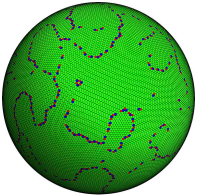
Universal lower bounds for the energy of spherical codes: lifting the Levenshtein framework



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Linear Programming Bounds: Notation

- $\mathbb{S}^{n-1}$: unit sphere in $\mathbf{R}^n$
- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$
- $r^2 = |x-y|^2 = 2 - 2\langle x, y\rangle = 2 - 2t$.
- **Interaction potential** $h : [-1, 1) \to \mathbf{R}$
- Riesz s-potential: $h(t) = (2-2t)^{-s/2} = |x-y|^{-s}$
- The h-**energy** of a spherical code C:

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

  where $t = \langle x, y\rangle$ denotes Euclidean inner product of x and y.
- $\mathcal{E}(n, h; N) = \min\{E_h(C) \mid C \subset \mathbb{S}^{n-1}, |C| = N\}$.
- **Absolutely monotone** h: $h^{(k)}(t) \geq 0$ for all $t \in [-1, 1)$ and all $k \geq 0$.

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 surface measure on $\mathbb{S}^{n-1}$.

Gegenbauer polynomials

- The Gegenbauer polynomials and spherical harmonics can be defined through the **Addition Formula**:

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

- $\{P_k^{(n)}(t)\}_{k=0}^{\infty}$ is orthogonal with respect to the weight $(1-t^2)^{(n-3)/2}$ on $[-1, 1]$ and normalized so that $P_k^{(n)}(1) = 1$.

Spherical Designs

- The **k-th moment** of a spherical code $C\mathbb{S}^{n-1}$ is

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

- $M_k(C) = 0$ 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

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

‘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:

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

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Let $A_{n,h} := \{f : f(t) \leq h(t), t \in [-1, 1), f_k \geq 0, k = 1, 2, \dots\}$.

Thm (Delsarte-Yudin LP Bound)

For any $C \subset \mathbb{S}^{n-1}$ with $|C| = N$

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

C satisfies $E(n, h; C) = E(n, f; C) = N^2(f_0 - \frac{f(1)}{N}) \iff$

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

(b) for all $k \geq 1$, either $f_k = 0$ or $M_k(C) = 0$.

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 $x \neq y \in C$.

- The first degree Gegenbauer polynomial $P_1^{(n)}(t) = t$.
- $M_1(C) = \sum_{x,y \in C} \langle x, y \rangle = |\sum_{x \in C} x|^2 = 0$.

If h is convex and increasing then linear interpolant

$$f(t) = h(\alpha_0) + h'(\alpha_0)(t + 1/n)$$

has (a) $f_1 = h'(\alpha_0) \geq 0$ and (b) $f(t) \leq h(t) \implies$ $\mathcal{E}(n, h; N = n + 1) = E(n, h; C)$.

Coding Problem: Separation

Consider $\Delta(C) := \min_{x \neq y \in C} |x - y|$ Suppose $f \in C[-1,1]$ has nonnegative Gegenbauer coefficients $f_k \geq 0$ and that $f(t) \leq 0$ for $t \in [-1, t_0)$ for some $t_0 \in (-1,1)$. Let $M = \max_t f(t)$ and define

$$h(t) = \begin{cases} 0 & -1 \leq t \leq t_0 \\ M & t_0 < t \leq 1 \end{cases}.$$

Then:

- $f \in A(n, h)$.
- $E(n, C; h) > 0 \iff \Delta(C) < \cos(t_0)$.
- $f_0 - \frac{f(1)}{N} > 0 \implies N \leq f(1)/f_0$ if there is any C with $\Delta(C) \geq \cos(t_0)$ and $|C| = N$.

Linear program: Maximize D-Y lower bound

Maximizing Delsarte-Yudin lower bound is a linear programming problem.

$$\text{Max } F(f) := N^2(f_0 - \frac{f(1)}{N}),$$
$$\text{subject to } f \in A_{n,h}.$$

For a subspace $\Lambda \subset C([-1,1])$, we consider

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

$1/N$-Quadrature Rules and Hermite Interpolation

- For a subspace $\Lambda \subset C([-1,1])$ and $N > 1$, we say $\{(\alpha_i, \rho_i)\}_{i=1}^k$ is a **$1/N$-quadrature rule exact for** Λ if $-1 \leq \alpha_i < 1$, $\rho_i > 0$ for $i = 1, 2, \ldots, k$, and

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

- For $f \in \Lambda \cap A_{n,h}$,

$$f_0 - \frac{f(1)}{N} = \sum_{i=1}^{k} \rho_i f(\alpha_i) \leq \sum_{i=1}^{k} \rho_i h(\alpha_i),$$

  and so

$$\mathcal{W}(n, N, \Lambda; h) \leq \sum_{i=1}^{k} \rho_i h(\alpha_i). \qquad (4)$$

- If there is some $f \in \Lambda \cap A_{n,h}$ such that $f(\alpha_i) = h(\alpha_i)$ for $i = 1, \ldots, k$, then equality holds in (4).

