Applications of orthogonal polynomials to minimal energy in polynomial metric spaces

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Outline

- Polynomial metric spaces (PM-spaces)
- Codes and designs in PM-spaces, energy, problems
- Delsarte bound, Levenshtein bound, $1/M$-quadrature
- Basic PM-spaces – overview
- LP bounds on energy of codes/designs in PM-spaces (folklore)
- Universal lower bound (ULB) – Main Theorem
- Two ways of improving ULB (if possible) – lifting the Levenshtein framework; subintervals
- ULB asymptotics in antipodal PM-spaces

Polynomial metric spaces (1)

A metric space $(\mathcal{M}, d)$ with diameter Δ, normalized (distance invariant) measure μ and standard (decreasing) substitution $\sigma = \sigma(d) = t \in [-1, 1]$ $(\sigma(0) = 1,\ \sigma(\Delta) = -1)$, is called *polynomial metric space* (PM-space) if:

- There is orthogonal decomposition V_i, $\dim V_i = r_i$, with orthonormal basis $\{v_{ij}\}_{j=1}^{r_i}$

$$\mathcal{L}_2(\mathcal{M}, \mu) = \bigoplus V_i;$$

- And polynomials $Q_i(t)$, $i = 0, 1, \ldots,$ such that

$$Q_i(\sigma(d(x, y)))) = \frac{1}{r_i} \sum_{j=1}^{r_i} v_{i,j}(x) \overline{v_{i,j}(y)}.$$

$\{Q_i(t)\}$ are orthogonal w.r.t. $\nu(t) = 1 - \mu(\sigma^{-1}(t))$, $Q_i(1) = 1$.

Polynomial metric spaces (2)

- The Euclidean sphere $\mathbb{S}^{n-1}$ with the usual metric and inner product, standard substitution $\sigma(d) = 1 - \frac{d^2}{2}$, orthogonality weight $\nu(t) = (1-t^2)^{(n-3)/2}$, $Q_i(t)$ – the (normalized) Gegenbauer polynomials.
- Real, complex and quaternionic projective spaces $\mathbb{R}P^{n-1|}$, $\mathbb{C}P^{n-1}$ and $\mathbb{H}P^{n-1}$ with $\sigma(d) = 2(1-d^2)^2 - 1$, $Q_i(t)$ – the (normalized) Jacobi polynomials with parameters $(\alpha, \beta) = (\frac{m(n-1)}{2} - 1, \frac{m}{2} - 1)$, where $m = 1, 2, 4$, respectively.
- Hamming space $H(n, q)$ with $\sigma(d) = 1 - \frac{2d}{n}$, $Q_i(t)$ – the (normalized) Krawtchouk polynomials.
- Johnson space $J(n, w)$ with $\sigma(d) = 1 - \frac{2d}{w}$, $Q_i(t)$ – the (normalized) Hahn polynomials.

Polynomial metric spaces (2)

$\mathcal{M}$	$d(x,y)$	$\mu(x)$, $\overline{\mu}(d)$	$\sigma(d)$
$\mathbb{S}^{n-1}$	$\lvert x-y\rvert$	$\mu(x)=d\sigma_{n-1}(x)$	$1-\frac{d^2}{2}$
$H(n,q)$	$\lvert i:(x_i\neq y_i\}\rvert$	$\overline{\mu}(d)=\frac{1}{q^n}\sum_{i=0}^{d}(q-1)^i\binom{n}{i}$	$1-\frac{2d}{n}$
$J(n,w)$	$w-wt(x*y)$	$\overline{\mu}(d)=\frac{1}{\binom{n}{w}}\sum_{i=0}^{d}\binom{w}{i}\binom{n-i}{i}$	$1-\frac{2d}{w}$
$\mathbb{F}P^{n-1}$	$\sqrt{2}\sin\frac{\varphi(X,Y)}{2}$	$\overline{\mu}(d)=\gamma_{m,n}\int_{\cos^2\varphi}^{1}(1-z)^{\frac{m(n-1)}{2}-1}z^{\frac{m}{2}-1}dz$	$2(1-d^2)^2-1$

