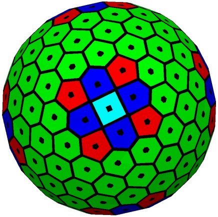
Universal lower bounds for potential energy of spherical codes



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Midwestern Workshop on Asymptotic Analysis

Notation

- $\mathbb{S}^{n-1}$: unit sphere in $\mathbf{R}^n$
- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$
- **Interaction potential** $h : [-1, 1] \to \mathbf{R} \cup \{+\infty\}$ (low. semicont.)
- The *h*-**energy** of a spherical code C:

$$E(n, C; h) := \sum_{x,y \in C, y \neq x} h(\langle x, y \rangle),$$

  where $t = \langle x, y \rangle$ denotes Euclidean inner product of x and y.
- Riesz s-potential: $h(t) = (2 - 2t)^{-s/2} = |x - y|^{-s}$
- Log potential: $h(t) = -\log(2 - 2t) = -\log |x - y|$
- 'Kissing' potential:

$$h(t) = \begin{cases} 0, & -1 \leq t \leq 1/2 \\ \infty, & 1/2 \leq t \leq 1 \end{cases}$$

Problem

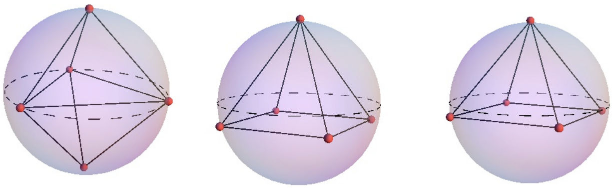
Determine

$$\mathcal{E}(n, N; h) := \min\{E(n, C; h) : |C| = N, C \subset \mathbb{S}^{n-1}\}$$

and find (prove) configuration that achieves minimal h-energy.

- Code fishing.
- Even if one 'knows' an optimal code, it is usually difficult to prove optimality–need lower bounds on $\mathcal{E}(n, N; h)$.
- Delsarte-Yudin linear programming bounds: Find a potential f such that $h \geq f$ for which we can obtain lower bounds for the minimal f-energy $\mathcal{E}(n, N; f)$.
- Discuss optimal codes for $N = 2, 3, 4$, and 5 points on S^2.

Optimal five point log and Riesz s-energy code on S^2



(a) (b) (c)

Figure : 'Optimal' 5-point configurations on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) optimal square-base pyramid SBP ($s = 16$).

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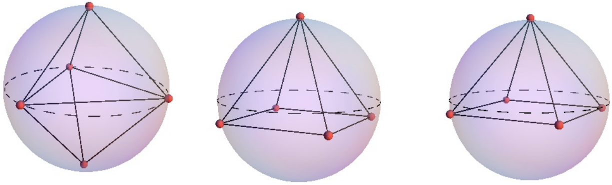

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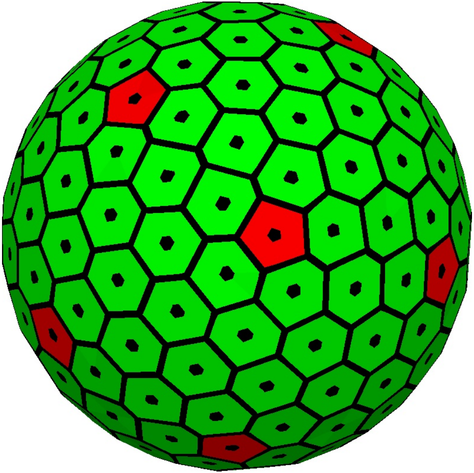
Figure : 'Optimal' 5-point configurations on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) optimal square-base pyramid SBP ($s = 16$).

- P. D. Dragnev, D. A. Legg, and D. W. Townsend, **Discrete logarithmic energy on the sphere**, Pacific J. Math. **207** (2002), 345–357.
- R. E. Schwartz, **The Five-Electron Case of Thomson?s Problem**, Exp. Math. **22** (2013), 157–186.

