# IMPROVED DELSARTE BOUNDS FOR SPHERICAL CODES IN SMALL DIMENSIONS

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ABSTRACT. We present an extension of the Delsarte linear programming method for spherical codes. For several dimensions it yields improved upper bounds including some new bounds on kissing numbers. Musin's recent work on kissing numbers in dimensions three and four can be formulated in our framework.

## 1. INTRODUCTION

A *spherical* $(n, N, \alpha)$*-code* is a set $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ of unit vectors in $\mathbb{R}^n$ such that the pairwise angular distance betweeen the vectors is at least $\alpha$. One tries to find codes which maximize $N$ or $\alpha$ if the other two values are fixed. The *kissing number problem* asks for the maximum number $k(n)$ of non-overlapping unit balls touching a central unit ball in $n$-space. This corresponds to the special case of spherical codes that maximize $N$, for $\alpha = \frac{\pi}{3}$.

In the early seventies Philippe Delsarte pioneered an approach that yields upper bounds on the cardinalities of binary codes and association schemes [3][4]. In 1977, Delsarte, Goethals and Seidel [5] adapted this approach to the case of spherical codes. The "Delsarte linear programming method" subsequently led to the exact resolution of the kissing number for dimensions 8 and 24, but also to the best upper bounds available today on kissing numbers, binary codes, and spherical codes (see Conway & Sloane [2]).

Here we suggest and study strengthenings of the Delsarte method, for the setting of spherical codes and kissing numbers: We show that one can sometimes improve the Delsarte bounds by extending the space of functions to be used.

Let $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N) \in \mathbb{R}^{n\times N}$ be an $(n, N, \alpha)$-code, and let

$$\mathbf{M} = (x_{ij}) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = \mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{N\times N}$$

be the Gram matrix of scalar products of the $\mathbf{x}_i$. Then

- $x_{ii} = 1$, while $x_{ij} \le \cos\alpha$ for $i \ne j$,
- $\mathbf{M}$ is symmetric and positive semidefinite, and
- $\mathbf{M}$ has rank $\le n$.

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Moreover, any matrix $\mathbf{M} \in \mathbb{R}^{N\times N}$ with these properties corresponds to a spherical $(n, N, \alpha)$-code. The following is a variant of a theorem by Delsarte, Goethals and Seidel [5] with a one-line proof.

**Theorem 1.1.** *Let* $\mathbf{M} = (x_{ij}) = \mathbf{X}^\top\mathbf{X}$ *for an* $(n, N, \alpha)$*-code* $\mathbf{X} \in \mathbb{R}^{n\times N}$. *Let* $c > 0$ *and let* $f : [-1, 1] \to \mathbb{R}$ *be a function such that*

(i) $\sum_{i,j=1}^{N} f(x_{ij}) \geq 0$,
(ii) $f(t) + c \leq 0$ *for* $-1 \leq t \leq \cos\alpha$, *and*
(iii) $f(1) + c \leq 1$.

*Then* $N \leq 1/c$.

*Proof.* Let $g(t) = f(t) + c$. Then

$$N^2 c \leq N^2 c + \sum_{i,j\leq N} f(x_{ij}) = \sum_{i,j\leq N} g(x_{ij}) \leq \sum_{i\leq N} g(x_{ii}) = N\, g(1) \leq N.$$

□

To prove a bound on $N$ with the help of this theorem, we need to find a "good" function $f$ that works for every conceivable code.

We follow an approach presented by Conway and Sloane [2]. Start with a finite set $\mathcal{S}$ of functions that satisfy (i) for every $(n, N, \alpha)$-code for given $n$ and $\alpha$. As (i) is preserved if we take linear combinations of functions in $\mathcal{S}$ with non-negative coefficients, (i) holds for all functions in the cone spanned by $\mathcal{S}$. Condition (ii) is discretized, and we formulate the following linear program. Let $\mathcal{S} = \{f_1, f_2, \ldots, f_k\}$, and $t_1, t_2, \ldots, t_s$ be a subdivision of $[-1, \cos\alpha]$.

$$\begin{array}{lllll} \max\ c: & \sum_{i=1}^{k} c_i f_i(1) & \leq & 1 - c, & \\ & \sum_{i=1}^{k} c_i f_i(t_j) & \leq & -c, & \text{for } 1 \leq j \leq s, \\ & c_i & \geq & 0, & \text{for } 1 \leq i \leq k. \end{array}$$

Minor inaccuracies stemming from the discretization have to be dealt with. Theorem 1.1 then yields a bound on $N$.

In Section 2, we look at the set $\mathcal{S}$ which is classically used in this method. All functions in this set have the stronger property that for a fixed $n$, the matrix $(f(x_{ij}))$ is positive semidefinite for all $(n, N, \alpha)$-codes independently of $\alpha$, which implies condition (i).

In Section 3 we explore functions one could add to this set satisfying condition (i) independently of $n$ and $\alpha$. However, we found no substantial improvements to known bounds through the help of the functions described in that section.

In Section 4 we present a family of functions $f_\alpha$. These functions have the property that the matrix $(f_\alpha(x_{ij}))$ is diagonally dominant and thus positive semidefinite for all $(n, N, \alpha)$-codes for all $n$ and $N$, implying condition (i). This yields improvements to some best known bounds. In particular, we obtain improved upper bounds for the kissing number in the dimensions $10,\ 16,\ 17,\ 25$ and $26$, and a number of new bounds for spherical codes in dimensions $3$, $4$ and $5$.

