

IMPROVED DELSARTE BOUNDS VIA EXTENSION OF THE FUNCTION SPACE

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

1. INTRODUCTION

A *spherical* (n, N, α) -code is a set $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of unit vectors in \mathbb{R}^n such that the pairwise angular distance between the vectors is at least α . One tries to find codes which maximize N or α 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 by extending the space of functions to be used, one can in some cases/dimensions improve the bounds that are achievable by the Delsarte method.

Let $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{n \times N}$ be an (n, N, α) -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 $x_{ij} \leq \cos \alpha$ for $i \neq j$,
- \mathbf{M} is symmetric and positive semidefinite, and
- \mathbf{M} has rank $\leq n$.

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Moreover, any matrix $\mathbf{M} \in \mathbb{R}^{N \times N}$ with these properties corresponds to a spherical (n, N, α) -code. We get the following theorem with a one-line proof.

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

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

Then $N \leq 1/c$.

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

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

To prove a bound on N with the help of this theorem, we need to find a “good” function f (and it needs to work for every conceivable code).

We follow an approach by Conway and Sloane [2]. Start with a finite set \mathcal{S} of functions that satisfy (i) for every (n, N, α) -code. 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 $\mathcal{S} = \{f_1, f_2, \dots, f_k\}$, and t_1, t_2, \dots, t_s be a subdivision of $[-1, \cos \alpha]$.

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

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

In Section 2, we will take a closer 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 $(n, N, 0)$ -codes, which implies condition (i).

In Sections 3 and 4 we explore further functions one could add to this set, asking only for condition (i) to hold. However, we found no substantial improvements to known bounds through the help of the functions described in these sections.

In Section 5 we present a family of functions f_α which can be added to \mathcal{S} . These functions have the property that the matrix $(f_\alpha(x_{ij}))$ is diagonally dominant and thus positive semidefinite for all (n, N, α) -codes for all n and N , which is a strengthening of condition (i) slightly different from the condition used classically. 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, which have not seen any improvements in the last 25 years.

We will explore the limits to this approach in Section 6, and in the final section we show how Musin's recent work [7][8] on the kissing numbers in three and four dimensions can be reformulated in our framework.

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2. THE CLASSICAL APPROACH

To guarantee the 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 sets of unit vectors (\mathbf{x}_i) . The 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 $G_0^n(t) = 1$, $G_1^n(t) = t$, $G_2^n(t) = \frac{nt^2-1}{n-1}$, \dots are orthogonal with respect to the scalar product

$$\langle g(t), h(t) \rangle := \int_{-1}^{+1} g(t)h(t)(1-t^2)^{\frac{n-3}{2}} dt$$

on the vector space $\mathbb{R}[t]$ of polynomials; this product arises naturally in integration over S^{n-1} (see for instance [1, Sect. 6.4]).

Theorem 2.1 (Schoenberg [9]). *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 $(G_k^n(x_{ij}))$ is positive semidefinite as well.*

Schoenberg also proved a converse implication: If application of a continuous function $f : [-1, 1] \rightarrow \mathbb{R}$ 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 $k \geq 0$.

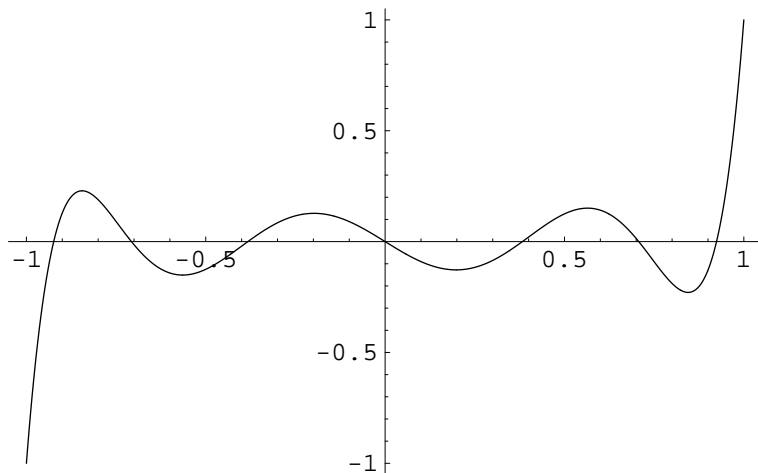


FIGURE 1. A plot of $G_7^4(t)$

The Delsarte Method. To obtain bounds on N , given n and α , 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 α for given n and N , a similar technique is used. One repeatedly uses the method from before with varying α until one finds the smallest α , for which Theorem 1.1 forbids an (n, N, α) -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 lower bounds can be achieved this way. The true values are 12 and 24, respectively, but the proofs are much more complicated. See section 7 for more details.

3. EXTENDING THE FUNCTION SPACE

Instead of limiting ourselves to Gegenbauer polynomials, let us consider the bigger space of candidates for f given by condition (i) in Theorem 1.1, i.e. we look for other functions with $\sum_{i,j \leq N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \geq 0$ for every (n, N, α) -code $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$.

