Upper bounds for energies of codes of given cardinality and separation

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Abstract. We introduce a linear programming framework for obtaining upper bounds for potential energy of spherical codes of fixed cardinality and minimum distance. Using Hermite interpolation we construct polynomials to derive corresponding bounds. Our bounds are universal in the sense that they are valid for all absolutely monotone potential functions as the required interpolation nodes do not depend on the potentials.

1 Introduction

Let $\mathbb{S}^{n-1}$ denote the unit sphere in $\mathbb{R}^n$ and $C \subset \mathbb{S}^{n-1}$ be a spherical code. Given an (extended real-valued) function $h(t) : [-1, 1] \to [0, +\infty]$, the *potential energy* (or *h-energy*) of C is given by

$$E_h(C) := \sum_{x,y \in C, x \neq y} h(\langle x, y \rangle), \tag{1}$$

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

Denote by

$$C(n, M, s) := \{C \subset \mathbb{S}^{n-1} : |C| = M, s(C) = s\}$$

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the family of all spherical codes on $\mathbb{S}^{n-1}$ of given cardinality M and given maximal inner product $s(C) = \max\{\langle x, y\rangle : x, y \in C, x \neq y\}$. Equivalently, minimum distance $d(C) = \min\{d(x, y) : x, y \in C, x \neq y\}$ is investigated in coding theory.

Given, n, M, s, and $h(t)$, we are interested in upper bounds on the quantity

$$\mathcal{G}_h(n, M, s) := \sup_{C \in C(n,M,s)} \{E_h(C)\}. \tag{2}$$

Hereafter we consider only *absolutely monotone* potentials $h(t)$; i.e. real valued extended functions $h(t) : [-1, 1] \to (0, +\infty]$ such that $h^{(k)}(t) \geq 0$ for every $t \in [-1, 1)$ and every integer $k \geq 0$, and $h(1) = \lim_{t\to 1^-} h(t)$. Among the more prominent absolutely monotone potentials we list the *Newton potential* (when $h(t) = [2(1 - t)]^{1-n/2}$); the *Riesz potential* (when $h(t) = [2(1 - t)]^{-\alpha/2},\ \alpha > 0$); the *Exponential potential* (when $h(t) = e^{-2\alpha(1-t)}$); and the *Logarithmic potential* (when $h(t) = -\log[2(1 - t)]$).

In this article a general linear programming bound in the spirit of the Delsarte-Yudin approach is proposed for obtaining upper bounds on $\mathcal{G}_h(n, M, s)$. Polynomials which work in wide areas are constructed and tested in cases where good codes are known. We point out that upper bounds on the minimal energy for Riesz ($0 < \alpha < 2$) and Logarithmic potentials on $\mathbb{S}^2$ have been considered by G. Wagner in [10].

2 Linear programming for upper bounds for $\mathcal{G}_h(n, M, s)$

Let $P_i^{(n)}(t)$, $i = 0, 1, \ldots$, be the Gegenbauer polynomials normalized by $P_i^{(n)}(1) = 1$. Denote by $U_{n,s;h}$ the set of the real polynomials which satisfy the following two conditions:

(F1) $f(t) \geq h(t)$ for every $t \in [-1, s]$;

(F2) the coefficients in the expansion $f(t) = \sum_{i=0}^{r} f_i P_i^{(n)}(t)$ in terms of Gegenbauer polynomials satisfy $f_i \leq 0$ for $i = 1, \ldots, r$.

Upper bounds for the quantity $\mathcal{G}_h(n, M, s)$ can be obtained by the following linear programming theorem.

Theorem 1. *Let $n \geq 3$, $M \geq 2$ be positive integers, $s \in [-1, 1)$, and $h(t)$ be a function defined on $[-1, 1)$. If $f \in U_{n,s;h}$, then $\mathcal{G}_h(n, M, s) \leq M(f_0 M - f(1))$.*

Proof. For a spherical code $C \in C(n, M, s)$ and a polynomial $f \in U_{n,s;h}$ we consider the identity

$$f(1)M + \sum_{x \in C} \sum_{y \in C\setminus\{x\}} f(\langle x, y\rangle) = f_0 M^2 + \sum_{i=1}^{\deg(f)} f_i M_i(C), \tag{3}$$

where $M_i(C) = \sum_{x,y\in C} P_i^{(n)}(\langle x, y\rangle) \geq 0$ are the moments of C (see, for example [2]). Then (F1) together with $s(C) = s$ imply that the the left hand side of (3) is at least $Mf(1) + E_h(C)$ and (F2) together with $M_i \geq 0$ for all i give that the right hand side is at most $M^2 f_0$. Therefore $E_h(C) \leq M(f_0 M - f(1))$. Since these estimations are valid for every code $C \in C(n, M, s)$ we conclude that $\mathcal{G}_h(n, M, s) \leq M(f_0 M - f(1))$.