In the final section we show how Musin's recent work [8, 9] on the kissing numbers in three and four dimensions can be formulated in our framework.

## 2. The classical approach

To guarantee condition (i) in Theorem 1.1, one looks for a function $f$ that will return a matrix $(f(x_{ij}))$ which is positive semidefinite for all finite sets of unit vectors $\mathbf{x}_i$. One reason for this restriction is that one knows a lot about these functions, by the following theorem of Schoenberg about Gegenbauer polynomials. These polynomials (also known as the *spherical* or the *ultraspherical* polynomials) may be defined in a variety of ways. One compact description is that for any $n \geq 2$ and $k \geq 0$, $G_k^n(t)$ is a polynomial of degree $k$, normalized such that $G_k^n(1) = 1$, and such that $G_0^n(t) = 1$, $G_1^n(t) = t$, $G_2^n(t) = \frac{nt^2-1}{n-1}$, $\ldots$ are orthogonal with respect to the scalar product

$$\langle\, g, h \,\rangle \;:=\; \iint_{S^{n-1}} g(\langle \mathbf{x}, \mathbf{y}\rangle) h(\langle \mathbf{x}, \mathbf{y}\rangle)\; d\omega(\mathbf{x})\; d\omega(\mathbf{y})$$

on the vector space $\mathbb{R}[t]$ of polynomials, where $d\omega(\mathbf{x})$ is the invariant measure on the surface of the sphere.

FIGURE 1. A plot of $G_7^4(t)$

**Theorem 2.1** (Schoenberg [10]). *If $(x_{ij}) \in \mathbb{R}^{N\times N}$ is a positive semidefinite matrix of rank at most $n$ with ones on the diagonal, then the matrix $\big(G_k^n(x_{ij})\big)$ is positive semidefinite as well.*

Schoenberg also proved a converse implication: If application of a continuous function $f : [-1, 1] \to \mathbb{R}$ to any positive semidefinite matrix $(x_{ij})$ of rank at most $n$ with ones on the diagonal yields a positive semidefinite matrix $(f(x_{ij}))$, then $f$ is a non-negative combination of the Gegenbauer polynomials $G_k^n$, for $k \geq 0$.

**The Delsarte Method.** To obtain bounds on $N$, given $n$ and $\alpha$, one takes for $\mathcal{S}$ the Gegenbauer polynomials up to some degree $k$, and uses the linear program described in the introduction. The minor inaccuracies arising from the discretization can be dealt with by selecting a slightly smaller $c$. Then Theorem 1.1 yields a bound.

To obtain bounds on $\alpha$ for given $n$ and $N$, a similar technique is used. One repeatedly uses the method from before with varying $\alpha$ in order to find a small $\alpha$ for which Theorem 1.1 forbids an $(n, N, \alpha)$-code.

In most dimensions, the Delsarte method gives the best known upper bound for the kissing number; in dimensions 2, 8 and 24 this bound is optimal. In dimension three and four, this method gives the bounds $k(3) \leq 13$ and $k(4) \leq 25$, and it was proven that no better bounds can be achieved this way. The true values are 12 and 24, respectively, but the proofs are much more complicated.

## 3. Extending the function space

Let us consider the space $\mathcal{P}(n, \alpha)$ of candidates for $f$ given by condition (i) in Theorem 1.1, i.e. we look for functions with $\sum_{i,j \leq N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \geq 0$ for every $(n, N, \alpha)$-code $\{\mathbf{x}_1, \ldots \mathbf{x}_N\}$.

It is easy to see that $\mathcal{P}(n, \alpha)$ contains all non-negative functions, the Gegenbauer polynomials $G_k^n$ (by Theorem 2.1), and all convex combinations of these functions for all $\alpha$. But the addition of non-negative functions to the set $\mathcal{S}$ will not improve the bounds we get from applying Delsarte's method. The interesting question is if there are any other functions in $\mathcal{P}(n, \alpha)$.

We will say that a function has the *average property on* $S^{n-1}$ if for every code $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \subset S^{n-1}$ we have

$$\frac{1}{N^2} \sum_{i,j=1}^{N} f(x_{ij}) \geq \frac{1}{\omega_n^2} \iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) \, d\omega(\mathbf{x}) \, d\omega(\mathbf{y}),$$

where $\omega_n$ is the $(n-1)$-dimensional area of $S^{n-1}$. Obviously, every function with this property and $\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) \, d\omega(\mathbf{x}) \, d\omega(\mathbf{y}) \geq 0$ is in $\mathcal{P}(n, \alpha)$ for all $\alpha$. Non-negative combinations of Gegenbauer polynomials have this property, and the next result says that there are no other such functions.

**Theorem 3.1.** *Let $f : [-1, 1] \to \mathbb{R}$ be a continuous function with the average property, and with $\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) \, d\omega(\mathbf{x}) \, d\omega(\mathbf{y}) \geq 0$. Then $f$ is a non-negative combination of the Gegenbauer polynomials $G_k^n$.*

For the proof we will need two other results. First, the classical addition theorem for spherical harmonics (see [1, Chap. 9], which credits Müller [7], who in turn says that this goes back to Gustav Herglotz (1881–1925)).

