Universal lower bounds on energy for spherical codes, test functions and LP optimality

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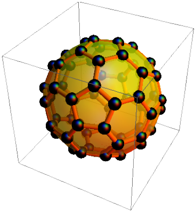
Outline

- Why minimize energy?
- Delsarte-Yudin LP approach
- DGS bounds for spherical τ-desings
- Levenshtein bounds for codes
- $1/N$ quadrature and Levenshtein nodes
- Universal lower bound for energy (ULB)
- Improvements of ULB and LP universality
- Examples
- ULB for $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$
- Conclusions and summary of future work

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

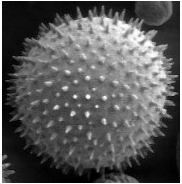
$$E_s(C) := \sum_{j \neq k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad s > 0, \qquad E_{\log}(\omega_N) := \sum_{j \neq k} \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

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

Why Minimize Potential Energy? Coding:

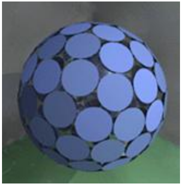
Tammes Problem (1930)

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.



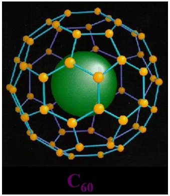
Definition

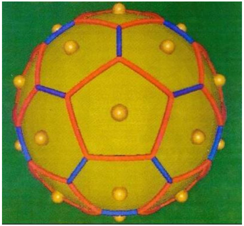
Codes that maximize the minimum distance are called **optimal (maximal) codes**. Hence our choice of terms.

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 $N = 1 - 12,\ 13, 14,\ 24$)

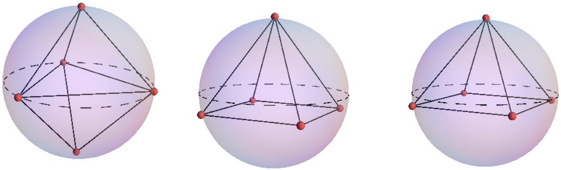
Limiting case - Best packing

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.

Optimal five point log and Riesz s-energy code on $\mathbb{S}^2$



(a) (b) (c)

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

- P. Dragnev, D. Legg, and D. Townsend, *Discrete logarithmic energy on the sphere*, Pacific J. Math. **207** (2002), 345–357.
- X. Hou, J. Shao, *Spherical Distribution of 5 Points with Maximal Distance Sum*, Discr. Comp. Geometry, **46** (2011), 156–174
- R. E. Schwartz, *The Five-Electron Case of Thomson's Problem*, Exp. Math. **22** (2013), 157–186.

Optimal five point log and Riesz s-energy code on $\mathbb{S}^2$

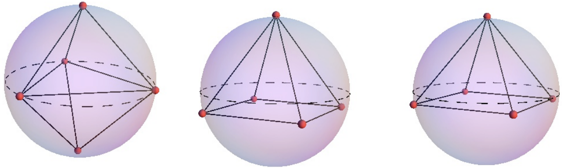


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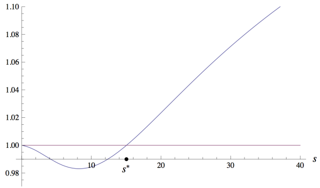
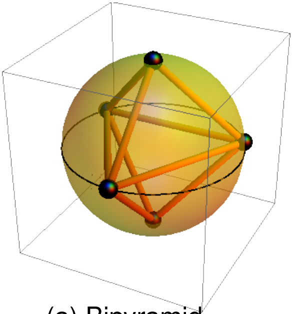
Figure : 'Optimal' 5-point code on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) 'optimal' SBP ($s = 16$).



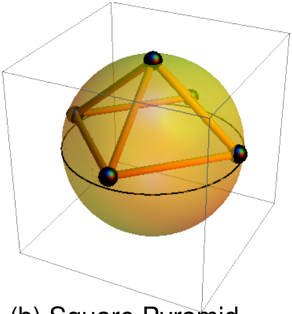
Melnik et.el. 1977 $s^* = 15.048\ldots?$

