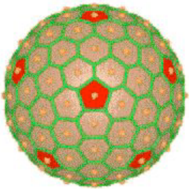

Minimal Discrete Energy and Maximal Polarization

E. B. Saff

https://my.vanderbilt.edu/edsaff/

Center for Constructive Approximation

Vanderbilt University

Imperial College, March 14, 2017

Best-Packing vs. Best-Covering

Best-Packing vs. Best-Covering

Two Trivial Problems: For $A = [0, 1] \subset \mathbb{R}$ **solve**

Best-packing (maximize min separation) of 5 points on A

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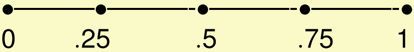

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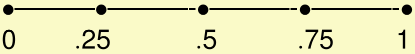

Best-covering (minimize largest gap on A) for 5 points on A

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●———●———-●———-●———-●
0 .25 .5 .75 1

Best-covering (minimize largest gap on A) for 5 points on A

—-x———x———x———x———x—-
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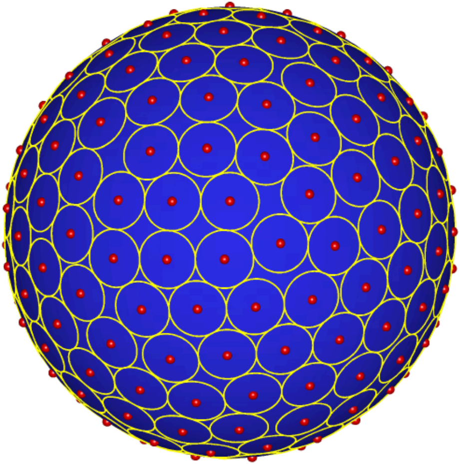
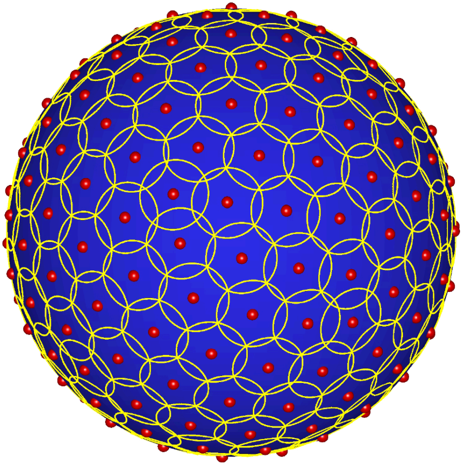
Challenge Question: Same problems for $N = 5$ points, but $[0, 1]$ is replaced by the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$?

Best-packing on $\mathbb{S}^2$



200 points in near best-packing on $\mathbb{S}^2$

Best-covering on $\mathbb{S}^2$



200 points in near best-covering on $\mathbb{S}^2$

Motivation

Questions from physics

- How does global order (crystalline structure) arise out of simple pairwise particle interactions?
- How does the structure depend on the geometry of the manifold A (dimension, curvature, ...) in which the particles live?

Generating good node sets

- How to generate a large number of points on a set A that have a given density and good local properties (packing and covering)?

Discrete energy

Let (A, m) be an infinite compact metric space.
K a **symmetric** and **lower semi-continuous kernel** on $A \times A$.
K-energy of $\omega_N = (x_1, \dots, x_N) \in A^N$ is

$$E_K(\omega_N) := \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} K(x_i, x_j) = \sum_{i \neq j} K(x_i, x_j)$$

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Minimal N-point K-energy of the set A is

$$\mathcal{E}_K(A, N) := \inf\{E_K(\omega_N) : \omega_N \subset A,\ \#\omega_N = N\}.$$

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$$\mathcal{E}_K(A, N) := \inf\{E_K(\omega_N) : \omega_N \subset A, \#\omega_N = N\}.$$

If $E_K(\omega_N^*) = \mathcal{E}_K(A, N)$, then ω_N^* is called N-point K-equilibrium configuration for A or a set of optimal K-energy points.
In general, ω_N^* is not unique.

Continuous Energy Problem

$\mathcal{M}(A)$ is set of all probability measures with support on A.
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$$I_K[\mu] := \iint\limits_{A\times A} K(x, y)\, d\mu(x) d\mu(y).$$

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If $W_K(A) = \infty$, (i.e. $\mathrm{cap}_K(A) := 1/W_K(A) = 0$), then every $\mu \in \mathcal{M}(A)$ is an equilibrium measure.