**Theorem 3.2** (Addition Theorem [1, Thm. 9.6.3])**.**
*The Gegenbauer polynomial* $G_k^{(n)}(t)$ *can be written as*

$$G_k^{(n)}(\langle \mathbf{x}, \mathbf{y} \rangle) \;=\; \frac{\omega_n}{m} \sum_{\ell=1}^{m} S_{k,\ell}(\mathbf{x}) S_{k,\ell}(\mathbf{y}),$$

*where the functions* $S_{k,1}, S_{k,2}, \ldots, S_{k,m}$ *form an orthonormal basis for the space of "spherical harmonics of degree* $k$*," which has dimension* $m = m(k,n) = \binom{k+n-2}{k} + \binom{k+n-3}{k-1}$.

Further, we will use the following lemma.

**Lemma 3.3.** *For a continuous function* $f : [-1,1] \to \mathbb{R}$*, the following are equivalent:*

(i) $\sum_{i,j=1}^{N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \geq 0$ *for every code* $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \subset S^{n-1}$.
(ii) $\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) h(\mathbf{x}) h(\mathbf{y})\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) \geq 0$ *for every non-negative continuous function* $h : S^{n-1} \to \mathbb{R}_{\geq 0}$.

*Proof.* Statement (ii) is trivial for $h = 0$, so we may assume that in fact $\int_{S^{n-1}} h(\mathbf{x})\ d\omega(\mathbf{x}) = 1$. Treat $h(\mathbf{x})$ as a probability density for picking random vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \subset S^{n-1}$. Then we get in expectation

$$\begin{aligned} &E\left[\frac{1}{N^2} \sum_{i,j=1}^{N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle)\right] \\ &= \frac{1}{N} f(1) + E\left[\frac{1}{N^2} \sum_{i \neq j}^{N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle)\right] \\ &= \frac{1}{N} f(1) + \frac{N-1}{N} E\left[f(\langle \mathbf{x}_1, \mathbf{x}_2 \rangle)\right] \\ &= \frac{1}{N} f(1) + \frac{N-1}{N} \iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) h(\mathbf{x}) h(\mathbf{y})\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}). \end{aligned}$$

Choosing $N$ sufficiently large we see that (i) implies (ii).

For $\mathbf{x}_i \in S^{n-1}$ and $\epsilon > 0$, let

$$h_i^{\epsilon}(\mathbf{y}) = \begin{cases} c(\epsilon)(\epsilon - |\mathbf{x}_i - \mathbf{y}|), & \text{for } |\mathbf{x}_i - \mathbf{y}| < \epsilon, \\ 0, & \text{otherwise,} \end{cases}$$

where $c(\epsilon)$ is chosen such that $\int_{S^{n-1}} h_i^{\epsilon}(\mathbf{y})\ d\omega(\mathbf{y}) = 1$. Given a code $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \subset S^{n-1}$, let $h^{\epsilon} = \frac{1}{N} \sum h_i^{\epsilon}$. For $\epsilon \to 0$, the integral in (ii) approaches the sum in (i), and thus (ii) implies (i). □

*Proof of Theorem 3.1.* We may write $f$ as sum of Gegenbauer polynomials

$$f(t) = c_0 G_0^{(n)}(t) + c_1 G_1^{(n)}(t) + c_2 G_2^{(n)}(t) + \dots\ ,$$

with $c_i \in \mathbb{R}$ for $i \geq 0$. Then

$$\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle)\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) = \iint_{S^{n-1}} c_0\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}),$$

and $f$ has the average property if and only if $f - c_0$ has the average property. Thus we may assume that $c_0 = 0$.

For $r \geq 1$, let

$$h_r(\mathbf{x}) := S_{r,1}(\mathbf{x}) + d_r,$$

with $d_r \geq 0$ such that $h_r(\mathbf{x}) \geq 0$ for $|\mathbf{x}| \leq 1$. Then

$$\begin{aligned}
&\iint_{S^{n-1}} S_{k,\ell}(\mathbf{x}) S_{k,\ell}(\mathbf{y}) h_r(\mathbf{x}) h_r(\mathbf{y})\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) \\
&\qquad = \int S_{k,\ell}(\mathbf{x}) S_{r,1}(\mathbf{x})\, d\omega(\mathbf{x}) \int S_{k,\ell}(\mathbf{y}) S_{r,1}(\mathbf{y})\, d\omega(\mathbf{y}) \\
&\qquad\quad + d_r \int S_{k,\ell}(\mathbf{x}) S_{r,1}(\mathbf{x})\, d\omega(\mathbf{x}) \int S_{k,\ell}(\mathbf{y})\, d\omega(\mathbf{y}) \\
&\qquad\quad + d_r \int S_{k,\ell}(\mathbf{x})\, d\omega(\mathbf{x}) \int S_{k,\ell}(\mathbf{y}) S_{r,1}(\mathbf{y})\, d\omega(\mathbf{y}) \\
&\qquad\quad + d_r^2 \int S_{k,\ell}(\mathbf{x})\, d\omega(\mathbf{x}) \int S_{k,\ell}(\mathbf{y})\, d\omega(\mathbf{y}) \\
&\qquad = \begin{cases} 0, & \text{if } (k,\ell) \neq (r,1), \\ 1, & \text{if } (k,\ell) = (r,1). \end{cases}
\end{aligned}$$

Therefore by Theorem 3.2,

$$\iint_{S^{n-1}} G_k^{(n)}(\langle \mathbf{x}, \mathbf{y} \rangle) h_r(\mathbf{x}) h_r(\mathbf{y})\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) = \begin{cases} 0, & \text{if } k \neq r, \\ \frac{\omega_n}{m}, & \text{if } k = r, \end{cases}$$

and thus

$$\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle) h_r(\mathbf{x}) h_r(\mathbf{y})\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) = c_r \frac{\omega_n}{m}.$$

This implies by Lemma 3.3 that $c_r \geq 0$, proving the theorem. □

By Theorem 3.1, if we want to find new functions which are in $\mathcal{P}(n, \alpha)$ for all $\alpha$, we may restrict ourselves to functions which do not have the average property, and thus $\iint_{S^{n-1}} f(\langle \mathbf{x}, \mathbf{y} \rangle)\, d\omega(\mathbf{x})\, d\omega(\mathbf{y}) > 0$. The following family shows that such functions exist. This family is very general in the sense that it is in $\mathcal{P}(n, \alpha)$ for all $n$ and $\alpha$.

