \times \Omega \rightarrow (-\infty, \infty]$, the **(continuous) energy** of a Borel probability measure $\mu \in \mathbb{P}(\Omega)$ is

$$I_K(\mu) = \int_{\Omega} \int_{\Omega} K(x, y) d\mu(x) d\mu(y).$$

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- What measure(s) minimize I_K ?
- Is the equilibrium measure unique?
- Is it the uniform measure/volume form? Does it have “nice” symmetries?
- Is the support full dimensional, or lower dimensional?
- Is it discrete?

Discrete and Continuous Energy

Minimization of the discrete and continuous energies

$$E_K(\omega_N) = \sum_{i \neq j} K(z_i, z_j), \quad I_K(\mu) = \int_{\Omega} \int_{\Omega} K(x, y) d\mu(x) d\mu(y).$$

are related:

$$\lim_{N \rightarrow \infty} \min_{\omega_N \subset \Omega} \frac{E_K(\omega_N)}{N^2} = \min_{\mu \in \mathbb{P}(\Omega)} I_K(\mu),$$

and if $\mu_{\omega_N} = \frac{1}{N} \sum_{j=1}^N \delta_{z_j}$, then

$$I_K(\mu_{\omega_N}) = \frac{1}{N^2} \left(E_K(\omega_N) + \sum_{j=1}^N K(z_j, z_j) \right).$$

If $\{\omega_N^*\}_{N=2}^{\infty}$ are minimizers of E_K and $\mu_{\omega_N^*} \xrightarrow{*} \mu$, then μ minimizes I_K .

Compact Connected Two-Point Homogeneous Spaces

We call Ω **two-point homogeneous** if for all $x_1, x_2, y_1, y_2 \in \Omega$ s.t. $\rho(x_1, x_2) = \rho(y_1, y_2)$, there exists an isometry h such that $h(x_i) = y_i$.
Examples include Hamming Spaces and \mathbb{R}^d . The only such spaces that are also compact and connected are \mathbb{S}^d , \mathbb{RP}^d , \mathbb{CP}^d , \mathbb{HP}^d , \mathbb{OP}^1 , and \mathbb{OP}^2 .

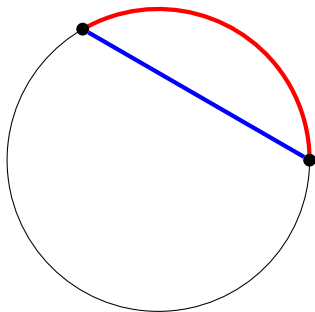
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Each of these spaces has a **geodesic metric** $\theta(x, y) \leq \pi$ and a **chordal metric**



$$\rho(x, y) = \sin \left(\frac{\theta(x, y)}{2} \right) = \sqrt{\frac{1 - \cos(\theta(x, y))}{2}},$$

and can be embedded via a map $A : \Omega \rightarrow \mathbb{S}^{d'}$ such that

$$\rho(x, y) = c \|A(x) - A(y)\|.$$

Chordal Riesz Energy on the Sphere

For each space Ω , the (chordal) Riesz s -kernels and logarithmic kernel are

$$R_s(x, y) = \begin{cases} \frac{\rho(x, y)^{-s}}{s}, & s \in \mathbb{R} \setminus \{0\} \\ -\log(\rho(x, y)), & s = 0 \end{cases}.$$

Theorem (Classical; Riesz, '38; Björck, '56)

Let $s < d$. Then the minimizers of $I_{R, s}$ on \mathbb{S}^d are:

- *If $-2 < s$, σ (uniquely).*
- *If $s = -2$, every measure with center of mass at the origin, i.e.*

$$\int_{\mathbb{S}^d} \cos(\theta(x, y)) d\mu(x) = \int_{\mathbb{S}^d} \langle x, y \rangle d\mu(x) = 0, \quad \forall y \in \mathbb{S}^d.$$

- *If $s < -2$, every measure of the form $\frac{1}{2} (\delta_p + \delta_{-p})$, $p \in \mathbb{S}^d$.*

Chordal Riesz Energy on Projective Spaces

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Theorem (Chen, Hardin, Saff '21; Anderson, Dostert, Grabner, M., Stepaniuk, '23; Bilyk, M., Nathe, '24)

Let $s < \dim(\mathbb{F}\mathbb{P}^d)$. Then the minimizers of $I_{R,s}$ are:

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- *If $s < -2$, every measure of the form $\frac{1}{d+1} \sum_{j=1}^{d+1} \delta_{e_j}$, where $\{e_1, \dots, e_{d+1}\} \subset \mathbb{F}\mathbb{P}^d$ is a set where all element are diameter apart, i.e. points corresponding to an orthonormal basis in \mathbb{F}^{d+1} .*

Discrete Chordal Riesz Energy on Projective Spaces

- $s = -2$: If $\mathbb{F} = \mathbb{R}, \mathbb{C}$, minimizers of $E_{R,-2}$ correspond to tight frames in \mathbb{F}^{d+1} :

$$R_{-2}(x, y) = \frac{\cos(\theta(x, y)) - 1}{2} = \frac{|\langle x, y \rangle|^2 - 1}{2}$$

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- $s \rightarrow \infty$: Minimizers of $E_{R,s}$ become best line-packings/Grassmannian frames, i.e. they minimize coherence, $\max_{i \neq j} |\langle z_i, z_j \rangle|$ (Chen, Hardin, Saff '21).

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- $s \geq 0$: As $N \rightarrow \infty$, the minimizers of $E_{R,s}$ are “nearly tight” (Chen, Hardin, Saff '21), i.e. $Z_N = [z_1, \dots, z_N]$

$$\lim_{N \rightarrow \infty} \frac{1}{N} Z_N Z_N^* = \frac{1}{d+1} I_{d+1}.$$

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$$G_s(x, y) = \begin{cases} \frac{\theta(x, y)^{-s}}{s} & s \in \mathbb{R} \setminus \{0\} \\ -\log(\theta(x, y)) & s = 0 \end{cases}.$$

Theorem (Brauchart, Hardin, Saff '12; Bilyk, Dai, M. '18; Bilyk, Dai '19)

Let $s < d$. Then the minimizers of $I_{G,s}$ on \mathbb{S}^d are:

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- Minimizing $E_{G,-1}$ (maximizing the sum of distances) was another problem posed by Fejes Tóth (solved by Kelly '70).
 - Minimizing $E_{G,-1}$ is equivalent to minimizing the L^2 discrepancy with respect to hemispheres (Bilyk, Dai, M. '18).

Geodesic Riesz Energy on Projective Spaces

Since $\mathbb{R}P^1 \simeq S^1$, $\mathbb{C}P^1 \simeq S^2$, $\mathbb{H}P^1 \simeq S^4$, $\mathbb{O}P^1 \simeq S^8$, only consider $d \geq 2$.

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Theorem (Lim, McCann (plus Bilyk, Glazyrin, M., Park, Vlasiuk) '22; Bilyk, M., Nathe)

Let $d \geq 2$, $s < \dim(\mathbb{F}P^d) = D$. Then the minimizers of $I_{G,s}$ are:

- If $\Omega = \mathbb{R}P^d$ ($D = d$) and $D - 2 \leq s$, σ (uniquely).
- If $\Omega = \mathbb{C}P^d$ ($D = 2d$) and $D - 3 \leq s$, σ (uniquely).
- If $\Omega = \mathbb{H}P^d$ ($D = 4d$) and $D - 5 \leq s$, σ (uniquely).
- If $\Omega = \mathbb{O}P^2$ ($D = 16$) and $D - 9 \leq s$, σ (uniquely).
- If $s \leq -2$, every measure of the form $\frac{1}{d+1} \sum_{j=1}^{d+1} \delta_{e_j}$, where $\{e_1, \dots, e_{d+1}\} \subset \mathbb{F}P^d$ is a set where all element are diameter apart, i.e. points corresponding to an orthonormal basis in \mathbb{F}^{d+1} .

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Let $\alpha = \frac{\dim_{\mathbb{R}}(\Omega)}{2} - 1$ and $\beta = \frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$ if $\Omega = \mathbb{F}\mathbb{P}^d$ and $\beta = \alpha$ if $\Omega = \mathbb{S}^d$

Theorem (Bilyk, M., Nathe)

The minimizers of $I_{G,s}$ are:

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For $\mathbb{F}\mathbb{P}^d$, $d \geq 2$:

- We believe the bound $s \leq -2$ can be improved to $s < -1$.