Definition 3.1. Let $\mathcal{P}_N^n(\alpha)$ be the set of all functions $f : [-1, 1] \rightarrow \mathbb{R}$, for which

- (i) $f(1) = 1$,
- (ii) $\sum_{i,j \leq N} f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) \geq 0$ for every (n, N, α) -code $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$.

We define

$$\begin{aligned}
\mathcal{P}_N^n &:= \mathcal{P}_N^n(0), \\
\mathcal{P}^n(\alpha) &:= \bigcap_N \mathcal{P}_N^n(\alpha), \\
\mathcal{P}_N(\alpha) &:= \bigcap_n \mathcal{P}_N^n(\alpha), \\
\mathcal{P}_N, \mathcal{P}^n, \mathcal{P}(\alpha) &\text{ and } \mathcal{P} \text{ accordingly.}
\end{aligned}$$

Fact 3.2.

- (i) $\mathcal{P}_N^n(\alpha) \subseteq \mathcal{P}_N^n(\alpha')$ for $\alpha \leq \alpha'$.
- (ii) $\mathcal{P}_N^n(\alpha) \subseteq \mathcal{P}_N^{n-1}(\alpha)$.
- (iii) If $f \in \mathcal{P}^n$ is Riemann integrable, then $\int_{S^{n-1}} f(\langle \mathbf{e}_1, x \rangle) dx \geq 0$.
- (iv) If $f \in \mathcal{P}_N^n(\alpha)$ and $N < n$, then $f(x) \geq -\frac{1}{N}$ for $-\frac{1}{N} \leq x \leq \cos \alpha$.
- (v) If $f, g \in \mathcal{P}_N^n(\alpha)$, and $0 \leq c \leq 1$, then $cf + (1-c)g \in \mathcal{P}_N^n(\alpha)$.
- (vi) All functions with $f(x) \geq 0$ for $-1 \leq x \leq 1$ are in \mathcal{P} .
- (vii) $G_k^n \in \mathcal{P}^n$.

Proof. (i), (ii), (v) and (vi) follow directly from the definitions, (vii) follows from Theorem 2.1. To show (iii), observe that if $N \rightarrow \infty$, and the \mathbf{x}_i are uniformly distributed over S^{n-1} , then the sum in Definition 3.1 divided by N approaches the integral. To see (iv), note that for $-\frac{1}{k} \leq x \leq \cos \alpha$, there is a regular simplex on $k+1$ points with pairwise angular distance $\arccos x \geq \alpha$ inside S^{n-1} . \square

Statements (v)–(vii) show that $\mathcal{P}^n \subseteq \mathcal{P}_N^n$ contains all non-negative functions, the Gegenbauer polynomials G_k^n , and all convex combinations of these functions. Next, we will explore the space \mathcal{P}^n a little further. By the following lemma we may restrict our observations to functions with $f(x) \leq 1$.

Lemma 3.3. *For $f \in \mathcal{P}_N^n$, the function $g(x) = \min(f(x), 1)$ lies in \mathcal{P}_N^n .*

Proof. Suppose there are vectors $\mathbf{x}_1, \dots, \mathbf{x}_N \in S^{n-1}$ such that

$$S(g) := \sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) < 0.$$

Assume further that $S(g)$ is minimal among all multisets of N vectors selected from the set $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. As $f \in \mathcal{P}_N^n$, there are k, ℓ such that $f(\langle \mathbf{x}_k, \mathbf{x}_\ell \rangle) > 1$ and $\sum_{i \leq N} g(\langle \mathbf{x}_k, \mathbf{x}_i \rangle) \leq \sum_{i \leq N} g(\langle \mathbf{x}_\ell, \mathbf{x}_i \rangle)$.

Consider the configuration $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_N \in S^{n-1}$, obtained from $\mathbf{x}_1, \dots, \mathbf{x}_N$ when \mathbf{x}_ℓ is replaced by \mathbf{x}_k . Then

$$\begin{aligned}
\sum_{i,j \leq N} g(\langle \tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j \rangle) &= \\
&\sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle) - 2 \sum_{i \leq N} g(\langle \mathbf{x}_\ell, \mathbf{x}_i \rangle) + 2 \sum_{i \leq N} g(\langle \mathbf{x}_k, \mathbf{x}_i \rangle) \\
&\leq \sum_{i,j \leq N} g(\langle \mathbf{x}_i, \mathbf{x}_j \rangle).
\end{aligned}$$

Since $S(g)$ is minimal, equality must hold and thus $\sum_{i \leq N} g(\langle \mathbf{x}_k, \mathbf{x}_i \rangle) = \sum_{i \leq N} g(\langle \mathbf{x}_\ell, \mathbf{x}_i \rangle)$ whenever $f(\langle \mathbf{x}_k, \mathbf{x}_\ell \rangle) > 1$.

