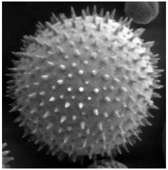
ESI MINIMAL ENERGY POINT SETS, LATTICES AND DESIGNS, 2014

Universal lower bounds for potential energy of spherical codes

Peter Dragnev
Indiana University-Purdue University Fort Wayne



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

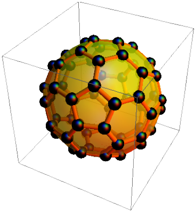
Outline

- 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
- Conclusions and summary of future work

Why Minimize Potential Energy? Electrostatics:

Thomson Problem (1904) -
("plum pudding" model of an atom)

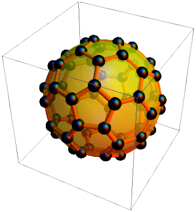
Find the (most) stable (ground state) energy configuration (**code**) of *N* classical electrons (Coulomb law) constrained to move on the sphere $\mathbb{S}^2$.



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**

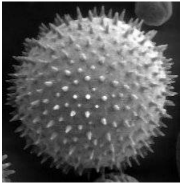
$$E_s(C) := \sum_{j \neq k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad s > 0, \qquad E_{\log}(\omega_N) := \sum_{j \neq k} \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

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

Why Minimize Potential Energy? Coding:

Tammes Problem (1930)

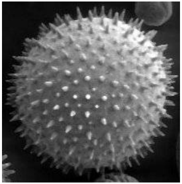
A Dutch botanist that studied modeling of the distribution of the orifices in pollen grain asked the following.



Why Minimize Potential Energy? Coding:

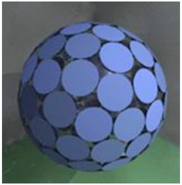
Tammes Problem (1930)

A Dutch botanist that studied modeling of the distribution of the orifices in pollen grain asked the following.



Tammes Problem (Best-Packing, $s = \infty$)

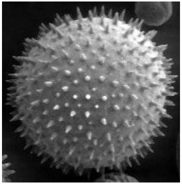
Place N points on the unit sphere so as to maximize the minimum distance between any pair of points.



Why Minimize Potential Energy? Coding:

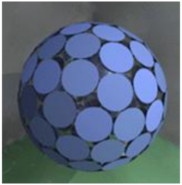
Tammes Problem (1930)

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.



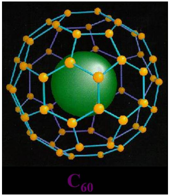
Definition

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

Why Minimize Potential Energy? Nanotechnology:

Fullerenes (1985) - (Buckyballs)

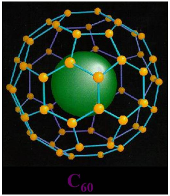
Vaporizing graphite, Curl, Kroto, Smalley, Heath, and O'Brian discovered C_{60} (Chemistry 1996 Nobel prize)

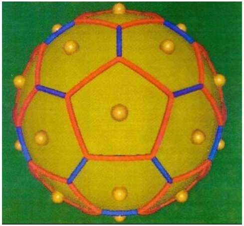


Why Minimize Potential Energy? Nanotechnology:

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

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 $\mathbb{S}^2$

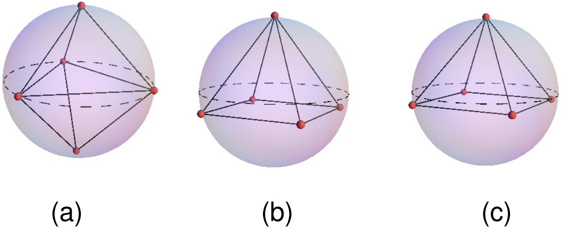


Figure : 'Optimal' 5-point codes on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) 'optimal' SBP ($s = 16$).