**Lemma 3.4.** *Let $\beta < \pi/2$, and let*

$$g_\beta(t) = \begin{cases} -1, & \text{if} \quad -1 \leq t < -\cos\frac{\beta}{2}, \\ 0, & \text{if} \quad -\cos\frac{\beta}{2} \leq t \leq \cos\beta, \\ 1, & \text{if} \quad \cos\beta < t \leq 1. \end{cases}$$

*Then $g_\beta \in \mathcal{P}(n, \alpha)$ for all $n$ and $\alpha$.*

FIGURE 2. A plot of $g_{\frac{\pi}{3}}(t)$ from Lemma 3.4

*Proof.* Suppose that $\beta < \frac{\pi}{2}$, $g := g_\beta \notin \mathcal{P}(n, \alpha)$, and $\mathbf{x}_1, \ldots, \mathbf{x}_N \in S^{n-1}$ is a minimal set with $\sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) < 0$. Then $\sum_{j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) < 0$ for some $i$; without loss of generality we may assume that $i = 1$. Let

$$I_i^+ := \{j \leq N : \langle \mathbf{x}_i, \mathbf{x}_j \rangle > \cos\beta\}, \; I_i^- := \{j \leq N : \langle \mathbf{x}_i, \mathbf{x}_j \rangle < -\cos\tfrac{\beta}{2}\}.$$

Then $\sum_{i \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_1 \rangle) = |I_1^+| - |I_1^-| < 0$. Let $j \in I_1^-$, we may assume that $j = 2$. Then $I_2^- \subseteq I_1^+$ and $I_1^- \subseteq I_2^+$, as a consequence of the spherical triangle inequality: If for unit vectors $\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k$ the angular distance between $\mathbf{x}_i$ and $-\mathbf{x}_j$ is at most $\frac{\beta}{2}$, and similarly between $-\mathbf{x}_j$ and $\mathbf{x}_k$, then the distance between $\mathbf{x}_i$ and $\mathbf{x}_k$ is at most $\beta$. Therefore,

$$\sum_{i \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_2 \rangle) = |I_2^+| - |I_2^-| \geq |I_1^-| - |I_1^+|.$$

By inclusion/exclusion we get

$$\sum_{3 \leq i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) = \sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) - 2\sum_{i \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_1 \rangle) - 2\sum_{i \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_2 \rangle) + 0 \leq \sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) < 0,$$

a contradiction to the minimality of the set. □

The following fact shows that these functions are truly an extension to the known elements of $\mathcal{P}(n, \alpha)$. If one is only interested in continuous functions, one can easily add a non-negative function $\tilde{p}$ with small support, such that $g_\beta + \tilde{p} \in \mathcal{P}(n, \alpha)$ is continuous, and the next fact will also apply to $g_\beta + \tilde{p}$.

**Fact 3.5.** *The function $g_\beta$ is not a convex combination of Gegenbauer polynomials and non-negative functions.*

*Proof.* Let

$$h(t) = c_{-1}p(t) + \sum_{k=0}^{\infty} c_k G_k^n(t)$$

with $p(t) \geq 0$, $c_k \geq 0$ and $\sum_{k=-1}^{\infty} c_k = 1$. By the linearity of the integral,

$$\int_{-1}^{-\cos\frac{\beta}{2}} h(t)\,dt \geq \min_{k\geq 1} \int_{-1}^{-\cos\frac{\beta}{2}} G_k^n(t)\,dt > \int_{-1}^{-\cos\frac{\beta}{2}} -1\,dt = \int_{-1}^{-\cos\frac{\beta}{2}} g_\beta(t)\,dt,$$

and thus $g_\beta(t) \neq h(t)$. □

## 4. THE MAIN RESULT

As noted above, the family $g_\beta$ is very general in the sense that $g_\beta \in \mathcal{P}(n, \alpha)$ for all $n$ and $\alpha$. Therefore, it may not come as a big surprise that we do not get significant improvements on the known Delsarte bounds through the use of $g_\beta$.

The Gegenbauer polynomials are specialized on the dimension at hand, $G_k^n \in \mathcal{P}(n, \alpha)$ for fixed $n$ and arbitrary $\alpha$. Next we will look at functions which are specialized on the minimum angular distance of the code instead, i.e., functions in $\mathcal{P}(n, \alpha)$ for fixed $\alpha$ and arbitrary $n$. Note that in this setting, there is not much sense in considering the average property since a sequence of $(n, \alpha, N)$-codes with fixed $\alpha$ can not converge towards the continuous case of the whole sphere. We will restrict ourselves to functions in the following smaller space.

