Asymptotic bounds for energy of spherical codes and designs

PETER BOYVALENKOV

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Joint work with:

P. Dragnev (Dept. Math. Sciences, IPFW, Fort Wayne, IN, USA)

D. Hardin, E. Saff (Dept. Math., Vanderbilt University, Nashville, TN, USA)

Maya Stoyanova Dept. Math. Inf. Sofia University, Sofia, Bulgaria

Midwestern Workshop on Asymptotic Analysis, October 7-9, 2016, Fort Wayne, USA

Energy of spherical codes (1)

- Let $\mathbb{S}^{n-1}$ denote the unit sphere in $\mathbb{R}^n$.
  A finite nonempty set $C \subset \mathbb{S}^{n-1}$ is called a spherical code.

Definition

For a given (extended real-valued) function $h(t) : [-1,1] \to [0,+\infty]$, we define the h-energy (or potential energy) of a spherical code C by

$$E(n,C;h) := \frac{1}{|C|} \sum_{x,y \in C, x \neq y} h(\langle x,y \rangle),$$

where $\langle x,y \rangle$ denotes the inner product of x and y.

- The potential function h is called k-absolutely monotone on $[-1,1)$ if its derivatives $h^{(i)}(t)$, $i = 0,1,\ldots,k$, are nonnegative for all $0 \leq i \leq k$ and every $t \in [-1,1)$.

Energy of spherical codes (2)

Problem

Minimize the potential energy provided the cardinality $|C|$ of C is fixed; that is, to determine

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

the minimum possible h-energy of a spherical code of cardinality M.

Energy of spherical codes (3)

Some interesting potentials:

- Riesz α-potential: $h(t) = (2-2t)^{-\alpha/2} = |x-y|^{-\alpha}$, $\alpha > 0$;
- Newton potential: $h(t) = (2-2t)^{-(n-2)/2} = |x-y|^{-(n-2)}$;
- Log potential: $h(t) = -(1/2)\log(2-2t) = -\log|x-y|$;
- Gaussian potential: $h(t) = \exp(2t-2) = \exp(-|x-y|^2)$;
- Korevaar potential: $h(t) = (1+r^2-2rt)^{-(n-2)/2}$, $0 < r < 1$.

Some references

- P. Delsarte, J.-M. Goethals, J. J. Seidel, Spherical codes and designs, *Geom. Dedicata* **6**, pp. 363-388, 1977.
- V. A. Yudin, Minimal potential energy of a point system of charges, *Discr. Math. Appl.* **3**, pp. 75-81, 1993.
- V. I. Levenshtein, Universal bounds for codes and designs, *Handbook of Coding Theory*, V. S. Pless and W. C. Huffman, Eds., Elsevier, Amsterdam, Ch. 6, pp. 499–648, 1998.
- H. Cohn, A. Kumar, Universally optimal distribution of points on spheres. Journal of AMS, **20**, no. 1, pp. 99-148, 2006.
- P. Boyvalenkov, P. Dragnev, D. Hardin, E. Saff, M. Stoyanova, Universal lower bounds for potential energy of spherical codes (arxiv1503.07228), to appear in Constructive Approximation.

Universal lower bound (ULB)

Theorem

Let n, $M \in (D(n,\tau), D(n,\tau+1)]$ and h be fixed. Then

$$\mathcal{E}(n,M;h) \geq M \sum_{i=0}^{k-1} \rho_i h(\alpha_i), \quad \mathcal{E}(n,M;h) \geq M \sum_{i=0}^{k} \gamma_i h(\beta_i).$$

These bounds can not be improved by using "good" polynomials of degree at most τ.

Note the universality feature – ρ_i, α_i (resp. γ_i, β_i) do not depend on the potential function h.

Next – to explain the above parameters and their connections and to investigate the bound in certain asymptotic process.

Gegenbauer polynomials

- For fixed dimension n, the (normalized) Gegenbauer polynomials are defined by $P_0^{(n)}(t) := 1$, $P_1^{(n)}(t) := t$ and the three-term recurrence relation

$$(i+n-2)\,P_{i+1}^{(n)}(t) := (2i+n-2)\,t\,P_i^{(n)}(t) - i\,P_{i-1}^{(n)}(t) \quad \text{for} \quad i \geq 1.$$

- Note that $\{P_i^{(n)}(t)\}$ are orthogonal in $[-1,1]$ with a weight $(1-t^2)^{(n-3)/2}$ and satisfy $P_i^{(n)}(1) = 1$ for all i and n.
- We have $P_i^{(n)}(t) = P_i^{((n-3)/2,(n-3)/2)}(t)/P_i^{((n-3)/2,(n-3)/2)}(1)$, where $P_i^{(\alpha,\beta)}(t)$ are the Jacobi polynomials in standard notation.