Figure : 5 points energy ratio

Optimal five point log and Riesz s-energy code on $\mathbb{S}^2$



(a) Bipyramid



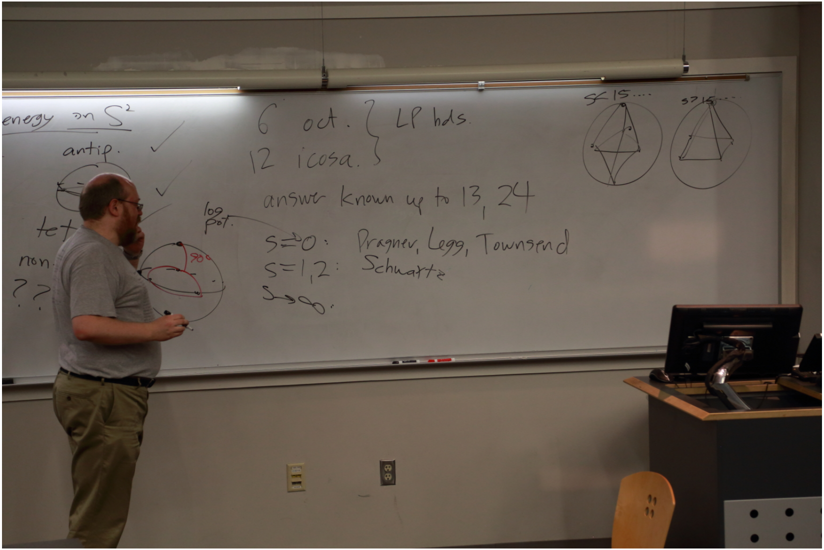
(b) Square Pyramid

Theorem (Bondarenko-Hardin-Saff)

Any limit as $s \to \infty$ of optimal s-energy codes of 5 points is a square pyramid with the square base in the Equator.

- A. V. Bondarenko, D. P. Hardin, E. B. Saff, *Mesh ratios for best-packing and limits of minimal energy configurations*, Acta Math. Hungarica, 142(1), (2014) 118–131.

Henry Cohn and the five-point energy problem



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: $h(t) = (1+r^2-2rt)^{-(n-2)/2}, \quad 0 < r < 1$.

Other potentials (low. semicont.);

'Kissing' potential: $h(t) = \begin{cases} 0, & -1 \le t \le 1/2 \\ \infty, & 1/2 \le t \le 1 \end{cases}$

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 potential f such that $h \ge f$ for which we can obtain lower bounds for the minimal f-energy $\mathcal{E}(n, N; f)$.

Spherical Harmonics and Gegenbauer polynomials

- $\mathrm{Harm}(k)$: 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 $\mathbb{S}^{n-1}$.
- For fixed dimension n, the Gegenbauer polynomials are defined by

$$P_0^{(n)} = 1, \quad P_1^{(n)} = t$$

and the three-term recurrence relation (for $k \geq 1$)

$$(k+n-2)P_{k+1}^{(n)}(t) = (2k+n-2)tP_k^{(n)}(t) - kP_{k-1}^{(n)}(t).$$

- Gegenbauer polynomials are orthogonal with respect to the weight $(1-t^2)^{(n-3)/2}$ on $[-1, 1]$ (observe that $P_k^{(n)}(1) = 1$).

Spherical Harmonics and Gegenbauer polynomials

- 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 $\mathbb{S}^{n-1}$,

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

‘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 $f : [-1, 1] \to \mathbf{R}$ 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)

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

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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 $f \in A_{n,h}$.

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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 shall solve the program for all $m \leq \tau(n, N)$.

Spherical designs and DGS Bound (Boyvalenkov)

- P. Delsarte, J.-M. Goethals, J. J. Seidel, Spherical codes and designs, Geom. Dedicata 6, 1977, 363-388.

Definition

A spherical τ-design $C \subset \mathbb{S}^{n-1}$ is a finite nonempty subset of $\mathbb{S}^{n-1}$ such that

$$\frac{1}{\mu(\mathbb{S}^{n-1})} \int_{\mathbb{S}^{n-1}} f(x) d\mu(x) = \frac{1}{|C|} \sum_{x \in C} f(x)$$

($\mu(x)$ is the Lebesgue measure) holds for all polynomials $f(x) = f(x_1, x_2, \ldots, x_n)$ of degree at most τ.

The strength of C is the maximal number $\tau = \tau(C)$ such that C is a spherical τ-design.

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- P. Delsarte, J.-M. Goethals, J. J. Seidel, Spherical codes and designs, Geom. Dedicata 6, 1977, 363-388.

Theorem (DGS - 1977)

For fixed strength τ and dimension n denote by

$$B(n,\tau) = \min\{|C| : \exists\ \tau\text{-design } C \subset \mathbb{S}^{n-1}\}$$

the minimum possible cardinality of spherical τ-designs $C \subset \mathbb{S}^{n-1}$.

$$B(n,\tau) \geq D(n,\tau) = \begin{cases} 2\binom{n+k-2}{n-1}, & \text{if } \tau = 2k-1, \\ \binom{n+k-1}{n-1} + \binom{n+k-2}{n-1}, & \text{if } \tau = 2k. \end{cases}$$

Levenshtein bounds for spherical codes (Boyvalenkov)

- V.I.Levenshtein, Designs as maximum codes in polynomial metric spaces, Acta Appl. Math. 25, 1992, 1-82.