**Definition 4.1.** *For $0 \leq \alpha \leq \pi$, let $\mathcal{R}(n, \alpha) \subseteq \mathcal{P}(n, \alpha)$ be the space of functions $f : [-1, 1] \to \mathbb{R}$, such that*

$$\sum_{i=0}^{N} f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle) \geq 0$$

*for every set $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in S^{n-1}$ with $\langle \mathbf{x}_i, \mathbf{x}_j \rangle \leq \cos\alpha$ for all $0 \leq i < j \leq N$.*

With the following lemma, we can reduce the vector combinations which have to be tested when we are searching for a function $f \in \mathcal{R}(n, \alpha)$.

**Lemma 4.2.** *Let $z = \cos\alpha$, let $\theta_0 < -\sqrt{z}$, and let $f : [-1, \theta_0] \to \mathbb{R}$ be some function. Let $n > N$ and let $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_N \in S^{n-1}$ be a set of $N+1$ points such that*

(i) $\langle \mathbf{x}_i, \mathbf{x}_j \rangle \leq z$ *for* $1 \leq i < j \leq N$,
(ii) $\langle \mathbf{x}_i, \mathbf{x}_0 \rangle \leq \theta_0$ *for* $1 \leq i \leq N$,
(iii) $\sum f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle)$ *is minimal with respect to* (i)-(ii),

(iv) $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ *is pointwise maximal with respect to* (i)-(iii).

*Then the* $\mathbf{x}_i$ *(*$i \geq 1$*) form a regular simplex with* $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = z$ *for* $i \neq j$.

*Proof.* For $N \leq 1$, the statement is trivial, so assume that $N \geq 2$. We may further assume that $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle$ is minimal among all the $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ ($1 \leq i < j \leq N$). Let $\mathbf{x}_i = (x_i^1, x_i^2, \ldots, x_i^n)^\top$.

By the symmetries of the sphere we may assume that

$$\begin{aligned} \mathbf{x}_0 &= \mathbf{e}_1, \\ x_i^j &= 0 \text{ for } j > i+1, \\ x_i^{i+1} &\geq 0 \text{ for } 1 \leq i \leq N. \end{aligned}$$

By (ii), $x_i^1 < -\sqrt{z}$, and thus, $x_i^1 \cdot x_j^1 > z$ for $1 \leq i \leq j \leq N$. By (i), $\langle \mathbf{x}_i, \mathbf{x}_j \rangle - x_i^1 \cdot x_j^1 < 0$, and therefore $x_1^2 > 0$ and $x_i^2 < 0$ for $i \geq 2$. This implies that $x_i^1 \cdot x_j^1 + x_i^2 \cdot x_j^2 > z$ for $i, j \geq 2$, and thus $x_2^3 > 0$ and $x_i^3 < 0$ for $i \geq 3$. Repeating this argument row by row we conclude that in fact

$$x_{i-1}^i > 0 \text{ and } x_j^i < 0 \text{ for } 1 \leq i \leq j \leq N,$$

and $\{\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{N-1}\}$ is linearly independent. The code looks as follows.

$$(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_N) = \begin{pmatrix} 1 & \leq \theta_0 & \ldots\ldots\ldots & & \leq \theta_0 \\ 0 & > 0 & < 0 & \ldots & < 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & > 0 & < 0 \\ 0 & \ldots\ldots\ldots\ldots & & 0 & \geq 0 \end{pmatrix}$$

If $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle < z$, adding a small $\varepsilon > 0$ to $x_N^N$ and adjusting $x_N^{N+1}$ accordingly (preserving $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle \leq z$ and $|\mathbf{x}_N| = 1$) will increase $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle$ without changing any of the other $\langle \mathbf{x}_i, \mathbf{x}_N \rangle$ (preserving (i)-(iii)), a contradiction to (iv). Thus, $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle = z$. By the minimality of $\langle \mathbf{x}_{N-1}, \mathbf{x}_N \rangle$, and (i), this proves the lemma. □

The following theorem will enable us to improve numerous bounds. Note that the definition of $f_\alpha$ for $z < t < 1$ is not important as $\langle x_i, x_j \rangle$ is never in this interval for an $(n, N, \alpha)$-code.

**Theorem 4.3.** *Let* $0 \leq z = \cos\alpha < 1$ *and*

$$f_\alpha(t) := \begin{cases} \frac{z-t^2}{1-z}, & \text{if } t < -\sqrt{z}, \\ 0, & \text{if } -\sqrt{z} \leq t \leq z, \\ \frac{t-z}{1-z}, & \text{if } t > z. \end{cases}$$

*Then* $f_\alpha \in \mathcal{R}(n, \alpha)$ *for all* $n$.

FIGURE 3. A plot of $f_{\frac{\pi}{3}}(t)$

*Proof.* For fixed $n > N_0$, let $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N, \mathbf{x}_0) \in \mathbb{R}^{n\times(N+1)}$ such that $\{\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N\}$ is a spherical $(n, N, \alpha)$-code and so that $S = \sum_{i=1}^N f_\alpha(\langle \mathbf{x}_0, \mathbf{x}_i\rangle)$ is minimal for all codes with $N \leq N_0$. If we choose $N$ minimal amongst such codes, we have $\langle \mathbf{x}_0, \mathbf{x}_i\rangle < -\sqrt{z}$ for $1 \leq i \leq N$.

