Universal Lower Bounds for the Energy of Spherical Codes

Edward B. Saff
Vanderbilt University

Joint work with: P. Boyvalenkov (BAS); P. Dragnev (IPFW), D. Hardin (Vanderbilt); and M. Stoyanova (Sofia) (BDHSS)
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 $C := \{x_1, \ldots, x_N\} \subset \mathbb{S}^{n-1} := \{x \in \mathbb{R}^n : |x| = 1\}$ 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 pairwise distance are called **optimal (maximal) codes**.
Why Minimize Potential Energy? Nanotechnology:

**Fullerenes** (1985) - (Buckyballs)
Vaporizing graphite, **Curl, Kroto, Smalley**, Heath, and O’Brien discovered $C_{60}$ (Chemistry 1996 Nobel prize)

Duality structure: 32 electrons and $C_{60}$. 
Optimal s-energy codes on $S^2$ ($1/r^s$ and $\log(1/r)$)

**Known optimal s-energy codes on $S^2$**

- $s = \log$, logarithmic points (known for $N = 2 – 6, 12$);
- $s = 1$, Thomson Problem (known for $N = 2 – 6, 12$)
- $s > 0$ arbitrary, (known for $N = 2, 3, 4, 6, 12$) sharp codes
- $s \rightarrow \infty$, Tammes Problem (known for $N = 1 – 14, 24$)

**Limiting case - Best packing**

For fixed $N$, any limit as $s \rightarrow \infty$ of optimal s-energy codes is an optimal (maximal) code.
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$

bipyramid

optimal square-base pyramid
Melnyk et al (1977) Bipyramid appears optimal for $0 < s < s^*$ where $s^* \approx 15.04808$.

Recently proved by R. Schwartz (over 150 pages + computer assist).

P. Dragnev et al. $s = \log$

Open problem for $s > s^* + \epsilon$
MORALS

Optimal Riesz $s$-energy configurations, in general, depend on $s$.

Rigorous proofs of computational observations can be quite difficult.
Minimal $h$-energy - preliminaries

- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$;
- Let the interaction potential $h : [-1, 1] \rightarrow \mathbb{R} \cup \{+\infty\}$ be an absolutely monotone\(^1\) function;
- The $h$-energy of a spherical code $C$:

$$E(n, C; h) := \sum_{x, y \in C, x \neq y} h(\langle x, y \rangle), \quad |x - y|^2 = 2 - 2\langle x, y \rangle = 2(1 - t),$$

where $t = \langle x, y \rangle$ denotes Euclidean inner product of $x$ and $y$.

---

\(^1\)A function $f$ is absolutely monotone on $I$ if $f^{(k)}(t) \geq 0$ for $t \in I$ and $k = 0, 1, 2, \ldots$
Minimal $h$-energy - preliminaries

- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$;
- Let the interaction potential $h : [-1, 1] \rightarrow \mathbb{R} \cup \{+\infty\}$ be an absolutely monotone\(^1\) function;
- The $h$-energy of a spherical code $C$:

$$E(n, C; h) := \sum_{x, y \in C, x \neq y} h(\langle x, y \rangle), \quad |x - y|^2 = 2 - 2\langle x, y \rangle = 2(1 - t),$$

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: \( h(t) = \exp(2t - 2) = \exp(-|x - y|^2) \);
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: $h(t) = \exp(2t - 2) = \exp(-| x - y |^2)$

Other potentials:

‘Best-packing’ potential: $h_\phi(t) = \begin{cases} 
0, & -1 \leq t \leq \cos \phi \\
\infty, & \cos \phi < t \leq 1
\end{cases}$
Absolutely monotone potentials - examples

- Newton potential: \( h(t) = (2 - 2t)^{-\left(\frac{n-2}{2}\right)} = |x - y|^{-\left(\frac{n-2}{2}\right)} \);
- 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: \( h(t) = \exp(2t - 2) = \exp(-|x - y|^2) \);

Other potentials:

- ‘Best-packing’ potential: \( h_\phi(t) = \begin{cases} 
0, & -1 \leq t \leq \cos \phi \\
\infty, & \cos \phi < t \leq 1 
\end{cases} \)

Remark

Even if one ‘knows’ an optimal code, it is often 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

\[
gr_{k,n} := \dim \text{Harm}(k) = \binom{k + n - 3}{n - 2} \binom{2k + n - 2}{k}.
\]

