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Universal upper and lower bounds on energy of spherical designs

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Abstract

Linear programming (polynomial) techniques are used to obtain lower and upper bounds for the potential energy of spherical designs. This approach gives unified bounds that are valid for a large class of potential functions. Our lower bounds are optimal for absolutely monotone potentials in the sense that for the linear programming technique they cannot be improved by using polynomials of the same or lower degree. When additional information about the structure (upper and lower bounds for the inner products) of the designs is known, improvements on the bounds are obtained. Furthermore, we provide ‘test functions’ for determining when the linear programming lower bounds for energy can be improved utilizing higher degree polynomials. We also provide some asymptotic results for these energy bounds.

1 Introduction

Let $\mathbb{S}^{n-1}$ be the unit sphere in $\mathbb{R}^n$. We refer to a finite set $C \subset \mathbb{S}^{n-1}$ as a *spherical code* and, for a given (extended real-valued) function $h : [-1,1] \to [0,+\infty]$, we consider the *h-energy* (or the potential energy) of C defined by

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

where $\langle x,y\rangle$ denotes the inner product of x and y. At times we shall require h to be *absolutely monotone* or *strictly absolutely monotone* on $[-1,1)$; i.e., its k-th derivative satisfies $h^{(k)}(t)\geq 0$ ($h^{(k)}(t)>0$, resp.) for all $k\geq 0$ and $t\in[-1,1)$.

A spherical τ-design $C\subset \mathbb{S}^{n-1}$, whose cardinality we denote by $|C|$, is a spherical code 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 surface area measure) holds for all polynomials $f(x)=f(x_1,x_2,\ldots,x_n)$ of total degree at most τ. The maximal number $\tau=\tau(C)$ such that C is a spherical τ-design is called the *strength* of C.

A commonly arising problem is to estimate the potential energy of certain sets of codes C (see [2, 8, 16, 23, 30, 36, 40]). In this paper we address this problem for the class of spherical designs of fixed dimension, strength and cardinality. Denote by

$$\mathcal{L}(n,N,\tau;h) := \inf\{E(n,C;h) : |C|=N,\ C\subset\mathbb{S}^{n-1} \text{ is a } \tau\text{-design}\} \tag{2}$$

and

$$\mathcal{U}(n,N,\tau;h) := \sup\{E(n,C;h) : |C|=N,\ C\subset\mathbb{S}^{n-1} \text{ is a } \tau\text{-design}\} \tag{3}$$

the minimum and the maximum possible h-energy of a spherical τ-design of N points on $\mathbb{S}^{n-1}$, respectively. In this paper we derive lower bounds on $\mathcal{L}(n,N,\tau;h)$ and upper bounds on $\mathcal{U}(n,N,\tau;h)$, which then define a strip where the energies of all designs of fixed dimension, strength and cardinality lie (see Theorem 3.7).

Concerning lower bounds for energy, a general linear programming technique originally introduced by Delsarte [19] for investigating codes over finite fields (see also [27]) has been utilized by Yudin [40], Kolushov and Yudin [30] and Andreev [2] (see also [1, 3, 29]) to prove the optimality of certain spherical codes among all possible codes. In 2007, Cohn and Kumar augmented this technique by introducing the notion of *conductivity* to prove the universal optimality of *sharp* codes. (A code is sharp if for some positive integer m, the code is a $2m-1$ design with at most m different values of the distance between distinct points in the code.) By *universal optimality of a code* we mean that among all codes of the same cardinality, it minimizes the

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energy for all absolutely monotone potentials. Essential to their method are certain quadrature rules associated with those sharp codes. Here, by combining the Delsarte method with quadrature formulas developed by Levenshtein, we derive lower bounds for general designs that are optimal for the linear programming technique when restricted to the use of polynomials of fixed maximal degree.

Since the collection of spherical designs is a special subclass of codes for a given dimension and cardinality, we expect that both larger lower bounds and lower upper bounds are possible when compared with minimal energy codes. Indeed we provide such examples in Section 5, where we discuss Mimura 2-designs (see Example 5.4). Our general upper bounds for $\mathcal{U}(n,N,\tau;h)$ are given in Theorems 3.6 and 3.7 in Section 3.

We remark that upper bounds for the Riesz s-energy of well-separated spherical designs of asymptotically optimal cardinality on $\mathbb{S}^2$ (that is, $|C| = \mathcal{O}(\tau^2)$ as $\tau \to \infty$) were obtained by Hesse and Leopardi in [25, 26]. The existence of such well-separated designs of asymptotically optimal cardinality on $\mathbb{S}^2$ (and more generally on $\mathbb{S}^{n-1}$) has been established recently by Bondarenko, Radchenko, and Viazovska in [6, 7].

An outline of our paper is as follows. Some preliminaries are explained in Section 2, where we refer to results and techniques developed by Delsarte, Goethals and Seidel [20] and Levenshtein [32, 33, 34] that will be needed for the statements of our main results. The relationship between the Delsarte-Goethals-Seidel bounds (6) for the minimum possible size of spherical designs of prescribed dimension and strength and the Levenshtein bounds for the maximum size of spherical codes of prescribed dimension and minimum distance will play a very important role in our investigation. Some results on the structure of designs of fixed dimension, strength and cardinality from [12, 10] are also discussed.

In Section 3 we formulate two general results that provide the framework for obtaining lower and upper bounds for the energy of spherical designs. Theorem 3.1 (lower bounds) is a slight modification of a known result (cf. [16, Proposition 4.1], [8, Chapter 5]), but Theorem 3.6 (upper bounds) is new.

Theorem 3.4 gives lower bounds that are optimal in the sense described in Theorem 3.5 – they cannot be improved by utilizing polynomials of the same or lower degree that satisfy the conditions of Theorem 3.1. Following Levenshtein [34] we call these bounds *universal*. Upper bounds for well-separated designs are derived in Theorem 3.7, which together with Theorem 3.4 determines a strip where the energies of such designs lie.

Some of the lower bounds on (2) from Theorem 3.4 can be further improved by either restricting the interval containing the inner products of even-strength designs (Theorems 4.1 and 4.2) or by allowing polynomials of higher degree for odd-strength designs (Theorems 4.3 and 4.4 and Corollary 4.5). For the latter case, Theorem 4.3 provides necessary and sufficient conditions for the global optimality of the bounds from Theorem 3.4.

Section 5 is devoted to improving upper bounds on (3) for spherical designs utilizing restrictions on their inner products. Some asymptotic results and numerical examples that illustrate these upper bounds are also included.

Finally, in Section 6 we derive an asymptotic lower bound for the energy of spherical designs of fixed strength as the dimension and cardinality grow to infinity in certain relation. An example (Euclidean realization of the Kerdock codes [28]) illustrating the tightness of these asymptotic bounds is presented.

2 Preliminaries

The results to be presented in Sections 3-7 utilize the notations and fundamental facts described in the subsections below. For Subsections 2.1-2.4 we extract notations and results from the Levenshtein's review chapter [34] (see also [33]) and in Subsection 2.5 we describe some results from [10, 12].

2.1 Gegenbauer polynomials and the linear programming framework

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

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

We 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 [39].

If $f(t) \in \mathbb{R}[t]$ is a real polynomial of degree r, then $f(t)$ can be uniquely expanded in terms of the Gegenbauer polynomials as

$$f(t) = \sum_{i=0}^{r} f_i P_i^{(n)}(t). \tag{4}$$

We use the identity (see, for example, [20, Corollary 3.8], [32, Equation (1.7)], [33, Equation (1.20)])

$$|C|f(1) + \sum_{x,y\in C, x\neq y} f(\langle x,y\rangle) = |C|^2 f_0 + \sum_{i=1}^{r} \frac{f_i}{r_i} \sum_{j=1}^{r_i} \left(\sum_{x\in C} Y_{ij}(x) \right)^2 \tag{5}$$

as a source of estimations by polynomial techniques. Here $C \subset \mathbb{S}^{n-1}$ is a spherical code, f is as in (4), $\{Y_{ij}(x) : j = 1,2,\ldots,r_i\}$ is an orthonormal basis of the space $\mathrm{Harm}(i)$ of homogeneous harmonic polynomials of degree i and $r_i = \dim \mathrm{Harm}(i)$.