Adjacent polynomials

- The (normalized) Jacobi polynomials

$$P_i^{(a+\frac{n-3}{2},b+\frac{n-3}{2})}(t), \quad a,b \in \{0,1\},$$

$P_i^{(a+\frac{n-3}{2},b+\frac{n-3}{2})}(1)=1$ and are called adjacent polynomials (Levenshtein). Short notation $P_i^{(a,b)}(t)$.

- $a=b=0 \to$ Gegenbauer polynomials.
- $P_i^{(a,b)}(t)$ are orthogonal in $[-1,1]$ with weight $(1-t)^a(1+t)^b(1-t^2)^{(n-3)/2}$. Many important properties follow, in particular interlacing of zeros.

Spherical designs (P. Delsarte, J.-M. Goethals, J. J. Seidel, 1977)

Definition

A spherical τ-design $C \subset \mathbb{S}^{n-1}$ is a spherical code of $\mathbb{S}^{n-1}$ such that

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

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

The strength of C is the maximal number $\tau = \tau(C)$ such that C is a spherical τ-design.

Delsarte-Goethals-Seidel bounds

For fixed strength τ 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 τ-designs $C \subset \mathbb{S}^{n-1}$.
Then Delsarte-Goethals-Seidel bound is

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

Levenshtein bounds for spherical codes (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 adjacent polynomial $P_i^{(a,b)}(t)$.
- The intervals $\mathcal{I}_m$ define partition of $\mathcal{I} = [-1, 1)$ to countably many non-overlapping closed subintervals.

Levenshtein bounds for spherical codes (2)

- For every $s \in \mathcal{I}_m$, Levenshtein used certain polynomial $f_m^{(n,s)}(t)$ of degree m which satisfy all conditions of the linear programming bounds for spherical codes. This yields the bound

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

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

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

is continuous in s.

Connections between DGS- and L-bounds (1)

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

$$L_{2k-2}(n, t_{k-1}^{1,1}) = L_{2k-1}(n, t_{k-1}^{1,1}) = D(n, 2k-1),$$

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

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

Connections between DGS- and L-bounds (2)

- For every fixed (cardinality) $M > D(n, 2k-1)$ there exist uniquely determined real numbers $-1 < \alpha_0 < \alpha_1 < \cdots < \alpha_{k-1} < 1$ and positive $\rho_0, \rho_1, \ldots, \rho_{k-1}$, such that the equality (quadrature formula)

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

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

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

where $s = \alpha_{k-1}$, $P_i(t) = P_i^{(1,0)}(t)$ is the $(1,0)$ adjacent polynomial.

Connections between DGS- and L-bounds (3)

- For every fixed (cardinality) $M > D(n, 2k)$ there exist uniquely determined real numbers $-1 = \beta_0 < \beta_1 < \cdots < \beta_k < 1$ and positive $\gamma_0, \gamma_1, \ldots, \gamma_k$, 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 β_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 $s = \beta_k$, $P_i(t) = P_i^{(1,1)}(t)$ is the $(1, 1)$ adjacent polynomial.

Connections between DGS- and L-bounds (4)

- So we always take care where the cardinality M is located with respect to the Delsarte-Goethals-Seidel bound. It follows that

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

where s and M are connected by the equality

$$M = L_\tau(n,s),$$

and

$$\tau := \tau(n,M)$$

is correctly defined.

- Therefore we associate M with the corresponding numbers

$$\alpha_0, \alpha_1, \ldots, \alpha_{k-1}, \rho_0, \rho_1, \ldots, \rho_{k-1} \text{ when } M \in [D(n,2k-1), D(n,2k)),$$

$$\beta_0, \beta_1, \ldots, \beta_k, \gamma_0, \gamma_1, \ldots, \gamma_k \text{ when } M \in [D(n,2k), D(n,2k+1)).$$

Asymptotic of ULB (1)

We consider the behaviour of our bounds in the asymptotic process where the strength τ is fixed, and the dimension n and the cardinality M tend simultaneously to infinity in certain relation. We consider sequence of codes of cardinalities (M_n) satisfying $M_n \in I_\tau = (R(n,\tau), R(n,\tau+1))$ for $n = 1, 2, 3, \ldots$ and

$$\lim_{n\to\infty} \frac{M_n}{n^{k-1}} = \begin{cases} \frac{2}{(k-1)!} + \gamma, & \tau = 2k-1, \\ \frac{1}{k!} + \gamma, & \tau = 2k, \end{cases}$$

(here $\gamma \geq 0$ is a constant and the terms $\frac{2}{(k-1)!}$ and $\frac{1}{k!}$ come from the Delsarte-Goethals-Seidel bound).