- **Spherical harmonics** (degree \(k\)): \(\{ Y_{kj}(x) : j = 1, 2, \ldots, r_{k,n} \}\) orthonormal basis of \(\text{Harm}(k)\) with respect to normalized \((n - 1)\)-dimensional surface area measure on \(S^{n-1}\).
Spherical Harmonics and Gegenbauer polynomials

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

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

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

- For fixed dimension $n$, the **Gegenbauer polynomials** are polys of a single real variable $t$ defined by

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

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

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

**Note:** $P_k^{(n)}(1) = 1$ for all $k = 0, 1, \ldots$. 
Spherical Harmonics and Gegenbauer polynomials

• Gegenbauer polynomials $P_k^{(n)}(t)$ are special types of Jacobi polynomials $P_k^{(\alpha,\beta)}(t)$ orthogonal w.r.t. weight $(1 - t)^\alpha(1 + t)^\beta$ on $[-1, 1]$, where $\alpha = \beta = (n - 3)/2$.

• The Gegenbauer polynomials and spherical harmonics are related through the **Addition Formula**:

$$
\sum_{j=1}^{r_{k,n}} Y_{kj}(x) Y_{kj}(y) = r_{k,n} P_k^{(n)}(t), \quad t = \langle x, y \rangle, \ x, y \in S^{n-1}.
$$
Spherical Harmonics and Gegenbauer polynomials

- Gegenbauer polynomials $P_k^{(n)}(t)$ are special types of Jacobi polynomials $P_k^{(\alpha,\beta)}(t)$ orthogonal w.r.t. weight $(1 - t)^\alpha(1 + t)^\beta$ on $[-1, 1]$, where $\alpha = \beta = (n - 3)/2$.

- The Gegenbauer polynomials and spherical harmonics are related through the Addition Formula:

$$\sum_{j=1}^{r_{k,n}} Y_{kj}(x) Y_{kj}(y) = r_{k,n} P_k^{(n)}(t), \quad t = \langle x, y \rangle, \ x, y \in S^{n-1}.$$ 

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

$$\sum_{x, y \in C} P_k^{(n)}(\langle x, y \rangle) = \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \sum_{x \in C} \sum_{y \in C} Y_{kj}(x) Y_{kj}(y)$$

$$= \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 \geq 0.$$
'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 good lower bounds for the minimal $f$-energy $E(n, N; f)$. 

Suppose $f : [-1, 1] \rightarrow \mathbb{R}$ is of the form

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

$$f(1) = \sum_{k=0}^{\infty} f_k < \infty \implies \text{convergence is absolute and uniform.}$$
‘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 good lower bounds for the minimal $f$-energy $E(n, N; f)$.

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

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

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

Then for $C \subset \mathbb{S}^{n-1}$, $|C| = N$,

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

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

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

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

(2)

An $N$-point spherical code $C$ satisfies $E(n, C; h) = N^2 (f_0 - f(1)/N)$ if and only if both of the following hold:

(a) $f(t) = h(t)$ for all $t \in \{ \langle x, y \rangle : x \neq y, \ x, y \in C \}$.

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

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

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

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

The full LP problem consists of maximizing the lower bound (2), that is the linear objective functional,

$$F(f) := N^2(f_0 - \frac{f(1)}{N}),$$

over all continuous $f$ 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

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

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

Full linear programming is too ambitious, truncate to a finite dimensional LP problem by maximizing

$$F(f) := N^2 (f_0 - \frac{f(1)}{N}),$$

subject to $f \in \mathcal{P}_m \cap A_{n,h}$ or more generally to $\Lambda \cap A_{n,h}$. 
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 for all $f \in \Lambda$,

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

Suppose there exists a $1/N$-quadrature rule $\{(\alpha_i, \rho_i)\}_{i=1}^k$ that is exact for a subspace $\Lambda \subset C([-1, 1])$.

(a) If $f \in \Lambda \cap A_{n,h}$ exists, then

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

(b) Furthermore, 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 (4) and we obtain

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

If such an $f \in \Lambda \cap A_{n,h}$ exists for every absolutely monotone functions $h$, then we say that $\Lambda$ is a ULB-space for $n$ and $N$. 
Where to find such $1/N$ quadrature rules?
Spherical Designs and DGS Bound


**Definition**

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

\[
\frac{1}{\sigma(\mathbb{S}^{n-1})} \int_{\mathbb{S}^{n-1}} p(x) \, d\sigma(x) = \frac{1}{|C|} \sum_{x \in C} p(x)
\]

(\( \sigma(x) \) is surface area measure on \( \mathbb{S}^{n-1} \)) holds for all polynomials \( p(x) = p(x_1, x_2, \ldots, x_n) \) of degree at most \( \tau \).