The Delsarte-Goethals-Seidel bound and the Levenshtein bound described in the next subsections are obtained after the sums on both sides of (5) are neglected for suitable polynomials.

2.2 Delsarte-Goethals-Seidel bound for spherical designs

Denote by $D(n,\tau)$ the Delsarte-Goethals-Seidel [20] bound for spherical designs

$$B(n,\tau) \geq D(n,\tau) := \begin{cases} 2\binom{n+k-2}{n-1}, \text{ if } \tau = 2k-1, \\ \binom{n+k-1}{n-1} + \binom{n+k-2}{n-1}, \text{ if } \tau = 2k, \end{cases} \tag{6}$$

where $B(n,\tau) := \min\{|C| : C \subset \mathbb{S}^{n-1}$ is a spherical τ-design$\}$. This bound plays an important role in our (initially heuristic) choice of applications of Theorems 3.1 and 3.6.

We shall utilize the values of the function $D(n,\tau)$ in (6) to decide the degrees of the polynomials to be used for the bounding of $\mathcal{L}(n,N,\tau;h)$ and $\mathcal{U}(n,N,\tau;h)$. The rule is the following – if we have dimension n, strength τ and cardinality $N \in (D(n,\tau), D(n,\tau+1)]$, then we use polynomials of degree τ for the lower bounds and τ or $\tau-1$ (depending on the parity of τ) for the upper bounds.

2.3 Levenshtein bounds for spherical codes

We now formulate and discuss the Levenshtein bounds [31, 32, 33, 34] on

$$A(n,s) := \max\{|C| : C \subset \mathbb{S}^{n-1}, \langle x,y\rangle \leq s \text{ for all } x,y \in C, x \neq y\}, \tag{7}$$

the maximal possible cardinality of a spherical code on $\mathbb{S}^{n-1}$ of prescribed maximal inner product s.

Denote by $P_i^{a,b}(t) := P_i^{(a+\frac{n-3}{2},b+\frac{n-3}{2})}(t)/P_i^{(a+\frac{n-3}{2},b+\frac{n-3}{2})}(1)$ the corresponding normalized Jacobi polynomials. These polynomials are called *adjacent* in [33, 34]. Note that $P_i^{0,0}(t) = P_i^{(n)}(t)$.

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 $t_0^{1,1} = -1$ by definition, and $t_i^{a,b}$, $a,b \in \{0,1\}$, $i \geq 1$, is the largest zero of the polynomial $P_i^{a,b}(t)$. The intervals $\{\mathcal{I}_m\}_{m=1}^{\infty}$ are well defined (see [34, Lemmas 5.29 and 5.30]) and therefore constitute a partition of $\mathcal{I} = [-1,1)$ into countably many closed subintervals with nonoverlapping interiors.

For every $s \in \mathcal{I}_m$, Levenshtein introduces a certain polynomial $f_m^{(n,s)}(t)$ of degree m that satisfies all the conditions of the corresponding linear programming bounds for spherical codes and yields the bound on (7)

$$A(n,s) \leq \begin{cases} L_{2k-1}(n,s) := \binom{k+n-3}{k-1}\Big[\frac{2k+n-3}{n-1} - \frac{P_{k-1}^{(n)}(s)-P_k^{(n)}(s)}{(1-s)P_k^{(n)}(s)}\Big] \text{ for } s \in \mathcal{I}_{2k-1}, \\ L_{2k}(n,s) := \binom{k+n-2}{k}\Big[\frac{2k+n-1}{n-1} - \frac{(1+s)(P_k^{(n)}(s)-P_{k+1}^{(n)}(s))}{(1-s)(P_k^{(n)}(s)+P_{k+1}^{(n)}(s))}\Big] \text{ for } s \in \mathcal{I}_{2k}. \end{cases} \tag{8}$$

The function

$$L(n,s) := \begin{cases} L_{2k-1}(n,s) & \text{for } s \in \mathcal{I}_{2k-1}, \\ L_{2k}(n,s) & \text{for } s \in \mathcal{I}_{2k} \end{cases} \tag{9}$$

is continuous in s.

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

$$L_{2k-2}(n,t_{k-1}^{1,1}) = L_{2k-1}(n,t_{k-1}^{1,1}) = D(n,2k-1) = 2\binom{n+k-2}{n-1}, \tag{10}$$

$$L_{2k-1}(n,t_k^{1,0}) = L_{2k}(n,t_k^{1,0}) = D(n,2k) = \binom{n+k-1}{n-1} + \binom{n+k-2}{n-1} \tag{11}$$

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

2.4 A useful quadrature

It follows from [34, Section 5] (see also [33, Section 4], [12]) that for every fixed (cardinality) $N > D(n, 2k-1)$ there exist uniquely determined real numbers $-1 < \alpha_0 < \alpha_1 < \cdots < \alpha_{k-1} < 1$ and $\rho_0, \rho_1, \ldots, \rho_{k-1}$, $\rho_i > 0$ for $i = 0, 1, \ldots, k-1$, such that the quadrature formula

$$f_0 = \frac{\Gamma(n-1)}{2^{n-2}\Gamma(\frac{n-1}{2})^2} \int_{-1}^{1} f(t)(1-t^2)^{\frac{n-3}{2}}\, dt = \frac{f(1)}{N} + \sum_{i=0}^{k-1} \rho_i f(\alpha_i) \tag{12}$$

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

The number $\alpha_{k-1} = \alpha_{k-1}(N)$ in (12) is the solution of the equation $L(n, s) = N$ (see (9)) for $s > t_{k-1}^{1,1}$. Once it is determined, it is known (and easily verified) that the remaining $\alpha_i = \alpha_i(N)$, $i = 0, 1, \ldots, k-2$, are roots of the equation

$$P_k^{1,0}(t) P_{k-1}^{1,0}(\alpha_{k-1}) - P_k^{1,0}(\alpha_{k-1}) P_{k-1}^{1,0}(t) = 0.$$

In fact, α_i, $i = 0, 1, \ldots, k-1$, are the roots of the Levenshtein polynomial [34, Eqs. (5.81) and (5.82)] (see also [34, Theorem 5.39])

$$f_{2k-1}^{(n,\alpha_{k-1})}(t) := (t - \alpha_{k-1}) \prod_{i=0}^{k-2} (t - \alpha_i)^2$$

used for obtaining the bound $L_{2k-1}(n, s)$, $s = \alpha_{k-1}$, in (8).

Similarly, for every fixed $N > D(n, 2k)$ there exist uniquely determined real numbers $-1 = \beta_0 < \beta_1 < \cdots < \beta_k < 1$ and $\gamma_0, \gamma_1, \ldots, \gamma_k$, $\gamma_i > 0$ for $i = 0, 1, \ldots, k$, such that the quadrature formula

$$f_0 = \frac{f(1)}{N} + \sum_{i=0}^{k} \gamma_i f(\beta_i) \tag{13}$$

is true for every real polynomial $f(t)$ of degree at most $2k$. The numbers $\beta_i = \beta_i(N)$, $i = 0, 1, \ldots, k$, are the roots of the Levenshtein polynomial

$$f_{2k}^{(n,\beta_k)}(t) := (t - \beta_0)(t - \beta_k) \prod_{i=1}^{k-1} (t - \beta_i)^2$$

(used for $L_{2k}(n, s)$, $s = \beta_k$, in (8)).