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

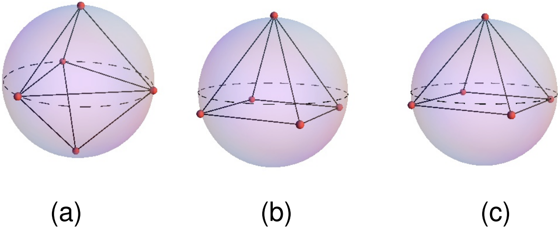
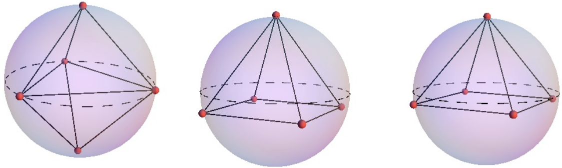


Figure : 'Optimal' 5-point codes on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) 'optimal' SBP ($s = 16$).

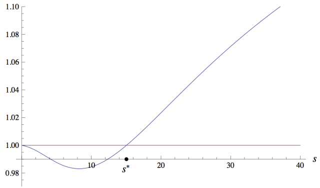
- P. Dragnev, D. Legg, and D. Townsend, *Discrete logarithmic energy on the sphere*, Pacific J. Math. **207** (2002), 345–357.
- X. Hou, J. Shao, *Spherical Distribution of 5 Points with Maximal Distance Sum*, Discr. Comp. Geometry, **46** (2011), 156–174
- R. E. Schwartz, *The Five-Electron Case of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

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



(a) (b) (c)

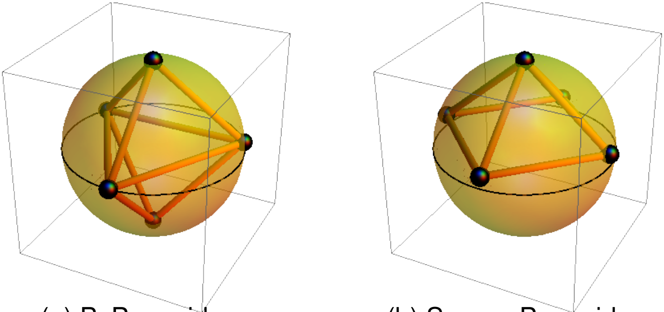
Figure : 'Optimal' 5-point code on $\mathbb{S}^2$: (a) bipyramid BP, (b) optimal square-base pyramid SBP ($s = 1$) , (c) 'optimal' SBP ($s = 16$).



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) ByPyramid (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.

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

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

Other potentials (low. semicont.);

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

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 $h \geq f$ 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

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

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

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

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

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

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

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

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

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

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

Spherical designs and DGS Bound

- 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.

Spherical designs and DGS Bound

- 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 (1)

- 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

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

- 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 (2)

Theorem (Levenshtein - 1979)

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

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

to derive the bound

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

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

Connections between DGS- and L-bounds

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

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

  is continuous in s.

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

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

$$L_{2e-1}(n, t_e^{1,0}) = L_{2e}(n, t_e^{1,0}) = D(n, 2e)$$

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

Levenshtein Function - $n = 4$

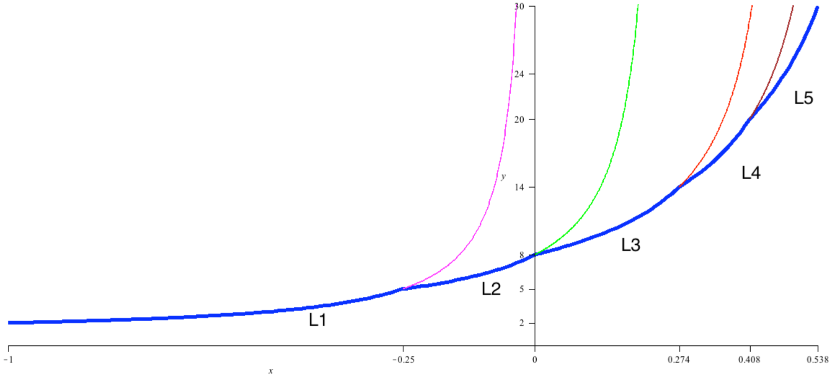


Figure : The Levenshtein function $L(4, s)$.

