Delsarte-Yudin LP method and Universal Lower Bound on energy

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Outline

- Why minimize energy?
- Delsarte-Yudin LP approach
- DGS bounds for spherical $\tau$-designs
- 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 $S^2$.

**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.

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 $S^2$

**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.
Optimal five point log and Riesz $s$-energy code on $S^2$

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

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

Figure: 5 points energy ratio
Optimal five point log and Riesz $s$-energy code on $S^2$

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.

Minimal $h$-energy - preliminaries

- Spherical Code: A finite set $C \subset S^{n-1}$ with cardinality $|C|$;
- Let the *interaction potential* $h : [-1, 1] \rightarrow \mathbb{R} \cup \{+\infty\}$ 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

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

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

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

- **Harm**(k): homogeneous harmonic polynomials in n variables of degree k restricted to $S^{n-1}$ with

$$r_k := \dim \text{Harm}(k) = \binom{k + n - 3}{n - 2} \binom{2k + n - 2}{k}.$$  

- **Spherical harmonics** (degree k): $\{Y_{kj}(x) : j = 1, 2, \ldots, r_k\}$ orthonormal basis of Harm(k) with respect to integration using $(n - 1)$-dimensional surface area measure on $S^{n-1}$.

- 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:

\[
\frac{1}{r_k} \sum_{j=1}^{r_k} Y_{kj}(x) Y_{kj}(y) = P^{(n)}_k(t), \quad t = \langle x, y \rangle, \ x, y \in S^{n-1}.
\]

- Consequence: If \( C \) is a spherical code of \( N \) points on \( S^{n-1} \),

\[
\sum_{x, y \in C} P^{(n)}_k(\langle x, y \rangle) = \frac{1}{r_k} \sum_{j=1}^{r_k} \sum_{x \in C} \sum_{y \in C} Y_{kj}(x) Y_{kj}(y) = \frac{1}{r_k} \sum_{j=1}^{r_k} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 \geq 0.
\]
Suppose $f: [-1, 1] \rightarrow \mathbb{R}$ is of the form

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

Then:

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

Then:

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

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

$$\geq f_0 N^2 - f(1)N = N^2 \left( f_0 - \frac{f(1)}{N} \right).$$
**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

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

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

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

An \( N \)-point spherical code \( C \) satisfies \( E(n, C; h) = N^2 \left( f_0 - f(1)/N \right) \) 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

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

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

Given \( n \) and \( N \) we shall solve the program for all \( m \leq \tau(n, N) \).
Spherical designs and DGS Bound


**Definition**

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

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

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

The strength of $C$ is the maximal number $\tau = \tau(C)$ such that $C$ is a spherical $\tau$-design.
Spherical designs and DGS Bound


Theorem (DGS - 1977)

For fixed strength $\tau$ 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 $\tau$-designs $C \subset \mathbb{S}^{n-1}$.

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

• For every positive integer \( m \) we consider the intervals

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

• 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 \( P_i^{(a+n/2, b+n/2)}(t) \).

• The intervals \( \mathcal{I}_m \) define partition of \( \mathcal{I} = [-1, 1) \) to countably many nonoverlapping closed subintervals.
Theorem (Levenshtein - 1979)

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

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

to derive the bound

$$A(n, s) \leq \begin{cases} 
L_{2k-1}(n, s) = \binom{k+n-3}{k-1} \frac{2k+n-3}{n-1} - \frac{P_{k-1}^{(n)}(s) - P_k^{(n)}(s)}{(1-s)P_k^{(n)}(s)} & \text{for } s \in I_{2k-1}, \\
L_{2k}(n, s) = \binom{k+n-2}{k} \frac{2k+n-1}{n-1} - \frac{(1+s)(P_k^{(n)}(s) - P_{k+1}^{(n)}(s))}{(1-s)(P_k^{(n)}(s) + P_{k+1}^{(n)}(s))} & \text{for } s \in I_{2k}, 
\end{cases}$$

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

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

is continuous in $s$.

- 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 $I_m$. 
Levenshtein Function - $n = 4$

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

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

(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 $\Lambda$ if $-1 \leq \alpha_i < 1$ and $\rho_i > 0$ for $i = 1, 2, \ldots, k$ if

$$f_0 = \gamma_n \int_{-1}^{1} f(t)(1 - t^2)^{(n-3)/2} dt = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i), \quad (f \in \Lambda).$$
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 $C \subset S^{n-1}$ is a spherical $\tau$ design, then choosing $
\{\alpha_1, \ldots, \alpha_k, 1\} = \{\langle x, y \rangle : x, y \in C\}$ and $
\rho_i =$ fraction of times $\alpha_i$ 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 $k$ 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 $C \subset S^{n-1}$ 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 $C \subset S^{n-1}$ 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 $\mathbb{R}^n$). 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.