$\mathcal{M}$	$\nu(t)=1-\overline{\mu}(\sigma^{-1}(t))$	$Q_i(t)$	r_i
$\mathbb{S}^{n-1}$	$\gamma_n(1-t^2)^{\frac{n-3}{2}}\,dt$	$P_i^{(\frac{n-3}{2},\frac{n-3}{2})}(t)$	$\frac{2i+n-2}{i+n-2}\binom{i+n-2}{i}$
$H(n,q)$	$\frac{1}{q^n}\sum_{i=0}^{d}(q-1)^i\binom{n}{i}\delta_{-1+\frac{2i}{n}}$	$\frac{1}{r_i}K_i^{n,q}(\frac{n(1-t)}{2})$	$(q-1)^i\binom{n}{i}$
$J(n,w)$	$\frac{1}{\binom{n}{w}}\sum_{i=0}^{d}\binom{w}{i}\binom{n-i}{i}\delta_{-1+\frac{2i}{w}}$	$J_i(\frac{w(1-t)}{2})$	$\binom{n}{i}-\binom{n}{i-1}$
$\mathbb{F}P^{n-1}$	$c_{m,n}(1-t)^{\frac{m(n-1)}{2}-1}(1+t)^{\frac{m}{2}-1}\,dt$	$P_i^{(\alpha,\beta)}(t)$ $\alpha=\frac{m(n-1)}{2}-1,$ $\beta=\frac{m}{2}-1$	$\frac{(2i+\alpha+\beta+1)\binom{i+\alpha+\beta}{i}\binom{i+\alpha}{i}}{(\alpha+\beta+1)\binom{i+\beta}{i}}$ $\alpha=\frac{m(n-1)}{2}-1,$ $\beta=\frac{m}{2}-1$

Polynomial metric spaces (3)

- For any real polynomial $f(t)$ of degree r we have the unique expansion

$$f(t) = \sum_{i=0}^{r} f_i Q_i(t)$$

$$f_i = r_i \int_{-1}^{1} f(t) Q_i(t) d\nu(t)$$

- Denote by $F_{\geq}$ (respectively $F_{>}$) the set of polynomials such that $f_i \geq 0$ (respectively, $f_i > 0$) for every i (respectively for every $i \leq \deg(f)$).

Polynomial metric spaces (4)

- Adjacent measures $d\nu^{a,b}(t) = c^{a,b}(1-t)^a(1+t)^b d\nu(t)$, $a, b \in \{0, 1\}$
- Adjacent systems – polynomials $Q_i^{a,b}(t)$ orthogonal with respect to $\nu^{a,b}(t)$
- Corresponding parameters $r_i^{a,b} = ||Q_i^{a,b}||_{a,b}^{-1}$
- Fact:

$$Q_j^{1,0}(t) = \frac{1}{\sum_{i=0}^{j} r_i} \sum_{i=1}^{j} r_i Q_i(t) \in F_{\geq}$$

(then Christoffel-Darboux formula)

Codes and designs in PM-spaces (1)

- $C \subset \mathcal{M}$, $|C| < \infty$, is called code.
- A code C is called design iff

$$\sum_{x,y \in C} Q_i(\sigma(d(x,y))) = 0, \ i = 1, 2, \ldots, \tau$$

for some positive integer τ (equivalently, $\sum_{x \in C} v_{i,j}(x) = 0$)
- Example – spherical τ-designs are codes on $\mathbb{S}^{n-1}$ such that

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

holds for all polynomials $f(x) = f(x_1, x_2, \ldots, x_n)$ of total degree at most τ.

Codes and designs in PM-spaces (2)

- $C \subset \mathcal{M}$ – most important parameters are $|C|$, $s(C) := \max\{\sigma(d(x,y)) : x, y \in C, x \neq y\}$, $\tau(C) := \max\{\tau : C \text{ is a } \tau\text{-design}\}$.
- $A(\mathcal{M}, s) = \max\{|C| : s(C) = s\}$.
- $B(\mathcal{M}, \tau) = \min\{|C| : \tau(C) = \tau\}$.
- $A(\mathcal{M}, s)$ and $B(\mathcal{M}, \tau)$ are estimated by linear programming techniques – Levenshtein bounds and Delsarte bounds.