Connection between discrete and continuous energy

Fundamental Theorem (Frostman, Choquet, Fekete, Szegő,...)

With K as above,

$$\lim_{N\to\infty} \frac{\mathcal{E}_K(A,N)}{N^2} = W_K(A).$$

Moreover, if (ω_N^*) is any sequence of N-point K-energy minimizing configurations on A, then every weak* limit measure λ as $N \to \infty$ of the normalized counting measures

$$\nu(\omega_N^*) := \frac{1}{N} \sum_{x \in \omega_N^*} \delta_x$$

is an equilibrium measure for the continuous energy problem on A; i.e., $I_K[\lambda] = W_K(A)$.

Riesz s-Energy in Euclidean Space

Hereafter $A \subset \mathbb{R}^p$ and $m(x,y) = |x-y|$.

The **Riesz s-kernel** is defined by

$$K_s(x,y) := \frac{1}{|x-y|^s}, \;\; s > 0; \qquad K_{\log}(x,y) := \log\frac{1}{|x-y|}, \;\; x, y \in A.$$

We write

$$E_s(\omega) := E_{K_s}(\omega), \qquad \mathcal{E}_s(A,N) = \mathcal{E}_{K_s}(A,N), \;\; s > 0 \text{ or } s = \log.$$

For $p = 3$, $s = 1$, get Coulomb kernel.

For $A \subset \mathbb{R}^p$ and $s = p - 2$, we get Newton kernel.

Minimal Riesz s-Energy for $N = 5$ on $\mathbb{S}^2$

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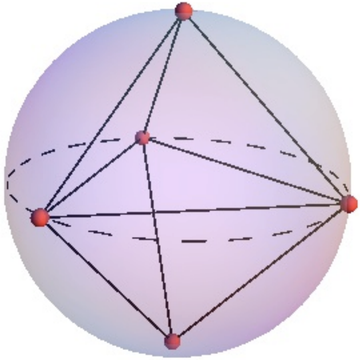
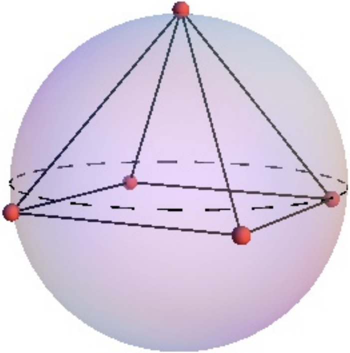
bipyramid

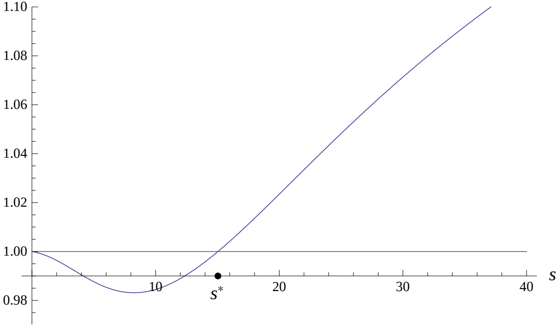


square-base pyramid



Minimal Riesz s-Energy for $N = 5$ on $\mathbb{S}^2$

Ratio of s-energy of **bipyramid** to s-energy of **optimal sq-base pyramid**



Melnyk et al (1977) Bipyramid appears optimal for $0 < s < s^*$ where $s^* \approx 15.04808$.

Recently proved by R. Schwartz (over 150 pages + computer assist).
Open problem for $s > s^* + \epsilon$

MORALS

Optimal Riesz s-energy configurations, in general, **depend on s.**

Rigorous proofs of computational observations **can be quite difficult.**

Best-Packing and Riesz Energy

Separation distance of $\omega_N = \{x_1, \ldots, x_N\} \subset A$

$$\delta(\omega_N) := \min_{1 \le i \ne j \le N} |x_i - x_j|.$$

N-point best-packing distance on A,

$$\delta_N(A) := \sup\{\delta(\omega_N) : \omega_N \subset A,\ \#\omega_N = N\},$$

ω_N^* *is best-packing configuration* if $\delta(\omega_N^*) = \delta_N(A)$.

