

# Bounds for Spherical Codes: The Levenshtein framework Lifted

PETER DRAGNEV

Purdue University Fort Wayne

Joint work with:

P. Boyvalenkov (Bulgarian Academy of Sciences), D. Hardin, E. Saff (Vanderbilt),  
M. Stoyanova (Sofia University, Bulgaria)

**Optimal Points Weminar, April 14, 2021**

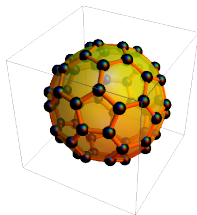
# Outline

- Why Minimize Energy?
- Minimal Energy, Spherical Harmonics, Gegenbauer Polynomials
- Delsarte-Yudin Linear Programming
- Dual Programming Heuristics
- $1/N$ -Quadrature and ULB space
- Levenshtein Framework - ULB Theorem
- Test Functions - Levenshtein Framework Lifted
- The Universality of the 600-cell Revisited

# 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  $\mathbb{S}^2$ .



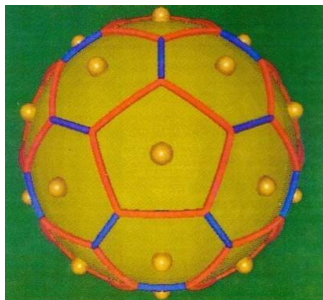
Generalized Thomson Problem ( $1/r^s$  potentials and  $\log(1/r)$ )

A code  $C := \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{S}^2$  that minimizes **Riesz  $s$ -energy**

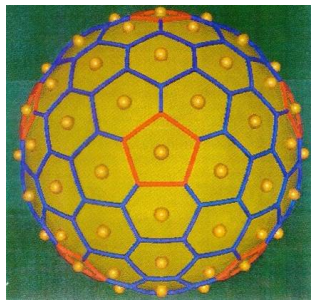
$$E_s(C) := \sum_{j \neq k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^s}, \quad s > 0, \quad E_{\log}(\omega_N) := \sum_{j \neq k} \log \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

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

# Electrostatics and Electrons in Equilibrium



32 Electrons

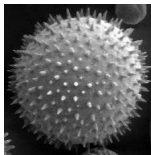


122 Electrons

# Why Minimize Potential Energy? Coding Theory:

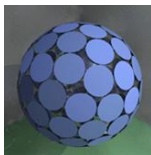
## Tammes Problem (1930)

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



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

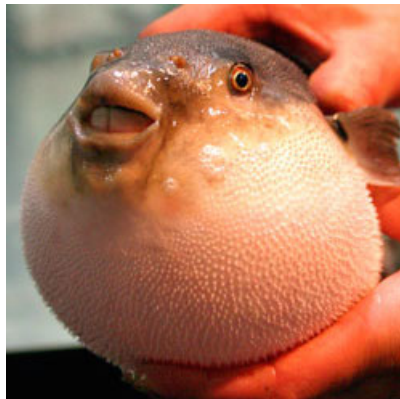
Place  $N$  points on the unit sphere so as to maximize the minimum distance between any pair of points.



## Definition

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

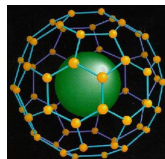
## More “Maximal Codes” from Biology



# Optimal Configurations in Chemistry

## Fullerenes (1985) - (Buckyballs)

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



# Richard Buckminster “Bucky” Fuller, 1895-1983



Montreal biosphere



# Florida "Fullerene"

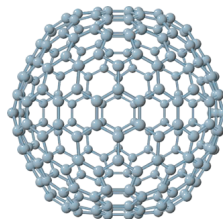
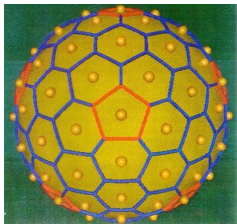
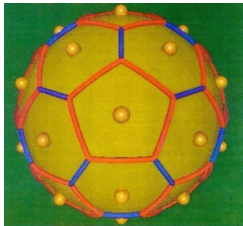