Energy of codes/designs in PM-spaces

- Let $h(t) : [-1,1) \to (0,+\infty)$ be given function. The h-energy (or potential energy) of $C \subset \mathcal{M}$ –

$$E(\mathcal{M},C;h) := \sum_{x,y\in C, x\neq y} h(\sigma(d(x,y))).$$

- h – (strictly) *absolutely monotone* on [-1,1); i.e., the k-th derivative of h satisfies

$$h^{(k)}(t) \geq 0$$

$(h^{(k)}(t) > 0)$ for all $k \geq 0$ and $t \in [-1,1)$.

Problems

- Find $A(\mathcal{M}, s)$.
- Find $B(\mathcal{M}, \tau)$.
- Minimize the potential energy provided the cardinality of C is fixed

$$\mathcal{E}(\mathcal{M}, N; h) := \inf\{E(\mathcal{M}, C; h) : |C| = N\}.$$

- Maximize the potential energy provided the cardinality and the strength of C are fixed

$$\mathcal{F}(\mathcal{M}, N, \tau; h) := \sup\{E(\mathcal{M}, C; h) : |C| = N, \tau(C) = \tau\}$$

(if the supremum exists).

Source of bounds in PM-spaces

Since $E(\mathcal{M}, C; Q_i) = \frac{1}{r_i} \sum_{j=1}^{r_i} |\sum_{x \in C} v_{ij}(x)|^2$, for a code $C \subset \mathcal{M}$ and polynomial potential $f(t) = \sum_{i=0}^{r} f_i Q_i^{(n)}(t)$ the following identity holds:

$$|C|f(1) + \sum_{x,y \in C, x \neq y} f(\sigma(d(x,y))) = |C|^2 f_0 + \sum_{i=1}^{r} \frac{f_i}{r_i} \sum_{j=1}^{r_i} \left| \sum_{x \in C} v_{ij}(x) \right|^2 .$$

Recall that $\{v_{ij}(x) : j = 1, 2, \ldots, r_i\}$ is an orthonormal basis of V_i and $r_i = \dim\ V_i$.

Delsarte bounds for minimal designs

For fixed space $\mathcal{M}$ and strength τ denote

$$B(\mathcal{M},\tau) = \min\{|C| : \exists\ \tau\text{-design } C \subset \mathcal{M}\}.$$

The Delsarte bound (obtained by Deslarte-Goethals-Seidel for $\mathbb{S}^{n-1}$, Rao for $H(n,q)$, Hoggar in the projective spaces, etc.) is

$$B(\mathcal{M},\tau) \geq D(\mathcal{M},\tau) = \left(1 - \frac{1}{Q_1(-1)}\right)^{\varepsilon} \sum_{i=0}^{k-\varepsilon} r^{0,\varepsilon},$$

Example – for $\mathbb{S}^{n-1}$

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

Levenshtein bounds for maximal codes (1)

- 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 so-called adjacent polynomial $Q_i^{(a,b)}(t)$.
- The intervals $\mathcal{I}_m$ define partition of $\mathcal{I} = [-1, 1)$ to countably/finitely many for infinite/finite $\mathcal{M}$ non-overlapping closed subintervals.

Levenshtein bounds for maximal codes (2)

- Levenshtein obtained in 1980's the bound

$$A(\mathcal{M},s) \leq L_{2k-1+\varepsilon}(\mathcal{M},s) = \left(1 - \frac{1}{Q_1(-1)}\right)^{\varepsilon} \left(1 - \frac{Q_{k-1}^{1,\varepsilon}(s)}{Q_k^{0,\varepsilon}(s)}\right) \sum_{i=0}^{k-1+\varepsilon} r_i^{0,\varepsilon}$$

  for all $s \in \mathcal{I}_{2k-1+\varepsilon}$

- For every fixed $\mathcal{M}$ each bound $L_m(\mathcal{M},s)$ is smooth and strictly increasing with respect to s. The function

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

  is continuous in s.