- For every positive integer m we consider the intervals

$$\mathcal{I}_m = \begin{cases} \left[t_{k-1}^{1,1}, t_k^{1,0}\right], & \text{if } m = 2k-1, \\ \left[t_k^{1,0}, t_k^{1,1}\right], & \text{if } m = 2k. \end{cases}$$

- Here $t_0^{1,1} = -1$, $t_i^{a,b}$, $a, b \in \{0,1\}$, $i \geq 1$, is the greatest zero of the Jacobi polynomial $P_i^{(a+\frac{n-3}{2}, b+\frac{n-3}{2})}(t)$.
- The intervals $\mathcal{I}_m$ define partition of $\mathcal{I} = [-1, 1)$ to countably many nonoverlapping closed subintervals.

Levenshtein bounds for spherical codes (Boyvalenkov)

Theorem (Levenshtein - 1979)

For every $s \in \mathcal{I}_m$, *Levenshtein used* $f_m^{(n,s)}(t) = \sum_{j=0}^{m} f_j P_j^{(n)}(t)$:

$$\text{(i) } f_m^{(n,s)}(t) \leq 0 \text{ on } [-1, s] \text{ and (ii) } f_j \geq 0 \text{ for } 1 \leq j \leq m$$

to derive the bound

$$A(n,s) \leq \begin{cases} L_{2k-1}(n,s) = \binom{k+n-3}{k-1}\left[\frac{2k+n-3}{n-1} - \frac{P_{k-1}^{(n)}(s) - P_k^{(n)}(s)}{(1-s)P_k^{(n)}(s)}\right] \\ \qquad\qquad \text{for } s \in \mathcal{I}_{2k-1}, \\ \\ L_{2k}(n,s) = \binom{k+n-2}{k}\left[\frac{2k+n-1}{n-1} - \frac{(1+s)(P_k^{(n)}(s) - P_{k+1}^{(n)}(s))}{(1-s)(P_k^{(n)}(s) + P_{k+1}^{(n)}(s))}\right] \\ \qquad\qquad \text{for } s \in \mathcal{I}_{2k}, \end{cases}$$

where $A(n,s) = \max\{|C| : \langle x, y\rangle \leq s \text{ for all } x \neq y \in C, \}$

Interplay between DGS- and L-bounds (Boyvalenkov)

- The connection between the Delsarte-Goethals-Seidel bound and the Levenshtein bounds are given by the equalities

$$L_{2k-2}(n, t_{k-1}^{1,1}) = L_{2k-1}(n, t_{k-1}^{1,1}) = D(n, 2k-1),$$

$$L_{2k-1}(n, t_{k}^{1,0}) = L_{2k}(n, t_{k}^{1,0}) = D(n, 2k)$$

at the ends of the intervals $\mathcal{I}_m$.

- For every fixed dimension n each bound $L_m(n, s)$ is smooth and strictly increasing with respect to s. The function

$$L(n,s) = \begin{cases} L_{2k-1}(n,s), & \text{if } s \in \mathcal{I}_{2k-1}, \\ L_{2k}(n,s), & \text{if } s \in \mathcal{I}_{2k}, \end{cases}$$

is continuous and piece-wise smooth in s.

Levenshtein Function - $n = 4$

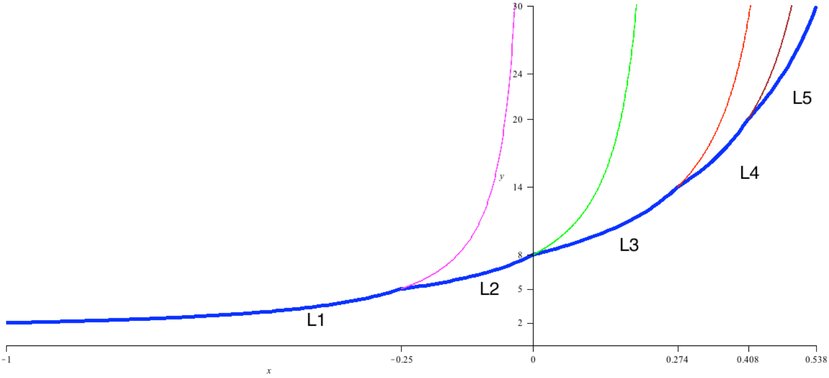


Figure : The Levenshtein function $L(4, s)$.