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Proposition

For each fixed $N \ge 2$,

$$\lim_{s \to \infty} \mathcal{E}_s(A, N)^{1/s} = \frac{1}{\delta_N(A)}.$$

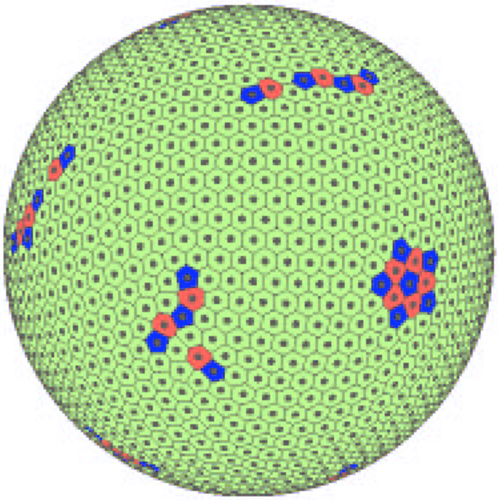
Moreover, every cluster point as $s \to \infty$ of s-energy minimizing N-point configurations on A is an N-point best-packing configuration on A.

What about **asymptotics** of
of the minimal energy as $N \to \infty$?

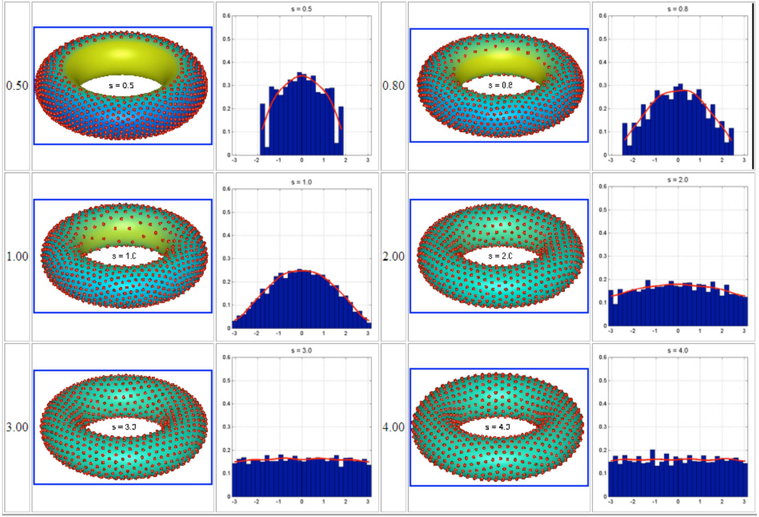
What do minimal energy points
“look like" for large N ?

$N = 1600, s = 4$

Red = heptagon, Green = hexagon, Blue = pentagon



An Example: Torus (Bagel), $N = 1000$



$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^2} = W_s(A) = I_s(\mu_A) < \infty, \ \text{for } 0 < s < d = \dim_{\mathcal{H}}(A).$$

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"Poppy-Seed Bagel" Theorem (HS (2005) and BHS (2008))

Suppose $s \geq d$ and $A \subset \mathbb{R}^p$ is a d-**rectifiable set** (i.e. Lipschitz image of a compact set in $\mathbb{R}^d$) . When $s = d$ we further assume A is a subset of a d-dimensional C^1 manifold. Then

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(A,N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(A)},$$

$$\lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^{1+s/d}} = \frac{C_{s,d}}{[\mathcal{H}_d(A)]^{s/d}}, \; s > d\,.$$

where $\mathcal{H}_d(\cdot)$ denotes d-dimensional Hausdorff measure.

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Furthermore, if $\mathcal{H}_d(A) > 0$, then optimal s-energy configurations for $s \geq d$ are asymptotically (as $N \to \infty$) **uniformly distributed** on A with respect to $\mathcal{H}_d$.