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Let $\alpha = \frac{\dim_{\mathbb{R}}(\Omega)}{2} - 1$ and $\beta = \frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$ if $\Omega = \mathbb{F}\mathbb{P}^d$ and $\beta = \alpha$ if $\Omega = \mathbb{S}^d$

Theorem (Bilyk, M., Nathe)

The minimizers of $I_{G,s}$ are:

- *If $-1 < s$ and $2\alpha - 2\beta - 1 \leq s < \dim(\Omega) = 2\alpha + 2$, σ (uniquely).*
- *If $s \leq -2$, every measure uniformly distributed on a maximal discrete set with all elements diameter apart.*

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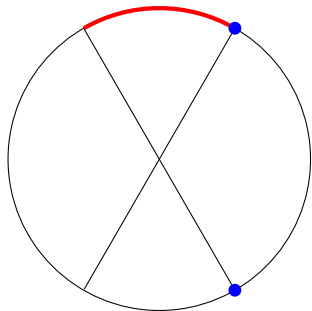
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- There cannot be a single transition point of minimizers: no minimizer of $I_{G,0}$ can have discrete support, but on $\mathbb{R}\mathbb{P}^4$, σ is not a minimizer.

Connection to Fejes Tóth Conjecture



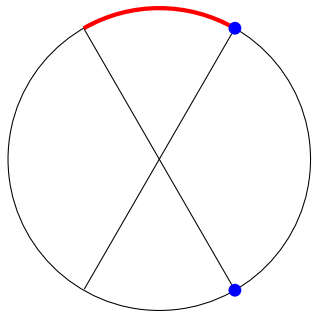
Fejes Tóth Conjecture '59

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

$$\begin{aligned}\phi(x, y) &= \arccos(|\langle x, y \rangle|) \\ &= \min\{\arccos(\langle x, y \rangle), \pi - \arccos(\langle x, y \rangle)\}\end{aligned}$$

Then $E_\phi(\omega_N) = \sum_{i \neq j} \phi(z_i, z_j)$ is maximized by periodically repeated elements of an orthonormal basis, i.e. $z_j = e_{j \bmod (d+1)}$.

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The acute angle ϕ on \mathbb{S}^d corresponds to θ on \mathbb{RP}^d .

Continuous Fejes Tóth Conjecture

The energy $I_{G, -1}$ on \mathbb{RP}^d is minimized by any measure of the form $\mu_{ONB} = \frac{1}{d+1} \sum_{j=1}^{d+1} \delta_{e_j}$, where $\{e_1, \dots, e_{d+1}\} \subset \mathbb{RP}^d$ is a set where all elements are diameter apart, i.e. points corresponding to an ONB in \mathbb{R}^{d+1} .

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The energy $I_{G,-1}$ on $\mathbb{R}\mathbb{P}^d$ is minimized by any measure of the form $\mu_{ONB} = \frac{1}{d+1} \sum_{j=1}^{d+1} \delta_{e_j}$, where $\{e_1, \dots, e_{d+1}\} \subset \mathbb{R}\mathbb{P}^d$ is a set where all elements are diameter apart, i.e. points corresponding to an ONB in \mathbb{R}^{d+1} .

If the conjecture holds true, $I_{G,-1}$ has minimizers other than those of the form μ_{ONB} . For instance, if A and B are copies of $\mathbb{R}\mathbb{P}^1$ in $\mathbb{R}\mathbb{P}^3$ and diameter apart, and σ_A, σ_B are uniform probability measures on each, $\frac{1}{2}(\sigma_A + \sigma_B)$ would minimize $I_{G,-1}$.

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Theorem (Lim, McCann (plus Bilyk, Glazyrin, M., Park, Vlasiuk) '22)

Let $d \geq 2$. For \mathbb{RP}^d , there exists a unique $s^ \in (-2, -1]$ such that for $s > s^*$, μ_{ONB} is not a minimizer of $I_{G,s}$, and for $s < s^*$, $I_{G,s}$ is exactly minimized by measures of the form μ_{ONB} .*

Discrete Minimizers

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$$2R_{-2}(x, y) = \frac{\cos(\theta(x, y)) - 1}{2} \leq -\frac{\theta(x, y)^2}{\pi^2} = \frac{2}{\pi^2} G_{-2}(x, y)$$

with equality iff $\theta(x, y) \in \{0, \pi\}$. Thus

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Similarly, for $s < s^*$,

$$I_{G,s}(\mu) \geq \pi^{s^* - s} \frac{s^*}{s} I_{G,s^*}(\mu) \geq \pi^{s^* - s} \frac{s^*}{s} I_{G,s^*}(\mu_{ONB}).$$

In both case, equality holds iff μ is of the form μ_{ONB} .