# "Mastodon" Fullerene – $C_{100}$ isolated



$C_{100}$  and Steven Stevenson

# Duality: 32/122 Electrons vs. $C_{60}/C_{240}$ Buckyballs



# Minimal Energy Problem

- Spherical Code: A finite set  $C \subset \mathbb{S}^{n-1}$  with cardinality  $|C| = N$ .
- $r^2 = |x - y|^2 = 2 - 2\langle x, y \rangle = 2 - 2t$ .
- **Interaction potential**  $h : [-1, 1) \rightarrow \mathbb{R}$
- The  $h$ -energy of a spherical code  $C \subset \mathbb{S}^{n-1}$ :

$$E(n, h; C) := \sum_{x, y \in C, y \neq x} h(\langle x, y \rangle),$$

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

**Minimal Energy Problem:** Find

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

# Absolutely Monotone Potentials

- **Interaction potential**  $h : [-1, 1) \rightarrow \mathbb{R}$
- **Absolutely monotone potentials:**

$$C_+^\infty := \{h \mid h^{(k)}(t) \geq 0, t \in [-1, 1), k \geq 0\}.$$

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

# Spherical Harmonics

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

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

- Spherical harmonics (degree  $k$ ):

$$\{Y_{kj}(x) : j = 1, 2, \dots, r_{k,n}\}$$

orthonormal basis of  $\text{Harm}(k)$  with respect to normalized  $(n-1)$ -dimensional surface area measure on  $\mathbb{S}^{n-1}$ .

# Spherical Harmonics and Gegenbauer Polynomials

- The **Gegenbauer polynomials** and spherical harmonics can be defined through the **Addition Formula** ( $t = \langle x, y \rangle$ ):

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

- $\{P_k^{(n)}(t)\}_{k=0}^{\infty}$  orthogonal w/weight  $(1-t^2)^{(n-3)/2}$  and  $P_k^{(n)}(1) = 1$ .
- 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  $\alpha = \beta = (n-3)/2$ .

# Spherical Designs

- The  $k$ -th moment of a spherical code  $C \subset \mathbb{S}^{n-1}$  is

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

- $M_k(C) = 0$  if and only if  $\sum_{x \in C} Y(x) = 0$  for all  $Y \in \text{Harm}(k)$ .
- If  $M_k(C) = 0$  for  $1 \leq k \leq \tau$ , then  $C$  is called a **spherical  $\tau$ -design** and

$$\int_{\mathbb{S}^{n-1}} p(y) d\sigma_n(y) = \frac{1}{N} \sum_{x \in C} p(x), \quad \forall p \in \Pi_\tau(\mathbb{R}^n).$$



## 'Good' potentials for lower bounds

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

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

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

## 'Good' potentials for lower bounds

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

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \quad f_k \geq 0 \text{ for all } k \geq 1. \quad (2)$$

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

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

## 'Good' potentials for lower bounds

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

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \quad f_k \geq 0 \text{ for all } k \geq 1. \quad (2)$$

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

$$\begin{aligned} E(n, C; f) &= \sum_{x, y \in C} f(\langle x, y \rangle) - f(1)N \\ &= \sum_{k=0}^{\infty} f_k M_k(C) - f(1)N \end{aligned}$$

## 'Good' potentials for lower bounds

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

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \quad f_k \geq 0 \text{ for all } k \geq 1. \quad (2)$$

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

$$\begin{aligned} E(n, C; f) &= \sum_{x, y \in C} f(\langle x, y \rangle) - f(1)N \\ &= \sum_{k=0}^{\infty} f_k M_k(C) - f(1)N \\ &\geq f_0 N^2 - f(1)N = N^2 \left( f_0 - \frac{f(1)}{N} \right). \end{aligned}$$

# Delsarte-Yudin LP Bound

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

## Thm (Delsarte-Yudin Lower Energy Bound)

For any  $C \subset \mathbb{S}^{n-1}$  with  $|C| = N$  and  $f \in A_{n,h}$ ,

$$E(n, h; C) \geq N^2(f_0 - \frac{f(1)}{N}). \quad (3)$$

$C$  satisfies  $E(n, h; C) = E(n, f; C) = N^2(f_0 - \frac{f(1)}{N}) \iff$

- (a)  $f(t) = h(t)$  for  $t \in \{\langle x, y \rangle : x \neq y, x, y \in C\}$ , and
- (b) for all  $k \geq 1$ , either  $f_k = 0$  or  $M_k(C) = 0$ .