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“Poppy-Seed Bagel” Theorem, continued

If $\{\omega_N^*\}_{N=2}^{\infty}$ is a sequence of minimal s-energy configurations on the d-rectifiable set A with $s > d$, then the sequence has "optimal order separation"; i.e.,

$$\delta(\omega_N^*) \asymp \frac{1}{N^{1/d}}, \quad N \to \infty.$$

Furthermore, if A is also d-regular, then the sequence $\{\omega_N^*\}$ provides "optimal order covering"; i.e.,

$$\rho(\omega_N^*, A) := \max_{y\in A} \min_{x\in\omega_N^*} |y - x| \asymp \frac{1}{N^{1/d}}, \quad N \to \infty.$$

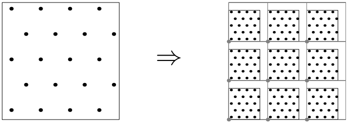
By "d-regular" we mean there is a positive measure μ supported on A and $c_1, c_2 > 0$ such that

$$c_1 r^d \leq \mu(B(x,r)) \leq c_2 r^d, \quad x \in A,\ 0 < r < \mathrm{diam}(A).$$

Proof that $\lim_{N\to\infty} \mathcal{E}_s([0,1]^d, N)/N^{1+s/d}$ exists for $s > d$

Let $U^d := [0,1]^d$, the unit cube in $\mathbb{R}^d$.

Start with N minimal s-energy points for U^d.



Let $0 < \gamma < 1$ and m a positive integer. Shrink U^d by a factor γ/m, creating m^d disjoint subcubes separated by $(1-\gamma)/m$.

$$\begin{aligned}\mathcal{E}_s(U^d, m^d N) &\leq m^d \mathcal{E}_s\left((\gamma/m)U^d, N\right) + \text{cube-cube interactions} \\ &\leq \gamma^{-s} m^s m^d \mathcal{E}_s\left(U^d, N\right) + K(1-\gamma)^{-s} m^{s+d} N^2,\end{aligned}$$

where $K := \sum_{\mathbf{k}\in\mathbb{Z}^d,\ \mathbf{k}\neq\mathbf{0}} |\mathbf{k}|^{-s} < \infty$ for $s > d$.

The Constant $C_{s,d}$

What is the constant $C_{s,d}$ for $s > d$?

$d = 1$: From optimality of the roots of unity on S^1,

$$C_{s,1} = 2\zeta(s) \quad \text{for} \quad s > 1,$$

where $\zeta(s)$ is the classical Riemann zeta function.

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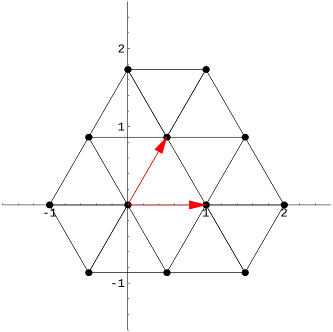
$d = 2$: From [KS] it is known that

$$C_{s,2} \leq \left(\sqrt{3}/2\right)^{s/2} \zeta_{\mathcal{L}}(s), \quad s > 2,$$

where $\zeta_{\mathcal{L}}(s)$ is the zeta function for the unit hexagonal lattice.

The Constant $C_{s,2}$



Conjecture: $C_{s,2} = \left(\sqrt{3}/2\right)^{s/2} \zeta_{\mathcal{L}}(s)$, $s > 2$,

where $\zeta_{\mathcal{L}} := \sum_{0 \neq \mathbf{v} \in \mathcal{L}} |\mathbf{v}|^{-s}$,

$\mathcal{L} = \{k_1 \mathbf{v}_1 + k_2 \mathbf{v}_2 : \ k_1, k_2 \in \mathbb{Z}\}$.

This is equivalent to the conjecture that the “equi-triangular” lattice describes the ground state for particles in the plane interacting through a Riesz potential r^{-s}.

Similar conjectures for $d = 8$ (E_8 lattice) and $d = 24$ (Leech lattice).

Connection to Best-packing Problem in $\mathbb{R}^d$

- The d-dimensional packing density Δ_d is the maximum fraction of d space that can be covered by a collection of non-overlapping balls of the same radius.
- Connection between $C_{s,d}$ and Δ_d:

$$(C_{s,d})^{1/s} \to (1/2)\left(\frac{\mathrm{Vol}(\mathcal{B}_d)}{\Delta_d}\right)^{1/d} \text{ as } s \to \infty,.$$

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$\Delta_1 = 1,$

$\Delta_2 = \pi/\sqrt{12}$ (Fejes-Toth),

$\Delta_3 = \pi/\sqrt{18}$ (Hales)

Δ_8 Solved

The sphere packing problem in dimension 8

Maryna S. Viazovska

March 15, 2016

In this paper we prove that no packing of unit balls in Euclidean space $\mathbb{R}^8$ has density greater than that of the E_8-lattice packing.