Asymptotic of ULB (2)

Recall that the nodes $\alpha_i = \alpha_i(n, 2k-1, M)$, $i = 0, \ldots, k-1$, are defined for positive integers n, k, and M satisfying $M > R(n, 2k-1)$ and that the nodes $\beta_i = \beta_i(n, 2k, M)$, $i = 0, \ldots, k$, are defined if $M > R(n, 2k)$.

Lemma

If $\tau = 2k-1$ for some integer k, then

$$\lim_{n\to\infty} \alpha_0(n, 2k-1, M_n) = -1/(1+\gamma(k-1)!), \text{ and}$$

$$\lim_{n\to\infty} \alpha_i(n, 2k-1, M_n) = 0, \qquad i = 1, \ldots, k-1.$$

If $\tau = 2k$ for some integer k, then

$$\lim_{n\to\infty} \beta_i(n, 2k, M_n) = 0, \qquad i = 1, \ldots, k.$$

Asymptotic of ULB (3)

Sketch of the proof

$\lim_{n\to\infty} \alpha_i = 0$, $i = 1, \dots, k-1$, follow from the inequalities

$$t_k^{1,1} > |\alpha_{k-1}| > |\alpha_1| > |\alpha_{k-2}| > |\alpha_2| > \cdots .$$

For α_0 – use the Vieta formula

$$\sum_{i=0}^{k-1} \alpha_i = \frac{(n+2k-1)(n+k-2)}{(n+2k-2)(n+2k-3)} \cdot \frac{P_k^{1,0}(s)}{P_{k-1}^{1,0}(s)} - \frac{k}{n+2k-2}$$

to conclude that

$$\lim_{n\to\infty} \alpha_0 = \lim_{n\to\infty} \frac{P_k^{(1,0)}(s)}{P_{k-1}^{(1,0)}(s)}.$$

Asymptotic of ULB (4)

The behavior of the ratio $P_k^{(1,0)}(s)/P_{k-1}^{(1,0)}(s)$ can be found by using certain identities by Levenshtein:

$$M_n = \left(1 - \frac{P_{k-1}^{(1,0)}(s)}{P_k^{(n)}(s)}\right) D(n, 2k-2) = \left(1 - \frac{P_k^{(1,0)}(s)}{P_k^{(n)}(s)}\right) D(n, 2k).$$

These imply

$$\lim_{n\to\infty} \frac{P_k^{(n)}(s)}{P_{k-1}^{(1,0)}(s)} = -\frac{1}{1+\gamma(k-1)!}, \quad \lim_{n\to\infty} \frac{P_k^{(1,0)}(s)}{P_k^{(n)}(s)} = 1,$$

correspondingly. Therefore

$$\lim_{n\to\infty} \alpha_0 = \frac{P_k^{(1,0)}(s)}{P_{k-1}^{(1,0)}(s)} = -\frac{1}{1+\gamma(k-1)!}.$$

Asymptotic of ULB (5)

Similarly, $\lim_{n\to\infty} \beta_i = 0$ follows easy for $i \geq 2$, then $\lim_{n\to\infty} \beta_1 = 0$ is obtained by using the formula

$$\sum_{i=1}^{k-1} \beta_i = \frac{(n-k-1)P_k^{(1,1)}(s)}{nP_{k-1}^{(1,1)}(s)}$$

and investigation of the ratio $P_k^{(1,1)}(s)/P_{k-1}^{(1,1)}(s)$ in the interval $\mathcal{I}_{2k}$ – it is non-positive, increasing, equal to zero in the right end $s = t_k^{1,1}$, and tending to 0 as n tends to infinity in the left end $s = t_k^{1,0}$.

Asymptotic of ULB (6)

Recall that in the case $\tau = 2k-1$ there are associated weights $\rho_i = \rho_i(n, 2k-1, M_n)$, $i = 0, \ldots, k-1$, and, similarly, in the case $\tau = 2k$ there are weights $\gamma_i = \gamma_i(n, 2k-1, M_n)$, $i = 0, \ldots, k$.