## Linear program: Maximize D-Y lower bound

Maximizing Delsarte-Yudin lower bound is a linear programming problem.

$$\begin{aligned} &\text{Maximize } N^2(f_0 - \frac{f(1)}{N}) \\ &\text{subject to } f \in A_{n,h}. \end{aligned}$$

## Linear program: Maximize D-Y lower bound

Maximizing Delsarte-Yudin lower bound is a linear programming problem.

$$\begin{aligned} &\text{Maximize } N^2(f_0 - \frac{f(1)}{N}) \\ &\text{subject to } f \in A_{n,h}. \end{aligned}$$

For a subspace  $\Lambda \subset C([-1, 1])$ , we consider

$$\mathcal{W}(n, N, \Lambda; h) := \sup_{f \in \Lambda \cap A_{n,h}} N^2(f_0 - \frac{f(1)}{N}). \quad (4)$$

## Linear program: Maximize D-Y lower bound

Maximizing Delsarte-Yudin lower bound is a linear programming problem.

$$\begin{aligned} &\text{Maximize } N^2(f_0 - \frac{f(1)}{N}) \\ &\text{subject to } f \in A_{n,h}. \end{aligned}$$

For a subspace  $\Lambda \subset C([-1, 1])$ , we consider

$$\mathcal{W}(n, N, \Lambda; h) := \sup_{f \in \Lambda \cap A_{n,h}} N^2(f_0 - \frac{f(1)}{N}). \quad (5)$$

Usually,  $\Lambda = \text{span}\{P_i^{(n)}\}_{i \in I}$  for some finite  $I$ ,

and we replace  $f(t) \leq h(t)$  with  $f(t_j) \leq h(t_j)$ ,  $j \in J$  for finite  $J$ .



# Dual Programming Heuristics

## Primal Program

Maximize  $c^T x$

subject to  $Ax \leq b, x \geq 0$

## Dual Program

Minimize  $b^T y$

subject to  $A^T y \geq b, y \geq 0$

# Dual Programming Heuristics

## Primal Program

Maximize  $c^T x$

subject to  $Ax \leq b, x \geq 0$

## Dual Program

Minimize  $b^T y$

subject to  $A^T y \geq b, y \geq 0$

**Primal**    Maximize     $f_0 - \frac{1}{N} \sum_{i \in I} f_i$

subject to:  $\sum_{i \in I} f_i P_i^{(n)}(t_j) \leq h(t_j), j \in J, f_i \geq 0.$

# Dual Programming Heuristics

## Primal Program

Maximize  $c^T x$

subject to  $Ax \leq b, x \geq 0$

## Dual Program

Minimize  $b^T y$

subject to  $A^T y \geq b, y \geq 0$

**Primal**    Maximize     $f_0 - \frac{1}{N} \sum_{i \in I} f_i$

subject to:  $\sum_{i \in I} f_i P_i^{(n)}(t_j) \leq h(t_j), j \in J, f_i \geq 0.$

**Dual**    Minimize     $\sum_{j \in J} \rho_j h(t_j)$

subject to:  $\frac{1}{N} + \sum_{j \in J} \rho_j P_i^{(n)}(t_j) \geq 0, i \in I \setminus \{0\}, \rho_j \geq 0.$

# Dual Programming Heuristics - complementary slackness

Add slack variables  $\{u_j\}_{j \in J}$  and  $\{w_i\}_{i \in I}$ .

**Primal**    Maximize     $f_0 - \frac{1}{N} \sum_{i \in I} f_i$

subject to:  $\sum_{i \in I} f_i P_i^{(n)}(t_j) + u_j = h(t_j), j \in J, f_i \geq 0.$

**Dual**    Minimize     $\sum_{j \in J} \rho_j h(t_j)$

subject to:  $\frac{1}{N} + \sum_{j \in J} \rho_j P_i^{(n)}(t_j) - w_i = 0, i \in I \setminus \{0\}, \rho_j \geq 0.$

Complementary slackness condition for Primal Objective=Dual Objective:  
 $f_i \cdot w_i = 0, i \in I$ , and  $\rho_j \cdot u_j = 0, j \in J$ .