3 Construction and investigation of polynomials for Theorem 1

3.1 Levenshtein framework parameters

It is customary in this field to use certain parameters which were introduced by Levenshtein in [7] (see also [8, Section 5]) and generalized in [2] by the notion of a $1/N$-quadrature rule over subspaces.

Definition 1. *A finite sequence of ordered pairs* $\{(\alpha_i,\rho_i)\}_{i=1}^k$, $-1 \le \alpha_1 < \alpha_2 < \cdots < \alpha_k < 1$, $\rho_i > 0$ *for* $i = 1, 2, \ldots, k$, *forms a* $1/N$-quadrature rule, $N > 0$, that is exact for the subspace $\Lambda \subset C[-1, 1]$ *if*

$$f_0 = \gamma_n \int_{-1}^{1} f(t)(1-t^2)^{(n-3)/2}dt = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i), \tag{4}$$

for all $f \in \Lambda$.

Levenshtein's Theorem 5.39 in [8] defines a Gauss-Jacobi quadrature formula which is a $1/L_m(n,s)$-quadrature rule exact for the subspace of real polynomials of degree at most m. Hereafter $L_m(n,s)$, $m = 1, 2, \ldots$, is the Levenshtein upper bound on the maximal possible cardinality of spherical codes on $\mathbb{S}^{n-1}$ with $s(C) = s$.

The nodes in the Levenshtein's $1/L_m(n,s)$-quadrature rule are the roots of certain polynomial $f_m^{(n,s)}(t)$ of degree m (see [8, Theorem 5.39]). The explicit form of $f_m^{(n,s)}(t)$ can be found for example in [7, Eqs. (1.35-36)] or [8, Eq. (3.82)].

3.2 Construction of working polynomials

Denote by T the multiset of the roots of $f_m^{(n,s)}(t)$; i.e.,

$$T = \begin{cases} \{\alpha_0, \alpha_0, \alpha_1, \alpha_1, \ldots, \alpha_{k-2}, \alpha_{k-2}, \alpha_{k-1}\} & \text{if } m = 2k-1 \\ \{-1, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_{k-1}, \alpha_{k-1}, \alpha_k\} & \text{if } m = 2k \end{cases},$$

where $-1 < \alpha_i < \alpha_{i+1}$ for every i and s is equal to α_{k-1} for $m = 2k-1$ and to α_k for $m = 2k$.

Let n, M and s be such that the set $C(n, M, s)$ is nonempty. We consider the polynomial

$$f(t) := -\alpha f_m^{(n,s)}(t) + H_{h,T}(t) = \sum_{i=0}^{m} f_i P_i^{(n)}(t), \tag{5}$$

where $\alpha > 0$ is a parameter (to be determined later) and $H_{h,T}(t)$ is the Hermite interpolation polynomial to the function $h(t)$ that agrees with $h(t)$ exactly in the points of T (counted with their multiplicities). Note that the degree of $g(t)$ is at most $m - 1$.

Theorem 2. *Let $h(t)$ be absolutely monotone. We have $f(t) \in U_{n,s;h}$ for any large enough α, where $f(t)$ is defined as in (5). In particular, if*

$$\alpha = \max \left\{ \frac{g_i}{\ell_i} : 1 \leq i \leq m-1 \right\},$$

then $f(t) \in U_{n,s;h}$ and

$$\mathcal{G}_h(n,M,s) \leq M(f_0 M - f(1)).$$

A code $C \in C(n,M,s)$ attains this bound if and only if all inner products of C are in T and $f_i M_i = 0$ for every $i \geq 1$.

Proof. The absolute monotonicity of $h(t)$ and the interpolation conditions for $g(t)$ imply that $g(t) \geq h(t)$ for $t \in [-1,s]$. Since $f_m^{(n,s)}(t) \leq 0$ for $t \in [-1,s]$ and $f(\alpha_i) = g(\alpha_i) = h(\alpha_i)$ for every i (note also that $f'(\alpha_i) = g'(\alpha_i) = h'(\alpha_i)$ in the double roots of $f_m^{(n,s)}(t)$), if follows from (5) that $f(t) \geq h(t)$ for every $t \in [-1,s]$; i.e. (F1) is satisfied (whatever $\alpha > 0$ is).