Lower Bounds 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

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

- 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

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

Proposition

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

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

(b) We have

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

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).

$1/N$-Quadrature Rules

Quadrature Rules from Spherical Designs

If $C \subset \mathbb{S}^{n-1}$ is a spherical τ design, then choosing $\{\alpha_1, \dots, \alpha_k, 1\} = \{\langle x, y\rangle \colon x, y \in C\}$ and $\rho_i =$ fraction of times α_i occurs in $\{\langle x, y\rangle \colon x, y \in C\}$ gives a $1/N$ quadrature rule exact for $\Lambda = \mathcal{P}_\tau$.

Levenshtein Quadrature Rules

Of particular interest is when the number of nodes k satisfies $m = 2k - 1$ or $m = 2k$. Levenshtein gives bounds on N and m for the existence of such quadrature rules.

Sharp Codes

Definition

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

Theorem (Cohn and Kumar, 2007)

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 $[-1, 1]$.*

Theorem (Cohn and Kumar, 2007)

Let C be the 600*-cell (*120 *in $\mathbf{R}^n$). Then there is $f \in \Lambda \cap A_{n,h}$, s.t. $f(\langle x, y\rangle) = h(\langle x, y\rangle)$ for all $x \neq y \in C$, where $\Lambda = \mathcal{P}_{17} \cap \{f_{11} = f_{12} = f_{13} = 0\}$. Hence it is a universal code.*

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

n	N	M	Inner products	Name
2	N	$N-1$	$\cos(2\pi j/N)$ $(1 \le j \le N/2)$	N-gon
n	$N \le n$	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 : H. Cohn, A. Kumar, JAMS 2007.

Levenshtein $1/N$-Quadrature Rule - odd interval case

- For every fixed (cardinality) $N > D(n, 2k-1)$ there exist uniquely determined 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 $f_{2k-1}^{(n,\alpha_k)}(t)$.

Levenshtein $1/N$-Quadrature Rule - even interval case

- Similarly, for every fixed (cardinality) $N > D(n,2k)$ there exist uniquely determined real numbers $-1 = \beta_0 < \beta_1 < \cdots < \beta_k < 1$ and $\gamma_0, \gamma_1, \ldots, \gamma_k$, $\gamma_i > 0$ for $i = 0, 1, \ldots, k$, such that the equality

$$f_0 = \frac{f(1)}{N} + \sum_{i=0}^{k} \gamma_i f(\beta_i) \qquad (6)$$

  is true for every real polynomial $f(t)$ of degree at most $2k$.
- The numbers β_i, $i = 0, 1, \ldots, k$, are the roots of the Levenshtein's polynomial $f_{2k}^{(n,\beta_k)}(t)$.
- Sidelnikov (1980) showed the *optimality* of the Levenshtein polynomials $f_{2k-1}^{(n,\alpha_{k-1})}(t)$ and $f_{2k}^{(n,\beta_k)}(t)$.

Universal Lower Bound (ULB)

Main Theorem - (BDHSS - 2014)

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 $\{\alpha_i\}$, respectively $\{\beta_i\}$, provide the bounds

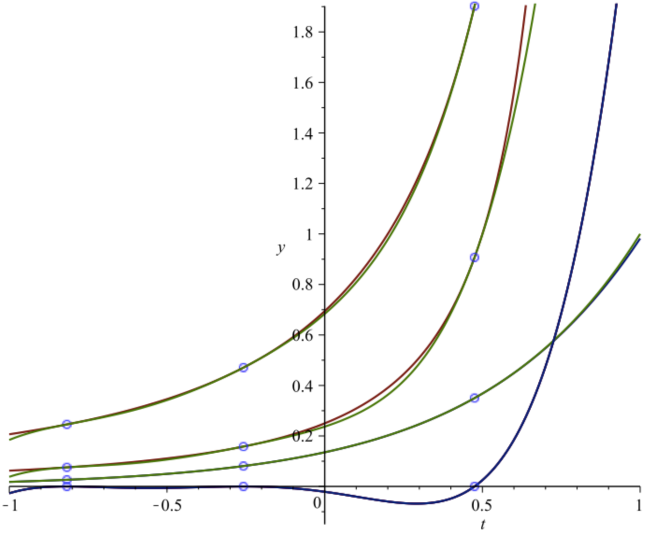
$$\mathcal{E}(n, N, h) \geq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i),$$