# 1/ $N$ -Quadrature Rules

- For a subspace  $\Lambda \subset C[-1, 1]$  we say  $\{(\alpha_i, \rho_i)\}_{i=1}^k$  with  $-1 \leq \alpha_i < 1$ ,  $\rho_i > 0$  for  $i = 1, 2, \dots, k$  is a **1/ $N$ -quadrature rule exact for  $\Lambda$**  if

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

$$\implies f_0 - \frac{f(1)}{N} = \sum_{i=1}^k \rho_i f(\alpha_i).$$

# 1/ $N$ -Quadrature Rules

- **Example:** Given a spherical  $\tau$ -design  $C$  and  $|C| = N$ .

Then  $\{\alpha_0 = 1, \alpha_1, \dots, \alpha_k\} := \{\langle x, y \rangle \mid x, y \in C\}$  and

$$\rho_i := \frac{|\{(x, y) \in C \times C \mid \langle x, y \rangle = \alpha_i\}|}{N^2}, \quad i = 0, \dots, k$$

is a  $1/N$ -QR exact for  $\Pi_\tau$ . If  $p \in \Pi_\tau([-1, 1])$  then for any  $y \in \mathbb{S}^{n-1}$  we have

$$\gamma_n \int_{-1}^1 p(t)(1-t^2)^{(n-3)/2} dt = \int_{\mathbb{S}^{n-1}} p(\langle x, y \rangle) d\sigma_n(x) = \frac{1}{N} \sum_{x \in C} p(\langle x, y \rangle)$$

# ULB space

- For  $f \in \Lambda \cap A_{n,h}$  and  $\{(\alpha_i, \rho_i)\}_{i=1}^k$  exact for  $\Lambda$ :

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

and so

$$\mathcal{W}(n, N, \Lambda; h) \leq N^2 \sum_{i=1}^k \rho_i h(\alpha_i), \quad (6)$$

# ULB space

- For  $f \in \Lambda \cap A_{n,h}$  and  $\{(\alpha_i, \rho_i)\}_{i=1}^k$  exact for  $\Lambda$ :

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

and so

$$\mathcal{W}(n, N, \Lambda; h) \leq N^2 \sum_{i=1}^k \rho_i h(\alpha_i), \quad (7)$$

- with " $=$ "  $\iff \left( \begin{array}{l} \exists f \in \Lambda \cap A_{n,h} \text{ such that} \\ f(\alpha_i) = h(\alpha_i), i = 1, \dots, k \end{array} \right)$
- If equality holds in (7) for **all**  $h \in C_+^\infty$ , we call  $\Lambda$  (with associated QR) a  **$(n, N)$ -ULB space**.



# Hermite Interpolation

Suppose  $f, h \in C^1([-1, 1))$ ,  $f \leq h$  and  $f(\alpha) = h(\alpha)$  for some  $\alpha \in [-1, 1)$ .

- If  $\alpha > -1$  then  $f'(\alpha) = h'(\alpha)$ .
- If  $\alpha = -1$  then  $f'(\alpha) \leq h'(\alpha)$ .

If  $f(\alpha_i) = h(\alpha_i)$ ,  $i = 1, \dots, k$  and  $\alpha_i > -1$ , then  $2k$  necessary conditions.

# Sharp Codes

Observe that a spherical  $\tau$ -design  $C$  yields a  $1/|C|$ -quadrature rule that is exact for  $\Lambda = \Pi_\tau$  with nodes  $\{\langle x, y \rangle \mid x \neq y \in C\}$ .

## Definition

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

Idea of proof: Show Hermite interpolant to  $h$  is in  $A_{n,h}$ ; i.e.,  $\Pi_\tau$  is a  $(n, |C|)$ -ULB space.

# Levenshtein Framework - $1/N$ -Quadrature Rule

- For every fixed  $N > D(n, 2k - 1)$  (the DGS bound) there exists a  $1/N$ -QR that is exact on  $\Lambda = \Pi_{2k-1}$ .
- The numbers  $\alpha_i$ ,  $i = 1, 2, \dots, k$ , are the roots of the equation

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

where  $P_i(t) = P_i^{(n-1)/2, (n-3)/2}(t)$  is a Jacobi polynomial and  $s = \alpha_k$  is chosen to get weight  $1/N$  at node 1.