As mentioned in the Introduction we always take into consideration where the cardinality N is located with respect to the Delsarte-Goethals-Seidel bound. It follows from the properties of the bounds $D(n, \tau)$ and $L_\tau(n, s)$ (see (10) and (11)) that

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

where n, s and N are connected by the equality

$$N = L_\tau(n, s).$$

Therefore we can always associate N with the corresponding numbers:

$$\alpha_0, \alpha_1, \ldots, \alpha_{k-1}, \rho_0, \rho_1, \ldots, \rho_{k-1} \text{ when } N \in (D(n, 2k-1), D(n, 2k)] \tag{14}$$

or with

$$\beta_0, \beta_1, \ldots, \beta_k, \gamma_0, \gamma_1, \ldots, \gamma_k \text{ when } N \in (D(n, 2k), D(n, 2k+1)]. \tag{15}$$

2.5 Bounds on smallest and largest inner products of spherical designs

Denote

$$u(n, N, \tau) := \sup\{u(C) : C \subset \mathbb{S}^{n-1} \text{ is a } \tau\text{-design}, |C| = N\}, \tag{16}$$

where $u(C) := \max\{\langle x, y\rangle : x, y \in C, x \neq y\}$, and

$$\ell(n, N, \tau) := \inf\{\ell(C) : C \subset \mathbb{S}^{n-1} \text{ is a } \tau\text{-design}, |C| = N\}, \tag{17}$$

where $\ell(C) := \min\{\langle x, y\rangle : x, y \in C, x \neq y\}$.

For every n, τ and cardinality $N \in [D(n, \tau), D(n, \tau+1)]$ non-trivial upper bounds on $u(n, N, \tau)$ can be obtained (cf. [12, 10]). Similarly, for even $\tau = 2k$ and cardinality $N \in [D(n, 2k), D(n, 2k+1))$ non-trivial lower bounds on $\ell(n, N, 2k)$ are possible [12, 10]. We describe here explicitly the cases $\tau = 2$ and $\tau = 4$.

In [12, 10] the quantities $u(n, N, \tau)$ and $\ell(n, N, \tau)$ are estimated by using the following equivalent definition of spherical designs (see [22]), which is a consequence of (5): a spherical τ-design $C \subset \mathbb{S}^{n-1}$ is a spherical code such that for any point $x \in \mathbb{S}^{n-1}$ and any real polynomial of the form $f(t) = \sum_{i=0}^{\tau} f_i P_i^{(n)}(t)$, the equality

$$\sum_{x \in C} f(\langle x, y\rangle) = f_0 |C| \tag{18}$$

holds.

Lemma 2.1 ([10]). *Let $n \geq 3$.*

(a) *For every $N \in [D(n,2), D(n,3)] = [n+1, 2n]$ we have*

$$u(n,N,2) \leq \frac{N-2}{n} - 1. \tag{19}$$

(b) *For every $N \in [D(n,4), D(n,5)] = [n(n+3)/2, n(n+1)]$ we have*

$$u(n,N,4) \leq \frac{2(3+\sqrt{(n-1)[(n+2)N-3(n+3)]})}{n(n+2)} - 1. \tag{20}$$

Proof. To prove (a) one can use the polynomial $f(t) = \left(t + \sqrt{\frac{2}{n(N-2)}}\right)^2$ in (18) with y being the midpoint of the geodesic arc between two of the closest points in C as in Theorem 3.2 from [10]. The bound (20) in (b) is proved in the example following Theorem 3.2 from [10]. □

Lemma 2.2 ([10]). *Let $n \geq 3$.*

(a) *For every $N \in [D(n,2), D(n,3)) = [n+1, 2n)$ we have*

$$\ell(n,N,2) \geq 1 - \frac{N}{n}. \tag{21}$$

(b) *For every $N \in [D(n,4), D(n,5)) = [n(n+3)/2, n(n+1))$ we have*

$$\ell(n,N,4) \geq 1 - \frac{2}{n}\left(1 + \sqrt{\frac{(n-1)(N-2)}{n+2}}\right). \tag{22}$$

Proof. The bound in (a) can be proved by utilizing the polynomial $f(t) = t^2$ in (18) with y being the midpoint of the geodesic arc between points $-x$ and $z \in C$, where x, z is a pair of points of C with smallest inner product (see Theorem 3.3 from [10]). The bound in (b) is proved as in the example after Theorem 3.3 from [10]. □

We remark that different bounds on $u(n,N,\tau)$ and $\ell(n,N,\tau)$ can be obtained by a technique from [12, Sections 2 and 3]. For $\tau \geq 4$ such bounds are better in higher dimensions than those from Lemmas 2.1 and 2.2. More generally, when $\tau = 2k$ we establish in Lemma 2.3 lower bounds on $\ell(n,N,\tau)$ that will be used in Section 4 to establish Theorem 4.1.

Lemma 2.3 ([12, Lemma 4.1]). *Let $N \in (D(n,2k), D(n,2k+1))$ and*

$$f(t) := (t-\beta_1)^2 \cdots (t-\beta_k)^2,$$

where $\beta_0, \ldots, \beta_k$ are as in (15). Let ξ and η denote the smallest and largest roots, respectively, of $f(t) = \gamma_0 N f(-1)$. Then $\xi \leq \ell(n,N,2k) \leq u(n,N,2k) \leq \eta$.

Proof. For the convenience of the reader, we provide a proof of Lemma 2.3. Let C be a spherical design of strength $\tau = 2k$ on $\mathbb{S}^{n-1}$ with $|C| = N$. Let x and y be distinct points in C. Since $f(t) \geq 0$ for all t and f vanishes at $\beta_1, \ldots, \beta_k$, it follows from (18) and (13) that

$$f(1) + f(\langle x,y\rangle) \leq \sum_{z\in C} f(\langle x,z\rangle) = N f_0 = f(1) + N\gamma_0 f(-1),$$

and so $f(\langle x,y\rangle) \leq N\gamma_0 f(-1)$. Since $f(t)$ is strictly decreasing for $t < \beta_1$ and strictly increasing for $t > \beta_k$, we must have $\xi \leq \langle x,y\rangle \leq \eta$. □

Note that Lemma 2.3 will produce a non-trivial bound $\xi > -1$ if and only if $\gamma_0 N < 1$ and the next assertion, implicit in [14, Section 4] (see also Remark 5.58 in [34]), shows that this is indeed true for $N \in (D(n,2k), D(n,2k+1))$. We use the kernel

$$T_k(u,v) := \sum_{i=0}^{k} r_i P_i^{(n)}(u) P_i^{(n)}(u)$$

(see [34, Equation (5.14)]) and its obvious properties.

Lemma 2.4. *If $N \in (D(n,2k), D(n,2k+1))$, then $\gamma_0 N \in (0,1)$. Hence, $\ell(n,N,2k) > -1$.*

Proof. We have the formulas (Equation (5.113) in [34])

$$\gamma_0 = \frac{T_k(s,1)}{T_k(-1,-1)T_k(s,1) - T_k(-1,1)T_k(s,-1)}$$

and (the equation in the last line of page 594 in [34])

$$N = L_{2k}(n,s) = \frac{T_k(1,1)T_k(s,-1) - T_k(1,-1)T_k(s,1)}{T_k(s,-1)}.$$

A little algebra then shows that

$$\gamma_0 N = \frac{T - A(s)}{T - 1/A(s)},$$

where $A(s) := T_k(s,1)/T_k(s,-1)$ as in [14] and $T := T_k(1,1)/T_k(1,-1)$. Moreover, we have

$$A(s) = T \cdot \frac{P_k^{1,0}(s)}{P_k^{0,1}(s)}$$

from [34, Lemma 5.24], where $P_k^{1,0}(s) > 0$ and $P_k^{0,1}(s) < 0$ for every $s \in \left(t_k^{1,0}, t_k^{1,1}\right)$ (see Lemmas 5.29 and 5.30 in [34]). Therefore the signs of $A(s)$ and T are opposite. We conclude that

$$\gamma_0 N = \frac{|T| + |A(s)|}{|T| + 1/|A(s)|}.$$

The ratio $\frac{P_k^{1,0}(s)}{P_k^{0,1}(s)}$ is decreasing in s in the interval $\left(t_k^{1,0}, t_k^{1,1}\right)$ (see [34, Lemma 5.31]), i.e. $|A(s)|$ is increasing in $s \in \left(t_k^{1,0}, t_k^{1,1}\right)$. Since $\gamma_0 N = 0$ and 1 for $s = t_k^{1,0}$ and $t_k^{1,1}$, respectively, we obtain that $\gamma_0 N$ increases from 0 to 1 when s increases from $s = t_k^{1,0}$ to $t_k^{1,1}$. □

3 General lower and upper bounds

The general framework of the linear programming bounds for the quantities $\mathcal{L}(n,N,\tau;h)$ and $\mathcal{U}(n,N,\tau;h)$ is given by the next two theorems. Theorem 3.1 is an adaptation of known results (cf. [40, 16]) to spherical designs, we are not aware of any prior use of linear programming techniques for obtaining upper bounds on the potential energy as in Theorem 3.6.