By Lemma 4.2, we may assume that the $\mathbf{x}_i$ $(i \geq 1)$ form a regular simplex with $\langle \mathbf{x}_i, \mathbf{x}_j\rangle = z$ for $i \neq j$. By symmetry we may assume that

$$\mathbf{x}_i = \sqrt{z}\,\mathbf{e}_{N+1} + \sqrt{1-z}\,\mathbf{e}_i \in S^{n-1} \text{ for } 1 \leq i \leq N.$$

Let $\mathbf{x}_0 = (x_0^1, x_0^2, \ldots, x_0^n)^\top$. Note that the choice of the $\mathbf{x}_i$ implies that $x_0^i \leq 0$ for $i \leq N+1$; if $x_0^i > 0$, then using $-x_0^i$ instead would decrease $S$. Further, $x_0^i = 0$ for $i > N+1$; otherwise we could decrease $S$ by setting $x_0^i = 0$ and decreasing $x_0^{N+1}$.

Next we will show that we can choose $\mathbf{x}_0$ such that $x_0^i = x_0^j$ for all $i, j \leq N$. Let $\tilde{\mathbf{x}}_0 \in S^{n-1}$ be defined as

$$\tilde{\mathbf{x}}_0 = -\sqrt{\frac{\sum_{i=1}^N (x_0^i)^2}{N}} \sum_{i=1}^N \mathbf{e}_i + x_0^{N+1}\,\mathbf{e}_{N+1}.$$

Then

$$\begin{aligned}
&\sum_{i=1}^N f_\alpha\left(\langle \tilde{\mathbf{x}}_0, \mathbf{x}_i\rangle\right) - \sum_{i=1}^N f_\alpha\left(\langle \mathbf{x}_0, \mathbf{x}_i\rangle\right) = \\
&\qquad N\, f_\alpha\left(x_0^{N+1}\sqrt{z} - \sqrt{\frac{\sum_{i=1}^N (x_0^i)^2}{N}}\sqrt{1-z}\right) \\
&\qquad\qquad - \sum_{i=1}^N f_\alpha\left(x_0^{N+1}\sqrt{z} + x_0^i\sqrt{1-z}\right) \\
&\qquad\qquad = \frac{2N\, x_0^{N+1}\sqrt{z}}{\sqrt{1-z}}\left(\sqrt{\frac{\sum_{i=1}^N (x_0^i)^2}{N}} + \frac{\sum_{i=1}^N x_0^i}{N}\right) \leq 0,
\end{aligned}$$

where the last inequality is true since $x_0^{N+1} \leq 0$, and all other factors are non-negative. Thus, $\tilde{\mathbf{x}}_0$ minimizes $S$ and we may assume that $\mathbf{x}_0 = \tilde{\mathbf{x}}_0$.

This implies that

$$\langle \mathbf{x}_0, \mathbf{x}_i \rangle = x_0^i \sqrt{1-z} + x_0^{N+1}\sqrt{z}$$
$$= -\sqrt{(1-z)\frac{1-(x_0^{N+1})^2}{N}} + x_0^{N+1}\sqrt{z},$$

which is minimized for $x_0^{N+1} = -\sqrt{\frac{zN}{1-z+zN}}$. Thus,

$$\langle \mathbf{x}_0, \mathbf{x}_i \rangle \geq -\sqrt{z + \frac{1-z}{N}}$$

for $1 \leq i \leq N$, and therefore

$$S = \sum_{i=0}^{N} f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle) \geq 1 + N\, f\left(-\sqrt{z + \frac{1-z}{N}}\right) = 0,$$

proving the theorem. □

Note that in fact, the matrix $(f_\alpha(x_{ij}))$ is positive semidefinite for every $(n, N, \alpha)$-code $\mathbf{X}$. This is an easy consequence of Geršgorin's circle theorem (see [6]), combined with the fact that $(f_\alpha(x_{ij}))$ is symmetric and diagonally dominant (i.e., $2f_\alpha(x_{ii}) \geq \sum_{j=1}^{N} |f_\alpha(x_{ij})|$ for $1 \leq i \leq N$).

We can add $f_{\frac{\pi}{3}}$ to the Gegenbauer polynomials in dimension $n$ to get new bounds on the kissing numbers $k(n)$ through linear programming as in Section 1. This yields the new bounds in Table 1, where the known bounds are taken from [2] (with the exception of the bound $k(9) \leq 379$ from [13]). For other $n \leq 30$, the best currently known bounds were not improved.

| $n$ | lower bound | Delsarte bound | new upper bound |
|---|---|---|---|
| 9 | 306 | 380* | 379 |
| 10 | 500 | 595 | 594 |
| 16 | 4320 | 8313 | 8312 |
| 17 | 5346 | 12218* | 12210 |
| 25 | 196656 | 278363 | 278083 |
| 26 | 196848 | 396974 | 396447 |

* : 379 and 12215 with some extra inequalities

TABLE 1. New upper bounds for the kissing number

Similarly, new bounds for the minimal angular separation in spherical codes can be achieved. Some of them are shown in Table 2 (here, the lower bounds are from [12]). We express our bounds in degrees as this is the usual notation in the literature.

| $n$ | $N$ | lower bound | Delsarte bound | new upper bound |
|---|---|---|---|---|
| 3 | 13 | 57.13 | 60.42 | 60.34 |
| 3 | 14 | 55.67 | 58.09 | 58.00 |
| 3 | 15 | 53.65 | 56.13 | 56.10 |
| 3 | 24 | 43.69 | 44.45 | 44.43 |
| 4 | 9 | 80.67 | 85.60 | 83.65 |
| 4 | 10 | 80.40 | 82.19 | 80.73 |
| 4 | 11 | 76.67 | 79.46 | 78.73 |
| 4 | 22 | 60.13 | 63.41 | 63.38 |
| 4 | 23 | 60.00 | 62.36 | 62.30 |
| 4 | 24 | 60.00 | 60.50 | 60.38 |
| 5 | 11 | 82.36 | 87.30 | 85.39 |
| 5 | 12 | 81.14 | 84.94 | 83.14 |
| 5 | 13 | 79.20 | 82.92 | 81.54 |
| 5 | 14 | 78.46 | 81.20 | 80.30 |
| 5 | 15 | 78.46 | 79.73 | 79.30 |

TABLE 2. New upper bounds for $\alpha$ in $(n, N, \alpha)$-codes

As an example for the proofs of the values in Tables 1 and 2, we prove the following theorem. The proofs for all other values are similar, and the exact functions used are stated in the appendix.