<table>
<thead>
<tr>
<th>n</th>
<th>N</th>
<th>M</th>
<th>Inner products</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>N</td>
<td>N-1</td>
<td>$\cos(2\pi j/N)$ (1 ≤ j ≤ N/2)</td>
<td>N-gon</td>
</tr>
<tr>
<td>n</td>
<td>N ≤ n</td>
<td>1</td>
<td>$-1/(N-1)$</td>
<td>simplex</td>
</tr>
<tr>
<td>n</td>
<td>n+1</td>
<td>2</td>
<td>$-1/n$</td>
<td>simplex</td>
</tr>
<tr>
<td>n</td>
<td>2n</td>
<td>3</td>
<td>$-1, 0$</td>
<td>cross polytope</td>
</tr>
<tr>
<td>3</td>
<td>12</td>
<td>5</td>
<td>$-1, \pm 1/\sqrt{5}$</td>
<td>icosahedron</td>
</tr>
<tr>
<td>4</td>
<td>120</td>
<td>11</td>
<td>$-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4$</td>
<td>600-cell</td>
</tr>
<tr>
<td>8</td>
<td>240</td>
<td>7</td>
<td>$-1, \pm 1/2, 0$</td>
<td>$E_8$ roots</td>
</tr>
<tr>
<td>7</td>
<td>56</td>
<td>5</td>
<td>$-1, \pm 1/3$</td>
<td>kissing</td>
</tr>
<tr>
<td>6</td>
<td>27</td>
<td>4</td>
<td>$-1/2, 1/4$</td>
<td>kissing/Schlafli</td>
</tr>
<tr>
<td>5</td>
<td>16</td>
<td>3</td>
<td>$-3/5, 1/5$</td>
<td>kissing</td>
</tr>
<tr>
<td>24</td>
<td>196560</td>
<td>11</td>
<td>$-1, \pm 1/2, \pm 1/4, 0$</td>
<td>Leech lattice</td>
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<td>23</td>
<td>4600</td>
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<td>$-1, \pm 1/3, 0$</td>
<td>kissing</td>
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<td>891</td>
<td>5</td>
<td>$-1/2, -1/8, 1/4$</td>
<td>kissing</td>
</tr>
<tr>
<td>23</td>
<td>552</td>
<td>5</td>
<td>$-1, \pm 1/5$</td>
<td>equiangular lines</td>
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<tr>
<td>22</td>
<td>275</td>
<td>4</td>
<td>$-1/4, 1/6$</td>
<td>kissing</td>
</tr>
<tr>
<td>21</td>
<td>162</td>
<td>3</td>
<td>$-2/7, 1/7$</td>
<td>kissing</td>
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<tr>
<td>22</td>
<td>100</td>
<td>3</td>
<td>$-4/11, 1/11$</td>
<td>Higman-Sims</td>
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<tr>
<td>$q^{3+1}_{q+1}$</td>
<td>(q + 1)(q^3 + 1)</td>
<td>3</td>
<td>$-1/q, 1/q^2$</td>
<td>isotropic subspaces</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4 if q = 2)</td>
<td>(q a prime power)</td>
</tr>
</tbody>
</table>

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 $\alpha_i$, $i = 1, 2, \ldots, k$, 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 $f_{2k-1}^{(n, \alpha_k)}(t)$. 
• 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

\[
f_0 = \frac{f(1)}{N} + \sum_{i=0}^{k} \gamma_i f(\beta_i)
\]  

is true for every real polynomial \( f(t) \) of degree at most \( 2k \).

• The numbers \( \beta_i, i = 0, 1, \ldots, k \), 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 \( f_{2k}^{(n,\beta_k)}(t) \).
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

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

respectively,

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

The Hermite interpolants at these nodes are the optimal polynomials which solve the finite LP in the class $P_\tau \cap A_{n,h}$. 
Gaussian, Korevaar, and Newtonian potentials
Newtonian energy comparison (BBCGKS 2006) - $N = 5 - 64$, $n = 4$. 

