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

Peter D. Dragnev
Indiana University-Purdue University Fort Wayne

Joint work with: P. Boyvalenkov (BAS); D. Hardin, Ed Saff (Vanderbilt); and M. Stoyanova (Sofia) (BDHSS)

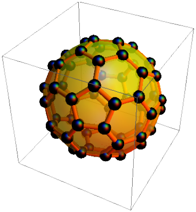
Outline

- 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

Why Minimize Potential Energy? Electrostatics:

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 $\mathbb{S}^2$.



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

A code $C := \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^{n-1}$ that minimizes **Riesz *s*-energy**

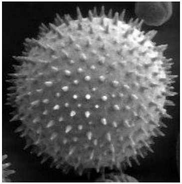
$$E_s(C) := \sum_{j \neq k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad s > 0, \qquad E_{\log}(\omega_N) := \sum_{j \neq k} \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

is called an **optimal *s*-energy code**.

Why Minimize Potential Energy? Coding:

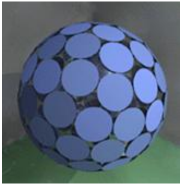
Tammes Problem (1930)

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.



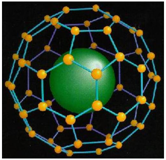
Definition

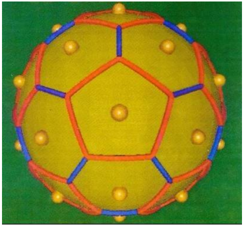
Codes that maximize the minimum distance are called **optimal (maximal) codes**. Hence our choice of terms.

Why Minimize Potential Energy? Nanotechnology:

Fullerenes (1985) - (Buckyballs)

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





Duality structure: 32 electrons and C_{60}.

Optimal s-energy codes on $\mathbb{S}^2$

Known optimal s-energy codes on $\mathbb{S}^2$

- $s = \log$, 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*.

[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 $\mathcal{E}(n, N; f)$.

Suppose $f : [-1, 1] \to \mathbf{R}$ has a Gegenbauer expansion 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)

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

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

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

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

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 $\sum_{x,y \in C} P_k^{(n)}(\langle x, y\rangle) = 0$.

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

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

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 $\sum_{x,y\in C} P_k^{(n)}(\langle x, y\rangle) = 0$.

Infinite linear programming is too ambitious, truncate the program

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

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 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.
- In fact, α_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)

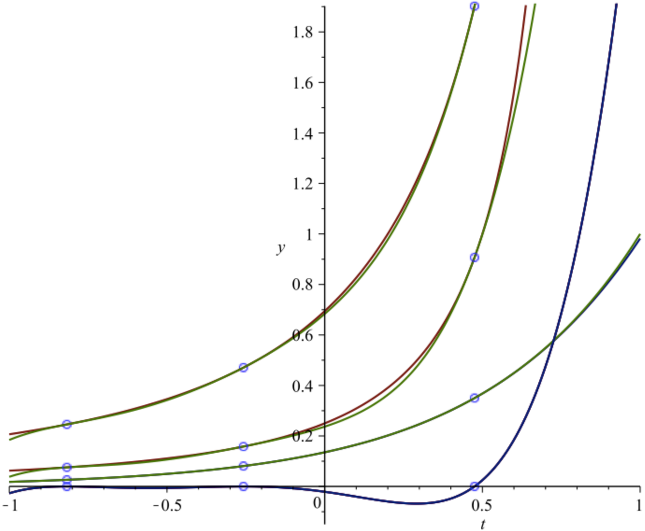
ULB Theorem - (BDHSS - Constructive Approximation, 2016)

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 polinomials 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 Λ of $C([-1,1])$ of real-valued functions continuous on $[-1,1]$, let

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

- 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 $-1 \leq \alpha_i < 1$ 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 $f \in \Lambda \cap A_{n,h}$,

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

(b) We have

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

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

Improvement of ULB and Test Functions

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

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

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

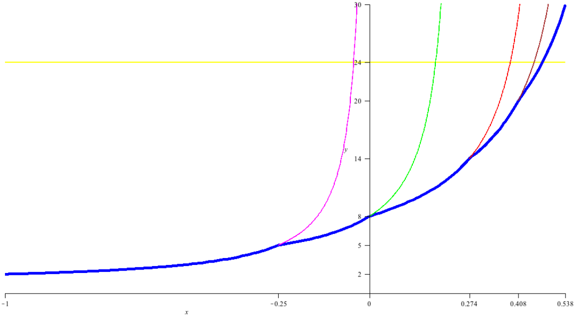
The case $n = 4$, $N = 24$ is important.

- 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.

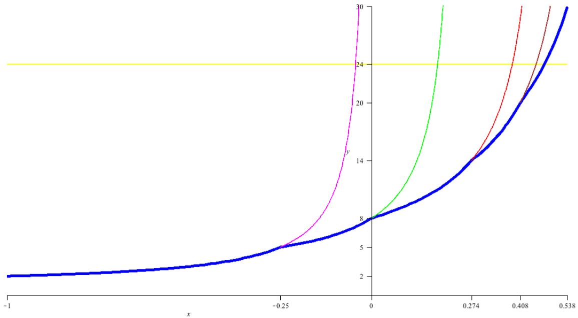
Suboptimal LP solutions for $m \leq m(N, n)$



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 $\mathcal{P}_m \cap A_{n,h}$ is given by the Hermite interpolants at the Levenshtein nodes determined by $N = L_m(n, s)$.

Suboptimal LP solutions for $N = 24$, $n = 4$, $m = 1 - 5$



$$f_1(t) = .499P_0(t) + .229P_1(t)$$
$$f_2(t) = .581P_0(t) + .305P_1(t) + 0.093P_2(t)$$
$$f_3(t) = .658P_0(t) + .395P_1(t) + .183P_2(t) + 0.069P_3(t)$$
$$f_4(t) = .69P_0(t) + .43P_1(t) + .23P_2(t) + .10P_3(t) + 0.027P_4(t)$$
$$f_5(t) = .71P_0(t) + .46P_1(t) + .26P_2(t) + .13P_3(t) + 0.05P_4(t) + 0.01P_5(t).$$

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:

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

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 Polinomial for (4, 24)-code

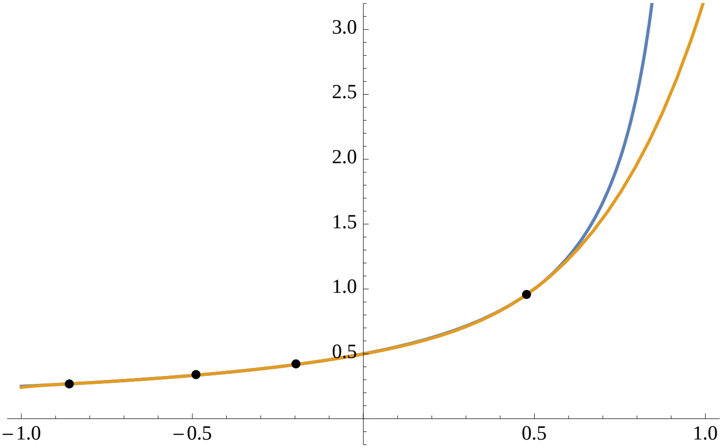


Figure : The (4, 24)-code optimal interpolant - Coulomb potential

Sketch of the proof

Step 1: Find a Quadrature Rule exact on Λ

- 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 Λ.

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.

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 1.

Lemma

Suppose $T := \{t_1 \leq \cdots \leq t_k\} \subset [a, b]$ *is a set of nodes and* $B := \{g_1, \dots, g_k\}$ *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*

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

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

THANK YOU!