Keywords: Sphere packing, Modular forms, Fourier analysis
AMS subject classification: 52C17, 11F03, 11F30

1 Introduction

The sphere packing constant measures which portion of d-dimensional Euclidean space can be covered by non-overlapping unit balls. More precisely, let $\mathbb{R}^d$ be the Euclidean vector space equipped with distance $\|\cdot\|$ and Lebesgue measure $\mathrm{Vol}(\cdot)$. For $x \in \mathbb{R}^d$ and $r \in \mathbb{R}_{>0}$ we denote by $B_d(x, r)$ the ball in $\mathbb{R}^d$ with center x and radius r. Let $X \subset \mathbb{R}^d$ be a discrete set of points such that $\|x - y\| \geq 2$ for any distinct $x, y \in X$. Then the union

$$\mathcal{P} = \bigcup_{x \in X} B_d(x, 1)$$

is a *sphere packing*. If X is a lattice in $\mathbb{R}^d$ then we say that $\mathcal{P}$ is a *lattice sphere packing*. The *finite density* of a packing $\mathcal{P}$ is defined as

Δ_{24} Solved

THE SPHERE PACKING PROBLEM IN DIMENSION 24

HENRY COHN, ABHINAV KUMAR, STEPHEN D. MILLER, DANYLO RADCHENKO, AND MARYNA VIAZOVSKA

Abstract. Building on Viazovska's recent solution of the sphere packing problem in eight dimensions, we prove that the Leech lattice is the densest packing of congruent spheres in twenty-four dimensions, and that it is the unique optimal periodic packing. In particular, we find an optimal auxiliary function for the linear programming bounds, which is an analogue of Viazovska's function for the eight-dimensional case.

1. Introduction

The sphere packing problem asks how to arrange congruent balls as densely as possible without overlap. The *density* is the fraction of space covered by the balls, and the problem is to find the maximal possible density. This problem plays an important role in geometry, number theory, and information theory. See [4] for background and references on sphere packing and its applications.

Although many interesting constructions are known, provably optimality is very rare. Aside from the trivial case of one dimension, the optimal density was previously known only in two [8], three [6, 7], and eight [9] dimensions, with the latter result being a recent breakthrough due to Viazovska. Building on her work, we prove the following theorem:

Theorem 1.1. *The Leech lattice achieves the optimal sphere packing density in* $\mathbb{R}^{24}$*, and it is the only periodic packing in* $\mathbb{R}^{24}$ *with that density.*

Generalized CHEBYSHEV CONSTANTS

Riesz s-Polarization

and Best-Covering

Riesz s-Polarization: Definition

Let $A \subset \mathbb{R}^p$ be infinite compact set.

s-Polarization of $\omega_N = (x_1, ..., x_N) \in A^N$ is defined by

$$P_s(\omega_N; A) := \min_{\mathbf{x} \in A} \sum_{j=1}^{N} K_s(\mathbf{x}, \mathbf{x}_j) = \min_{\mathbf{x} \in A} \sum_{j=1}^{N} \frac{1}{|\mathbf{x} - \mathbf{x}_j|^s}, \quad s > 0.$$

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N-point s-Polarization (s-Chebyshev constant) of A

$$\mathcal{P}_s(A, N) := \max_{\omega_N \in A^N} P_s(\omega_N; A) = \max_{\omega_N\in A^N} \min_{\mathbf{x}\in A} \sum_{j=1}^{N} \frac{1}{|\mathbf{x}-\mathbf{x}_j|^s}$$

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Let $A \subset \mathbb{R}^p$ be infinite compact set.

s-Polarization of $\omega_N = (x_1, \dots, x_N) \in A^N$ is defined by

$$P_s(\omega_N; A) := \min_{\mathbf{x} \in A} \sum_{j=1}^{N} K_s(\mathbf{x}, \mathbf{x}_j) = \min_{\mathbf{x} \in A} \sum_{j=1}^{N} \frac{1}{|\mathbf{x} - \mathbf{x}_j|^s}, \quad s > 0.$$