Connections between Delsarte and Levenshtein bounds

- Important connections between the Delsarte bounds and Levenshtein bounds are given by the equalities

$$L_{2k-2}(\mathcal{M}, t_{k-1}^{1,1}) = L_{2k-1}(\mathcal{M}, t_{k-1}^{1,1}) = D(\mathcal{M}, 2k-1),$$

$$L_{2k-1}(\mathcal{M}, t_{k}^{1,0}) = L_{2k}(\mathcal{M}, t_{k}^{1,0}) = D(\mathcal{M}, 2k)$$

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

- It is important where the cardinality N is located with respect to the Delsarte bound. Since

$$N \in [D(\mathcal{M}, \tau), D(\mathcal{M}, \tau+1)] \iff s \in \mathcal{I}_\tau,$$

  where s and N are connected by $N = L_\tau(\mathcal{M}, s)$, we define

$$\tau = \tau(\mathcal{M}, N).$$

Examples – Euclidean spheres $\mathbb{S}^{n-1}$ (1)

$x = (x_1, x_2, \dots, x_n), y = (y_1, y_2, \dots, y_n) \in \mathbb{S}^{n-1}$

$$d(x, y) = \left((x_1 - y_1)^2 + \cdots + (x_n - y_n)^2\right)^{1/2},$$

$$\langle x, y \rangle = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n,$$

connected by

$$\langle x, y \rangle = 1 - \frac{d^2(x, y)}{2}.$$

Substitution $\sigma(d) = 1 - d^2/2 : [0, 2] \to [-1, 1]$, measure μ – the normalized Lebesgue measure on $\mathbb{S}^{n-1}$.

V_i – the homogeneous harmonic polynomials in n variables of total degree i and basis the spherical harmonics $v_{ij} = Y_{ij}$;

$$r_i = \dim(V_i) = \frac{2i + n - 2}{i + n - 2} \cdot \binom{i + n - 2}{i}.$$

Examples – Euclidean spheres $\mathbb{S}^{n-1}$ (2)

The Q-system – normalized by $Q_i(1) = 1$ Gegenbauer polynomials, orthogonal on $[-1, 1]$ with respect to

$$d\nu(t) = c_n(1 - t^2)^{(n-3)/2} dt,$$

where $c_n := \Gamma(\frac{n}{2})/\sqrt{\pi}\Gamma(\frac{n-1}{2})$ is a normalizing constant.
Three term recurrence relation

$$(i + n - 2)Q_{i+1}(t) = (2i + n - 2)tQ_i(t) - iQ_{i-1}(t),$$

with initial conditions $Q_0(t) = 1$ and $Q_1(t) = t$.
The codes/designs on $\mathbb{S}^{n-1}$ are finite sets of points of the sphere and are naturally called spherical codes/designs.

Examples – Euclidean spheres $\mathbb{S}^{n-1}$ (3)

The bound for designs – by Delsarte, Goethals, and Seidel (1977)

$$B(n,\tau) \geq D(n,\tau) := \binom{n+k-1-\varepsilon}{n-1} + \binom{n+k-2}{n-1},$$

where $\tau = 2k-1+\varepsilon$, $\varepsilon \in \{0,1\}$.
The Levenshtein bound (1979)

$$L_\tau(n,s) = \binom{k+n-3+\varepsilon}{n-2} A,$$

$$A = \frac{2k+n-3+2\varepsilon}{n-1} - \frac{(1+s)^\varepsilon \left(Q_{k-1+\varepsilon}(s) - Q_{k+\varepsilon}(s)\right)}{(1-s)\left(Q_k(s) + \varepsilon Q_{k+\varepsilon}(s)\right)},$$

τ, ε as above.