The **strength** of \( C \) is the maximal number \( \tau = \tau(C) \) such that \( C \) is a spherical \( \tau \)-design.
How many points are needed for a $\tau$-design?

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 $C \subset \mathbb{S}^{n-1}$.

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

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

This follows from the fact that for a $\tau$-design $C$,
\[
\sum_{x, y \in C} P_k^{(n)}(\langle x, y \rangle) = \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 = 0, \text{ for } 1 \leq k \leq \tau
\]

and so if $f \in \mathcal{P}_\tau$, then
\[
\sum_{x, y \in C} f(\langle x, y \rangle) = \sum_{k=0}^{\tau} \sum_{x, y \in C} f_k P_k^{(n)}(\langle x, y \rangle) = N^2 f_0,
\]
or
\[
f_0 = \frac{1}{N^2} \sum_{x, y \in C} f(\langle x, y \rangle) = \frac{1}{N} f(1) + \sum_{i=1}^{k} \rho_i f(\alpha_i).
\]
Sharp Codes

**Definition**

A spherical code $C \subset \mathbb{S}^{n-1}$ is a *sharp* 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 as above, then $C$ is universally optimal; i.e., $C$ is $h$-energy optimal for any $h$ that is absolutely monotone on $[-1, 1]$. Hermite interpolant to $h$ at the $m$ inner products belongs to $A_{n,h}$ and $P_{2m-1}$ is a ULB subspace for $n$, and $N = |C|$.***

**Theorem (Cohn and Kumar, 2007)**

*Let $C$ be the 600-cell (120 in $\mathbb{R}^4$). Then there is $f \in \Lambda \cap A_{4,h}$, s.t. $f(\langle x, y \rangle) = h(\langle x, y \rangle)$ for all $x \neq y \in C$, where $
abla = P_{17} \cap \{f_{11} = f_{12} = f_{13} = 0\}$. Hence it is a universal code.*
Another valuable source of $1/N$-quadrature rules...
Another valuable source of $1/N$-quadrature rules...

Levenshtein
Main Theorem - (BDHSS - Constr. Approx., 2016)

Let \( h \) be a fixed absolutely monotone potential, \( n \) and \( N \) be fixed, and \( \tau = \tau(n, N) \) be such that \( N > D(n, \tau) \). Then for \( \tau = 2k - 1 \) the nodes \( \{\alpha_i\}_{i=1}^k \) for the Levenshtein \( 1/N \)-quadrature rule that is exact for \( \mathcal{P}_\tau \) provide the bounds