respectively,

$$\mathcal{E}(n, N, h) \geq N^2 \sum_{i=0}^{k} \gamma_i h(\beta_i).$$

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

Gaussian, Korevaar, and Newtonian potentials



ULB comparison - BBCGKS 2006 Newton Energy

N	Harmonic Energy	ULB Bound	%	N	Harmonic Energy	ULB Bound	%	N	Harmonic Energy	ULB Bound	%
5	4.00	4.00	0.00	25	182.99	182.38	0.34	45	664.48	663.00	0.22
6	6.50	6.42	1.28	26	199.69	199.00	0.35	46	697.26	695.40	0.27
7	9.50	9.42	0.88	27	217.15	216.38	0.36	47	730.75	728.60	0.29
8	13.00	13.00	0.00	28	235.40	234.50	0.38	48	764.59	762.60	0.26
9	17.50	17.33	0.95	29	254.38	253.38	0.39	49	799.70	797.40	0.29
10	22.50	22.33	0.74	30	274.19	273.00	0.43	50	835.12	833.00	0.25
11	28.21	28.00	0.74	31	294.79	293.51	0.43	51	871.98	869.40	0.30
12	34.42	34.33	0.26	32	315.99	314.80	0.38	52	909.19	906.60	0.28
13	41.60	41.33	0.64	33	337.79	336.86	0.28	53	947.15	944.60	0.27
14	49.26	49.00	0.53	34	360.52	359.70	0.23	54	985.88	983.40	0.25
15	57.62	57.48	0.24	35	384.54	383.31	0.32	55	1025.76	1023.00	0.27
16	66.95	66.67	0.42	36	409.07	407.70	0.33	56	1066.62	1063.53	0.29
17	76.98	76.56	0.54	37	434.19	432.86	0.31	57	1108.17	1104.88	0.30
18	87.62	87.17	0.51	38	460.28	458.80	0.32	58	1150.43	1147.05	0.29
19	98.95	98.48	0.48	39	487.25	485.51	0.36	59	1193.38	1190.03	0.28
20	110.80	110.50	0.27	40	514.90	513.00	0.37	60	1236.91	1233.83	0.25
21	123.74	123.37	0.30	41	543.16	541.40	0.32	61	1281.38	1278.45	0.23
22	137.52	137.00	0.38	42	572.16	570.60	0.27	62	1326.59	1323.88	0.20
23	152.04	151.38	0.44	43	601.93	600.60	0.22	63	1373.09	1370.13	0.22
24	167.00	166.50	0.30	44	632.73	631.40	0.21	64	1420.59	1417.20	0.24

Newtonian energy comparison (BBCGKS 2006) - $N = 5 - 64$, $n = 4$.

ULB comparison - BBCGKS 2006 Gauss Energy

N	Gaussian Energy	ULB Bound	%	N	Gaussian Energy	ULB Bound	%	N	Gaussian Energy	ULB Bound	%
5	0.82085	0.82085	0.0000	25	54.83402	54.81419	0.0362	45	195.4712	195.46	0.0042
6	1.51674	1.469024	3.1460	26	59.8395	59.7986	0.0684	46	204.7676	204.76	0.0049
7	2.351357	2.303011	2.0561	27	65.02733	64.99832	0.0446	47	214.2834	214.27	0.0075
8	3.3213094	3.321309	0.0000	28	70.43742	70.41329	0.0343	48	223.994	223.99	0.0007
9	4.6742772	4.614371	1.2816	29	76.06871	76.0435	0.0332	49	233.9421	233.93	0.0040
10	6.1625802	6.123668	0.6314	30	81.9183	81.88889	0.0359	50	244.0939	244.09	0.0022
11	7.9137359	7.85	0.8517	31	87.99142	87.95307	0.0436	51	254.4665	254.46	0.0028
12	9.8040902	9.780806	0.2375	32	94.26767	94.2326	0.0372	52	265.0585	265.05	0.0049
13	11.975434	11.92615	0.4116	33	100.75	100.7275	0.0223	53	275.8551	275.85	0.0030
14	14.353614	14.28178	0.5005	34	107.4465	107.4377	0.0082	54	286.8694	286.86	0.0020
15	16.90261	16.88487	0.1049	35	114.3862	114.3632	0.0202	55	298.1012	298.1	0.0019
16	19.742184	19.70346	0.1962	36	121.5266	121.504	0.0186	56	309.5522	309.54	0.0030
17	22.795437	22.73703	0.2562	37	128.874	128.86	0.0109	57	321.2188	321.21	0.0041
18	26.046099	25.98526	0.2336	38	136.4529	136.4314	0.0158	58	333.0979	333.08	0.0043
19	29.510614	29.44794	0.2124	39	144.244	144.218	0.0180	59	345.1882	345.18	0.0033
20	33.161221	33.12489	0.1096	40	152.2451	152.2199	0.0165	60	357.497	357.49	0.0033
21	37.051623	37.03121	0.0551	41	160.4628	160.4379	0.0155	61	370.0202	370.01	0.0030
22	137.52	137.00	0.3753	42	168.8894	168.8713	0.0107	62	382.7551	382.75	0.0019
23	41.177514	41.15351	0.0583	43	177.5346	177.5199	0.0083	63	395.7039	395.7	0.0004
24	45.537431	45.49154	0.1008	44	186.3928	186.3839	0.0048	64	408.8804	408.87	0.0021