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

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

- 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

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

Proposition

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

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

(b) We have

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

If there is some $f \in \Lambda \cap A_{n,h}$ such that $f(\alpha_i) = h(\alpha_i)$ for $i = 1, \ldots, e-1$, 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 $\{\alpha_0, \ldots, \alpha_{e-1}, 1\} = \{\langle x, y\rangle : x, y \in C\}$ and $\rho_i =$ fraction of times α_i occurs in $\{\langle x, y\rangle : x, y \in C\}$ gives a $1/N$ quadrature rule exact for $\Lambda = \mathcal{P}_\tau$.

Levenshtein Quadrature Rules

Of particular interest is when the number of nodes e satisfies $m = 2e - 1$ or $m = 2e$. 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 : From: H.Cohn, A.Kumar, JAMS 2007.

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

- For every fixed (cardinality) $N > D(n, 2e-1)$ there exist uniquely determined real numbers $-1 \leq \alpha_0 < \alpha_1 < \cdots < \alpha_{e-1} < 1$ and $\rho_0, \rho_1, \ldots, \rho_{e-1}$, $\rho_i > 0$ for $i = 0, 1, \ldots, e-1$, such that the equality

$$f_0 = \frac{f(1)}{N} + \sum_{i=0}^{e-1} \rho_i f(\alpha_i)$$

  holds for every real polynomial $f(t)$ of degree at most $2e-1$.
- The numbers α_i, $i = 0, 1, \ldots, e-1$, are the roots of the equation

$$P_e(t)P_{e-1}(s) - P_e(s)P_{e-1}(t) = 0,$$

  where $s = \alpha_{e-1}$, $P_i(t) = P_i^{(n-1)/2,(n-3)/2}(t)$ is a Jacobi polynomial.
- In fact, α_i, $i = 0, 1, \ldots, e-1$, are the roots of the Levenshtein's polynomial $f_{2e-1}^{(n,\alpha_{e-1})}(t)$.

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

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

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

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

Universal Lower Bound (ULB)

Main Theorem - (BDHSS - 2014)

Let h be a fixed absolutely monotone potential, N and n be fixed, and $m = m(N,n)$ be such that $N \in [D(n,m), D(n,m+1))$. Then the Levenshtein nodes $\{\alpha_i\}$, respectively $\{\beta_i\}$, provide the bounds

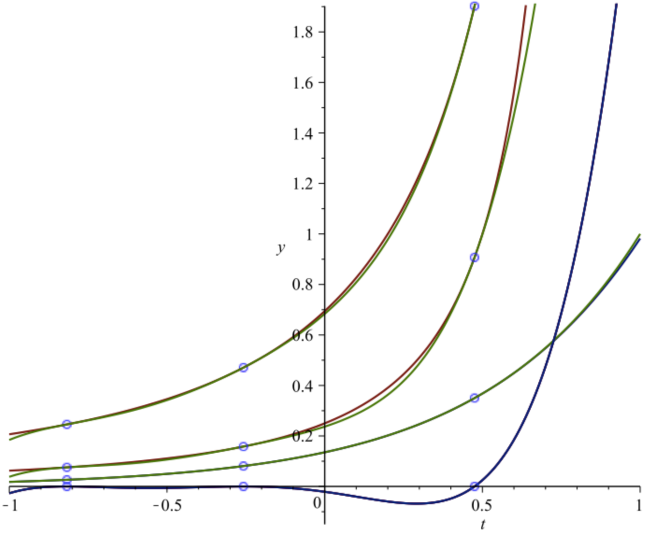
$$\mathcal{E}(n,N,h) \geq N^2 \sum_{i=0}^{e-1} \rho_i h(\alpha_i),$$