In view of the Lemma we need the asymptotic of $\rho_0(n, 2k-1, M_n)M_n$ only.

Lemma

If $\tau = 2k-1$, then

$$\lim_{n\to\infty} \rho_0(n, 2k-1, M_n)M_n = (1+\gamma(k-1)!)^{2k-1}.$$

Asymptotic of ULB (7)

This follows from the asymptotic of α_0 and the formula

$$\rho_0(n, 2k-1, M_n) M_n = -\frac{(1-\alpha_1^2)(1-\alpha_2^2)\cdots(1-\alpha_{k-1}^2)}{\alpha_0(\alpha_0^2-\alpha_1^2)(\alpha_0^2-\alpha_2^2)\cdots(\alpha_0^2-\alpha_{k-1}^2)}$$

(can be derived by setting $f(t) = t, t^3, \ldots, t^{2k-1}$ in the quadrature rule and resolving the obtained linear system with respect to $\rho_0, \ldots, \rho_{k-1}$).

Asymptotic of ULB (8)

Theorem

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

Asymptotic of ULB (9)

Let $\tau = 2k-1$. We deal with the odd branch of our ULB

$$\begin{aligned}
\mathcal{E}(n, M_n; h) &\geq M_n \sum_{i=0}^{k-1} \rho_i h(\alpha_i) \\
&= M_n \left(\rho_0 h(\alpha_0) + h(0) \sum_{i=1}^{k-1} \rho_i + o(1) \right) \\
&= M_n \left(\rho_0 (h(\alpha_0) - h(0)) + h(0) \left(1 - \frac{1}{M_n} + o(1) \right) \right) \\
&= h(0) M_n + c_3 + M_n o(1),
\end{aligned}$$

where $o(1)$ is a term that goes to 0 as $n \to \infty$ and

$$c_3 = \left((1 + \gamma(k-1)!)^{2k-1} \right) \left(h \left(-\frac{1}{1+\gamma(k-1)!} \right) - h(0) \right) - h(0).$$

Asymptotic of ULB (10)

Similarly, in the even case we obtain

$$\begin{aligned}\mathcal{E}(n, M_n; h) &\geq M_n \left(\gamma_0(h(-1) - h(0)) + h(0)\left(1 - \frac{1}{M_n}\right) + o(1)\right) \\ &= h(0)M_n + c_4 + M_n o(1),\end{aligned}$$

where $c_4 = \gamma_0 M_n(h(-1) - h(0)) - h(0)$ (here $\gamma_0 M_n \in (0, 1)$).

More precise asymptotic (1)

Theorem

If $\tau = 2k-1$ *then*

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

where $b_{2j} = \int_{-1}^{1} t^{2j}(1-t^2)^{(n-3)/2} dt = \frac{(2j-1)!!}{n(n+2)\ldots(n+2j-2)}$,
$\gamma_k = 1 + \gamma(k-1)!$ *and* $P_{2k-1}(t) = \sum_{j=0}^{k-1} \frac{h^{(2j)}(0)}{(2j)!} t^j$.

More precise asymptotic (2)

Observe that $h(t) \geq P_{2k-1}(t)$ for every $t \in [-1, 1)$, and, furthermore,

$$0 \leq h(\alpha_i^{(n)}) - P_{2k-1}(\alpha_i^{(n)}) \leq \frac{h^{(2k)}(\xi)}{(2k)!} \cdot |\alpha_i^{(n)}|^{2k}, \tag{1}$$

where $|\xi| \in (0, |\alpha_i^{(n)}|)$, $i = 1, 2 \ldots, k-1$, by the Taylor expansion formula. Since $\frac{c_1}{\sqrt{n}} \leq t_k^{1,1} \leq \frac{c_2}{\sqrt{n}}$ for some constants c_1 and c_2, and for every n, it follows that

$$M_n \sum_{i=1}^{k-1} \rho_i^{(n)} \left(h(\alpha_i^{(n)}) - P_{2k-1}(\alpha_i^{(n)}) \right) = O(1/n).$$

More precise asymptotic (3)

Corollary

If $\tau = 2k - 1$ *then*

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

and

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

What next?

We do not know the asymptotic of our bounds in the case when the dimension n is fixed, and the cardinality M tends to infinity (with τ).

Thank you for your attention!