Theorem 3.1. *Let n, N, τ be positive integers with $N \geq D(n,\tau)$ and let $h : [-1,1] \to [0,+\infty]$. Suppose I is a subset of $[-1,1)$ and $f(t) = \sum_{i=0}^{\deg(f)} f_i P_i^{(n)}(t)$ is a real polynomial such that*

(A1) *$f(t) \leq h(t)$ for $t \in I$, and*

(A2) *the Gegenbauer coefficients satisfy $f_i \geq 0$ for $i \geq \tau + 1$.*

If $C \subset \mathbb{S}^{n-1}$ is a spherical τ-design of $|C| = N$ points such that $\langle x, y\rangle \in I$ for distinct points $x, y \in C$, then

$$E(n,C;h) \geq N(f_0 N - f(1)). \tag{23}$$

In particular, if $I = [\ell(n,N,\tau), u(n,N,\tau)]$, then

$$\mathcal{L}(n,N,\tau;h) \geq N(f_0 N - f(1)). \tag{24}$$

Proof. Using (1), (5) and the conditions of the theorem we consecutively have

$$\begin{aligned} Nf(1) + E(n,C;h) &= Nf(1) + \sum_{x,y\in C, x\neq y} h(\langle x,y\rangle) \\ &\geq |C|f(1) + \sum_{x,y\in C, x\neq y} f(\langle x,y\rangle) \\ &= |C|^2 f_0 + \sum_{i=1}^{\deg(f)} \frac{f_i}{r_i} \sum_{j=1}^{r_i} \left(\sum_{x\in C} Y_{ij}(x)\right)^2 \\ &\geq N^2 f_0, \end{aligned}$$

which implies (23). If $I = [\ell(n,N,\tau), u(n,N,\tau)]$, the assertion (24) follows immediately from the definitions (2), (16), and (17). □

Our choice of polynomials for Theorem 3.1 follows from ideas of Levenshtein [33, 34] and the connections (10) and (11). We start with fixed dimension n, cardinality N and strength τ under the assumption that $N \in (D(n,\tau), D(n,\tau+1)]$. Now the equation $N = L_\tau(n,s)$ determines all necessary parameters as explained in subsections 2.3 and 2.4.

Definition 3.2. We denote by $A_{n,\tau,I;h}$ the set of polynomials satisfying conditions (A1) and (A2) of Theorem 3.1. For convenience we shall write $A_{n,\tau;h} := A_{n,\tau,[-1,1];h}$.

Next we need Hermite interpolation as follows. If $h \in C^1([-1,1])$, we define the Hermite interpolant $F(t)$ as follows:

(i) for odd $\tau = 2k-1$ the polynomial $F(t)$ of degree at most $2k-1$ by

$$F(\alpha_i) = h(\alpha_i),\ F'(\alpha_i) = h'(\alpha_i),\ i = 0, 1, \ldots, k-1;$$

(ii) for even $\tau = 2k$ the polynomial $F(t)$ of degree at most $2k$ 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, as in [16] (see also [2, 30, 40]), a Hermite interpolation problem that requires the graph of $F(t)$ to intersect and be tangent to the graph of the potential function $h(t)$ at all points α_i and all β_i except for $\beta_0 = -1$ where only intersection is required.

Lemma 3.3. *Suppose h is absolutely monotone on $[-1,1]$ and that F satisfies* (i) *or* (ii)*. Then $F(t) \le h(t)$ for all $t \in [-1,1]$.*

Proof. The proof follows from the well-known error formula for Hermite interpolation (see [18, Theorem 3.5.1]), namely

$$h(t) - F(t) = \begin{cases} \frac{h^{(\tau+1)}(\xi)}{(\tau+1)!}(t-\alpha_0)^2 \cdots (t-\alpha_{k-1})^2, & \tau = 2k-1, \\ \\ \frac{h^{(\tau+1)}(\xi)}{(\tau+1)!}(t-\beta_0)(t-\beta_1)^2 \cdots (t-\beta_k)^2, & \tau = 2k, \end{cases}$$

for some $\xi = \xi(t) \in (-1,1)$ and the fact that $h^{(\tau+1)}(t) \ge 0$ for $t \in [-1,1]$. □

In [15, Theorem 3.1], the following result was established by the authors, which provides a lower bound on the h-energy of *general* codes.

Theorem 3.4. *Let n, N and τ be positive integers with $N \in (D(n,\tau), D(n,\tau+1)]$ and suppose h is absolutely monotone on $[-1,1]$. Then, for any positive integer τ, we have*

$$\mathcal{L}(n,N,\tau;h) \ge \inf_C E(n,C;h) \ge \begin{cases} N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i), & \tau = 2k-1, \\ \\ N^2 \sum_{i=0}^{k} \gamma_i h(\beta_i), & \tau = 2k, \end{cases} \quad (25)$$

where the infimum is over spherical codes $C \subset \mathbb{S}^{n-1}$ with $|C| = N$.

Utilizing Theorems 3.1 and 3.4 we provide a sufficient condition for the optimality of the bounds in (25) for a class of spherical designs.

Theorem 3.5. *Suppose n, τ, and I are as in Theorem 3.1, $N \in (D(n,\tau), D(n,\tau+1)]$, h is absolutely monotone on $[-1,1]$ and that $\alpha_i \in I$ for $i = 0, \ldots, k-1$ in the case that $\tau = 2k-1$ and that $\beta_i \in I$ for $i = 0, \ldots, k$ in the case that $\tau = 2k$. If $C \subset \mathbb{S}^{n-1}$ is a spherical τ-design with $|C| = N$ and inner products $\langle x, y \rangle \in I$ for $x \neq y \in C$, then the linear programming lower bounds in* (25) *cannot be improved by utilizing polynomials of degree at most τ satisfying* (A1)*; i.e., for any such polynomial f we have*

$$N(f_0 N - f(1)) \le N(F_0 N - F(1)) = \begin{cases} N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i), & \tau = 2k-1, \\ \\ N^2 \sum_{i=0}^{k} \gamma_i h(\beta_i), & \tau = 2k, \end{cases} \quad (26)$$

where $F(t)$ is the Hermite interpolating polynomial from (i) *and* (ii)*.*

Proof. We shall consider only the case $\tau = 2k-1$ since the $\tau = 2k$ case is analogous. Notice that (i) and (12) allow us to rewrite (25) as

$$E(n,C;h) \ge N^2 \sum_{i=0}^{k-1} \rho_i F(\alpha_i) = N(F_0 N - F(1)).$$

Lemma 3.3 implies that $F(t) \le h(t)$ for every $t \in [-1,1]$; in particular $F(t)$ satisfies the condition (A1) of Theorem 3.1. The condition (A2) is trivially satisfied and therefore $F \in A_{n,2k-1,I;h}$.

Furthermore, for any polynomial $f(t) \in A_{n,2k-1,I;h}$ of degree at most $2k-1$, we have from the quadrature formula (12) for $f(t)$ and the fact that $\{\alpha_i\} \subset I$

$$N(F_0 N - F(1)) = N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i) \ge N^2 \sum_{i=0}^{k-1} \rho_i f(\alpha_i) = N(f_0 N - f(1)),$$

which proves (26) and the theorem. □

In Theorem 4.1 we show that the bound for $\mathcal{L}(n,N,\tau;h)$ in (25) can be improved over the whole range $D(n,\tau) < N < D(n,\tau+1)$ in the case of even τ.