# Universal Lower Bound (ULB)

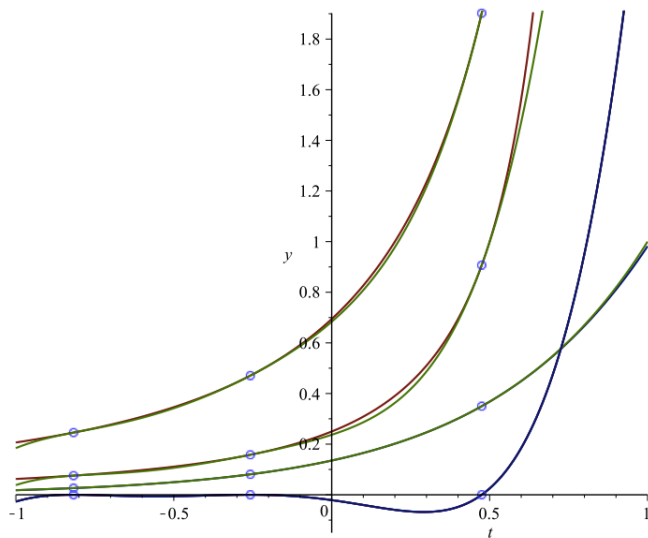
## ULB Theorem - (BDHSS, 2016)

Let  $h \in C_+^\infty$  and  $n, k$ , and  $N$  such that  $N \geq D(n, 2k - 1)$ . Then  $\Lambda = \Pi_{2k-1}$  is a  $(n, N)$ -ULB space with the Levenshtein QR  $\{\alpha_i, \rho_i\}_{i=1}^k$ ; i.e.,

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

The Hermite interpolants at these nodes are the optimal polynomials which solve the finite LP in the class  $\Pi_{2k-1} \cap A_{n,h}$ .

# 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 Gaussian Energy

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

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

# Improvement of ULB and Test Functions

Test functions (Boyvalenkov, Danev, Boumova, '96)

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



# Improvement of ULB and Test Functions

Test functions (Boyvalenkov, Danev, Boumova, '96)

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

# Improvement of ULB and Test Functions

Test functions (Boyvalenkov, Danev, Boumova, '96)

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

## Subspace ULB Improvement Theorem (BDHSS, 2016)

Let  $\Lambda \subset C([-1, 1])$  be a ULB space with  $1/N$ -QR  $\{(\alpha_i, \rho_i)\}_{i=1}^k$ . Suppose  $\Lambda' = \Lambda \oplus \text{span} \{P_j^{(n)} : j \in \mathcal{I}\}$  for some index set  $\mathcal{I} \subset \mathbb{N}$ . If  $Q_j(n, \{\alpha_i, \rho_i\}) \geq 0$  for  $j \in \mathcal{I}$ , then

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

If there is  $j : Q_j(n, \{\alpha_i, \rho_i\}) < 0$ , then  $\mathcal{W}(n, N, \Lambda'; h) < \mathcal{W}(n, N, \Lambda; h)$ .

# Test functions - examples

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

## Example: ULB's for $N = 24$ , $n = 4$ codes

$D_4$  lattice =  $\{v \in \mathbf{Z}^4 \mid \text{sum of components is even}\}$ .

$C_{24}$  consists of the 24 minimal length vectors in  $D_4$  lattice (scaled to unit sphere) and is a kissing configuration:  $T(C_{24}) = 0.5$ .

- $C_{24}$  is 5-design with 4 distinct inner products:  $\{-1, -1/2, 0, 1/2\}$ .
- Kissing number problem in  $\mathbb{R}^4$  – solved by Musin (2003) using modification of linear programming bounds.
- $C_{24}$  is conjectured to be maximal code but not yet proved.
- $C_{24}$  is not universally optimal – Cohn, Conway, Elkies, Kumar (2008); however,  $D_4$  is conjectured to be universally optimal in  $\mathbb{R}^4$ .