Gaussian energy comparison (BBCGKS 2006) - $N = 5 - 64$, $n = 4$.

Sketch of the proof - $\{\alpha_i\}$ case

- Let $f(t)$ be the Hermite's interpolant of degree $m = 2k - 1$ s.t.

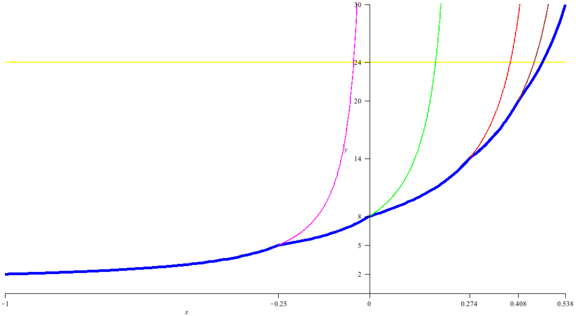
$$f(\alpha_i) = h(\alpha_i),\ f'(\alpha_i) = h'(\alpha_i),\ i = 1, 2, \ldots, k;$$

- The absolute monotonicity implies $f(t) \leq h(t)$ on $[-1, 1]$;
- The nodes $\{\alpha_i\}$ are zeros of $P_k(t) + cP_{k-1}(t)$ with $c > 0$;
- Since $\{P_k(t)\}$ are orthogonal (Jacobi) polynomials, the Hermite interpolant at these zeros has positive Gegenbauer coefficients (shown in Cohn-Kumar, 2007). So, $f(t) \in \mathcal{P}_\tau \cap A_{n,h}$;
- If $g(t) \in \mathcal{P}_\tau \cap A_{n,h}$, then by the quadrature formula

$$g_0 - \frac{g(1)}{N} = \sum_{i=1}^{k} \rho_i g(\alpha_i) \leq \sum_{i=1}^{k} \rho_i h(\alpha_i) = \sum_{i=1}^{k} \rho_i f(\alpha_i) = f_0 - \frac{f(1)}{N}$$

$\square$

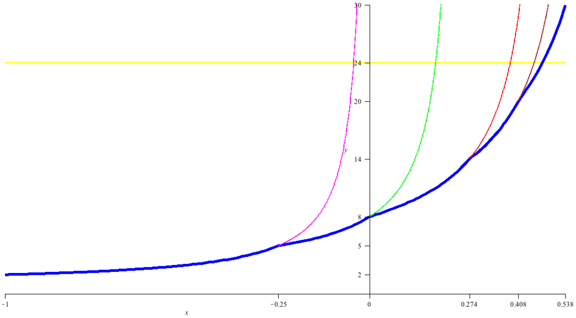
Suboptimal LP solutions for $m \leq m(N, n)$



Theorem - (BDHSS - 2014)

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 $N = 24$, $n = 4$, $m = 1 - 5$



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

Some Remarks

- The bounds do not depend (in certain sense) from the potential function h.
- The bounds are attained by all configurations called universally optimal in the Cohn-Kumar's paper apart from the 600-cell (a 120-point 11-design in four dimensions).
- Necessary and sufficient conditions for ULB global optimality and LP-universally optimal codes.
- Analogous theorems hold for other polynomial metric spaces (H_q^n, J_w^n, $\mathbb{RP}^n$, $\mathbb{CP}^n$, $\mathbb{HP}^n$).

Improvement of ULB (details in Stoyanova's talk)

P.B., D. Danev, S. Bumova, *Upper bounds on the minimum distance of spherical codes*, IEEE Trans. Inform. Theory, 41, 1996, 1576–1581.