As mentioned above, the specific properties of the spherical designs, namely the existence of nontrivial upper bounds on $u(n,N,\tau)$, allows further application of the linear programming techniques. We are able to derive upper bounds on $\mathcal{U}(n,N,\tau;h)$ thus setting a strip for the energies of the spherical designs under consideration.

Theorem 3.6. *Let n, N, τ be positive integers with $N \geq D(n,\tau)$ and let $h:[-1,1]\to[0,+\infty]$. Suppose I is a subset of $[-1,1)$ and $g(t)=\sum_{i=0}^{\deg(g)} g_i P_i^{(n)}(t)$ is a real polynomial such that*

(B1) *$g(t)\geq h(t)$ for $t\in I$, and*

(B2) *the Gegenbauer coefficients satisfy $g_i \leq 0$ for $i\geq \tau+1$.*

If $C\subset \mathbb{S}^{n-1}$ is a spherical τ-design of $|C|=N$ points such that $\langle x,y\rangle \in I$ for distinct points $x,y\in C$, then

$$E(n,C;h)\leq N(g_0N-g(1)). \tag{27}$$

In particular, if $I=[\ell(n,N,\tau),u(n,N,\tau)]$, then

$$\mathcal{U}(n,N,\tau;h)\leq N(g_0N-g(1)). \tag{28}$$

Proof. Let $C\subset\mathbb{S}^{n-1}$ be an arbitrary spherical τ-design of $|C|=N$ points. Using (1), (5) and the conditions of the theorem we consecutively have

$$\begin{aligned} Ng(1)+E(n,C;h) &= Ng(1)+\sum_{x,y\in C, x\neq y} h(\langle x,y\rangle) \\ &\leq Ng(1)+\sum_{x,y\in C, x\neq y} g(\langle x,y\rangle) \\ &= N^2 g_0 + \sum_{i=1}^{\deg(g)} \frac{g_i}{r_i}\sum_{j=1}^{r_i}\left(\sum_{x\in C} Y_{ij}(x)\right)^2 \\ &\leq N^2 g_0, \end{aligned}$$

which implies (27). Since the design C was arbitrary, we conclude that (28) holds. □

We utilize Theorem 3.6 to determine an upper bound that in conjunction with the lower bound (26) in Theorem 3.5 defines a strip where the energy of designs lives. We shall formulate the theorem for the odd case $\tau=2k-1$, but a similar assertion holds for the even case $\tau=2k$.

Theorem 3.7. *Let n, N, and $\tau=2k-1$ be positive integers with $N>D(n,\tau)$ and let $h:[-1,1]\to[0,+\infty]$ be absolutely monotone. For $\alpha_{k-1}<u<1$ (see (14)) and every $j\in\{0,1,\dots,k-1\}$, let $G(t)=G_{j,u}(t)$ be the Hermite interpolant of h of degree $2k-1$ that satisfies*

$$G(\alpha_i)=h(\alpha_i),\ G'(\alpha_i)=h'(\alpha_i),\ i\in\{0,1,\dots,k-1\}\setminus\{j\}, G(-1)=h(-1),\ G(u)=h(u).$$

Then, for any spherical τ-design C with $|C|=N$ and $u(C)=\max_{x,y\in C,x\neq y}\langle x,y\rangle\leq u$,

$$E(n,C;h)\leq N(G_0N-G(1))=N^2\sum_{i=0}^{k-1}\rho_i h(\alpha_i)+N^2\rho_j\left[G(\alpha_j)-h(\alpha_j)\right]. \tag{29}$$

In particular, if $u:=u(n,N,\tau)<1$, then

$$\mathcal{U}(n,N,\tau;h)-\mathcal{L}(n,N,\tau;h)\leq N^2\min_{0\leq j\leq k-1}\rho_j[G_{j,u}(\alpha_j)-h(\alpha_j)]. \tag{30}$$

Proof. It follows from the Hermite error formula

$$h(t)-G(t)=\frac{h^{(2k)}(\xi)}{(2k)!}(t+1)(t-u)\prod_{i\neq j}(t-\alpha_i)^2,$$

that $G(t)\geq h(t)$ for $t\in[-1,u]$. We next apply the quadrature formula (13) to the polynomial $G(t)$ and utilize Theorem 3.6 to conclude (29). For $N\in(D(n,\tau),D(n,\tau+1)]$ the estimate (30) follows from Theorem 3.4 and (29). When $N>D(n,\tau+1)$, we utilize [15, Theorem 3.4] instead. □

Remark 1. Theorem 3.7 and its counterpart for even τ give upper bounds for well separated τ-designs with $N>D(n,\tau+1)$. In this case, the lower end of the energy strip is given by lower bounds coming from higher degree polynomials. Indeed, the cardinality N is located in some interval $(D(n,\tau'),D(n,\tau'+1)]$, where $\tau'\geq\tau+1$, and the corresponding expression from (25) can be calculated. It turns out that this is a valid lower bound (cf. [15, Theorem 3.1]).

4 Improving the linear programming lower bounds

4.1 Even strength

We show that the bounds from Theorem 3.4 can be improved when some additional information about the distribution of the inner products of the designs under consideration is available. This is exactly the case for designs of even strength $2k$ and cardinality N in the interval $(D(n,2k), D(n,2k+1))$. In fact, $N = D(n,2k)$ is possible only for $k = 1$ (the regular simplex) and $k = 2$ (see [4, 5]).

It follows from Lemmas 2.3 and 2.4 that $-1 < \ell(n,N,2k)$ for every $N \in (D(n,2k), D(n,2k+1))$. We next use this fact to improve the bound (25) for the case of even strength $\tau = 2k$, where $N \in (D(n,2k), D(n,2k+1))$.

Theorem 4.1. *Suppose $N \in (D(n,2k), D(n,2k+1))$ and h is absolutely monotone on $[-1,1]$. Let $G(t)$ be the Hermite interpolant of $h(t)$ of degree at most $2k$ such that*

$$G(\ell) = h(\ell),\ G(\beta_i) = h(\beta_i),\ G'(\beta_i) = h'(\beta_i),\ i = 1,\ldots,k,$$

where $\ell := \ell(n,N,2k)$. Then

$$\mathcal{L}(n,N,2k;h) \geq N(G_0N - G(1)) = N^2\sum_{i=0}^{k}\gamma_i G(\beta_i) > N^2\sum_{i=0}^{k}\gamma_i h(\beta_i).$$

Proof. We note that $\ell \leq \beta_1$ (see [12, Theorem 4.5]). Using Theorem 3.1 with $f = G$ and $I = [\ell,1]$, we obtain $\mathcal{L}(n,N,2k;h) \geq N(G_0N - G(1))$. Since the degree of $G(t)$ is at most $2k$ we can apply the quadrature formula (13) and so

$$\begin{aligned} G_0N - G(1) &= N\sum_{i=0}^{k}\gamma_i G(\beta_i) = N\left(\gamma_0 G(-1) + \sum_{i=1}^{k}\gamma_i h(\beta_i)\right) \\ &= N\left(\gamma_0(G(-1) - h(-1)) + \sum_{i=0}^{k}\gamma_i h(\beta_i)\right) \\ &> N\sum_{i=0}^{k}\gamma_i h(\beta_i), \end{aligned}$$

(the inequality $G(-1) > h(-1)$ follows from the interpolation). □

We remark that the choice of the polynomial $G(t)$ in Theorem 4.1 is not usually optimal for maximizing the lower bound in Theorem 4.1. In a forthcoming paper, we shall develop methods for choosing optimal interpolation points.

Next we show that the inequality for $\ell(n,N,2)$ from Lemma 2.2(a) can be used for obtaining a lower bound for $\mathcal{L}(n,N,2;h)$ that is better than (25) in the whole range $n+1 = D(n,2) < N < 2n = D(n,3)$.