**Theorem 4.4.** *The kissing number in dimension* 10 *is at most* 594.

*Proof.* Let

$$\begin{aligned} f(x) &= 0.013483\, G_1^{(10)}(x) + 0.0519007\, G_2^{(10)}(x) + 0.1256323\, G_3^{(10)}(x) \\ &\quad + 0.2121789\, G_4^{(10)}(x) + 0.2486231\, G_5^{(10)}(x) + 0.2032308\, G_6^{(10)}(x) \\ &\quad + 0.09343\, G_7^{(10)}(x) + 0.04367\, G_{11}^{(10)}(x) + 0.006165\, f_{\frac{\pi}{3}}(x). \end{aligned}$$

On both $[-1, -\frac{1}{\sqrt{2}}]$ and $[-\frac{1}{\sqrt{2}}, 0.5]$, this is a polynomial of degree 11. It is readily checked that for $-1 \leq x \leq \frac{1}{2}$,

$$f(x) + \frac{1}{594.9} < 0 \text{ and } f(1) + \frac{1}{594.9} < 1,$$

so $k(10) < 594.9$ by Theorem 1.1. □

## 5. MUSIN REVISITED: $k(3) = 12$ AND $k(4) = 24$

For dimensions three and four, using $f_{\frac{\pi}{3}}$ gives marginal improvements to the bounds on the kissing numbers achieved with the Delsarte method, but not enough to show that $k(3) = 12$ and $k(4) = 24$. Several proofs for

$k(3) = 12$ are known, the first one by Schütte and van der Waerden [11]. For dimension four, only recently a proof for $k(4) = 24$ was found by Musin [8]. The same techniques also yield the arguably simplest proof for dimension three [9].

Our techniques give a new framework for Musin's proofs. As mentioned above, Gegenbauer polynomials $G_k^{(n)}$ are in $\mathcal{P}(n, \alpha)$ for a specific $n$ and arbitrary $\alpha$. Similarly, the functions $f_\alpha$ are in $\mathcal{P}(n, \alpha)$ for a specific $\alpha$ and arbitrary $n$. To get the strongest bounds one should look for functions which are specialized for the $n$ and $\alpha$ at hand, though.

As a consequence of Lemma 3 in [9] and Section 5 in [8], we get the following two lemmas stated in our framework.

**Lemma 5.1.** *Let*

$$\begin{aligned} g_3(t) &= 1 + 1.6\, G_1^{(3)}(t) + 3.48\, G_2^{(3)}(t) + 1.65\, G_3^{(3)}(t) \\ &\quad + 1.96\, G_4^{(3)}(t) + 0.1\, G_5^{(3)}(t) + 0.32\, G_9^{(3)}(t), \end{aligned}$$

*and let*

$$\hat{g}_3(t) = \begin{cases} \min\left\{-\frac{1}{2.89} g_3(t), 0\right\}, & \textit{for } t \leq \frac{1}{2}, \\ 2t - 1, & \textit{for } t > \frac{1}{2}. \end{cases}$$

*Then* $\hat{g}_3 \in \mathcal{R}\left(3, \frac{\pi}{3}\right)$.

**Lemma 5.2.** *Let*

$$\begin{aligned} g_4(t) &= 1 + 2\, G_1^{(4)}(t) + 6.12\, G_2^{(4)}(t) + 3.484\, G_3^{(4)}(t) \\ &\quad + 5.12\, G_4^{(4)}(t) + 1.05\, G_9^{(4)}(t), \end{aligned}$$

*and let*

$$\hat{g}_4(t) = \begin{cases} \min\left\{-\frac{1}{6.226} g_4(t), 0\right\}, & \textit{for } t \leq \frac{1}{2}, \\ 2t - 1, & \textit{for } t > \frac{1}{2}. \end{cases}$$

*Then* $\hat{g}_4 \in \mathcal{R}\left(4, \frac{\pi}{3}\right)$.

With the help of these two functions, we can show that $k(3) = 12$ and $k(4) = 24$ using the same method as before.