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

and similarly for \( \tau = 2k \) with Levenshtein nodes \( \{\alpha_i\}_{i=0}^k \). The Hermite interpolants at these nodes are the optimal polynomials that solve the finite LP in the class \( \mathcal{P}_\tau \cap A_{n,h} \).
<table>
<thead>
<tr>
<th>N</th>
<th>Harmonic Energy</th>
<th>ULB Bound</th>
<th>%</th>
<th>N</th>
<th>Harmonic Energy</th>
<th>ULB Bound</th>
<th>%</th>
<th>N</th>
<th>Harmonic Energy</th>
<th>ULB Bound</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4.00</td>
<td>4.00</td>
<td>0.00</td>
<td>25</td>
<td>182.99</td>
<td>182.38</td>
<td>0.34</td>
<td>45</td>
<td>664.48</td>
<td>663.00</td>
<td>0.22</td>
</tr>
<tr>
<td>6</td>
<td>6.50</td>
<td>6.42</td>
<td>1.28</td>
<td>26</td>
<td>199.69</td>
<td>199.00</td>
<td>0.35</td>
<td>46</td>
<td>697.26</td>
<td>695.40</td>
<td>0.27</td>
</tr>
<tr>
<td>7</td>
<td>9.50</td>
<td>9.42</td>
<td>0.88</td>
<td>27</td>
<td>217.15</td>
<td>216.38</td>
<td>0.36</td>
<td>47</td>
<td>730.75</td>
<td>728.60</td>
<td>0.29</td>
</tr>
<tr>
<td>8</td>
<td>13.00</td>
<td>13.00</td>
<td>0.00</td>
<td>28</td>
<td>235.40</td>
<td>234.50</td>
<td>0.38</td>
<td>48</td>
<td>764.59</td>
<td>762.60</td>
<td>0.26</td>
</tr>
<tr>
<td>9</td>
<td>17.50</td>
<td>17.33</td>
<td>0.95</td>
<td>29</td>
<td>254.38</td>
<td>253.38</td>
<td>0.39</td>
<td>49</td>
<td>799.70</td>
<td>797.40</td>
<td>0.29</td>
</tr>
<tr>
<td>10</td>
<td>22.50</td>
<td>22.33</td>
<td>0.74</td>
<td>30</td>
<td>274.19</td>
<td>273.00</td>
<td>0.43</td>
<td>50</td>
<td>835.12</td>
<td>833.00</td>
<td>0.25</td>
</tr>
<tr>
<td>11</td>
<td>28.21</td>
<td>28.00</td>
<td>0.74</td>
<td>31</td>
<td>294.79</td>
<td>293.51</td>
<td>0.43</td>
<td>51</td>
<td>871.98</td>
<td>869.40</td>
<td>0.30</td>
</tr>
<tr>
<td>12</td>
<td>34.42</td>
<td>34.33</td>
<td>0.26</td>
<td>32</td>
<td>315.99</td>
<td>314.80</td>
<td>0.38</td>
<td>52</td>
<td>909.19</td>
<td>906.60</td>
<td>0.28</td>
</tr>
<tr>
<td>13</td>
<td>41.60</td>
<td>41.33</td>
<td>0.64</td>
<td>33</td>
<td>337.79</td>
<td>336.86</td>
<td>0.28</td>
<td>53</td>
<td>947.15</td>
<td>944.60</td>
<td>0.27</td>
</tr>
<tr>
<td>14</td>
<td>49.26</td>
<td>49.00</td>
<td>0.53</td>
<td>34</td>
<td>360.52</td>
<td>359.70</td>
<td>0.23</td>
<td>54</td>
<td>985.88</td>
<td>983.40</td>
<td>0.25</td>
</tr>
<tr>
<td>15</td>
<td>57.62</td>
<td>57.48</td>
<td>0.24</td>
<td>35</td>
<td>384.54</td>
<td>383.31</td>
<td>0.32</td>
<td>55</td>
<td>1025.76</td>
<td>1023.00</td>
<td>0.27</td>
</tr>
<tr>
<td>16</td>
<td>66.95</td>
<td>66.67</td>
<td>0.42</td>
<td>36</td>
<td>409.07</td>
<td>407.70</td>
<td>0.33</td>
<td>56</td>
<td>1066.62</td>
<td>1063.53</td>
<td>0.29</td>
</tr>
<tr>
<td>17</td>
<td>76.98</td>
<td>76.56</td>
<td>0.54</td>
<td>37</td>
<td>434.19</td>
<td>432.86</td>
<td>0.31</td>
<td>57</td>
<td>1108.17</td>
<td>1104.88</td>
<td>0.30</td>
</tr>
<tr>
<td>18</td>
<td>87.62</td>
<td>87.17</td>
<td>0.51</td>
<td>38</td>
<td>460.28</td>
<td>458.80</td>
<td>0.32</td>
<td>58</td>
<td>1150.43</td>
<td>1147.05</td>
<td>0.29</td>
</tr>
<tr>
<td>19</td>
<td>98.95</td>
<td>98.48</td>
<td>0.48</td>
<td>39</td>
<td>487.25</td>
<td>485.51</td>
<td>0.36</td>
<td>59</td>
<td>1193.38</td>
<td>1190.03</td>
<td>0.28</td>
</tr>
<tr>
<td>20</td>
<td>110.80</td>
<td>110.50</td>
<td>0.27</td>
<td>40</td>
<td>514.90</td>
<td>513.00</td>
<td>0.37</td>
<td>60</td>
<td>1236.91</td>
<td>1233.83</td>
<td>0.25</td>
</tr>
<tr>
<td>21</td>
<td>123.74</td>
<td>123.37</td>
<td>0.30</td>
<td>41</td>
<td>543.16</td>
<td>541.40</td>
<td>0.32</td>
<td>61</td>
<td>1281.38</td>
<td>1278.45</td>
<td>0.23</td>
</tr>
<tr>
<td>22</td>
<td>137.52</td>
<td>137.00</td>
<td>0.38</td>
<td>42</td>
<td>572.16</td>
<td>570.60</td>
<td>0.27</td>
<td>62</td>
<td>1326.59</td>
<td>1323.88</td>
<td>0.20</td>
</tr>
<tr>
<td>23</td>
<td>152.04</td>
<td>151.38</td>
<td>0.44</td>
<td>43</td>
<td>601.93</td>
<td>600.60</td>
<td>0.22</td>
<td>63</td>
<td>1373.09</td>
<td>1370.13</td>
<td>0.22</td>
</tr>
<tr>
<td>24</td>
<td>167.00</td>
<td>166.50</td>
<td>0.30</td>
<td>44</td>
<td>632.73</td>
<td>631.40</td>
<td>0.21</td>
<td>64</td>
<td>1420.59</td>
<td>1417.20</td>
<td>0.24</td>
</tr>
</tbody>
</table>