Theorem 4.2. *Let $n \geq 2$ and $N \in [n+1, 2n]$. If h is absolutely monotone on $[-1,1]$, then*

$$\mathcal{L}(n,N,2;h) \geq \frac{N[h(0)N(N-n-1) + nh(1-N/n)]}{N-n}. \tag{31}$$

In particular, if $\zeta := N/n$, then

$$\mathcal{L}(N/\zeta,N,2;h) \geq h(0)N^2 + \frac{N[h(1-\zeta) - \zeta h(0)]}{\zeta - 1}. \tag{32}$$

Proof. If $N = n+1$, then the regular simplex is a universally optimal code that is also a two-design, and (31) and (32) hold with equality. Therefore, we may assume that $n+1 < N \leq 2n$.

Let $\kappa \leq 1 - N/n$. By Lemma 2.2(a), $\ell(n,N,2) \geq 1 - N/n$. Therefore, we can apply Theorem 3.1 with $I = [\kappa, 1]$ and a second degree polynomial $f(t)$ such that $f(\kappa) = h(\kappa)$, $f(a) = h(a)$ and $f'(a) = h'(a)$, where

$$a := \frac{n(1-\kappa) - N}{n(1-\kappa) + \kappa N n}. \tag{33}$$

Observe that $a \in I$. Choosing $\kappa = 1 - N/n$ gives $a = 0$ and, hence, the bounds (31) and (32) follow. □

Remark 2. For any $\kappa \leq 1-N/n$, the choice of a in (33) maximizes the functional $f_0 - f(1)/N$ over all polynomials $f(t)$ of degree two such that $f(t) \leq h(t)$ on $I = [\kappa, 1]$. Indeed, the nodes $\{\kappa, a, 1\}$ define a quadrature rule

$$g_0 = \frac{g(1)}{N} + w_1 g(a) + w_0 g(\kappa),$$

that is exact for all polynomials $g(t) \in \mathcal{P}_2$. The weights

$$w_1 = \frac{(1+\kappa(N-1))^2}{N(N(\frac{1}{n}+\kappa^2)-(1-\kappa)^2)}, \quad w_0 = \frac{N-n-1}{n(N-1)\kappa^2+2n\kappa+N-n}$$

are strictly positive for $n+1 < N \leq 2n$. The optimality of the node a now follows as in Theorem 3.5.

The independence of the optimal touching point a in (33) on the potential function h is a phenomenon similar to the universality of the Levenshtein nodes $\{\alpha_i\}$ (respectively $\{\beta_i\}$) considered in Section 3. We shall consider the problem for bounding cardinalities and energies of spherical codes and designs with inner products in some interval $[\ell, u] \subset [-1, 1]$ in a future work.

Lower bounds for the energy of 4-designs by Theorem 3.1 can be obtained by interpolation with polynomials of degree four:

$$f(\kappa) = h(\kappa), \ \ f(a) = h(a), \ \ f'(a) = h'(a), \ \ f(b) = h(b), \ \ f'(b) = h'(b),$$

where κ is the expression on the right-hand side of (22) and the touching points a and b are chosen to maximize $f_0 N - f(1)$.

4.2 Odd strength

In contrast to the even strength case, non-trivial lower bounds on $\ell(n, N, 2k-1)$ seem impossible for $N \in [D(n, 2k-1), D(n, 2k)]$ without further constraints. Instead we show that higher degree polynomials can lead to improving the lower bound (25) for $\tau = 2k-1$.

Let n, $N \in [D(n, 2k-1), D(n, 2k)]$ and $\tau = 2k-1$ be fixed and j be a positive integer. Taking the necessary parameters from $N = L_{2k-1}(n, s)$ we consider the following functions in n and $s \in \mathcal{I}_{2k-1}$

$$Q_j(n,s) := \frac{1}{N} + \sum_{i=0}^{k-1} \rho_i P_j^{(n)}(\alpha_i). \tag{34}$$

Note that $Q_j(n, s)$ is the same as the quadrature rule expression on the right-hand side of (12) applied to $f = P_j^{(n)}$ since $P_j^{(n)}(1) = 1$.

The functions $Q_j(n, s)$ were firstly introduced and investigated in [13]. The applications in [13] target the upper bounds on $A(n, s)$ and, in particular, the possibilities for improving the Levenshtein bounds. We are going to see that the functions $Q_j(n, s)$ are useful for our purposes as well. The next theorem shows that (the signs of) the functions $Q_j(n, s)$ give necessary and sufficient conditions for existence of improving polynomials of higher degrees.

Theorem 4.3. *Assume that h is strictly absolutely monotone. Then the bound (25) can be improved by a polynomial from $A_{n,2k-1;h}$ of degree at least $2k$ if and only if one has $Q_j(n, s) < 0$ for some $j \geq 2k$.*

Moreover, if $Q_j(n, s) < 0$ for some $j \geq 2k$, then (25) can be improved by a polynomial from $A_{n,2k-1;h}$ of degree exactly j.

Proof. The necessity mirrors the spherical codes' analog [15, Theorem 4.1] (see also [15, Theorem 2.6]). We include the simplified proof of the sufficiency in the context of the spherical designs for completeness.

Let us assume $Q_j(n, s) < 0$ for some $j \geq 2k$. We prove that the bound (25) can be improved by using the polynomial $f(t) = \varepsilon P_j^{(n)}(t) + g(t)$ for suitable $\varepsilon > 0$, where the polynomial $g(t)$ is such that $\deg(g) = 2k-1$ and

$$g(\alpha_i) = h(\alpha_i) - \varepsilon P_j^{(n)}(\alpha_i), \ g'(\alpha_i) = h'(\alpha_i) - \varepsilon (P_j^{(n)})'(\alpha_i), \ i = 0, 1, \ldots, k-1 \tag{35}$$

(i.e. $g(t)$ is Hermite interpolant of $h(t) - \varepsilon P_j^{(n)}(t)$ in the points $\alpha_0, \alpha_1, \ldots, \alpha_{k-1}$. We denote $g(t) = \sum_{\ell=0}^{2k-1} g_\ell P_\ell^{(n)}(t)$. Note that $f_0 = g_0$ and $f(1) = g(1) + \varepsilon$.

We first prove that $f(t) = \varepsilon P_j^{(n)}(t) + g(t) \in A_{n,2k-1;h}$ for some $\varepsilon > 0$. For condition (A2) we need to see only that $f_j = \varepsilon > 0$. For condition (A1), let us choose $\varepsilon > 0$ such that $\left(h - \varepsilon P_j^{(n)}\right)^{(\ell)}(t) \geq 0$ for every $\ell \geq 0$ and for every $t \in [-1, 1]$. It is clear that such ε exists because h is strictly absolutely monotone and this leaves finitely many ℓ to generate inequalities for ε. Moreover, since the function $\tilde{h}(t) := h(t) - \varepsilon P_j^{(n)}(t)$ is absolutely monotone by the choice of ε, we could infer as in Lemma 3.3 that g satisfies $g(t) \leq \tilde{h}(t)$ for every $t \in [-1, 1)$ which implies that $f(t) \leq h(t)$ for every $t \in [-1, 1]$ and hence $f(t) \in A_{n,2k-1;h}$.

It remains to see that the bound given by $f(t)$ is better than (25). This follows by combining equalities from (35) and applying (12) and (34) to obtain

$$N(Nf_0 - f(1)) = N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i) - \varepsilon N^2 Q_j(n, s)$$

Since $Q_j(n, s) < 0$, we have $N(Nf_0 - f(1)) > N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i)$, i.e. the polynomial $f(t)$ indeed gives a better bound. □

As mentioned above, the test functions $Q_j(n,s)$ were initially defined in [13] as related to the Levenshtein bounds $\mathcal{L}(n,s)$ on maximal spherical codes. Theorem 4.3 shows that $Q_j(n,s)$ prove to be very useful tool in the context of potential energy as well. In particular, the signs of the test functions $Q_{2k+3}(n,s)$, where $\tau = 2k-1$, were investigated in detail in [13] (see also [9]). Denote

$$k_0 := \frac{k^2 - 4k + 5 + \sqrt{k^4 - 8k^3 - 6k^2 + 24k + 25}}{4}$$

for short (k_0 is well defined for $k \geq 9$).