- Let n and N be fixed, $N \in [D(n, 2k-1), D(n, 2k))$, $L_m(n,s) = N$ and j be positive integer.
- [BDB] introduce the following **test functions** in n and $s \in \mathcal{I}_{2k-1}$

$$Q_j(n,s) = \frac{1}{N} + \sum_{i=1}^{k} \rho_i P_j^{(n)}(\alpha_i) \qquad (7)$$

  (note that $P_j^{(n)}(1) = 1$).
- Observe that $Q_j(n,s) = 0$ for every $1 \le j \le 2k-1$.
- We shall use the functions $Q_j(n,s)$ to give necessary and sufficient conditions for existence of improving polynomials of higher degrees.

Necessary and sufficient conditions (2)

Theorem (Optimality characterization (BDHSS-2014))

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 $Q_j(n, s) < 0$ for some $j \geq 2k$.

Moreover, if $Q_j(n, s) < 0$ 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 $Q_j(n, \alpha_k) \geq 0$, $j \geq j_0(n, N)$.

Corollary

If $Q_j(n, s) \geq 0$ for all $j > \tau(n, N)$, then $f^h_{\tau(n,N)}(t)$ solves the (LP).

Sketch of the proof - $\{\alpha_i\}$ case

"$\Longrightarrow$" Suppose $Q_j(n,s) \geq 0$, $j \geq 2e$. For any $f \in \mathcal{P}_r \cap A_{n,h}$ we write

$$f(t) = g(t) + \sum_{2e}^{r} f_i P_i^{(n)}(t)$$

with $g \in \mathcal{P}_{2e-1} \cap A_{n,h}$. Manipulation yields

$$Nf_0 - f(1) = N\sum_{i=0}^{e-1} \rho_i f(\alpha_i) - N\sum_{j=2e}^{r} f_j Q_j(n,s) \leq N\sum_{i=0}^{k} \rho_i h(\alpha_i).$$

"$\Longleftarrow$" Let now $Q_j(n,s) < 0$, $j \geq 2e$. Select $\epsilon > 0$ s.t. $h(t) - \epsilon P_j^{(n)}(t)$ is absolutely monotone. We improve using $f(t) = \epsilon P_j^{(n)}(t) + g(t)$, where

$$g(\alpha_i) = h(\alpha_i) - \epsilon P_j^{(n)}(\alpha_i),\ g'(\alpha_i) = h'(\alpha_i) - \epsilon (P_j^{(n)})'(\alpha_i) \qquad \square$$

Examples

Definition

A universal configuration is called **LP universal** if it solves the finite LP problem.

Remark

Ballinger, Blekherman, Cohn, Giansiracusa, Kelly, and Shűrmann, conjecture two universal codes $(40, 10)$ *and* $(64, 14)$.

Theorem

The spherical codes $(N, n) = (40, 10)$, $(64, 14)$ *and* $(128, 15)$ *are not LP-universally optimal.*

Proof.

We prove $j_0(10, 40) = 10$, $j_0(14, 64) = 8$, $j_0(15, 128) = 9$. $\square$

Test functions - examples

j	(4, 24)	(10, 40)	(14, 64)	(15, 128)	(7, 182)	(4, 120)
0	1	1	1	1	1	1
1	0	0	0	0	0	0
2	0	0	0	0	0	0
3	0	0	0	0	0	0
4	0	0.021943574	0.013744273	0.000659722	0	0
5	0	0.043584477	0.023867606	0.012122396	0	0
6	0.085714286	0.024962302	0.015879248	0.010927837	0	0
7	0.16	0.015883951	0.012369147	0.005957261	0	0
8	-0.024	0.026086948	0.015845575	0.006751842	0.022598277	0
9	-0.02048	0.02824122	0.016679926	0.008493915	0.011864096	0
10	0.064232727	0.024663991	0.015516168	0.00811866	-0.00835109	0
11	0.036864	0.024338487	0.015376208	0.007630277	0.003071311	0
12	0.059833108	0.024442076	0.01558101	0.007746238	0.009459538	0.053050398
13	0.06340608	0.024976926	0.015644873	0.007809405	0.0065461	0.066587396
14	0.054456422	0.025919671	0.015734138	0.007817465	0.005369545	-0.046646712
15	-0.003869491	0.02498472	0.015637274	0.007865499	0.006137772	-0.018428319
16	0.008598724	0.024214119	0.015521057	0.007815602	0.005268455	0.020868837
17	0.091970863	0.025123445	0.01562458	0.007761374	0.005134928	-0.000422871
18	0.049262707	0.025449746	0.015694798	0.007812225	0.004722806	0.012656294
19	0.035330484	0.024905002	0.015617497	0.00784714	0.003857119	0.006371173
20	0.048230925	0.024837415	0.015589583	0.00781076	0.007863772	0.011244953

ULB for projective spaces $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$ (1)

Denote $\mathbb{T}_\ell\mathbb{P}^{n-1}$, $\ell = 1, 2, 4$ – projective spaces $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$.