# Levenshtein Framework lifted for $(4, 24)$ -codes

For  $n = 4$ ,  $N = 24$  Levenshtein nodes and weights (exact for  $\Pi_5$ ) are:

$$\{\alpha_1, \alpha_2, \alpha_3\} = \{-.817352..., -.257597..., .474950...\}$$

$$\{\rho_1, \rho_2, \rho_3\} = \{0.138436..., 0.433999..., 0.385897...\},$$

The test functions for  $(4, 24)$ -codes are:

$Q_6$	$Q_7$	$Q_8$	$Q_9$	$Q_{10}$	$Q_{11}$	$Q_{12}$
0.0857	0.1600	-0.0239	-0.0204	0.0642	0.0368	0.0598

# Levenshtein Framework lifted for (4, 24)-codes

Motivated by this we consider the following space

$$\Lambda := \text{span}\{P_0^{(4)}, \dots, P_5^{(4)}, P_8^{(4)}, P_9^{(4)}\}.$$

## Theorem

*The space  $\Lambda$  with 1/24-QR  $\{(\alpha_i, \rho_i)\}_{i=1}^4$  given by*

$$\begin{aligned}\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\} &\approx \{-0.86029, -0.48984, -0.19572, 0.47854\} \\ \{\rho_1, \rho_2, \rho_3, \rho_4\} &\approx \{0.09960, 0.14653, 0.33372, 0.37847\},\end{aligned}$$

*is a (4, 24)-ULB space. All (relevant) test functions  $Q_j$  are now positive so this solves full LP.*

Arestov and Babenko (2000) arrive at these nodes, weights in the context of maximal codes.

# Levenshtein Framework lifted for (4, 24)-codes

Motivated by this we consider the following space

$$\Lambda := \text{span}\{P_0^{(4)}, \dots, P_5^{(4)}, P_8^{(4)}, P_9^{(4)}\}.$$

## Theorem

*The space  $\Lambda$  with 1/24-QR  $\{(\alpha_i, \rho_i)\}_{i=1}^4$  given by*

$$\begin{aligned}\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\} &\approx \{-0.86029, -0.48984, -0.19572, 0.47854\} \\ \{\rho_1, \rho_2, \rho_3, \rho_4\} &\approx \{0.09960, 0.14653, 0.33372, 0.37847\},\end{aligned}$$

*is a (4, 24)-ULB space. All (relevant) test functions  $Q_j$  are now positive so this solves full LP.*

Arestov and Babenko (2000) arrive at these nodes, weights in the context of maximal codes.

# LP Optimal Polynomial for (4, 24)-code

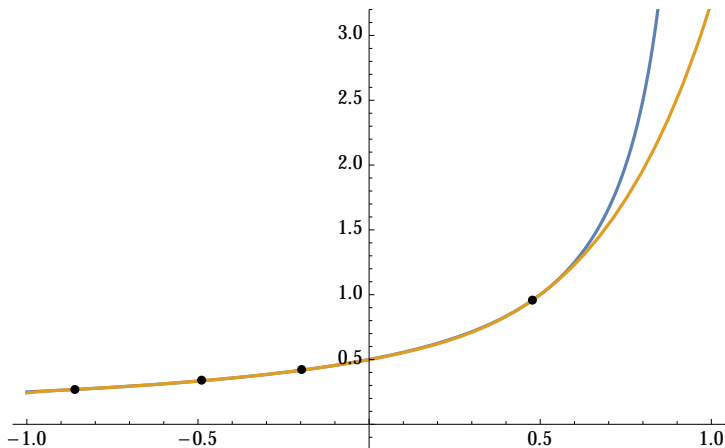


Figure: The (4, 24)-code optimal interpolant - Coulomb potential



## Sufficient Condition: Partial products

Following ideas from Cohn and Woo (2012) we consider partial products associated with a multi-set  $T := \{t_1 \leq \dots \leq t_m\} \subset [-1, 1]$

$$p_j(t) := \prod_{i \leq j} (t - t_i).$$

### Lemma

*Let  $\{\alpha_i, \rho_i\}$  be a  $1/N$ -QR with nodes  $-1 \leq \alpha_1 < \dots < \alpha_k$  that is exact for  $\Lambda$ . If  $\alpha_1 > -1$ , let  $T := \{\alpha_1, \alpha_1, \alpha_2, \alpha_2, \dots, \alpha_k, \alpha_k\}$ , else only take one  $\alpha_1$  once.*

*Suppose for each  $j \leq m = |T|$  there exists  $q_j \in A_{n,p_j}$  such that  $q_j(\alpha_i) = p_j(\alpha_i)$  for  $i = 1, \dots, k$ . Then  $\Lambda$  is a  $(n, N)$ -ULB space.*

# Sufficient Condition: Partial products

## Lemma

Let  $\{\alpha_i, \rho_i\}$  be a  $1/N$ -QR with nodes  $-1 \leq \alpha_1 < \dots < \alpha_k$  that is exact for  $\Lambda$ . If  $\alpha_1 > -1$ , let  $T := \{\alpha_1, \alpha_1, \alpha_2, \alpha_2, \dots, \alpha_k, \alpha_k\}$ , else only take one  $\alpha_1$  once.