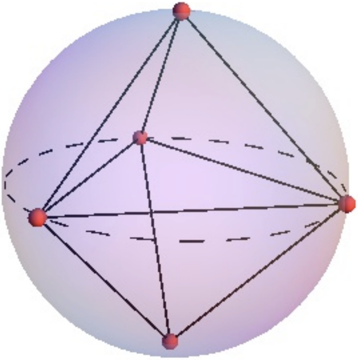
N-point s-Polarization (s-Chebyshev constant) of A

$$\mathcal{P}_s(A, N) := \max_{\omega_N \in A^N} P_s(\omega_N; A) = \max_{\omega_N \in A^N} \min_{\mathbf{x} \in A} \sum_{j=1}^{N} \frac{1}{|\mathbf{x} - \mathbf{x}_j|^s}$$

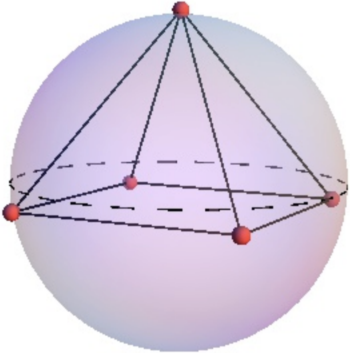
Fact: $\mathcal{P}_s(A, N) \geq \frac{1}{N-1} \mathcal{E}_s(A, N)\,, \qquad N \geq 2\,.$

Maximal Riesz s-Polarization for $N = 5$ on $\mathbb{S}^2$

bipyramid

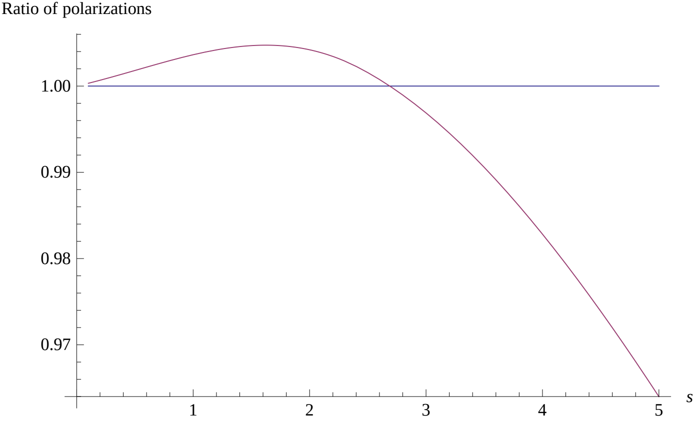


square-base pyramid



Maximal Riesz s-Polarization for $N = 5$ on $\mathbb{S}^2$

Ratio of s-polar of **optimal sq-base pyramid** to s-polar of **bipyramid**



Square-base pyramid appears optimal for s up to $s \approx 2.69$

Regular simplices of 2,3, 4 points are optimal for all s.

Connection to Best-Covering as $s \to \infty$

Covering radius of $\omega_N \in A^N$ is given by

$$\rho(\omega_N; A) := \max_{y \in A} \min_{x \in \omega_N} |y - x|.$$

Proposition

For each fixed N,

$$\lim_{s \to \infty} \mathcal{P}_s(A, N)^{1/s} = \frac{1}{\rho_N(A)},$$

where $\rho_N(A)$ is the ***N*-point covering radius of** A :

$$\rho_N(A) = \inf\{\rho(\omega_N; A) : \omega_N \in A^N\}.$$

Furthermore, every cluster point as $s \to \infty$ of optimal $N-$point s-polarization configurations ω_N^s is an $N-$point best-covering configuration.

Conjecture of Ambrus, K. Ball, Erdélyi (2011)

For unit circle $\mathbb{S}^1$ and every $s > 0$ and $N \geq 1$ the max polarization is attained for equally spaced points. [True for $s = 2$ (Ambrus) and $s = 4$ (Erdélyi, S)].

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Theorem (Hardin, Kendall,S)(2012)

Let $f : [0, \pi] \to [0, \infty]$ be non-increasing and strictly convex. For a configuration $\omega_N = (z_1, ..., z_N)$ on $\mathbb{S}^1$, set

$$P_f(\omega_N, \mathbb{S}^1) := \min_{z \in \mathbb{S}^1} \sum_{k=1}^{n} f(d(z, z_k)),$$

$$\mathcal{P}_f(\mathbb{S}^1, N) := \max\{P_f(\omega_N, \mathbb{S}^1) : \omega_N \in (\mathbb{S}^1)^N\},$$

where $d(z, w)$ denotes geodesic distance on $\mathbb{S}^1$. Then $P_f(\omega_N; \mathbb{S}^1) = \mathcal{P}_f(\mathbb{S}^1, N)$ if and only if ω_N consists of N distinct points equally spaced on $\mathbb{S}^1$.