Newtonian energy comparison (Ballinger et al 2006) - \( N = 5 – 64, \ n = 4 \).
### ULB comparison - Ballinger et al 2006 Gauss Energy

<table>
<thead>
<tr>
<th>N</th>
<th>Gaussian Energy</th>
<th>ULB Bound</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.82085</td>
<td>0.82085</td>
<td>0.000</td>
</tr>
<tr>
<td>6</td>
<td>1.51674</td>
<td>1.469024</td>
<td>3.146</td>
</tr>
<tr>
<td>7</td>
<td>2.351357</td>
<td>2.303011</td>
<td>2.056</td>
</tr>
<tr>
<td>8</td>
<td>3.321309</td>
<td>3.321309</td>
<td>0.000</td>
</tr>
<tr>
<td>9</td>
<td>4.6742772</td>
<td>4.614371</td>
<td>1.2816</td>
</tr>
<tr>
<td>10</td>
<td>6.1625802</td>
<td>6.123668</td>
<td>0.6314</td>
</tr>
<tr>
<td>11</td>
<td>7.9137359</td>
<td>7.85</td>
<td>0.8517</td>
</tr>
<tr>
<td>12</td>
<td>9.8040902</td>
<td>9.780806</td>
<td>0.2375</td>
</tr>
<tr>
<td>13</td>
<td>11.975434</td>
<td>11.92615</td>
<td>0.4116</td>
</tr>
<tr>
<td>14</td>
<td>14.353614</td>
<td>14.28178</td>
<td>0.5005</td>
</tr>
<tr>
<td>15</td>
<td>16.902015</td>
<td>16.88487</td>
<td>0.1049</td>
</tr>
<tr>
<td>16</td>
<td>19.742184</td>
<td>19.70346</td>
<td>0.1962</td>
</tr>
<tr>
<td>17</td>
<td>22.795437</td>
<td>22.73793</td>
<td>0.2562</td>
</tr>
<tr>
<td>18</td>
<td>26.046009</td>
<td>25.98526</td>
<td>0.2336</td>
</tr>
<tr>
<td>19</td>
<td>29.510614</td>
<td>29.44794</td>
<td>0.2124</td>
</tr>
<tr>
<td>20</td>
<td>33.161221</td>
<td>33.12489</td>
<td>0.1096</td>
</tr>
<tr>
<td>21</td>
<td>37.051623</td>
<td>37.03121</td>
<td>0.0551</td>
</tr>
<tr>
<td>22</td>
<td>317.52</td>
<td>137.00</td>
<td>0.3753</td>
</tr>
<tr>
<td>23</td>
<td>41.177514</td>
<td>41.15351</td>
<td>0.0583</td>
</tr>
<tr>
<td>24</td>
<td>45.537431</td>
<td>45.49154</td>
<td>0.1008</td>
</tr>
</tbody>
</table>

### Gaussian energy comparison (BBCGKS 2006) - $N = 5 - 64, n = 4$. 
To Be Continued ...
Sketch of the proof - \{\alpha_i\} case

- Let $f(t)$ be the Hermite 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, $f(t) \in P_{\tau} \cap A_{n,h};$

- If $g(t) \in P_{\tau} \cap A_{n,h}$, then by the quadrature formula
  \[ g_0 - \frac{g(1)}{N} = \sum_{i=1}^{k} \rho_i g(\alpha_i) \leq \sum_{i=1}^{k} \rho_i h(\alpha_i) = \sum_{i=1}^{k} \rho_i f(\alpha_i) = f_0 - \frac{f(1)}{N} \quad \square \]
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 $(H_q^n, J_w^n, \mathbb{RP}^n, \mathbb{CP}^n, \mathbb{HP}^n)$.

