Asymptotic bounds for energy of spherical codes and designs

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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 $h(t) : [-1, 1] \rightarrow [0, +\infty]$, 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 $t \in [-1, 1)$.
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 $\alpha$-potential: $h(t) = (2 - 2t)^{-\alpha/2} = |x - y|^{-\alpha}$, $\alpha > 0$;
- Newton potential: $h(t) = (2 - 2t)^{-\frac{n-2}{2}} = |x - y|^{-(n-2)}$;
- 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: $h(t) = (1 + r^2 - 2rt)^{-(n-2)/2}$, $0 < r < 1$. 

PB, PD, DH, ES, MS

Asymptotic bounds for energy of spherical...
Some references

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 $\tau$.

Note the universality feature – $\rho_i, \alpha_i$ (resp. $\gamma_i, \beta_i$) 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.
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

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

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 \( P_{i}^{(a, b)}(t) \).

- \( a = b = 0 \rightarrow \) 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.
A spherical $\tau$-design $C \subset S^{n-1}$ is a spherical code of $S^{n-1}$ such that

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

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

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

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

$$\mathcal{I}_m = \begin{cases} 
[t_{k-1}^{1,1}, t_k^{1,0}], & \text{if } m = 2k - 1, \\
[t_k^{1,0}, t_k^{1,1}], & \text{if } m = 2k.
\end{cases}$$

- 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

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

- 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 \( s \).
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 \( \alpha_i, \ i = 0, 1, \ldots, k - 1 \), 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 $\beta_i, i = 1, 2, \ldots, k$, 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

$$M \in [D(n, \tau), D(n, \tau + 1)] \iff s \in I_\tau,$$

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 \( \tau \) 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

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

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

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

$$\lim_{n \to \infty} \beta_i(n, 2k, M_n) = 0, \quad i = 1, \ldots, k.$$
Asymptotic of ULB (3)

Sketch of the proof

\[ \lim_{n \to \infty} \alpha_i = 0, \ i = 1, \ldots, k - 1, \]  follow from the inequalities

\[ t_{k}^{1,1} > |\alpha_{k-1}| > |\alpha_1| > |\alpha_{k-2}| > |\alpha_2| > \cdots. \]

For \( \alpha_0 \) – 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 $P^{(1,0)}_k(s)/P^{(1,0)}_{k-1}(s)$ can be found by using certain identities by Levenshtein:

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

These imply

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

correspondingly. Therefore

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

\[
\sum_{i=1}^{k-1} \beta_i = \frac{(n - k - 1) P_k^{(1,1)}(s)}{nP_k^{(1,1)}(s)}
\]

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 $\alpha_0$ 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

$$E(n, M_n; h) \geq M_n \sum_{i=0}^{k-1} \rho_i h(\alpha_i)$$

$$= M_n \left( \rho_0 h(\alpha_0) + h(0) \sum_{i=1}^{k-1} \rho_i + o(1) \right)$$

$$= M_n \left( \rho_0 (h(\alpha_0) - h(0)) + h(0) \left( 1 - \frac{1}{M_n} + o(1) \right) \right)$$

$$= h(0) M_n + c_3 + M_n o(1),$$

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

\[
\mathcal{E}(n, M_n; h) \geq M_n \left( \gamma_0(h(-1) - h(0)) + h(0) \left( 1 - \frac{1}{M_n} \right) + o(1) \right) \\
= h(0)M_n + c_4 + M_n o(1),
\]

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 \( b_{2j} = \int_{-1}^{1} t^{2j}(1 - t^2)^{(n-3)/2} \, dt = \frac{(2j-1)!!}{n(n+2)...(n+2j-2)} \),

\( \gamma_k = 1 + \gamma(k - 1) \) 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,

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

(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

\[
M_n \sum_{i=1}^{k-1} \rho_i^{(n)} (h(\alpha_i^{(n)}) - P_{2k-1}(\alpha_i^{(n)})) = O(1/n).
\]
More precise asymptotic (3)

**Corollary**

If $\tau = 2k - 1$ then

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

and

$$\lim \inf_{n \to \infty} \frac{\mathcal{E}(n, M_n; h) - h(0)M_n}{M_n} \cdot n = \frac{h''(0)}{2}.$$
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 $\tau$).
Thank you for your attention!