Examples – Hamming spaces $H(n, q)$ (1)

$n \geq 2$, $q \geq 2$ – positive integers. The q-ary Hamming space $H(n, q)$ consists of vectors $x = (x_1, x_2, \ldots, x_n)$, where $x_i \in \{0, 1, \ldots, q-1\}$, and the distance between $x, y \in H(n, q)$ is the Hamming distance, i.e. the number of coordinates in which x and y differ

$$\overline{\mu}(d) = \frac{1}{q^n} \sum_{i=0}^{d} (q-1)^i \binom{n}{i}$$

is the normalized volume of a ball of radius d. The standard substitution is

$$\sigma(d) = 1 - \frac{2d}{n},$$

$$r_i = (q-1)^i \binom{n}{i}.$$

Examples – Hamming spaces $H(n,q)$ (2)

The Q-system is defined by

$$Q_i = \frac{1}{r_i} K_i^{n,q}(n(1-t)/2),$$

where

$$K_i^{n,q}(z) = \sum_{j=0}^{i} (q-1)^{i-j} \binom{z}{j} \binom{n-z}{i-j}$$

are the q-ary Krawtchouk polynomials.
The Hamming analog of the spherical harmonics is as follows. Let V_0 consist of the constant function 1 and, for $i = 1, \ldots, n$, let V_i consist of the r_i functions

$$V_i = \{u(x) : H(n,q) \to \mathbb{C} \mid u(x) = \xi^{\alpha_1 x_{j_1} + \cdots + \alpha_i x_{j_i}},$$
$$1 \le j_1 < \cdots < j_i \le n, \alpha_1, \ldots, \alpha_i \in \{1, \ldots, q-1\}\},$$

where ξ is a (complex) primitive q-th root of unity.

Examples – Hamming spaces $H(n,q)$ (3)

The addition formula relates the Krawtchouk polynomials and the orthonormal systems V_i, $i = 0, \ldots, n$,

$$Q_i^{(n,q)}(\sigma(d(x,y))) = \frac{1}{r_i} \sum_{j=1}^{r_i} Y_{ij}(x) \overline{Y_{ij}(y)}.$$

The binary space $H(n,2)$ is antipodal while the spaces $H(n,q)$ with $q \geq 3$ are clearly not antipodal.
The codes in $H(n,q)$ are known as error-correcting codes since they are capable to correct $[(d-1)/2]$ errors if their minimum distance is d. The τ-designs are widely known as orthogonal arrays.

Examples – Hamming spaces $H(n,q)$ (4)

The bound for designs in $H(n,q)$ can be proved by combinatorial arguments; first obtained by Rao (1947)

$$B(n,\tau) \geq R(n,\tau) := q^{1-\varepsilon} \sum_{i=0}^{k-1+\varepsilon} \binom{n-1+\varepsilon}{i} (q-1)^i,$$

where $\tau = 2k-1+\varepsilon$, $\varepsilon \in \{0,1\}$. The Levenshtein bound for $\mathcal{A}(H(n,q),s) := A_q(n,s)$

$$A_q(n,s) \leq L_\tau(n,s) = q^\varepsilon \left(1 - \frac{Q_{k-1}^{1,\varepsilon}(s)}{Q_k^{0,\varepsilon}(s)}\right) \sum_{i=0}^{k-1} \binom{n-\varepsilon}{i} (q-1)^i,$$

τ, ε as above.

Radau Quadrature Rule – $\tau = 2k - 1$

- For every fixed (cardinality) $N > D(\mathcal{M}, 2k-1)$ there exist uniquely determined real numbers (nodes)

$$-1 < \alpha_0 < \alpha_1 < \cdots < \alpha_{k-1} < 1$$

  and (weights) $\rho_0, \rho_1, \ldots, \rho_{k-1}$, $\rho_i > 0$ for $i = 0, 1, \ldots, k-1$, such that the equality

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

  holds for every real polynomial $f(t)$ of degree at most $2k-1$.

- The numbers α_i, $i = 0, 1, \ldots, k-1$, are the roots of the equation

$$Q_k^{1,0}(t)Q_{k-1}^{1,0}(s) - Q_k^{1,0}(s)Q_{k-1}^{1,0}(t) = 0.$$

Lobato Quadrature Rule – $\tau = 2k$

- Similarly, for every fixed (cardinality) $N > D(\mathcal{M}, 2k)$ there exist uniquely determined real numbers (nodes)

$$-1 = \beta_0 < \beta_1 < \cdots < \beta_k < 1$$

and (weights) $\gamma_0, \gamma_1, \ldots, \gamma_k$, $\gamma_i > 0$ 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 $2k$.