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

\[
Q_j(n, s) = \frac{1}{N} + \sum_{i=1}^{k} \rho_i P_j^{(n)}(\alpha_i) \tag{5}
\]

(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 - CA, 2016))

The ULB bound

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

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

\[
g(\alpha_i) = h(\alpha_i) - \epsilon P_{j}^{(n)}(\alpha_i), \quad g'(\alpha_i) = h'(\alpha_i) - \epsilon (P_{j}^{(n)})'(\alpha_i)
\]
Examples

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

Remark
Ballinger, Blekherman, Cohn, Giansiracusa, Kelly, and Shūrmann, 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 \(j_0(10, 40) = 10, j_0(14, 64) = 8, j_0(15, 128) = 9\).
### Test functions - examples

<table>
<thead>
<tr>
<th>j</th>
<th>(4, 24)</th>
<th>(10, 40)</th>
<th>(14, 64)</th>
<th>(15, 128)</th>
<th>(7, 182)</th>
<th>(4, 120)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0.021943574</td>
<td>0.013744273</td>
<td>0.00659722</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0.043584477</td>
<td>0.023867606</td>
<td>0.012122396</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0.085714286</td>
<td>0.024962302</td>
<td>0.015879248</td>
<td>0.010927837</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0.16</td>
<td>0.015883951</td>
<td>0.012369147</td>
<td>0.005957261</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>-0.024</td>
<td>0.026086948</td>
<td>0.015845575</td>
<td>0.006751842</td>
<td>0.022598277</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>-0.02048</td>
<td>0.02824122</td>
<td>0.016679926</td>
<td>0.008493915</td>
<td>0.011864096</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>0.064232727</td>
<td>0.024663991</td>
<td>0.015516168</td>
<td>0.00811866</td>
<td>-0.00835109</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>0.036864</td>
<td>0.024338487</td>
<td>0.015376208</td>
<td>0.007630277</td>
<td>0.003071311</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>0.059833108</td>
<td>0.024442076</td>
<td>0.01558101</td>
<td>0.007746238</td>
<td>0.009459538</td>
<td>0.053050398</td>
</tr>
<tr>
<td>13</td>
<td>0.06340608</td>
<td>0.024976926</td>
<td>0.015644873</td>
<td>0.007809405</td>
<td>0.0065461</td>
<td>0.066587396</td>
</tr>
<tr>
<td>14</td>
<td>0.054456422</td>
<td>0.025919671</td>
<td>0.015734138</td>
<td>0.007817465</td>
<td>0.005369545</td>
<td>-0.046646712</td>
</tr>
<tr>
<td>15</td>
<td>-0.003869491</td>
<td>0.02498472</td>
<td>0.015637274</td>
<td>0.007865499</td>
<td>0.006137772</td>
<td>-0.018428319</td>
</tr>
<tr>
<td>16</td>
<td>0.008598724</td>
<td>0.024214119</td>
<td>0.015521057</td>
<td>0.007815602</td>
<td>0.005268455</td>
<td>0.020868837</td>
</tr>
<tr>
<td>17</td>
<td>0.091970863</td>
<td>0.025123445</td>
<td>0.01562458</td>
<td>0.007761374</td>
<td>0.005134928</td>
<td>-0.000422871</td>
</tr>
<tr>
<td>18</td>
<td>0.049262707</td>
<td>0.025449746</td>
<td>0.015694798</td>
<td>0.007812225</td>
<td>0.004722806</td>
<td>0.012656294</td>
</tr>
<tr>
<td>19</td>
<td>0.035330484</td>
<td>0.024905002</td>
<td>0.015617497</td>
<td>0.00784714</td>
<td>0.003857119</td>
<td>0.006371173</td>
</tr>
<tr>
<td>20</td>
<td>0.048230925</td>
<td>0.024837415</td>
<td>0.015589583</td>
<td>0.00781076</td>
<td>0.007863772</td>
<td>0.011244953</td>
</tr>
</tbody>
</table>