Universal Lower Bounds on Energy and LP-Extremal Polynomials for (4,24)-Codes

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Outline

- Why minimize energy?
- Delsarte-Yudin LP Energy Bound
- Universal Lower Bound for Energy (ULB)
- Subspace ULB
- Improvements of ULB via Test Functions
- \((4, 24)\)-code significance
- ULB for \((4, 24)\)-code
**Thomson Problem** (1904) -
(“plum pudding” model of an atom)

Find the (most) stable (ground state) energy configuration (code) of $N$ classical electrons (Coulomb law) constrained to move on the sphere $S^2$.

**Generalized Thomson Problem** ($1/r^s$ potentials and $\log(1/r)$)

A code $C := \{x_1, \ldots, x_N\} \subset S^{n-1}$ that minimizes **Riesz $s$-energy**

$$E_s(C) := \sum_{j \neq k} \frac{1}{|x_j - x_k|^s}, \quad s > 0, \quad E_{\log(\omega_N)} := \sum_{j \neq k} \log \frac{1}{|x_j - x_k|}$$

is called an **optimal $s$-energy code**.
Why Minimize Potential Energy? Coding:

**Tammes Problem (1930)**
A Dutch botanist that studied modeling of the distribution of the orifices in pollen grain asked the following.

**Tammes Problem (Best-Packing, \(s = \infty\))**
Place \(N\) points on the unit sphere so as to maximize the minimum distance between any pair of points.

**Definition**
Codes that maximize the minimum distance are called **optimal (maximal) codes**. Hence our choice of terms.
**Fullerenes** (1985) - (Buckyballs)

Vaporizing graphite, Curl, Kroto, Smalley, Heath, and O’Brien discovered $C_{60}$
(Chemistry 1996 Nobel prize)

Duality structure: 32 electrons and $C_{60}$. 
Optimal s-energy codes on $S^2$

**Known optimal s-energy codes on $S^2$**

- $s = \log$, Smale’s problem, logarithmic points (known for $N = 2 – 6, 12$);
- $s = 1$, Thomson Problem (known for $N = 2 – 6, 12$)
- $s = -1$, Fejes-Toth Problem (known for $N = 2 – 6, 12$)
- $s \to \infty$, Tammes Problem (known for $N = 1 – 12, 13, 14, 24$)

**Limiting case - Best packing**

For fixed $N$, any limit as $s \to \infty$ of optimal s-energy codes is an optimal (maximal) code.

**Universally optimal codes**

The codes with cardinality $N = 2, 3, 4, 6, 12$ are special (sharp codes) and minimize large class of potential energies. First "non-sharp" is $N = 5$ and very little is rigorously proven.
Minimal $h$-energy - preliminaries

- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$;
- Let the interaction potential $h : [-1, 1] \to \mathbb{R} \cup \{+\infty\}$ be an absolutely monotone\(^1\) function;
- The $h$-energy of a spherical code $C$:

$$E(n, C; h) := \sum_{x,y \in C, y \neq x} h(\langle x, y \rangle), \quad |x - y|^2 = 2 - 2\langle x, y \rangle = 2(1 - t),$$

where $t = \langle x, y \rangle$ denotes Euclidean inner product of $x$ and $y$.

**Problem**

Determine

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

and find (prove) optimal $h$-energy codes.

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\(^1\)A function $f$ is absolutely monotone on $I$ if $f^{(k)}(t) \geq 0$ for $t \in I$ and $k = 0, 1, 2, \ldots$
Absolutely monotone potentials - examples

- Newton potential: \( h(t) = (2 - 2t)^{-(n-2)/2} = |x - y|^{-(n-2)} \);
- Riesz s-potential: \( h(t) = (2 - 2t)^{-s/2} = |x - y|^{-s} \);
- Log potential: \( h(t) = -\log(2 - 2t) = -\log |x - y| \);
- Gaussian potential: \( h(t) = \exp(2t - 2) = \exp(-|x - y|^2) \);
- Korevaar potential: \( h(t) = (1 + r^2 - 2rt)^{-(n-2)/2}, \quad 0 < r < 1 \).

Remark

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 subpotential \( f \) such that \( h \geq f \) for which we can obtain lower bounds for the minimal \( f \)-energy \( \mathcal{E}(n, N; f) \). Usually \( f \) is chosen to be appropriate polynomial.
‘Good’ potentials for lower bounds - Delsarte-Yudin LP

**Delsarte-Yudin approach:**

Find a potential \( f \) such that \( h \geq f \) for which we can obtain lower bounds for the minimal \( f \)-energy \( E(n, N; f) \).