Example: $A = S^2$; $N = 174$; s=1

Red = pentagon, Green = hexagon, Blue = heptagon



Example: $A = S^2$; $N = 174$; s=0

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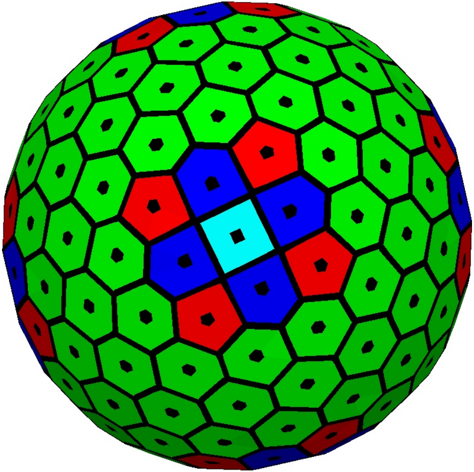
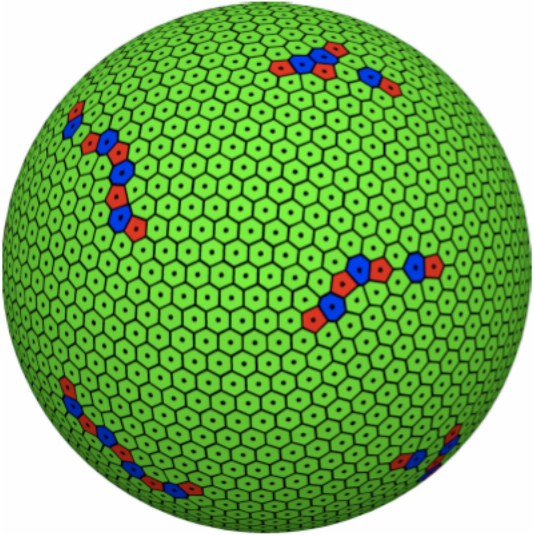


Example: $A = S^2$; $N = 1600$; s=4

Red = pentagon, Green = hexagon, Blue = heptagon



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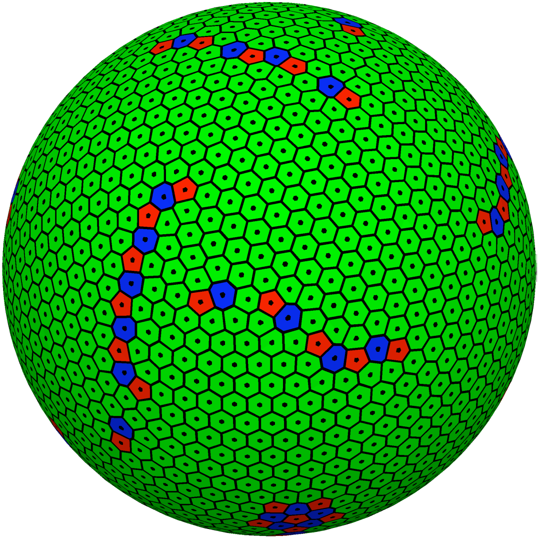

Spherical Harmonics

- $\mathrm{Harm}(k)$: homogeneous harmonic polynomials in n variables of degree k restricted to $\mathbb{S}^{n-1}$ with

$$r_k := \dim \mathrm{Harm}(k) = \binom{k+n-3}{n-2}\left(\frac{2k+n-2}{k}\right).$$

- Spherical harmonics (degree k): $\{Y_{kj}(x) : j = 1, 2, \ldots, r_k\}$ orthonormal basis of $\mathrm{Harm}(k)$ with respect to integration using $(n-1)$-dimensional surface area measure on $\mathbb{S}^{n-1}$.

Gegenbauer polynomials

- Gegenbauer polynomials: For fixed dimension n, $\{P_k^{(n)}(t)\}_{k=0}^{\infty}$ is family of orthogonal polynomials with respect to the weight $(1-t^2)^{(n-3)/2}$ on $[-1,1]$ normalized so that $P_k^{(n)}(1)=1$.
- The Gegenbauer polynomials and spherical harmonics are related through the well-known **Addition Formula**:

$$\frac{1}{r_k}\sum_{j=1}^{r_k} Y_{kj}(x)Y_{kj}(y) = P_k^{(n)}(t), \qquad t=\langle x,y\rangle,\ x,y\in\mathbb{S}^{n-1}.$$

- Consequence: If C is a spherical code of N points on $\mathbb{S}^{n-1}$,

$$\sum_{x,y\in C} P_k^{(n)}(\langle x,y\rangle) = \frac{1}{r_k}\sum_{j=1}^{r_k}\sum_{x\in C}\sum_{y\in C} Y_{kj}(x)Y_{kj}(y) = \frac{1}{r_k}\sum_{j=1}^{r_k}\left(\sum_{x\in C} Y_{kj}(x)\right)^2 \geq 0.$$

‘Good’ potentials for lower bounds

Suppose $f : [-1, 1] \to \mathbf{R}$ is of the form

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \qquad f_k \geq 0 \text{ for all } k \geq 1. \tag{1}$$

$f(1) = \sum_{k=0}^{\infty} f_k < \infty \implies$ convergence is absolute and uniform.