Suppose for each  $j \leq m = |T|$  there exists  $q_j \in A_{n,p_j}$  such that  $q_j(\alpha_i) = p_j(\alpha_i)$  for  $i = 1, \dots, k$ . Then  $\Lambda$  is a  $(n, N)$ -ULB space.

## Proof.

For  $h \in C_+^\infty$  define

$$f(t) = \sum_{j=1}^m h[t_1, \dots, t_j] q_{j-1}(t),$$

where  $h[t_1, \dots, t_i]$  are the divided differences of  $h$ . Then  $f \in A_{n,h}$  and  $f(\alpha_i) = h(\alpha_i)$ ,  $i = 1, \dots, k$ . □

## Levenshtein framework lifted - skip2/add2

Motivated by (4, 24)-code, let  $\tau(n, N) = 2k - 1$  and  $Q_{2k+2}^{(n, N)} < 0$  or  $Q_{2k+3}^{(n, N)} < 0$ . In this case the **skip-two/add-two** subspace is

$$\Lambda_{n,k} := \mathcal{P}_{2k-1} \oplus \text{span} \left( P_{2k+2}^{(n)}, P_{2k+3}^{(n)} \right). \quad (8)$$

### Lemma

*Any  $1/N$ -quadrature rule that is exact on  $\Lambda_{n,k}$  has at least  $k + 1$  distinct nodes.*

Let  $\{(\beta_i, \theta_i)\}_{i=1}^{k+1}$  be a  $1/N$ -quadrature rule with exactly  $k + 1$  exact on  $\Lambda_{n,k}$ , namely,  $-1 \leq \beta_1 < \dots < \beta_{k+1} < 1$ ,  $\theta_i > 0$ ,  $i = 1, \dots, k + 1$ , and

$$f_0 = \int_{-1}^1 f(t) d\mu(t) = \frac{f(1)}{N} + \sum_{i=1}^{k+1} \theta_i f(\beta_i) \quad (9)$$

holds for every polynomial from the subspace  $\Lambda_{n,k}$  defined in (8).

# Levenshtein framework lifted - skip2/add2 quadrature nodes

Define the *partial products*

$$q_j(t) := (t - \beta_1) \cdots (t - \beta_j), \quad j = 1, 2, \dots, k+1, \quad q_0(t) \equiv 1. \quad (10)$$

## Theorem

*There are constants  $c_1$ ,  $c_2$ , and  $c_3$  such that*

$$a_{k+1,k+1}^{1,0} q_{k+1}(t) = P_{k+1}^{1,0}(t) + c_1 P_k^{1,0}(t) + c_2 P_{k-1}^{1,0}(t) + c_3 P_{k-2}^{1,0}(t), \quad (11)$$

*where  $a_{k+1,k+1}^{1,0}$  denotes the leading coefficient of the polynomial  $P_{k+1}^{1,0}(t)$ . Moreover,  $(\beta_i)_{i=1}^{k+1}$  interlace with the nodes  $(\alpha_i)_{i=1}^k$  of the Levenshtein quadrature for  $\mathcal{P}_{2k-1}$ ; i.e.,*

$$-1 \leq \beta_1 < \alpha_1 < \cdots < \beta_k < \alpha_k < \beta_{k+1} < 1. \quad (12)$$

# Levenshtein framework lifted - Examples

Dimension	Cardinality	Lev: $\Lambda = \Pi_k$	new: $\Lambda = \Pi_k$
3	14	5	9
3	22	7	11
3	23	7	11
3	32	9	13
3	34	9	13
3	44	11	15
3	47	11	15
3	59	13	17
3	62	13	17
4	24	5	9
4	44	7	11
4	48	7	11
4	120	11	15
5	36	5	9
5	38	5	9

# The Universality of the 600-cell Revisited

- $C_{600} = 120$  points in  $\mathbb{R}^4$ . Each  $x \in C_{600}$  has 12 nearest neighbors forming an icosahedron (Voronoi cells are spherical dodecahedra).
- 8 inner products between distinct points in  $C_{600}$ :  
 $\{-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4\}$ .
- $2^7+1$  or  $2^8$  interpolation conditions (would require 14 or 15 design)
- $C_{600}$  is an 11 design, but almost a 19 design (only 12-th moment is nonzero); i.e.,  $M_k(C_{600}) = 0$  for  $k \in \{1, \dots, 19\} \setminus \{12\}$ .