- V. I. Levenshtein, Designs as maximum codes in polynomial metric spaces, Acta Appl. Math. 25, 1992, 1-82.

All parameters together

- Given $\mathcal{M}$ and N, define $\tau = \tau(\mathcal{M}, n)$ and s, where $N = L_\tau(n, s)$.
- Then get all corresponding numbers:

$$\alpha_0, \alpha_1, \ldots, \alpha_{k-1}, \rho_0, \rho_1, \ldots, \rho_{k-1} \text{ if } N \in (D(\mathcal{M}, 2k-1), D(\mathcal{M}, 2k)]$$

or with

$$\beta_0, \beta_1, \ldots, \beta_k, \gamma_0, \gamma_1, \ldots, \gamma_k \text{ if } N \in (D(\mathcal{M}, 2k), D(\mathcal{M}, 2k+1)].$$

Linear programming bounds for energy of codes

- **Theorem 1.**
  Let $\mathcal{M}$ and N be fixed and $f(t)$ be a real polynomial such that

  (A1) $f(t) \leq h(t)$ for $-1 \leq t \leq 1$.

  (A2) $f(t) \in F_{\geq}$.

  Then $\mathcal{E}(\mathcal{M}, N; h) \geq N(f_0 N - f(1))$.

- $A_{\mathcal{M},N;h}$ – the set of good polynomials.

- **Theorem 2.**
  Let $\mathcal{M}$, N, τ and h be fixed. Suppose that there exists $t_0 = t_0(\mathcal{M}, N, \tau) \in [-1, 1]$ such that no τ-design $C \subset \mathcal{M}$ of size N can have inner products $\sigma(d(x, y)) \in (t_0, 1)$. Let $g(t)$ be a real polynomial such that

  (B1) $g(t) \geq h(t)$ for every $t \in [-1, t_0]$,

  (B2) the coefficients in the expansion $g(t) = \sum_{i=0}^{\deg(g)} g_i Q_i(t)$ satisfy $g_i \leq 0$ for $i \geq \tau + 1$.

  Then $\mathcal{F}(\mathcal{M}, N, \tau; h) \leq N(g_0 N - g(1))$.

Universal lower bound (ULB) (1)

- Consider Hermite's interpolation to $h(t)$ as follows:
  (i) the polynomial $f(t)$ of degree $\tau = 2k - 1$ by

$$f(\alpha_i) = h(\alpha_i),\ f'(\alpha_i) = h'(\alpha_i),\ i = 0, 1, \ldots, k-1.$$

  (ii) the polynomial $f(t)$ of degree $\tau = 2k$ by

$$f(\beta_0) = h(\beta_0),\ f(\beta_i) = h(\beta_i),\ f'(\beta_i) = h'(\beta_i),\ i = 1, \ldots, k.$$

- These conditions define a Hermite's interpolation problem for $f(t)$ to intersect and touch the graph of the potential function $h(t)$.
- This and the absolute monotonicity of h imply that the condition (A1) is satisfied (Rolle's theorem). (A2) – later

Universal lower bound (ULB) (2)

- **Theorem 3.** Let $\mathcal{M}$, $N \in (D(\mathcal{M},\tau), D(\mathcal{M},\tau+1)]$ and h be fixed. Then the polynomials from (i) and (ii) give the bounds

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

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

respectively.
These bounds can not be improved by using polynomials from $A_{\mathcal{M},N;h}$ of degree at most $2k-1$ and $2k$, respectively.

Sketch of the proof of the ULB (1)

We have to prove that our polynomial is positive definite, i.e. (A2) is satisfied.
The Q-system of $\mathcal{M}$ satisfies the Krein condition if

$$Q_i(t)Q_j(t) \in F_{\geq}$$

for every i and j.
If $f \in F_{\geq}$ and $g \in F_{\geq}$, then $fg \in F_{\geq}$. We apply this for combinations of $Q_i^{1,0} \in F_{\geq}$.
The Q-system of $\mathcal{M}$ satisfies the strengthened Krein condition if it satisfies the Krein condition and, in addition,

$$(t+1)Q_i^{1,1}(t)Q_j^{1,1}(t) \in F_{\geq}$$

for every i and j.
The strengthened Krein condition is satisfied in all major PM-spaces.