The Levenshtein intervals are

$$\mathcal{I}_m = \begin{cases} \left[t_{k-1,\ell}^{1,1}, t_{k,\ell}^{1,0}\right], & \text{if } m = 2k-1, \\ \left[t_{k,\ell}^{1,0}, t_{k,\ell}^{1,1}\right], & \text{if } m = 2k, \end{cases}$$

where $t_{i,\ell}^{a,b}$ is the greatest zero of $P_i^{(a+\frac{\ell(n-1)}{2}-1, b+\frac{\ell}{2}-1)}(t)$.
The Levenshtein function is given as

$$L(n,s) = \begin{cases} \binom{k+\frac{\ell(n-1)}{2}-1}{k-1} \frac{\binom{k+\frac{\ell n}{2}-2}{k-1}}{\binom{k+\frac{\ell}{2}-2}{k-1}} \left[1 - \frac{P_k^{(\frac{\ell(n-1)}{2}, \frac{\ell}{2}-1)}(s)}{P_k^{(\frac{\ell(n-1)}{2}-1, \frac{\ell}{2}-1)}(s)}\right], & s \in \mathcal{I}_{2k-1} \\ \binom{k+\frac{\ell(n-1)}{2}-1}{k-1} \frac{\binom{k+\frac{\ell n}{2}-1}{k}}{\binom{k+\frac{\ell}{2}-1}{k}} \left[1 - \frac{P_k^{(\frac{\ell(n-1)}{2}, \frac{\ell}{2})}(s)}{P_k^{(\frac{\ell(n-1)}{2}-1, \frac{\ell}{2})}(s)}\right], & s \in \mathcal{I}_{2k}. \end{cases}$$

ULB for projective spaces $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$ (2)

The Delasarte-Goethals-Seidel numbers are:

$$D_\ell(n,\tau) = \begin{cases} \dfrac{\binom{k+\frac{\ell(n-1)}{2}-1}{k}\binom{k+\frac{\ell n}{2}-1}{k}}{\binom{k+\frac{\ell}{2}-1}{k}}, & \text{if } \tau = 2k-1, \\ \\ \dfrac{\binom{k+\frac{\ell(n-1)}{2}-1}{k}\binom{k+\frac{\ell n}{2}-1}{k}}{\binom{k+\frac{\ell}{2}-1}{k}}, & \text{if } \tau = 2k. \end{cases}$$

The Levenshtein $1/N$-quadrature nodes $\{\alpha_{i,\ell}\}_{i=1}^{k}$ (respectively $\{\beta_{i,\ell}\}_{i=1}^{k}$), are the roots of the equation

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

where $s = \alpha_k$ (respectively $s = \beta_k$) and $P_i(t) = P_i^{(\frac{\ell(n-3)}{2},\frac{\ell}{2}-1)}(t)$ (respectively $P_i(t) = P_i^{(\frac{\ell(n-3)}{2},\frac{\ell}{2})}(t)$) are Jacobi polynomials.

ULB for projective spaces $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$ (3)

ULB for $\mathbb{RP}^{n-1}$, $\mathbb{CP}^{n-1}$, $\mathbb{HP}^{n-1}$ - (BDHSS - 2015)

Given the projective space $\mathbb{T}_\ell\mathbb{P}^{n-1}$, $\ell = 1, 2, 4$, let h be a fixed absolutely monotone potential, n and N be fixed, and $\tau = \tau(n, N)$ be such that $N \in [D_\ell(n, \tau), D_\ell(n, \tau + 1))$. Then the Levenshtein nodes $\{\alpha_{i,\ell}\}$, respectively $\{\beta_{i,\ell}\}$, provide the bounds

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

respectively,

$$\mathcal{E}(n, N, h) \geq N^2 \sum_{i=0}^{k} \gamma_i h(\beta_{i,\ell}).$$

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

Conclusions and future work

- ULB works for all absolutely monotone potentials
- Particularly good for analytic potentials
- Necessary and sufficient conditions for improvement of the bound

Future work:

- Johnson polynomial metric spaces
- Asymptotics of ULB for all polynomial metric spaces
- Relaxation of the inequality $f(t) \leq h(t)$ on $[-1, 1]$
- ULB and the analytic properties of the potential function

THANK YOU!