From Two-point Homogeneous Spaces to the Interval

Let $\alpha = \frac{\dim_{\mathbb{R}}(\Omega)}{2} - 1$ and $\beta = \frac{\dim_{\mathbb{R}}(\mathbb{F})}{2} - 1$ if $\Omega = \mathbb{F}\mathbb{P}^d$ and $\beta = \alpha$ if $\Omega = \mathbb{S}^d$.

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$$\int_{\Omega} \int_{\Omega} F(\cos(\theta(x, y))) d\sigma(x) d\sigma(y) = \int_{-1}^1 F(t) d\nu(t) = \widehat{F}_0$$

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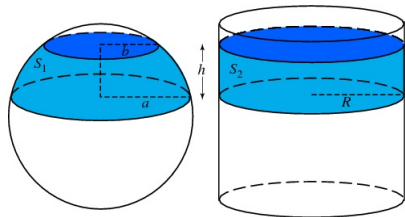
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For the sphere, $\alpha = \beta$, giving us the Gegenbauer polynomials, with weight $d\nu(t) = \gamma(1-t^2)^{\frac{d-2}{2}} dt$.



Conditional Strict Positive Definiteness

We call a real-valued kernel conditionally positive definite if for any set of points $\omega_N = \{z_1, \dots, z_N\} \subset \Omega$

$$\sum_{i,j=1}^N K(z_i, z_j) c_i c_j \geq 0 \quad \text{for all } c_i \in \mathbb{R}, \text{ with } \sum_{j=1}^N c_j = 0.$$

Extending this, a kernel K is conditionally positive definite if for any finite signed Borel measure τ on Ω satisfying $\nu(\Omega) = 0$,

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The kernel is called conditionally strictly positive definite (CSPD) if equality occurs iff $\tau \equiv 0$.

Theorem

If K is conditionally strictly positive definite on Ω , then I_K has a unique minimizer.

Conditional Strict Positive Definiteness

We call $F : [-1, 1] \rightarrow (-\infty, \infty]$ conditionally strictly positive definite (CSPD) on Ω if for any finite signed Borel measure τ on Ω satisfying $\tau(\Omega) = 0$ and $\tau \not\equiv 0$,

$$I_F(\tau) := \int_{\Omega} \int_{\Omega} F(\cos(\theta(x, y))) d\tau(x) d\tau(y) > 0.$$

Theorem

If $F(\cos(\theta(x, y)))$ is conditionally strictly positive definite on Ω , then I_F is uniquely minimized by σ .

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Theorem

If $F(\cos(\theta(x, y)))$ is conditionally strictly positive definite on Ω , then I_F is uniquely minimized by σ .

For the unique minimizer μ of I_F and any isometry g of Ω ,

$$\begin{aligned} I_F(\mu) &= \int_{\Omega} \int_{\Omega} F(\cos(\theta(x, y))) d\mu(x) d\mu(y) \\ &= \int_{\Omega} \int_{\Omega} F(\cos(\theta(g(x), g(y)))) d\mu(x) d\mu(y) = I_F(g\#\mu). \end{aligned}$$

Theorem (Bochner '41; Schoenberg '42; Bilyk, M., Vlasiuk '22; Anderson, Dostert, Grabner, M., Stepaniuk '23)

Let $F \in C([-1, 1])$. Then the following are equivalent:

- 1 σ is the unique minimizer of I_F over $\mathcal{P}(\Omega)$.
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For general $F \in L^1([-1, 1], \nu)$, the only known implications are

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Goal: Want the most general class of functions F such that $\widehat{F}_n > 0$ for all $n \in \mathbb{N}$ implies F is CSPD and/or σ is the unique minimizer.

Continuous Approximation

For any non-negative $F \in L^1([-1, 1], \nu)$ and $\varepsilon > 0$, let

$$F^{(\varepsilon)}(\cos(\theta(x, y))) := \frac{1}{(\sigma(B_\varepsilon))^2} \int_{B_\varepsilon(x)} \int_{B_\varepsilon(y)} F(\cos(\theta(u, v))) d\sigma(u) d\sigma(v).$$

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Theorem (Mercer 1909)

If $F \in C([-1, 1])$ is conditionally positive definite, then

$$F(t) = \sum_{n=0}^{\infty} \widehat{F}_n P_n^{(\alpha, \beta)}(t),$$

where the series converges absolutely and uniformly on $[-1, 1]$.