Sketch of the proof of the ULB (2)

We explain the case $\varepsilon = 0$. Consider the interpolation polynomial $f(t) = H_T(h)$, where

$$\begin{aligned} T &= (\alpha_0, \alpha_0, \alpha_1, \alpha_1, \ldots, \alpha_{k-1}, \alpha_{k-1}) \\ &= (t_1, t_2, \ldots, t_{2k-1}, t_{2k}) \end{aligned}$$

is the ordered multiset (i.e. $t_{2i+1} = t_{2i+2} = \alpha_i$) of the touching points of f and h. Then Lemma 10 from Cohn-Woo (2012) states that f is a nonnegative linear combination of the constant 1 and the partial products

$$\prod_{j=1}^{m}(t - t_j), \;\; m = 1, 2, \ldots, 2k-1. \qquad (1)$$

Sketch of the proof of the ULB (3)

By Theorem 3.1 from Cohn-Kumar (2007) all partial products

$$(t-\alpha_0)(t-\alpha_1)\dots(t-\alpha_i),\ \ i=0,1,\dots,k-2$$

expand in the system $\{Q_i^{1,0}(t)\}$ with nonnegative coefficients (because α_i are roots of $Q_i^{1,0}(t)+cQ_{i-1}^{1,0}(t)$).

The interlacing properties of the zeros of $Q_{k-1}^{1,0}$ and $Q_k^{1,0}$ yield that

$$Q_k^{1,0}(t)+\frac{Q_k^{1,0}(s)}{Q_{k-1}^{1,0}(s)}Q_{k-1}^{1,0}=C(t-\alpha_0)(t-\alpha_1)\dots(t-\alpha_{k-1}),\ \ C>0$$

is also positive definite. The Krein condition implies that all partial products (1) belong to $F_>$ and hence $f(t)=H_T(h)\in F_\geq$.

Sketch of the proof of the ULB (4)

Computation of the ULB – use the $(1/M)$-quadrature rule

$$f_0 M - f(1) = \sum_{i=0}^{k-1} \rho_i f(\alpha_i)$$

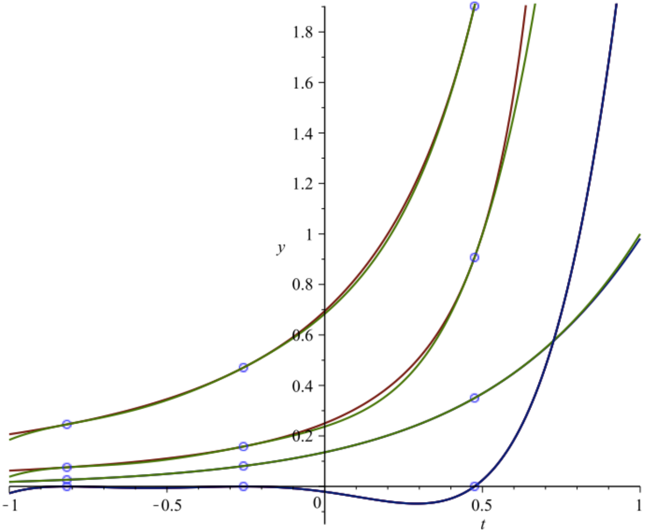
and then the interpolation conditions $f(\alpha_i) = h(\alpha_i)$.

Optimality of the ULB – again by the $1/M$-quadrature rule. Let $F(t) = \sum_{i=0}^{r} F_i Q_i(t)$ of degree $r \leq 2k - 1 + \varepsilon$ satisfies $F(t) \leq h(t)$ for every $t \in [-1, 1)$. Then

$$f_0 M - f(1) = M \sum_{i=0}^{k-1} \rho_i h(\alpha_i) \geq M \sum_{i=0}^{k-1} \rho_i F(\alpha_i) = F_0 M - F(1),$$

so $F(t)$ does not give better bound.