Sharp Codes

A spherical design C of degree m yields a quadrature rule that is exact for $\Lambda = \Pi_m$ (polynomials of degree m) with nodes $\{\langle x, y\rangle \mid x \neq y \in C\}$.

Definition

A spherical code $C \subset \mathbb{S}^{n-1}$ is **sharp** if there are m inner products between distinct points in it and C 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 $[-1, 1]$.*

Idea of proof: Show Hermite interpolant to h is in $A(n, h)$.

Levenshtein Framework - $1/N$-Quadrature Rule

- For every fixed (cardinality) $N > D(n, 2k-1)$(the DGS bound) there exist real numbers $-1 \leq \alpha_1 < \alpha_2 < \cdots < \alpha_k < 1$ and $\rho_1, \rho_2, \ldots, \rho_k$, $\rho_i > 0$ for $i = 1, 2, \ldots, k$, such that the equality

$$f_0 = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i)$$

  holds for every real polynomial $f(t)$ of degree at most $2k-1$.
- The numbers α_i, $i = 1, 2, \ldots, k$, are the roots of the equation

$$P_k(t)P_{k-1}(s) - P_k(s)P_{k-1}(t) = 0,$$

  where $s = \alpha_k$, $P_i(t) = P_i^{(n-1)/2,(n-3)/2}(t)$ is a Jacobi polynomial.

Universal Lower Bound (ULB)

ULB Theorem - (BDHSS, 2016)

Let h be a fixed absolutely monotone potential, n and N be fixed, and $N \geq D(n, 2k-1)$. Then the Levenshtein nodes $\{\alpha_i\}$ provide the bounds

$$\mathcal{E}(n, N, h) \geq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i).$$

The Hermite interpolants at these nodes are the optimal polynomials which solve the finite LP in the class $\mathcal{P}_\tau \cap A_{n,h}$.

Improvement of ULB and Test Functions

Test functions (Boyvalenkov, Danev, Boumova, '96)

$$Q_j(n, \alpha_k) := \frac{1}{N} + \sum_{i=1}^{k} \rho_i P_j^{(n)}(\alpha_i).$$

Subspace ULB Improvement Theorem (BDHSS, 2016)

Let $\{(\alpha_i, \rho_i)\}_{i=1}^{k}$ be a $1/N$-quadrature rule that is exact for a subspace $\Lambda \subset C([-1, 1])$ and such that equality holds in (4), namely

$$\mathcal{W}(n, N, \Lambda; h) = N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i).$$

Suppose $\Lambda' = \Lambda \bigoplus \text{span}\, \{P_j^{(n)} : j \in \mathcal{I}\}$ for some index set $\mathcal{I} \subset \mathbb{N}$. If $Q_j^{(n)} := \frac{1}{N} + \sum_{i=1}^{k} \rho_i P_j^{(n)}(\alpha_i) \geq 0$ for $j \in \mathcal{I}$, then

$$\mathcal{W}(n, N, \Lambda'; h) = \mathcal{W}(n, N, \Lambda; h) = N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i).$$

ULB Improvement for $(4, 24)$-codes

The case $n = 4$, $N = 24$ is important. C_4 consists of the minimal length vectors in D_4 lattice. $|C_4| = 24$.

- Kissing numbers in $\mathbb{R}^4$ - solved by Musin in 2003 using modification of linear programming bounds.
- C_4 is conjectured to be maximal code but not yet proved.
- C_4 is not universally optimal - Cohn, Conway, Elkies, Kumar - 2008.

ULB Improvement for $(4, 24)$-codes

For $n = 4$, $N = 24$ Levenshtein nodes and weights (exact for Π_5) are:

$$\{\alpha_1, \alpha_2, \alpha_3\} = \{-.817352..., -.257597..., .474950...\}$$
$$\{\rho_1, \rho_2, \rho_3\} = \{0.138436..., 0.433999..., 0.385897...\},$$

The test functions for $(4, 24)$-codes are:

Q_6	Q_7	Q_8	Q_9	Q_{10}	Q_{11}	Q_{12}
0.0857	0.1600	-0.0239	-0.0204	0.0642	0.0368	0.0598

Motivated by this we define

$$\Lambda := \mathrm{span}\{P_0^{(4)}, \dots, P_5^{(4)}, P_8^{(4)}, P_9^{(4)}\}.$$