Theorem 4.4. *[9, Theorem 3.5.9] We have $Q_{2k+3}(n,s) < 0$ for every $s \in \left(t_{k-1}^{1,1}, t_k^{1,0}\right)$ and for every $n \geq 3$ and $k \geq 9$ which satisfy $3 \leq n \leq k_0$.*

Corollary 4.5. *The bound (25) can be improved by using polynomials of degree $2k+3$ for every $s \in \left(t_{k-1}^{1,1}, t_k^{1,0}\right)$ and for every $n \geq 3$ and $k \geq 9$ that satisfy $3 \leq n \leq k_0$.*

Proof. This follows from Theorems 4.3 and 4.4. □

Remark 3. We note that test functions for the even case $\tau = 2k$ can be defined and investigated as well (see [13]). However, we conjecture that the linear programming in $[\ell(n,N,\tau), u(n,N,\tau)]$ by Theorem 3.1 is always better than the bounds which would come from higher degree polynomials.

5 Improved upper bounds for 2, 3, and 4-designs

In this section, we use bounds from Lemmas 2.1 and 2.2 to specify an interval I in Theorem 3.6 to obtain upper bounds for the energy of 2-, 3- and 4-designs. Our numerical experiments suggest that the use of even degree polynomials is not effective and so we turn our attention to polynomials of degrees 1 and 3.

5.1 Upper bounds for 2-designs

First we apply Theorem 3.6 for g a linear polynomial.

Theorem 5.1. *Let h be a convex non-negative function on $[-1,1]$ and let u and ℓ denote the upper and lower bounds in (19) and (21), respectively. For $N \in [n+1, 2n)$, if $\ell < u$ then*

$$\mathcal{U}(n,N,2;h) \leq \frac{N\left[(N-1)(uh(\ell) - \ell h(u)) + h(\ell) - h(u)\right]}{u - \ell}, \tag{36}$$

if $\ell = u$ then $\mathcal{U}(n,N,2;h) = Nh(-1/(N-1))$.

Proof. With $I = [\ell, u]$, the linear polynomial passing through the points $(\ell, h(\ell))$ and $(u, h(u))$ satisfies the conditions of Theorem 3.6 and gives the desired bound. If $u = \ell$, then we must also have $u = \ell = -1/(N-1)$ which implies that $\mathcal{U}(n,N,2;h) = Nh(-1/(N-1))$. □

Remark 4. Combining (31) and (36) gives a strip for the h-energy of any spherical 2-design of $N \in \{n+1, n+2, \ldots, 2n-1\}$ points when h is absolutely monotone. Note that if n and N tend simultaneously to infinity such that $N/n \to \zeta$ for some $\zeta \in (1,2)$, Theorem 4.2 and Theorem 5.1 give an asymptotic strip as $N \to \infty$:

$$h(0) + O\left(N^{-1}\right) \leq \frac{\mathcal{L}(n,N,2;h)}{N^2} \leq \frac{\mathcal{U}(n,N,2;h)}{N^2} \leq \frac{h(1-\zeta) + h(\zeta-1)}{2} + O\left(N^{-1}\right).$$

Example 5.1. Simple algebraic manipulations show that the bounds (31) and (36) for 2-designs coincide when $N = n+1$ or $N = n+2$ for every n and h (i.e. the strip becomes a point for these two cardinalities). The case $N = n+1$ leads to the regular simplex on $\mathbb{S}^{n-1}$.

The case $N = n+2$ is more interesting – Mimura [35] has proved that spherical 2-designs with $n+2$ points on $\mathbb{S}^{n-1}$ do exist if and only if n is even and Sali [37] (see also [38]) proved that there are no other (up to isometry) such 2-designs. Spherical 2-designs of $N = 2k$ points on $\mathbb{S}^{2k-3}$ are known as *Mimura spherical designs* and consist of two orthogonal k-simplices which we denote by $\{k,k\}$. This design has $k(k-1)$ distances of $\sqrt{2k/(k-1)}$ coming from edges within the two k-simplices and k^2 distances of $\sqrt{2}$ which are the edges joining the vertices from distinct simplices. The total number of various distances is $k(2k-1) = \binom{N}{2}$.

Sali's nonexistence result follows easily from the coincidence of our bounds. It also follows that the 2-designs of $n+2$ points for even n are unique and optimal – they have simultaneously minimum and maximum possible energy. The optimality cannot be extended to the larger class of spherical codes – Cohn and Kumar [16, Proposition 1.4] prove that if $n+1 < N < 2n$, then there is no N-point universally optimal spherical codes on $\mathbb{S}^{n-1}$. For the cases, $N \in \{n+3, n+4, \ldots, 2n-1\}$, there is a difference (increasing with N) between the bounds from (31) and (36).

Example 5.2 (Riesz s-energy of Mimura designs)**.** As mentioned above, Mimura designs clearly give the minimum energy over 2-designs with $2k$ points in $\mathbb{S}^{2k-3}$. The Riesz s-energy, that is the energy when $h(t) = (2(1-t))^{-s/2}$, is given by

$$E_s(\{k,k\}) = \frac{k^2}{2^{s/2}}\left(1 + \frac{k(k-1)}{k^2}\left(\frac{k-1}{k}\right)^{s/2}\right). \tag{37}$$

It is easy to see that Mimura designs are not universally optimal among general codes of cardinality $N = 2k$. Indeed, consider the competing configuration $\{2, 2k-2\}$ made of two orthogonal simplices, a 2-simplex and a $(2k-2)$-simplex (say the North Pole-South Pole diameter and a $(2k-2)$-simplex in the equatorial hyperplane). This configuration has 1 distance of length 2, $(2k-2)(2k-3)/2$ distances of length $\sqrt{2(2k-2)/(2k-3)}$ and $2(2k-2)$ distances of length $\sqrt{2}$. Thus the s-energy of this competing configuration is given by

$$E_s(\{2,2k-2\}) = \frac{2(2k-2)}{2^{s/2}}\left(1 + \frac{1}{2(2k-2)2^{s/2}} + \frac{2k-3}{4}\left(\frac{2k-3}{2k-2}\right)^{s/2}\right). \tag{38}$$

Comparison of (37) and (38) shows that for large enough s the Mimura design $\{k,k\}$ will have strictly larger energy than the competing configuration $\{2, 2k-2\}$. However, for $k = 3$ it was shown in [21] that the Mimura configuration minimizes, in particular, the logarithmic energy.

5.2 Upper bounds for 3 and 4-designs

For our estimates we shall apply Theorem 3.6 with $g(t)$ the Hermite interpolating polynomial of degree at most three satisfying

$$g(\ell) = h(\ell),\ g(a) = h(a),\ g'(a) = h'(a),\ g(u) = h(u), \tag{39}$$

where ℓ and u again denote lower and upper bounds, respectively, for the inner products of all spherical 3- or 4-designs under consideration. For $\tau = 3$ one can take $\ell = -1$ and u as in [12, Theorem 3.9]. For $\tau = 4$ the bounds u and ℓ are taken from Lemma 2.1(b) and 2.2(b), respectively.

Theorem 5.2. *Let $h \in C^4([-1,1])$ with $h^{(4)}(t) \geq 0$ for $t \in [-1,1]$. For $\tau = 3$ and $N \in [2n, \frac{n(n+3)}{2})$, and for $\tau = 4$ and $N \in [\frac{n(n+3)}{2}, n^2+n)$, we have*

$$\begin{aligned}\mathcal{U}(n,N,\tau;h) \quad \leq \quad & N(N-1)h(a_0) \\ & + \frac{(h(\ell)-h(a_0))\left[uN(1+na_0^2)+2Na_0+n(1-u)(1-a_0)^2\right]}{n(u-\ell)(\ell-a_0)^2} \\ & + \frac{(h(u)-h(a_0))\left[\ell N(1+na_0^2)+2Na_0+n(1-\ell)(1-a_0)^2\right]}{n(u-\ell)(u-a_0)^2},\end{aligned} \tag{40}$$

where

$$a_0 := \frac{N(\ell+u)+n(1-\ell)(1-u)}{n(1-\ell)(1-u)-N(1+\ell un)}, \tag{41}$$

and u and ℓ are chosen as described above.