Then:

$$\begin{aligned} E(n, C; f) &= \sum_{x,y \in C} f(\langle x, y \rangle) - f(1)N \\ &= \sum_{k=0}^{\infty} f_k \sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) - f(1)N \\ &\geq f_0 N^2 - f(1)N = N^2 \left(f_0 - \frac{f(1)}{N} \right). \end{aligned}$$

Thm (Delsarte-Yudin LP Bound)

Suppose f is of the form (1) and that $h(t) \geq f(t)$ for all $t \in [-1, 1]$. Then

$$\mathcal{E}(n, N; h) \geq N^2(f_0 - f(1)/N). \tag{2}$$

An N-point spherical code C satisfies $E(n, C; h) = N^2(f_0 - f(1)/N)$ if and only if both of the following hold:

(a) $f(t) = h(t)$ for all $t \in \{\langle x, y\rangle : x \neq y,\ x, y \in C\}$.

(b) for all $k \geq 1$, either $f_k = 0$ or $\sum_{x,y \in C} P_k^{(n)}(\langle x, y\rangle) = 0$.

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The **k-th moment** $M_k(C) := \sum_{x,y\in C} P_k^{(n)}(\langle x, y\rangle) = 0$ if and only if $\sum_{x\in C} Y(x) = 0$ for all $Y \in \mathrm{Harm}(k)$. If $M_k(C) = 0$ for $1 \leq k \leq \tau$, then C is called a **spherical τ-design** and

$$\int_{\mathbb{S}^{n-1}} p(y)\, d\sigma_n(y) = \frac{1}{N}\sum_{x\in C} p(x), \quad \forall \text{ polys } p \text{ of deg at most } \tau.$$

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(b) for all $k \geq 1$, either $f_k = 0$ or $\sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = 0$.

Maximizing the lower bound (2) can be written as maximizing the objective function

$$F(f_0, f_1, \ldots) := N \left(f_0(N-1) - \sum_{k=1}^{\infty} f_k \right),$$

subject to (i) $\sum_{k=0}^{\infty} f_k P_k^n(t) \leq h(t)$ and (ii) $f_k \geq 0$ for $k \geq 1$.

Lower Bounds and Quadrature Rules

- $A_{n,h}$: set of functions $f \leq h$ satisfying the conditions (1).
- For a subspace Λ of $C([-1,1])$ of real-valued functions continuous on $[-1,1]$, let

$$\mathcal{W}(n, N, \Lambda; h) := \sup_{f \in \Lambda \cap A_{n,h}} N^2(f_0 - f(1)/N). \qquad (3)$$

- For a subspace $\Lambda \subset C([-1,1])$ and $N > 1$, we say $\{(\alpha_i, \rho_i)\}_{i=0}^{e-1}$ is a $1/N$-**quadrature rule exact for** Λ if $-1 \leq \alpha_i < 1$ and $\rho_i > 0$ for $i = 0, 1, \ldots, e-1$ if

$$f_0 = \gamma_n \int_{-1}^{1} f(t)(1-t^2)^{(n-3)/2} dt = \frac{f(1)}{N} + \sum_{i=0}^{e-1} \rho_i f(\alpha_i), \quad (f \in \Lambda).$$

Theorem

Let $\{(\alpha_i, \rho_i)\}_{i=0}^{e-1}$ *be a* $1/N$*-quadrature rule that is exact for a subspace* $\Lambda \subset C([-1,1])$*.*

(a) *If* $f \in \Lambda \cap A_{n,h}$*,*

$$\mathcal{E}(n, N; h) \geq N^2 \left(f_0 - \frac{f(1)}{N} \right) = N^2 \sum_{i=0}^{e-1} \rho_i f(\alpha_i). \qquad (4)$$

(b) *We have*

$$\mathcal{W}(n, N, \Lambda; h) \leq N^2 \sum_{i=0}^{e-1} \rho_i h(\alpha_i). \qquad (5)$$

If there is some $f \in \Lambda \cap A_{n,h}$ *such that* $f(\alpha_i) = h(\alpha_i)$ *for* $i = 1, \ldots, e-1$*, then equality holds in* (5)*.*

Quadrature Rules

Quadrature Rules from Spherical Designs

If $C \subset \mathbb{S}^{n-1}$ is a spherical τ design, then choosing $\{\alpha_0, \ldots, \alpha_{e-1}, 1\} = \{\langle x, y\rangle : x, y \in C\}$ and ρ_i = fraction of times α_i occurs in $\{\langle x, y\rangle : x, y \in C\}$ gives a $1/N$ quadrature rule exact for $\Lambda = \Pi_\tau$.

Levenshtein Quadrature Rules

Of particular interest is when the number of nodes e satisfies $2e$ or $2e - 1 = \tau + 1$. Levenshtein gives bounds on N and τ for the existence of such quadrature rules. Can show that Hermite interpolant to an **absolutely monotone**[1] function h on $[-1, 1]$ is in $A_{n,h}$.

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[1] A function f is **absolutely monotone on an interval** I if $f^{(k)}(t) \geq 0$ for $t \in I$ and $k = 0, 1, 2, \ldots$.