Extending the Implication

Theorem (Bilyk, M., Nathe)

Suppose $F \in L^1([-1, 1], \nu)$ is bounded from below, $\widehat{F}_n > 0$ for all $n \in \mathbb{N}$, and for all $\mu \in \mathcal{P}(\Omega)$ such that $I_F(\mu) < \infty$, $\lim_{\varepsilon \rightarrow 0^+} I_{F(\varepsilon)}(\mu) = I_F(\mu)$. Then σ is the unique minimizer of I_F .

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If $\mu \neq \sigma$, there must be some $m \in \mathbb{N}$ such that $I_{P_m^{(\alpha, \beta)}}(\mu) > 0 = I_{P_m^{(\alpha, \beta)}}(\sigma)$.

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Since $I_G(\sigma) = \widehat{G}_0$,

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Domination of the Approximation

Proposition (Bilyk, M., Nathe)

Let $0 \leq s < \dim(\Omega)$. There exists constants $A, C > 0$ such that for all $x, y \in \Omega$ and $\varepsilon > 0$

$$G_s^{(\varepsilon)}(\cos(\theta(x, y))) \leq \begin{cases} CG_s(\cos(\theta(x, y))) & s > 0 \\ A + CG_0(\cos(\theta(x, y))) & s = 0 \end{cases}.$$

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Suppose a non-negative function $F \in L^1([-1, 1], \nu)$ is continuous for $t \in (-1, 1)$. Assume that for some $s \in [0, \dim(\Omega))$ there exist $a, a', c, c' > 0$ such that for all $t \in [-1, 1]$

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Minimizers of Riesz Energies

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Corollary

If $-2 < s \leq \dim(\Omega)$, $I_{R,s}$ is uniquely minimized by σ .

If $-1 < s$ and $2\alpha - 2\beta - 1 \leq s < \dim(\Omega)$, $I_{G,s}$ is uniquely minimized by σ .

Minimization for Absolutely Continuous Measures

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Suppose $F \in L^1([-1, 1], \nu)$, then

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- If for all $n \in \mathbb{N}$, $\widehat{F}_n > 0$, then σ is the unique minimizer of I_F over all $\mu \in \mathcal{P}(\Omega)$ of the form $d\mu(x) = h(x)d\sigma(x)$ for some $h \in L^\infty(\Omega)$.

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- If for all $n \in \mathbb{N}$, $\widehat{F}_n \geq 0$, then σ is a minimizer of I_F over all $\mu \in \mathcal{P}(\Omega)$ of the form $d\mu(x) = h(x)d\sigma(x)$ for some $h \in L^1(\Omega)$.
- If for all $n \in \mathbb{N}$, $\widehat{F}_n > 0$, then σ is the unique minimizer of I_F over all $\mu \in \mathcal{P}(\Omega)$ of the form $d\mu(x) = h(x)d\sigma(x)$ for some $h \in L^\infty(\Omega)$.

If $h \neq 1$, there is some $m \in \mathbb{N}$ such that $I_{P_m^{(\alpha, \beta)}}(\mu) > 0 = I_{P_m^{(\alpha, \beta)}}(\sigma)$.

Minimization for Absolutely Continuous Measures

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If $h \neq 1$, there is some $m \in \mathbb{N}$ such that $I_{P_m^{(\alpha, \beta)}}(\mu) > 0 = I_{P_m^{(\alpha, \beta)}}(\sigma)$. If

$$S_n^\delta F(t) := \frac{1}{A_n^\delta} \sum_{k=0}^n A_{n-k}^\delta \widehat{F}_k P_k^{(\alpha, \beta)}(t)$$

then for $\varepsilon > 0$, for $n \geq m$ sufficiently large,

$$I_F(\mu) \geq I_{S_n^\delta F}(\mu) - \left| I_F(\mu) - I_{S_n^\delta F}(\mu) \right| \geq I_{S_n^\delta F}(\sigma) + \frac{A_{n-m}^\delta}{A_n^\delta} \widehat{F}_m I_{P_k^{(\alpha, \beta)}}(\mu) - \varepsilon$$

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Open Problems/Questions

- Proving or disproving the Fejes Tóth conjecture.
- Determining the maximum value of s for which μ_{ONB} minimizes $I_{G,s}$
- Determining the minimum value of s for which σ minimized $I_{G,s}$.
- Determining what happens between these two values.
- How does the geometry of the space affect these values?
- Are there neat applications of the geodesic Riesz energies?
- Generalizing when positive Jacobi coefficient imply σ is a minimizer or F is CSPD.
- How well do these results extend to other spaces (Homogeneous spaces)?

Thank you!

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