respectively,

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

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

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	0.82084999	0.82084999	0.0000%	25	54.834017	54.814185	0.0362%	45	195.47125	195.4631	0.0042%
6	1.51673996	1.46902376	3.1460%	26	59.8395	59.798598	0.0684%	46	204.76757	204.7576	0.0049%
7	2.35135701	2.30301138	2.0561%	27	65.02733	64.998317	0.0446%	47	214.28344	214.2674	0.0075%
8	3.32130935	3.32130935	0.0000%	28	70.43742	70.413294	0.0343%	48	223.99398	223.9925	0.0007%
9	4.67427716	4.61437099	1.2816%	29	76.068713	76.043495	0.0332%	49	233.94211	233.9328	0.0040%
10	6.16258024	6.12366846	0.6314%	30	81.918295	81.888894	0.0359%	50	244.09388	244.0884	0.0022%
11	7.91373588	7.85	0.8517%	31	87.991423	87.953066	0.0436%	51	254.46646	254.4593	0.0028%
12	9.80409023	9.78080643	0.2375%	32	94.267668	94.232601	0.0372%	52	265.05852	265.0455	0.0049%
13	11.9754345	11.9261471	0.4116%	33	100.74997	100.72747	0.0223%	53	275.85509	275.8469	0.0030%
14	14.3536144	14.2817803	0.5005%	34	107.44648	107.43767	0.0082%	54	286.86944	286.8636	0.0020%
15	16.9026095	16.8848736	0.1049%	35	114.38622	114.36316	0.0202%	55	298.10119	298.0956	0.0019%
16	19.7421843	19.703455	0.1962%	36	121.5266	121.50395	0.0186%	56	309.55223	309.543	0.0030%
17	22.7954372	22.7370274	0.2562%	37	128.87404	128.86002	0.0109%	57	321.2188	321.2056	0.0041%
18	26.0460988	25.9852626	0.2336%	38	136.45288	136.43137	136.431	58	333.09792	333.0836	0.0043%
19	29.5106143	29.4479356	0.2124%	39	144.24399	144.21799	0.0180%	59	345.18817	345.1768	0.0033%
20	33.1612211	33.124887	0.1096%	40	152.24506	152.21987	0.0165%	60	357.49695	357.4852	0.0033%
21	37.0516229	37.0312077	0.0551%	41	160.46282	160.43793	0.0155%	61	370.02024	370.00899	0.0030%
22	137.52	137.00	0.3753%	42	168.88936	168.87128	0.0107%	62	382.75512	382.748	0.0019%
23	41.1775139	41.1535087	0.0583%	43	177.5346	177.51993	0.0083%	63	395.70391	395.7023	0.0004%
24	45.5374314	45.4915404	0.1008%	44	186.39278	186.38387	0.0048%	64	408.88043	408.8719	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 $m = 2e - 1$ s.t.

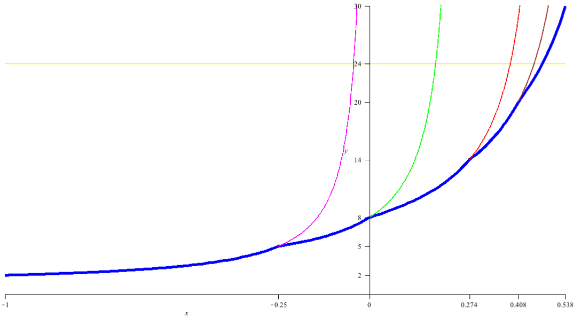
$$f(\alpha_i) = h(\alpha_i),\ f'(\alpha_i) = h'(\alpha_i),\ i = 0, 1, \ldots, e-1;$$

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

$$g_0 - \frac{g(1)}{N} = \sum_{i=0}^{e-1} \rho_i g(\alpha_i) \leq \sum_{i=0}^{e-1} \rho_i h(\alpha_i) = \sum_{i=0}^{e-1} \rho_i f(\alpha_i)$$