For (F2), observe that (5) implies that the coefficients f_i, $i = 1,2,\ldots,m-1$, in the Gegenbauer expansion of $f(t)$ are linear combinations $-\alpha\ell_i + g_i$, where $f_m^{(n,s)}(t) = \sum_{i=0}^{m} \ell_i P_i^{(n)}(t)$ and $g(t) = \sum_{i=0}^{m-1} g_i P_i^{(n)}(t)$. Since $\ell_i > 0$ for every i (see, for example, [8, Theorem 5.42]) it is clear that large enough α will make $f_i \leq 0$ for every $1 \leq i \leq m-1$. The inequality $f_i < 0$ follows for every $\alpha > 0$ since $\deg(F) = m$ and $\deg(g) = m-1$.

Since $f_0 M - f(1)$ is a linear function of α, the conditions $-\alpha\ell_i + g_i \leq 0$ for $i = 1,2,\ldots,m-1$ imply that the smallest value of α which works is $\alpha = \max\left\{\frac{g_i}{\ell_i} : 1 \leq i \leq m-1\right\}$. Moreover, the corresponding bound $\mathcal{G}_h(n,M,s) \leq M(f_0 M - f(1))$ will be best possible from this kind of f. This completes the proof.

Remark 1. Our numerical experiments suggest that the maximum for the parameter α in Theorem 2 is always attained at $i = 1$.

Remark 2. Construction with $g(t)$ of degree m is also possible by adding interpolation note at -1 for odd m and s for even m. Such approach gives sometimes slightly better bounds.

3.3 Investigation

We proceed with a representation of the bound from Theorem 2 in a ULB-form (see [2]) which may facilitate some further analysis. For simplicity we describe the odd case $m = 2k-1$ only.

Set $M_1 := L_{2k-1}(n,s)$. The number M_1 is not necessarily integer but the inequality $M_1 \geq M$ follows. Indeed, if $M > M_1$ is true, then the monotonicity of the Levenshtien bound implies $s(C) > s$, which contradicts to $C \in C(n,M,s)$.

Assume again that α is large enough as above for (F2) to be satisfied and express f_0 by the Levenshtein's $1/M_1$-quadrature rule. This gives

$$\begin{aligned}
\mathcal{G}_h(n,M,s) \leq M(f_0M - f(1)) &= M\left(M\left(\frac{f(1)}{M_1} + \sum_{i=0}^{k-1}\rho_i f(\alpha_i)\right) - f(1)\right) \\
&= M\left(\frac{M}{M_1} - 1\right) f(1) + M^2 \sum_{i=0}^{k-1}\rho_i f(\alpha_i) \\
&= M\left(\frac{M}{M_1} - 1\right) f(1) + M^2 \sum_{i=0}^{k-1}\rho_i h(\alpha_i),
\end{aligned}$$

where the last equality follows by using the interpolation conditions $f(\alpha_i) = h(\alpha_i)$, $i = 0, 1, \ldots, k-1$. The dependence of this bound on α comes from $f(1)$ only. Since $f(1)$ is linear with respect to α, the best bound is obtained again, of course, when α is chosen as in Theorem 2.

In the end of this section we put together the upper bound from Theorem 2 and the universal lower bound from [2]. We start now with $M = L_m(n,r)$ for a unique r (the uniqueness follows from the monotonicity of the Levenshtein bounds). Let the polynomial $f_{2k-1}^{(n,r)}(t)$ have roots $\alpha_0' < \alpha_1' < \cdots < \alpha_{k-1}' = r$ with corresponding weights $\rho_0', \rho_1', \ldots, \rho_{k-1}'$ in the Levenshtein's $1/M$-quadrature rule. Then the energy of any code $C \subset \mathbb{S}^{n-1}$ with cardinality $|C| = M$ is bounded from below by

$$E_h(C) \geq M^2 \sum_{i=0}^{k-1} \rho_i' h(\alpha_i')$$

(see [2, Theorem 3.1]). This, together with the bound from Theorem 2 implies

$$M^2 \sum_{i=0}^{k-1} \rho_i' h(\alpha_i') \leq E_h(C) \leq M\left(\frac{M}{M_1} - 1\right) f(1) + M^2 \sum_{i=0}^{k-1}\rho_i h(\alpha_i), \tag{6}$$

defining a strip where the energies of all codes from $C(n,M,s)$ lie and, in particular, a lower bound on $\mathcal{G}_h(n,M,s)$. Of course, lower bounds for $\mathcal{G}_h(n,M,s)$ can be extracted also from constructions of good codes.