Sharp Codes

Definition

A spherical code $C \subset \mathbb{S}^{n-1}$ is **sharp** if there are m inner products between distinct points in it and it is a spherical $(2m-1)$-design.

Theorem (Cohn and Kumar, 2006)

If $C \subset \mathbb{S}^{n-1}$ is a sharp code, then C is **universally optimal***; i.e., C is h-energy optimal for any h that is absolutely monotone on $[-1, 1]$.*

TABLE 1. The known sharp configurations, together with the 600-cell.

n	N	M	Inner products	Name
2	N	$N-1$	$\cos(2\pi j/N)$ $(1 \leq j \leq N/2)$	N-gon
n	$N \leq n$	1	$-1/(N-1)$	simplex
n	$n+1$	2	$-1/n$	simplex
n	$2n$	3	$-1, 0$	cross polytope
3	12	5	$-1, \pm 1/\sqrt{5}$	icosahedron
4	120	11	$-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4$	600-cell
8	240	7	$-1, \pm 1/2, 0$	E_8 roots
7	56	5	$-1, \pm 1/3$	kissing
6	27	4	$-1/2, 1/4$	kissing/Schläfli
5	16	3	$-3/5, 1/5$	kissing
24	196560	11	$-1, \pm 1/2, \pm 1/4, 0$	Leech lattice
23	4600	7	$-1, \pm 1/3, 0$	kissing
22	891	5	$-1/2, -1/8, 1/4$	kissing
23	552	5	$-1, \pm 1/5$	equiangular lines
22	275	4	$-1/4, 1/6$	kissing
21	162	3	$-2/7, 1/7$	kissing
22	100	3	$-4/11, 1/11$	Higman-Sims
$q\frac{q^3+1}{q+1}$	$(q+1)(q^3+1)$	3 (4 if $q=2$)	$-1/q, 1/q^2$	isotropic subspaces (q a prime power)

Figure : From: H.Cohn, A.Kumar, JAMS 2006.

Example: n-Simplex on $\mathbb{S}^{n-1}$

Let C be $N = n + 1$ points on $\mathbb{S}^{n-1}$ forming a regular simplex. Then there is only one inner product $\alpha_0 = \langle x, y \rangle$ for $x \neq y \in C$. Since $\sum_{x \in C} x = 0$, it easily follows that $\alpha_0 = -1/n$.

The first degree Gegenbauer polynomial $P_1^{(n)}(t) = t$.

If h is absolutely monotone (or just increasing and convex) then linear interpolant

$$f(t) = h(0) + h'(-1/n)(t + 1/n)$$

has $f_1 = h'(-1/n) \geq 0$ and, by convexity, stays below $h(t)$ and so shows that the n-simplex is a universally optimal spherical code.

D_4 lattice in $\mathbf{R}^4$

C = minimal length vectors from D_4 lattice in $\mathbf{R}^4$.

- $N = |C| = 24$
- $\{\langle x, y\rangle : x, y \in C\} = \{\pm 1, \pm 1/2, 0\}$
- C is a 5 design (not a 7 design). Use Levenshtein quadrature rule:

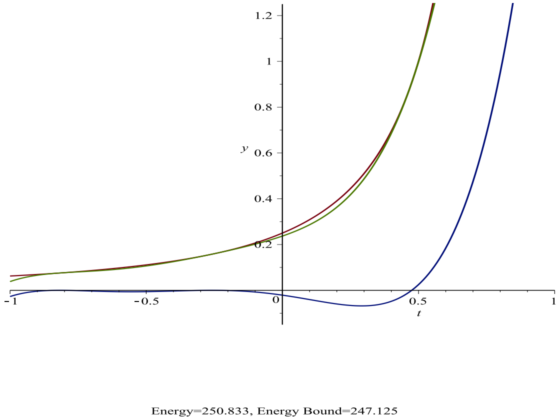

Figure : Figure by Peter Dragnev (yesterday). Upper graph is interpolant for Reisz $s = 4$ energy. Lower graph is for separation.

600 cell

- $C = 120$ points in $\mathbf{R}^4$. Each $x \in C$ has 12 nearest neighbors forming an icosahedron (Voronoi cells are dodecahedra).
- 8 inner products between distinct points in C: $\{-1, \pm 1/2, 0, (\pm 1 \pm 5)/4\}$.
- 2*7+1 interpolation conditions (would require $\tau = 14$ design)
- C is an 11 design, but almost a 19 design (only 12-th moment is nonzero). I.e. quadrature rule from C is exact on subspace Λ of Π_{19} that is $\perp$ to $P_{12}^{(4)}$.
- Cohn and Kumar find family of 17-th degree polynomials that proves universal optimality of 600 cell and they require $f_{11} = f_{12} = f_{13} = 0$. Why?