## 600 cell

- Coxeter (1963), Bórczky's (1978) bounds establish maximal code of 600-cell
- Andreev (1999) found polynomial in  $\Pi_{17}$  that shows 600-cell is maximal code.
- Danev, Boyvalenkov (2001) prove uniqueness (of spherical 11-design with 120 points).
- Cohn and Kumar(2007) find family of 17-th degree polynomials that proves **universal optimality** of  $C_{600}$  and they require  $f_{11} = f_{12} = f_{13} = 0$ ;  $\Lambda_{17}^0 = \Pi_{17} \cap \{P_{11}^{(4)}, P_{12}^{(4)}, P_{13}^{(4)}\}^\perp$  with Lagrange condition at -1. Partial product method doesn't work for this family.

## 600 cell - Levenshtein framework lift, 1<sup>st</sup> Step

- Levensthein:  $n = 4$ ,  $N = 120$ , quadrature: 6 nodes exact for  $\Pi_{11}$ :

$$\{\alpha_1, \dots, \alpha_6\} \approx \{-0.9356, -0.7266, -0.3810, 0.04406, 0.4678, 0.8073\}$$

$$\{\rho_1, \dots, \rho_6\} \approx \{0.02998, 0.1240, 0.2340, 0.2790, 0.2220, 0.1026\}$$

- Test functions:  $Q_{12}, Q_{13} > 0$ ,  $Q_{14}, Q_{15} < 0$ .
- Find quadrature rule for  $\Lambda_{15} = \Pi_{15} \cap \{P_{12}^{(4)}, P_{13}^{(4)}\}^\perp$ .

$$\{\beta_1, \dots, \beta_7\} \approx \{-0.981, -0.796, -0.476, -0.165, 0.097, 0.475, 0.808\}$$

$$C \prod (t - \beta_i) = P_7(t) + C_1 P_6(t) + C_2 P_5(t) + C_3 P_4(t), \quad P_k = P_k^{(\frac{1}{2}, \frac{3}{2})}.$$

- Verify Hermite interpolation works in  $\Lambda_{15}$ .
- New test functions  $Q_{12}, Q_{13} > 0$ , so this solves LP in  $\Pi_{15}$ .



## 600 cell - Levenshtein framework lift, 2<sup>nd</sup> Step

- Degree 17. Try  $\Lambda_{17}^1 = \Pi_{17} \cap \{P_{12}^{(4)}, P_{13}^{(4)}\}^\perp$ , double interpolation at -1. It works.
- Degree 17. Try  $\Lambda_{17}^2 = \Pi_{17} \cap \{P_{11}^{(4)}, P_{12}^{(4)}\}^\perp$ , double interpolation -1. It works.
- Degree 17. All solutions form triangle.

## 600 cell - Optimal Triangle in $\Pi_{17}$

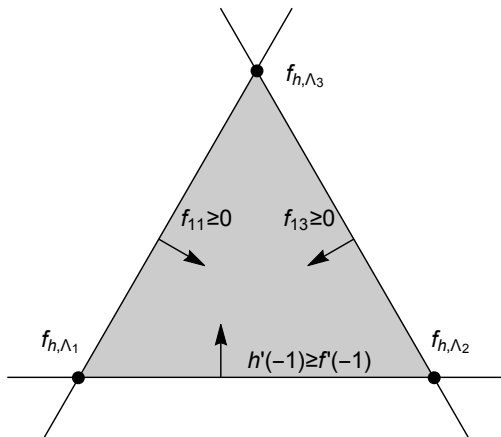


Figure: Set of LP-optimal polynomials for 600-cell and given  $h$  as in Theorem ??.

THANK YOU FOR YOUR ATTENTION !