<table>
<thead>
<tr>
<th>N</th>
<th>Harmonic Energy</th>
<th>ULB Bound</th>
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### Gaussian energy comparison (BBCGKS 2006) - \( N = 5 - 64, \ n = 4 \).

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Sketch of the proof - \( \{\alpha_i\} \) case

- Let \( f(t) \) be the **Hermite’s interpolant** of degree \( m = 2k - 1 \) s.t.

  \[
  f(\alpha_i) = h(\alpha_i), \quad f'(\alpha_i) = h'(\alpha_i), \quad i = 1, 2, \ldots, k;
  \]

- 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

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

  □
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 $N = 24$, $n = 4$, $m = 1 - 5$

\[ f_1(t) = 0.499P_0(t) + 0.229P_1(t) \]
\[ f_2(t) = 0.581P_0(t) + 0.305P_1(t) + 0.093P_2(t) \]
\[ f_3(t) = 0.658P_0(t) + 0.395P_1(t) + 0.183P_2(t) + 0.069P_3(t) \]
\[ f_4(t) = 0.69P_0(t) + 0.43P_1(t) + 0.23P_2(t) + 0.10P_3(t) + 0.027P_4(t) \]
\[ f_5(t) = 0.71P_0(t) + 0.46P_1(t) + 0.26P_2(t) + 0.13P_3(t) + 0.05P_4(t) + 0.01P_5(t). \]
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 $(H_q^n, J_w^n, \text{RP}_n, \text{CP}_n, \text{HP}_n)$. 

• 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 $s \in \mathcal{I}_{2k-1}$

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

(note that $P_j^{(n)}(1) = 1$).
• Observe that $Q_j(n, s) = 0$ for every $1 \leq j \leq 2k - 1$.
• We shall use the functions $Q_j(n, s)$ to give necessary and sufficient conditions for existence of improving polynomials of higher degrees.
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 \( f_{\tau(n,N)}^h(t) \) solves the (LP).
**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

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Denote $T_\ell P^{n-1}$, $\ell = 1, 2, 4$ – projective spaces $\mathbb{R}P^{n-1}$, $\mathbb{C}P^{n-1}$, $\mathbb{H}P^{n-1}$.

The Levenshtein intervals are

$$I_m = \begin{cases} 
[t_{k-1,\ell}^1, t_{k,\ell}^1], & \text{if } m = 2k - 1, \\
[t_{k,\ell}^1, t_{k,\ell}^0], & \text{if } m = 2k,
\end{cases}$$

where $t_{i,\ell}^{a,b}$ is the greatest zero of $P_i^{(a + \ell(n-1)/2 - 1, b + \ell/2 - 1)}(t)$.

The Levenshtein function is given as

$$L(n, s) = \begin{cases} 
(k + \ell(n-1)/2 - 1) \binom{k + \ell(n-1)/2}{k - 1} \left[ 1 - \frac{P_k^{(\ell(n-1)/2, \ell/2 - 1)}(s)}{P_k^{(\ell(n-1)/2 - 1, \ell/2 - 1)}(s)} \right], & s \in I_{2k-1} \\
(k + \ell(n-1)/2 - 1) \binom{k + \ell(n-1)/2}{k} \left[ 1 - \frac{P_k^{(\ell(n-1)/2, \ell/2)}(s)}{P_k^{(\ell(n-1)/2 - 1, \ell/2)}(s)} \right], & s \in I_{2k}. 
\end{cases}$$
The Delasarte-Goethals-Seidel numbers are:

\[ D_\ell(n, \tau) = \begin{cases} 
\frac{(k + \frac{\ell(n-1)}{2} - 1)(k + \frac{\ell(n-1)}{2} - 1)}{(k + \frac{\ell}{2} - 1)} \left( k + \frac{\ell}{2} - 1 \right), & \text{if } \tau = 2k - 1, \\
\frac{(k + \frac{\ell(n-1)}{2} - 1)(k + \frac{\ell(n-1)}{2} - 1)}{(k + \frac{\ell}{2} - 1)} \left( k + \frac{\ell}{2} - 1 \right), & \text{if } \tau = 2k.
\end{cases} \]

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 \( P_i(t) = P_i^{\left(\frac{\ell(n-3)}{2}, \frac{\ell}{2} - 1\right)}(t) \) (respectively \( P_i(t) = P_i^{\left(\frac{\ell(n-3)}{2}, \frac{\ell}{2}\right)}(t) \)) are Jacobi polynomials.
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 polynomials 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!