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 $\tau$-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.
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 $S^2$

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 $\mathbb{S}^2$

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 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 $s^* \approx 15.048 \ldots$?

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

(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.

Henry Cohn and the five-point energy problem
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.

\(^1\)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: \( h(t) = \begin{cases} 0, & -1 \leq t \leq 1/2 \\ \infty, & 1/2 \leq t \leq 1 \end{cases} \)

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

- **$\text{Harm}(k)$**: 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 $\text{Harm}(k)$ 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 $P_k^{(n)}(1) = 1$).
The Gegenbauer polynomials and spherical harmonics are related through the well-known *Addition Formula*:

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

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

\[
\sum_{x, y \in C} P_k^{(n)}(\langle x, y \rangle) = \frac{1}{r_k} \sum_{j=1}^{r_k} \sum_{x \in C} \sum_{y \in C} Y_{kj}(x) Y_{kj}(y)
\]

\[
= \frac{1}{r_k} \sum_{j=1}^{r_k} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 \geq 0.
\]
Delsarte-Yudin approach:

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

Suppose \( f : [-1, 1] \to \mathbb{R} \) is of the form

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

\( f(1) = \sum_{k=0}^{\infty} f_k < \infty \implies \) 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

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

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 $\sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = 0$. 
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)
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(b) for all $k \geq 1$, either $f_k = 0$ or $\sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = 0$.

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 (Boyvalenkov)


**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 (Boyvalenkov)


Theorem (DGS - 1977)

For fixed strength $\tau$ and dimension $n$ denote by

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

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

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


- 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.
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

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

where $A(n, s) = \max\{|C| : \langle x, y \rangle \leq s \text{ for all } x \neq y \in C, \}$
Interplay between DGS- and L-bounds (Boyvalenko)

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

\[
L_{2k-2}(n, t^1_{k-1}) = L_{2k-1}(n, t^1_{k-1}) = D(n, 2k - 1),
\]

\[
L_{2k-1}(n, t^1_0) = L_{2k}(n, t^1_0) = D(n, 2k)
\]

at the ends of the intervals \( I_m \).

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

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

is continuous and piece-wise smooth in \( s \).
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

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

(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
$\Lambda = P_\tau$.

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>$\cos(2\pi j/N)$ $(1 \leq j \leq N/2)$</td>
<td>$N$-gon</td>
</tr>
<tr>
<td>$n$</td>
<td>$N \leq n$</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>2$n$</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>
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<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>
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<tr>
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<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>$-1/2, -1/8, 1/4$</td>
<td>kissing</td>
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<tr>
<td>23</td>
<td>552</td>
<td>5</td>
<td>$-1, \pm 1/5$</td>
<td>equiangular lines</td>
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<td>$-4/11, 1/11$</td>
<td>Higman-Sims</td>
</tr>
</tbody>
</table>

\[ q^{q^3 + 1} \over q + 1 \] \( (q + 1)(q^3 + 1) \) \( 3 \) \( 4 \text{ if } q = 2 \) \( -1/q, 1/q^2 \) \( (q \text{ a prime power}) \)

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 $\alpha_i$, $i = 1, 2, \ldots, k$, 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 $f^{(n,\alpha_k)}_{2k-1}(t)$. 
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 \( f_{2k}^{(n,\beta_k)}(t) \).
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 polynomials which solve the finite LP in the class $\mathcal{P}_\tau \cap \mathcal{A}_{n,h}$. 

Main Theorem - (BDHSS - 2014)
Gaussian, Korevaar, and Newtonian potentials
Newtonian energy comparison (BBCGKS 2006) - $N = 5 - 64, n = 4$. 

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

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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

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

  $\square$
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 $P_m \cap A_{n,h}$ is given by the Hermite interpolants at the Levenshtein nodes determined by $N = L_m(n, s)$. 
Suboptimal LP solutions for $N = 24$, $n = 4$, $m = 1 - 5$

\[
\begin{align*}
  f_1(t) &= .499P_0(t) + .229P_1(t) \\
  f_2(t) &= .581P_0(t) + .305P_1(t) + 0.093P_2(t) \\
  f_3(t) &= .658P_0(t) + .395P_1(t) + .183P_2(t) + 0.069P_3(t) \\
  f_4(t) &= .69P_0(t) + .43P_1(t) + .23P_2(t) + .10P_3(t) + 0.027P_4(t) \\
  f_5(t) &= .71P_0(t) + .46P_1(t) + .26P_2(t) + .13P_3(t) + 0.05P_4(t) + 0.01P_5(t).
\end{align*}
\]
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 ($H_q^n$, $J_w^n$, $RP^n$, $CP^n$, $HP^n$).
Improvement of ULB (details in Stoyanova’s talk)


- 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 \( s \in \mathcal{I}_{2k - 1} \)

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

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

"\(\implies\)" 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

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

"\(\impliedby\)" 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

\[
g(\alpha_i) = h(\alpha_i) - \epsilon P_j^{(n)}(\alpha_i), \quad g'(\alpha_i) = h'(\alpha_i) - \epsilon (P_j^{(n)})'(\alpha_i)
\]
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 \(j_0(10, 40) = 10, j_0(14, 64) = 8, j_0(15, 128) = 9\). \(\square\)
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Denote $T_{\ell}P^{n-1}$, $\ell = 1, 2, 4$ – projective spaces $RP^{n-1}$, $CP^{n-1}$, $HP^{n-1}$.

The Levenshtein intervals are

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

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

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

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

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

Given the projective space $T_\ell \mathbb{P}^{n-1}$, $\ell = 1, 2, 4$, 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!