Suppose \( f : [-1, 1] \to \mathbb{R} \) has a Gegenbauer expansion of the form

\[
f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \quad f_k \geq 0 \text{ for all } k \geq 1. \quad (1)
\]

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

Then:

\[
E(n, C; f) = \sum_{x,y \in C} f(\langle x, y \rangle) - f(1)N
\]

\[
= \sum_{k=0}^{\infty} f_k \sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) - f(1)N
\]

\[
\geq f_0 N^2 - f(1)N = N^2 \left( f_0 - \frac{f(1)}{N} \right).
\]
Let $A_{n,h} = \{f : f(t) \leq h(t), \ t \in [-1, 1], f_k \geq 0, k = 1, 2, \ldots \}$. Then

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

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 $\sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = 0$. 
Thm (Delsarte-Yudin LP Bound)

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

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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 $f \in A_{n,h}$. 
Thm (Delsarte-Yudin LP Bound)

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

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Infinite linear programming is too ambitious, truncate the program

$$(LP) \quad \text{Maximize } F_m(f_0, f_1, \ldots, f_m) := N \left( f_0 (N - 1) - \sum_{k=1}^m f_k \right),$$

subject to $f \in \mathcal{P}_m \cap A_{n,h}$.

Given $n$ and $N$ we obtain ULB by solving LP for all $m \leq \tau(n, N)$. 
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 $\alpha_i$, $i = 1, 2, \ldots, k$, 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.

• In fact, $\alpha_i$, $i = 1, 2, \ldots, k$, are the roots of the Levenshtein’s polynomial $f_{2k-1}^{(n, \alpha_k)}(t)$. 
Universal Lower Bound (ULB)

ULB Theorem - (BDHSS - Constructive Approximation, 2016)

Let \( h \) be a fixed absolutely monotone potential, \( n \) and \( N \) be fixed, and \( \tau = \tau(n, N) \) be such that \( N \in [D(n, \tau), D(n, \tau + 1)) \). 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 \( \mathcal{P}_\tau \cap A_{n, h} \).
Gauss, Korevaar, and Newton potentials: (4,24)-codes
Subspace ULB and $1/N$-Quadrature Rules

- Recall that $A_{n,h}$ is the set of functions $f$ having positive Gegenbauer coefficients and $f \leq h$ on $[-1, 1]$. 
- For a subspace $\Lambda$ of $C([-1, 1])$ of real-valued functions continuous on $[-1, 1]$, let 
  \[
  \mathcal{W}(n, N, \Lambda; h) := \sup_{f \in \Lambda \cap A_{n,h}} N^2(f_0 - f(1)/N). 
  \]
- 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 $\Lambda$ if $-1 \leq \alpha_i < 1$ and $\rho_i > 0$ for $i = 1, 2, \ldots, k$ if 
  \[
  f_0 = \gamma_n \int_{-1}^{1} f(t)(1 - t^2)^{(n-3)/2}dt = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i), \quad (f \in \Lambda). 
  \]
Subspace ULB and $1/N$-Quadrature Rules

Subspace ULB Theorem [BDHSS, CA - 2016]

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

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

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

(b) We have

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

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 (5).
Define test functions (Boyvalenkov, Danev, Boumova - IEEE TIT ‘96)

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

**ULB Improvement Characterization Theorem (BDHSS, CA - 2016)**

The ULB bound

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

can be improved by a polynomial from \( A_{n,h} \) of degree at least \( 2k \) if and only if \( Q_j(n, \alpha_k) < 0 \) for some \( j \geq 2k \).

Moreover, if \( Q_j(n, \alpha_k) < 0 \) for some \( j \geq 2k \) and \( h \) is strictly absolutely monotone, then that bound can be improved by a polynomial from \( A_{n,h} \) of degree exactly \( j \).

Furthermore, there is \( j_0(n, N) \) such that \( Q_j(n, \alpha_k) \geq 0, j \geq j_0(n, N) \).
Subspace ULB and Test Functions

Subspace ULB Improvement Theorem (BDHSS, CA - 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 (5), namely

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

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

\[
W(n, N, \Lambda'; h) = W(n, N, \Lambda; h) = N^2 \sum_{i=1}^k \rho_i h(\alpha_i).
\]
The case $n = 4, N = 24$ is important.

- Kissing numbers in $\mathbb{R}^4$ - solved by Musin in 2003 in Math Annals paper.

- $D_4$ is conjectured to be maximal code but not yet proved.