Gauss, Korevaar, Newton potentials - $\mathcal{M} = \mathbb{S}^3$, $N = 24$



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) - $N = 5 - 64$, $n = 4$.

Two ways for improving ULB – shorter intervals and higher degrees

- The ULB bounds are optimal in some sense – they can not be improved by polynomials from $A_{\mathcal{M},N;h}$ of degree $\tau = \tau(\mathcal{M}, N)$ or lower.
- First way for obtaining better bounds – making better LP by subintervals of $[-1, 1)$ based on preliminary (nontrivial) information on inner products (for example, for designs in $\mathcal{M}$). This is exactly the case when τ is even and the space is antipodal.
- Second way for obtaining better bounds – using LP with higher degree polynomials. There are necessary and sufficient conditions for the global optimality of ULB, and we can do better when the ULB in not globally optimal.

Necessary and sufficient conditions for improvement

- Let $\mathcal{M}$ and N be fixed, $N \in [D(\mathcal{M}, 2k-1), D(\mathcal{M}, 2k))$, $L_\tau(n,s) = N$ and j be positive integer. We introduce the following functions

$$P_j(\mathcal{M}, s) = \frac{1}{N} + \sum_{i=0}^{k-1} \rho_i Q_j(\alpha_i).$$

- **Theorem 4.** The bound $N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i)$ can be improved by a polynomial from $A_{\mathcal{M},N;h}$ of degree at least $2k$ if and only if $P_j(n,s) < 0$ for some $j \geq 2e$. Moreover, if $P_j(n,s) < 0$ for some $j \geq 2k$, then that bound can be improved by a polynomial from $A_{\mathcal{M},N;h}$ of degree exactly j.

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

Asymptotic of ULB (1)

We consider the asymptotic behaviour of the ULB bound in the antipodal spaces $\mathbb{S}^{n-1}$ and $H(n,2)$ in the following process – consider sequence of codes of cardinalities (M_n) satisfying

$$M_n \in D_\tau = (D(n,\tau), D(n,\tau+1))$$

for $n = 1, 2, 3, \ldots$, $\tau = 2k - 1 + \varepsilon$, $\varepsilon \in \{0, 1\}$, and

$$\lim_{n\to\infty} \frac{M_n}{n^{k-1+\varepsilon}} = \frac{2-\varepsilon}{(k-1+\varepsilon)!} + \delta,$$

where $\delta \geq 0$. Denote $\delta_k := 1 + \delta(k-1)!$ for brevity.

Theorem 7. Let

$$R(t) := \sum_{j=0}^{2k-1+\varepsilon} \frac{h^{(j)}(0)}{j!} t^j.$$

a) Let $\tau = 2k-1$ (i.e. $\varepsilon = 0$) and M_n is as above. Then

$$\lim_{n\to\infty} M_n \left(\sum_{i=0}^{k-1} \rho_i h(\alpha_i) - \sum_{j=0}^{k-1} \frac{h^{(2j)}(0)}{(2j)!} \cdot b_{2j} \right)$$
$$= \delta_k^{2k-1} \left(h\left(-\frac{1}{\delta_k}\right) - R\left(-\frac{1}{\delta_k}\right)\right) - R(1).$$

Asymptotic of ULB (3)

b) Let $\tau = 2k$ (i.e. $\varepsilon = 1$), M_n is as above, and assume that

$$\lim_{n\to\infty} M_n \rho_0 = \rho \in [0,1].$$

Then

$$\lim_{n\to\infty} M_n \left(\sum_{i=0}^{k} \rho_i h(\alpha_i) - \sum_{j=0}^{k} \frac{h^{(2j)}(0)}{(2j)!} \cdot b_{2j} \right)$$
$$= \rho \left(h(-1) + R(-1) \right) - R(1).$$

Asymptotic of ULB (4)

Corollary. If M_n is as above, then

$$\liminf_{n\to\infty} \frac{\mathcal{E}(n, M_n; h)}{M_n} \geq h(0)$$

and

$$\liminf_{n\to\infty} \frac{\mathcal{E}(n, M_n; h) - h(0)M_n}{M_n} \cdot n \geq \frac{h''(0)}{2}.$$

Thank you for your attention!