$\square$

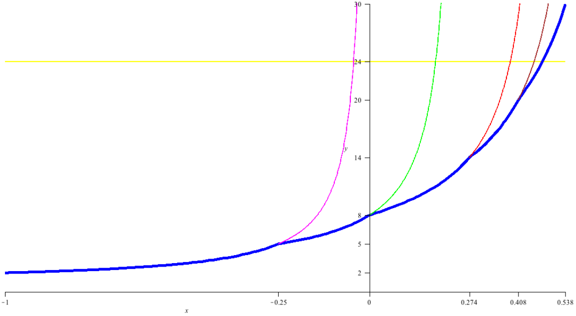
Suboptimal LP solutions for $m \le m(N, n)$



Theorem - (BDHSS - 2014)

The linear program (LP) can be solved for any $m \le m(N, n)$ 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

- Analogous theorems hold for other polynomial metric spaces (H_q^n, J_w^n, $\mathbb{RP}^n$, $\mathbb{CP}^n$, $\mathbb{HP}^n$). We are pursuing this in a separate work.
- 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).
- However, the bounds can be improved in other cases. There are necessary and sufficient conditions for their global optimality.

Improvement of ULB

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

$$Q_j(n,s) = \frac{1}{N} + \sum_{i=0}^{e-1} \rho_i P_j^{(n)}(\alpha_i) \tag{7}$$

(note that $P_j^{(n)}(1) = 1$).

- Observe that $Q_j(n,s) = 0$ for every $1 \leq j \leq 2e-1$.
- 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

$$L(n, N, 2e-1; h) \geq N^2 \sum_{i=0}^{e-1} \rho_i h(\alpha_i)$$

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

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

Proof – follows ideas from BDB-1996 where the test functions were first introduced w.r.t. optimal/maximal codes.

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

Cohn et.el. conjecture two universal codes $(40, 10)$ *and* $(64, 14)$*. Computational experiments show that all test functions* $Q_j(n, s) > 0$*, which suggests that unlike the* 600*-cell, these configurations are* **not** *LP universally optimal.*

Test functions - examples

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

Applications – asymptotic bounds (1)

- Let the dimension n and the cardinality N tend simultaneously to infinity in the relation

$$\lim \frac{N}{n^{e-1}} = \frac{1}{(e-1)!} + \gamma,$$

where $\gamma \geq 0$ is a constant, i.e. $N \sim n^{e-1}(\frac{1}{(e-1)!} + \gamma)$.

- We know (Boumova-Danev, ACCT2002) the asymptotic behaviour of the parameters:

$$\alpha_i \sim 0, \quad \text{for } i = 1, 2, \ldots, e-1,$$

$$\alpha_0 \sim -\frac{1}{1+\gamma(e-1)!},$$

$$\rho_0 N \sim (1+\gamma(e-1)!)^{2e-1}.$$

Applications – asymptotic bounds (2)

- Now the bounds are easy to be calculated –

$$\begin{aligned} W(n, N, 2e-1; h) &\geq N^2 \sum_{i=0}^{e-1} \rho_i h(\alpha_i) \\ &\sim N^2 \left(\rho_0 h(\alpha_0) + h(0) \sum_{i=1}^{e-1} \rho_i \right) \sim h(0) N^2. \end{aligned}$$

- Similarly, in the even case $W(n, N, 2e; h) \gtrsim h(0)N^2$.
- Kedrock codes mapped from the binary hamming space to the Euclidean sphere attain this bound.

Applications – asymptotic bounds (3)

- Let now n be fixed and $N \to \infty$. From $N \in [D(n,m), D(n,m+1))$ we have that $N \sim m^{n-1}$.
- For some special potentials, say Riesz $k_\alpha(t) = (2(1-t))^{-\alpha/2}$ with $\alpha > n-1$ we can derive the energy asymptotics

$$\mathcal{E}(n, N, k_\alpha) \sim N^{1+\frac{\alpha}{n-1}},$$

from the ULB bound

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:

- Other polynomial metric spaces, such as Binary Hamming, q-Hamming, Johnson, Projective
- Analytic investigation
- Relaxation of the inequality $f(t) \leq h(t)$ on $[-1, 1]$

THANK YOU!