- $D_4$ is not universally optimal - Cohn, Conway, Elkies, Kumar - 2008.
Suboptimal LP solutions for $m \leq m(N, n)$

Suboptimal LP Solutions Theorem - (BDHSS, CA - 2016)

The linear program (LP) can be solved for any $m \leq \tau(n, N)$ and the suboptimal solution in the class $\mathcal{P}_m \cap \mathcal{A}_{n,h}$ is given by the Hermite interpolants at the Levenshtein nodes determined by $N = L_m(n, s)$. 
Suboptimal LP solutions for $N = 24$, $n = 4$, $m = 1 - 5$

\[ f_1(t) = 0.499P_0(t) + 0.229P_1(t) \]
\[ f_2(t) = 0.581P_0(t) + 0.305P_1(t) + 0.093P_2(t) \]
\[ f_3(t) = 0.658P_0(t) + 0.395P_1(t) + 0.183P_2(t) + 0.069P_3(t) \]
\[ f_4(t) = 0.69P_0(t) + 0.43P_1(t) + 0.23P_2(t) + 0.10P_3(t) + 0.027P_4(t) \]
\[ f_5(t) = 0.71P_0(t) + 0.46P_1(t) + 0.26P_2(t) + 0.13P_3(t) + 0.05P_4(t) + 0.01P_5(t). \]

We seek optimal LP solution for $(4, 24)$-codes in all $\mathcal{P} \cap \mathcal{A}_{4,h}$. 
ULB Improvement for (4, 24)-codes

For $n = 4$, $N = 24$ Levenshtein nodes and weights are:

\[
\{\alpha_1, \alpha_2, \alpha_3\} = \{-0.817352..., -0.257597..., 0.474950...\}
\]
\[
\{\rho_1, \rho_2, \rho_3\} = \{0.138436..., 0.433999..., 0.385897...\},
\]

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

\[
\begin{array}{cccccc}
Q_6 & Q_7 & Q_8 & Q_9 & Q_{10} & Q_{11} & Q_{12} \\
0.0857 & 0.1600 & -0.0239 & -0.0204 & 0.0642 & 0.0368 & 0.0598 \\
\end{array}
\]

Motivated by this we define

\[
\Lambda := \text{span}\{P_0^{(4)}, \ldots, P_5^{(4)}, P_8^{(4)}, P_9^{(4)}\}.
\]
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 \( \Lambda \). A Hermite-type interpolant \( H(t) = H(h; (t - \alpha_1)^2 \ldots (t - \alpha_4)^2) \in \Lambda \cap A_{n,h} \) s. t.,

\[
H(\alpha_i) = h(\alpha_i), \quad H'(\alpha_i) = h'(\alpha_i), \quad i = 1, \ldots, 4
\]

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 \( Q_j^{(n)} \geq 0, j = 0, 1, \ldots, \) and hence \( H(t) \) is the optimal LP solution among all polynomials in \( A_{4,h} \).
LP Optimal Polynomial for (4, 24)-code

Figure: The (4, 24)-code optimal interpolant - Coulomb potential
Sketch of the proof

Step 1: Find a Quadrature Rule exact on $\Lambda$

- Determine $\{\rho_i\}$ in terms of $\{\alpha_i\}$ using $\{1, x, x^2, x^3\}$ as $f$ in QF

$$f_0 = \frac{f(1)}{24} + \sum_{i=1}^{4} \rho_i f(\alpha_i), \quad f \in \Lambda. \tag{6}$$

- Use Newton method to determine $\{\alpha_i\}$ using $P_4^{(4)}, P_5^{(4)}, P_8^{(4)}, P_9^{(4)}$.
  Verify (6) holds for $\{P_i^{(4)}, \ i = 0, \ldots, 5, 8, 9\}$ and hence on $\Lambda$.

Step 2: Find a Hermite-type interpolant

$$H(t) = \sum_{i=0}^{6} \beta_i P_i^{(4)}(t) + \beta_8 P_8^{(4)} + \beta_9 P_9^{(4)}.$$

- Hermite interpolation conditions define a non-degenerate linear system.
The following lemma plays an important role in the proof of the positive definiteness of the Hermite-type interpolants described in Theorem 1.

**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 $H(t, h; \text{span}(B))$ denote the Hermite-type interpolant associated with $T$. Then

$$H(t, h; \text{span}(B)) = \sum_{i=1}^{k} h[t_1, \ldots, t_i] H(t, (t-t_1) \cdots (t-t_{i-1}); \text{span}(B)), \quad (7)$$

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