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## APPENDIX A. FUNCTIONS USED TO PROVE THE VALUES IN TABLES 1 AND 2 IN SECTION 4

**Kissing numbers.** For $n \in \{9, 16, 17, 25, 26\}$, let

$$f(x) = c_f f_{\frac{\pi}{3}}(x) + \sum_{i=1}^{15} c_i G_i^{(n)}.$$

An argument similar to the proof of Theorem 4.4 using the following exact constants yields the bounds in Table 1.

| $n$ | 9 | 16 | 17 | 25 | 26 |
|---|---|---|---|---|---|
| $c_1$ | 0.019301 | 0.00150625 | 0.0010991163 | 0.000068346426 | 0.000050764918 |
| $c_2$ | 0.068796 | 0.00883013 | 0.0068289424 | 0.000597204273 | 0.000462456224 |
| $c_3$ | 0.151621 | 0.03241271 | 0.0264586211 | 0.003278765311 | 0.002637553785 |
| $c_4$ | 0.233218 | 0.08357928 | 0.0719084276 | 0.012746086882 | 0.010630533922 |
| $c_5$ | 0.242578 | 0.15818006 | 0.143361526 | 0.03727450386 | 0.032234603849 |
| $c_6$ | 0.173153 | 0.22396571 | 0.2142502303 | 0.084612203762 | 0.07583669717 |
| $c_7$ | 0.057219 | 0.22963948 | 0.2322459799 | 0.149967112742 | 0.139668776208 |
| $c_8$ | 0 | 0.16129212 | 0.17372837 | 0.207792862667 | 0.20110760134 |
| $c_9$ | 0 | 0.05703299 | 0.0656867748 | 0.213189306323 | 0.216300884031 |
| $c_{10}$ | 0.020652 | 0 | 0 | 0.15506047251 | 0.164792888823 |
| $c_{11}$ | 0.022367 | 0 | 0 | 0.052419478729 | 0.062508329517 |
| $c_{12}$ | 0 | 0.02211528 | 0.0310430395 | 0 | 0 |
| $c_{13}$ | 0 | 0.01792231 | 0.0309025515 | 0 | 0 |
| $c_{14}$ | 0 | 0 | 0 | 0.038614866776 | 0.042401423571 |
| $c_{15}$ | 0 | 0 | 0 | 0.039062690839 | 0.04958247785 |
| $c_f$ | 0.008455 | 0.00340331 | 0.0024045205 | 0.005312502853 | 0.00178248638 |

**Bounds on spherical codes.** Let

$$f(x) = c_f f_{\alpha}(x) + \sum_{i=1}^{15} c_i G_i^{(n)}.$$

An argument similar to the proof of Theorem 4.4 using the following exact constants yields the bounds in Table 2.

$n = 3$

| | | | | |
|---|---|---|---|---|
| $\alpha$ | 60.34 | 58.00 | 56.10 | 44.43 |
| $N$ | 13 | 14 | 15 | 24 |
| $c_1$ | 0.144628 | 0.17042 | 0.18047 | 0.11784 |
| $c_2$ | 0.264112 | 0.25438 | 0.24164 | 0.17644 |
| $c_3$ | 0.144806 | 0.19558 | 0.22834 | 0.1984 |
| $c_4$ | 0.145356 | 0.15492 | 0.15143 | 0.18525 |
| $c_5$ | 0 | 0.04105 | 0.06718 | 0.13696 |
| $c_6$ | 0 | 0 | 0 | 0.07768 |
| $c_7$ | 0 | 0 | 0 | 0.02916 |
| $c_8$ | 0.007163 | 0 | 0 | 0 |
| $c_9$ | 0.029096 | 0.02116 | 0.02355 | 0 |
| $c_{10}$ | 0 | 0.01089 | 0.01119 | 0 |
| $c_{11}$ | 0 | 0 | 0.00963 | 0.01056 |
| $c_{12}$ | 0 | 0 | 0 | 0.00582 |
| $c_{13}$ | 0 | 0 | 0 | 0.00593 |
| $c_{14}$ | 0.006433 | 0 | 0 | 0 |
| $c_{15}$ | 0 | 0.00451 | 0 | 0 |
| $c_f$ | 0.181467 | 0.07561 | 0.01986 | 0.01424 |

$n = 4$

| | | | | | | |
|---|---|---|---|---|---|---|
| $\alpha$ | 83.65 | 80.73 | 78.73 | 63.38 | 62.30 | 60.38 |
| $N$ | 9 | 10 | 11 | 22 | 23 | 24 |
| $c_1$ | 0.145068 | 0.15964 | 0.168 | 0.14776 | 0.13771 | 0.132654 |
| $c_2$ | 0.388785 | 0.39941 | 0.4074 | 0.25814 | 0.25131 | 0.241421 |
| $c_3$ | 0.036242 | 0.04195 | 0.0482 | 0.25129 | 0.24036 | 0.249607 |
| $c_4$ | 0 | 0 | 0 | 0.18154 | 0.18906 | 0.197614 |
| $c_5$ | 0 | 0 | 0 | 0.04859 | 0.05079 | 0.07055 |
| $c_8$ | 0 | 0 | 0 | 0.01237 | 0.00738 | 0 |
| $c_9$ | 0 | 0 | 0 | 0.01749 | 0.02374 | 0.024936 |
| $c_f$ | 0.318784 | 0.29896 | 0.2853 | 0.03731 | 0.05613 | 0.043207 |

$n = 5$

| | | | | | |
|---|---|---|---|---|---|
| $\alpha$ | 85.39 | 83.14 | 81.54 | 80.30 | 79.30 |
| $N$ | 11 | 12 | 13 | 14 | 15 |
| $c_1$ | 0.12887 | 0.144012 | 0.15234 | 0.1586 | 0.16383 |
| $c_2$ | 0.40902 | 0.416363 | 0.42226 | 0.4268 | 0.43007 |
| $c_3$ | 0.03922 | 0.044718 | 0.04976 | 0.056 | 0.06339 |
| $c_f$ | 0.33195 | 0.311568 | 0.29868 | 0.2871 | 0.276 |

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