It is clear from the above that $M = M_1$ implies the coincidence of the upper and lower bounds in (6). In this case the corresponding codes are sharp configurations (also universally optimal codes; see [5]) which means that they attain simultaneously the Levenshtein bound, the ULB bound [2] and the upper bound from Theorem 2.

4 Bounds for $(n, M) = (n, 2n+1)$ codes

It is natural to consider upper bounds for parameters where good codes are known. Here we show how our bound behaves for spherical codes $C_n \subset \mathbb{S}^{n-1}$ with $M = 2n+1$ points constructed in [6]. These codes are conjectured to be optimal (see [1, Section 3.3]) but this is proved in dimensions 3 [9] and 4 [11] only.

The maximal inner product of C_n is equal to the unique root $s \in (0, 1/n)$ of the equation

$$n(n-2)^2X^3 - n^2X^2 - nX + 1 = 0.$$

These parameters are in the region of the third Levenshtein bound; i.e., we use $m = 3$.

The universal lower bound [2] with parameters coming from $L_3(n, r) = M$ as in the last paragraph of the previous section is

$$R_h(n, 2n+1) := M^2 \left(\rho_0' h(\alpha_0') + \rho_1' h(r)\right). \tag{7}$$

To obtain upper bounds for $\mathcal{G}_h(n, M, s)$ we consider the corresponding Levenshtein polynomial $f_3^{(n,s)}(t)$ with zeros α_0 (double) and $\alpha_1 = s$ (simple). Then $T = \{\alpha_0, \alpha_0, \alpha_1\}$ and $g(t) := H_{h,T}(t)$ is the second degree interpolant to h in the nodes α_0 (doubly) and α_1. The polynomial from (5) is

$$f(t) = -\alpha f_3^{(n,s)}(t) + g(t) = \sum_{i=0}^{3} f_i P_i^{(n)}(t)$$

where $\alpha > 0$ has to be chosen to ensure $f_1 \leq 0$ and $f_2 \leq 0$ ($f_3 < 0$ follows for every $\alpha > 0$).

Here are the numerical results for $n = 5$, $M = 2n + 1 = 11$ and $s \approx 0.13285$ with the Newton potential $h(t) = 1/(2-2t)^{(n-2)/2}$.

The lower bound from (7) is

$$R_h(5, 11) = 11^2(\rho_0' h(\alpha_0') + \rho_1' h(\alpha_1')) \approx 37.484.$$

For the construction of the upper bound we find $f_3^{(5,s)}(t)$ with roots $(\alpha_0, \alpha_1 = s) \approx (-0.68069, 0.13285)$ and

$$g(t) = H(h; \alpha_0, \alpha_0, \alpha_1) \approx 0.23835t^2 + 0.46931t + 0.37128.$$

Then we search for α to satisfy the conditions $f_i \leq 0$ for $i = 1, 2, 3$. The computations show that all $\alpha \geq 0.661$ work as best the upper bound ≈ 41.906 from Theorem 2 (also the upper bound in (6)) is obtained with the smallest possible $\alpha = g_1/\ell_1 \approx 0.661$. For the representation of the upper bound in (6) we compute $M_1 = L_3(5, s) \approx 13.3014$ and

$$\mathcal{G}_h(n, M, s) \leq 11 \left(\frac{11}{M_1} - 1\right) f(1) + 11^2 \left(\rho_0 h(\alpha_0) + \rho_1 h(s)\right). \tag{8}$$

The Newton energy of the code C_5 is

$$E_h(C_5) = (3n^2 - n)h(s) + (n^2 - n)h(a) + 2nh(b) + 2nh(c) \approx 39.0225,$$

where $a \approx -0.22793$, $b \approx -0.553428$, and $c \approx -0.89904$. The best known (for the minimum Newton energy problem) code of 11 points on $\mathbb{S}^4$ has energy ≈ 38.0544 [1].

5 Conclusion and future work

The conditions of attaining the bound of Theorem 2 lead to the usual suspects – the universally optimal configurations [5]. In a broader view, our upper bounds set the range of all possible energies (or energy levels) of good spherical codes. Thus we impose restrictions on the structure of such code which could be useful for obtaining classification (or nonexistence) results.

It is also interesting if the optimality condition $f_1 = 0$ (see Remark 1) is true for every absolutely monotone potential function $h(t)$.

One more interesting object for investigation is the 600-cell in four dimensions which is an exceptional case among the universally optimal configurations (see [5, 4]). Here we expect to derive upper bound of next level.

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