Taking $f(\theta) = |e^{i\theta} - 1|^{-s}$ we get Euclidean distance, which proves conjecture of A,B,E.

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For the N-th roots of unity $\omega_N^* := \{e^{i2\pi k/N} : k = 1, 2, \ldots, N\}$

$$P_s(\omega_N^*; \mathbb{S}^1) = \frac{\mathcal{E}_s(\mathbb{S}^1; 2N)}{2N} - \frac{\mathcal{E}_s(\mathbb{S}^1; N)}{N} .$$

Corollary (for even integer $s = 2m$)

$$\mathcal{P}_{2m}(\mathbb{S}^1, N) = \frac{2}{(2\pi)^{2m}} \sum_{k=1}^{m} N^{2k} \zeta(2k) \alpha_{m-k}(2m)(2^{2k} - 1), \quad m \in \mathbb{N},$$

where $\alpha_j(p)$ is defined via the power series for $\operatorname{sinc} z = (\sin \pi z)/(\pi z)$:

$$(\operatorname{sinc} z)^{-p} = \sum_{j=0}^{\infty} \alpha_j(p) z^{2j} , \quad \alpha_0(p) = 1 .$$

Example $s = 2m = 6$

Given **any** N points $z_1, z_2, \ldots, z_N$ on $\mathbb{S}^1$, there exists a point z^* on $\mathbb{S}^1$ such that

$$\sum_{j=1}^{N} \frac{1}{|z^* - z_j|^6} \leq \frac{N^6}{480} + \frac{N^4}{192} + \frac{N^2}{120},$$

and this is best possible.

Riesz s-Polarization Asymptotics

Theorem (Ohtsuka, 1961)

$$\lim_{N\to\infty} \frac{\mathcal{P}_s(A,N)}{N} =: \mathcal{P}_s(A)$$

exists as an extended real number and $\mathcal{P}_s(A) \geq W_s(A)$. Furthermore,

$$\mathcal{P}_s(A) = \sup_{\mu} \inf_{x\in A} \int \frac{1}{|x-t|^s} d\mu(t),$$

where μ is prob. meas. on A.

$\mathcal{P}_s(A)$ is called the **Chebyshev-Riesz constant** for A.

Theorem (Farkas and Nagy 2008)

If the Maximum Principle holds on A for the Riesz s-potential, then

$$\mathcal{P}_s(A) = W_s(A).$$

Asymptotics for polarization on general sets

Proposition (BHS 2013)

For $d \in \mathbb{N}$, let $\mathcal{Q}_d := [0,1]^d$. Then for every $s > d$, the limit

$$\sigma_{s,d} := \lim_{N\to\infty} \frac{\mathcal{P}_s(\mathcal{Q}_d, N)}{N^{s/d}}$$

exists and is finite and positive.

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Polarization "Poppy-Seed Bagel" Theorem (s>d) (BHS 2013)

Let $A \subset \mathbb{R}^d$ be an infinite compact set of positive Lebesgue $\mathcal{L}_d$-measure whose boundary has measure zero. If $s > d$, then

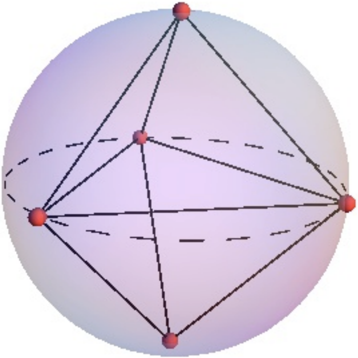
$$\lim_{N\to\infty} \frac{\mathcal{P}_s(A, N)}{N^{s/d}} = \frac{\sigma_{s,d}}{\mathcal{L}_d(A)^{s/d}}.$$

Furthermore, every asymptotically maximizing s-polarization sequence of N-point configurations on A is asymptotically uniformly distributed with respect to normalized $\mathcal{L}_d$-measure on A.

Answers to Challenge Question ?

Best-Packing and Best-Covering with $N = 5$ on $\mathbb{S}^2$

bipyramid



square-base pyramid