ULB Improvement for $(4,24)$-codes - Main Theorem

Theorem

The collection of nodes and weights $\{(\alpha_i,\rho_i)\}_{i=1}^4$

$$\{\alpha_1,\alpha_2,\alpha_3,\alpha_4\} = \{-0.86029..., -0.48984..., -0.19572, 0.478545...\}$$
$$\{\rho_1,\rho_2,\rho_3,\rho_4\} = \{0.09960..., 0.14653..., 0.33372..., 0.37847...\},$$

define a $1/N$*-quadrature rule that is exact for* Λ*. A Hermite-type interpolant* $H(t)=H(h;(t-\alpha_1)^2\dots(t-\alpha_4)^2)\in\Lambda\cap A_{n,h}$ *s. t. ,*

$$H(\alpha_i)=h(\alpha_i),\quad H'(\alpha_i)=h'(\alpha_i),\quad i=1,\dots,4$$

exists, and hence, improved ULB holds

$$\mathcal{E}(4,24;h)\geq N^2\sum_{i=1}^{4}\rho_i h(\alpha_i).$$

Moreover, the new test functions $Q_j^{(n)}\geq 0$, $j=0,1,\dots,$ *and hence* $H(t)$ *is the optimal LP solution among all polynomials in* $\mathcal{A}_{4,h}$.

LP Optimal Polynomial for $(4, 24)$-code

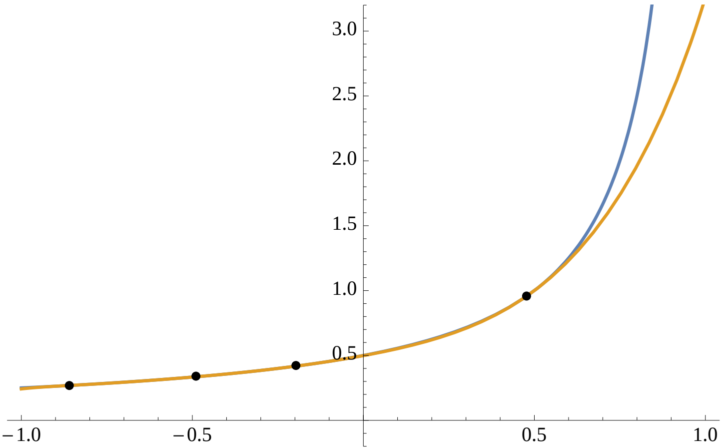

Figure: The $(4, 24)$-code optimal interpolant - Coulomb potential

Sketch of the proof

The following lemma plays an important role in the proof of the positive definiteness of the Hermite-type interpolants described in Theorem 2.

Lemma

Suppose $T := \{t_1 \leq \cdots \leq t_k\} \subset [a, b]$ *is a set of nodes and* $B := \{g_1, \ldots, g_k\}$ *is a linearly independent set of functions on* $[a, b]$ *such that the matrix* $g_B = (g_i(t_j))_{i,j=1}^{k}$ *is invertible (repetition of points in the multiset yields corresponding derivatives). Let* $H(t, h; \mathrm{span}(B))$ *denote the Hermite-type interpolant associated with* T*. Then*

$$H(t, h; \mathrm{span}(B)) = \sum_{i=1}^{k} h[t_1, \ldots, t_i] H(t, (t-t_1)\cdots(t-t_{i-1}); \mathrm{span}(B)), \quad (5)$$

where $h[t_1, \ldots, t_i]$ *are the divided differences of* h*.*

600 cell

- $C_{600} = 120$ 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_{600}: $\{-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4\}$.
- 2*7+1 or 2*8 interpolation conditions (would require 14 or 15 design)
- C_{600} 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 $\Lambda = \Pi_{19} \cap \{P_{12}^{(4)}\}^{\perp}$.
- Andreev (1999) found polynomial in Π_{17} to show 600-cell Cohn and Kumar find family of 17-th degree polynomials that proves universal optimality of C_{600} and they require $f_{11} = f_{12} = f_{13} = 0$; $\Lambda_{17}^{0} = \Pi_{17} \cap \{P_{11}^{(4)}, P_{12}^{(4)}, P_{13}^{(4)}\}^{\perp}$ with Lagrange condition at -1.

600 cell

- Levensthein: $n = 4$, $N = 120$, quadrature: 6 nodes exact for degree $= 11$.
- Test functions: $Q_{11}, Q_{12} > 0$, $Q_{13}, Q_{14} < 0$.
- Find quadrature rule for $\Lambda_{15} = \Pi_{15} \cap \{P_{12}^{(4)}, P_{13}^{(4)}\}^{\perp}$.
- Verify Hermite interpolation works in Λ_{15}.
- New test functions $Q_{11}, Q_{12} > 0$ so this solves the linear program in Π_{15}.
- Degree 17. Try $\Lambda_{17}^{1} = \Pi_{17} \cap \{P_{12}^{(4)}, P_{13}^{(4)}\}^{\perp}$, double interpolation at -1. It works.
- Degree 17. Try $\Lambda_{17}^{2} = \Pi_{17} \cap \{P_{11}^{(4)}, P_{12}^{(4)}\}^{\perp}$, double interpolation -1. It works.
- Degree 17. All solutions form triangle.