Proof. As in Lemma 3.3 we use (39) to see that $g(t) \geq h(t)$ for every $t \in [\ell, u]$, i.e. the condition (B1) is satisfied. Moreover, (B2) is trivially satisfied and therefore Theorem 3.6 can be applied. Standard calculations for optimization of $g_0 N - g(1)$ via derivatives show that the optimal value of a is given by (41). □

The asymptotic form of the bound (40) for $\tau = 4$ is easily determined when n and $N \in [D(n,4), D(n,5)) = [\frac{n(n+3)}{2}, n^2+n)$ tend simultaneously to infinity as described in the following corollary.

Corollary 5.3. *If n and N tend to infinity in relation $N = n^2\lambda + o(1)$ as $N \to \infty$, where $\lambda \in [1/2, 1)$ is a constant, then*

$$\mathcal{U}(n,N,4;h) \leq h(0)N^2 - h(0)N + c_1\sqrt{N} + c_2 + o(1), \qquad (N \to \infty), \tag{42}$$

where

$$c_1 = \frac{\sqrt{\lambda}[(2\sqrt{\lambda}-1)h(1-2\sqrt{\lambda}) + (1-2\sqrt{\lambda})h(2\sqrt{\lambda}-1)]}{2(2\sqrt{\lambda}-1)^3}$$

and

$$c_2 = \frac{(1-\sqrt{\lambda})h(1-2\sqrt{\lambda}) + \sqrt{\lambda}h(2\sqrt{\lambda}-1) - h(0)}{(2\sqrt{\lambda}-1)^3}.$$

Proof. The assertion follows from Theorem 5.2 and the asymptotic formulas below:

$$\begin{aligned} u(n,N,4) &= 2\sqrt{\lambda}-1+o(1) \text{ (from Lemma 2.1(b))}, \\ \ell(n,N,4) &= 1-2\sqrt{\lambda}+o(1) \text{ (from Lemma 2.2(b))}, \\ a_0 &= o(1) \text{ (from (41))}. \end{aligned}$$

□

6 Some asymptotic lower bounds

We consider the bounds (25) in the asymptotic process where the strength τ is fixed, and the dimension n and the cardinality N tend simultaneously to infinity in the relation

$$\lim_{n,N\to\infty} \frac{N}{n^{\lfloor \tau/2 \rfloor}} = \begin{cases} \frac{2}{(k-1)!}+\gamma, & \tau = 2k-1, \\ \frac{1}{k!}+\gamma, & \tau = 2k, \end{cases} \tag{43}$$

(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).

Theorem 6.1. *Let h be absolutely monotone on $[-1,1]$ and τ be fixed. If n and N tend to infinity as in (43), then*

$$\mathcal{L}(n,N,\tau;h) \geq h(0)N^2 + o(N^2). \tag{44}$$

Proof. Let $\tau = 2k-1$. From (43) and [11], the asymptotic behavior of the parameters from (25) is as follows: $\alpha_i = o(1)$, for $i = 1,2,\dots,k-1$, $\alpha_0 = -\frac{1}{1+\gamma(k-1)!} + o(1)$, $\rho_0 N = (1+\gamma(k-1)!)^{2k-1} + o(1)$ as $N \to \infty$. Now the lower bound of (25) is easily calculated:

$$\begin{aligned} \mathcal{L}(n,N,2k-1;h) &\geq N^2 \sum_{i=0}^{k-1} \rho_i h(\alpha_i) \\ &= N^2 \left(\rho_0 h(\alpha_0) + h(0) \sum_{i=1}^{k-1} \rho_i \right) + o(N^2) \\ &= N^2 \left(\rho_0 (h(\alpha_0) - h(0)) + h(0) \left(1 - \frac{1}{N}\right)\right) + o(N^2) \\ &= h(0)N^2 + o(N^2). \end{aligned}$$

Similarly, in the even case $\tau = 2k$, we obtain

$$\begin{aligned} \mathcal{L}(n,N,2k;h) &\geq N^2 \left(\gamma_0 (h(-1) - h(0)) + h(0) \left(1 - \frac{1}{N}\right)\right) + o(N^2) \\ &= h(0)N^2 + o(N^2). \end{aligned}$$

□

Remark 5. Our reason for considering the above asymptotic process is motivated by the observation that for fixed dimension n there may only be a finite number of τ's such that τ-designs of cardinalities in $(D(n,\tau), D(n,\tau+1)]$ exist. For example, it was conjectured in [24] that the minimum cardinality of τ-designs on $\mathbb{S}^2$ is greater than $D(n,\tau+1)$ for $\tau > 7$. Other asymptotics will be considered elsewhere.

Note that for $\tau = 4$ the main terms in the lower bound (44) and the upper bound (42) coincide. For odd τ, (44) also yields good energy estimates as shown in the next example.

Example 6.1. There is a standard construction (see [17, Chapter 5]) mapping binary codes from the Hamming space $H(n,2)$ to the sphere $\mathbb{S}^{n-1}$ – the coordinates 0 and 1 are replaced by $\pm 1/\sqrt{n}$, respectively. Denote by $\overline{x}$ and $\overline{C}$ the images of vector $x \in H(n,2)$ and code $C \subset H(n,2)$. Then the inner product $\langle \overline{x}, \overline{y} \rangle$ on $\mathbb{S}^{n-1}$ and the Hamming distance $d_H(x,y)$ in $H(n,2)$ are connected by

$$\langle \overline{x}, \overline{y} \rangle = 1 - \frac{2d_H(x,y)}{n}.$$

Levenshtein [33, pages 67-68] shows that spherical codes which are obtained by this construction from the Kerdock codes [28] are asymptotically optimal with respect to their cardinality. So it is natural to check them for energy optimality.

The Kerdock codes $K_\ell \subset H(2^{2\ell},2)$ are nonlinear. They exist in dimensions $n = 2^{2\ell}$ and their cardinality is $N = n^2 = 2^{4\ell}$. The Hamming distance (weight) distribution does not depend on the point and is as follows:

$$\begin{aligned} A_i &= 0 \text{ for } i \neq 0, i_1 = 2^{2\ell-1} - 2^{\ell-1}, i_2 = 2^{2\ell-1}, i_3 = 2^{2\ell-1} + 2^{\ell-1}, n = 2^{2\ell}, \\ A_0 &= 1, \\ A_{i_1} &= 2^{2\ell}(2^{2\ell-1} - 1), \\ A_{i_2} &= 2^{2\ell+1} - 2, \\ A_{i_3} &= 2^{2\ell}(2^{2\ell-1} - 1), \\ A_n &= 1. \end{aligned}$$

The weights $0, i_1, i_2, i_3, n$ correspond to the inner products $1, \frac{1}{\sqrt{n}}, 0, -\frac{1}{\sqrt{n}}, -1$, respectively. The spherical code $\overline{K}_\ell \subset \mathbb{S}^{2^{2\ell}-1}$ has energy

$$E(n, \overline{K}_\ell; h) = N\left(\left(2^{2\ell+1} - 2\right)h(0) + 2^{2\ell}(2^{2\ell-1} - 1)\left(h\left(\frac{1}{\sqrt{n}}\right) + h\left(-\frac{1}{\sqrt{n}}\right)\right) + h(-1)\right).$$

When n tends to infinity we obtain

$$E(n, \overline{K}_\ell; h) = \frac{N^2}{2}\left(h(\frac{1}{\sqrt{n}}) + h(-\frac{1}{\sqrt{n}})\right) + O(N) = h(0)N^2 + O(N^{3/2}) = h(0)n^4 + O(n^3),$$

where we assumed that h is differentiable at 0.

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