We may assume that $\mathbf{x}_1, \dots, \mathbf{x}_N \in S^{n-1}$ were chosen in a way that $\min\{Nk + \ell : f(\langle \mathbf{x}_k, \mathbf{x}_\ell \rangle) > 1\} \leq N^2$ is maximal among the multisets which achieve $S(g)$. But $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_N \in S^{n-1}$ has a higher value for this quantity, a contradiction. \square

The next two facts show that \mathcal{P}^n is substantially larger than just convex combinations of Gegenbauer functions and positive functions.

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

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

Then $f \in \mathcal{P}$.

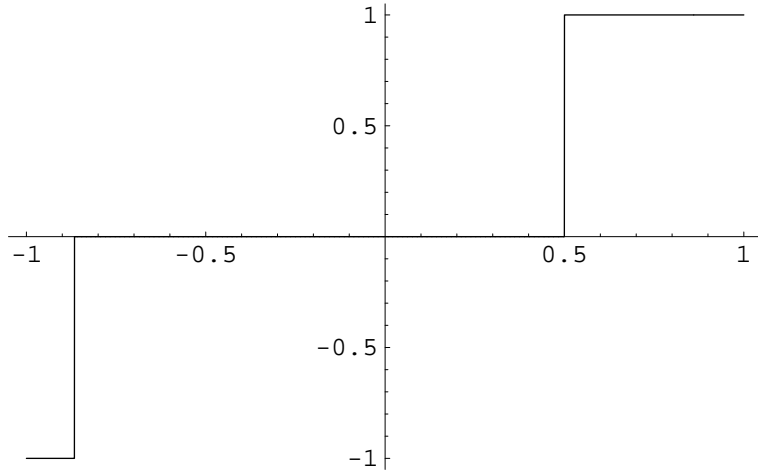


FIGURE 2. A plot of $f(t)$ from Fact 3.4 for $\beta = \frac{\pi}{3}$

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

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

Then $\sum_{i \leq N} f(\langle \mathbf{x}_i, \mathbf{x}_1 \rangle) = |I_1^+| - |I_1^-| < 0$. 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 β . Therefore,

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

By inclusion/exclusion we get

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

a contradiction to the minimality of the set. \square

Fact 3.5. *The function f from Fact 3.4 is not a convex combination of Gegenbauer polynomials and positive functions.*

Proof. Let

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

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

$$\int_{-1}^{-\cos \frac{\beta}{2}} g(x) dx \geq \min_k \int_{-1}^{-\cos \frac{\beta}{2}} G_k^n(x) dx > \cos \frac{\beta}{2} - 1 = \int_{-1}^{-\cos \frac{\beta}{2}} f(x) dx,$$

and thus $f(x) \neq g(x)$. \square

4. RESTRICTING THE FUNCTION SPACE

It is often difficult to test for a function $f : [-1, 1] \rightarrow \mathbb{R}$ whether $f \in \mathcal{P}_N^n(\alpha)$. We will focus on a smaller space reduce the difficulty.

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

$$1 + \sum_{i=1}^N f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle) \geq 0$$

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

Define $\mathcal{R}, \mathcal{R}^n$, etc. analogously to $\mathcal{P}, \mathcal{P}^n$, etc. in Definition 3.1.

So, instead of just requiring that the sum of all matrix entries in $(f(x_{ij}))$ is non-negative, we ask for all row sums to be non-negative. Again, we get a number of statements similar to Fact 3.2.

Fact 4.2.

- (i) $\mathcal{R}_N^n(\alpha) \subseteq \mathcal{R}_N^n(\alpha')$ for $\alpha \leq \alpha'$.
- (ii) $\mathcal{R}_N^n(\alpha) \subseteq \mathcal{R}_N^{n-1}(\alpha)$.
- (iii) Let $f \in \mathcal{R}_N^n(\alpha)$ and $N < n$, then $f(t) \geq -\frac{1}{N}$ for $-\frac{1}{N} \leq t \leq \cos \alpha$.
- (iv) If $f, g \in \mathcal{R}_N^n(\alpha)$, and $0 \leq c \leq 1$, then $cf + (1-c)g \in \mathcal{R}_N^n(\alpha)$.
- (v) All functions with $f(t) \geq 0$ for $-1 \leq t \leq 1$ are in \mathcal{R} .
- (vi) Let $f \in \mathcal{R}_N^n$, then $f(t) \geq -\frac{1}{N-1}$ for $-1 \leq t \leq 1$.
- (vii) Let $f \in \mathcal{R}^n$, then $f(t) \geq 0$ for $-1 \leq t \leq 1$.

Proof. Statements (i)-(v) follow directly from the definitions. For (vi), suppose that $f(t) < -\frac{1}{N-1}$ for some t . Then pick a point $\mathbf{x}_0 \in S^{n-1}$, and $N-1$ points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{N-1} \in S^{n-1}$ with $\langle \mathbf{x}_0, \mathbf{x}_i \rangle = t$, showing that $f \notin \mathcal{R}_N^n$. The same argument works for (vii), just pick N large enough. \square

Statement (vi) in Fact 4.2 shows that we have nothing to gain by adding functions in \mathcal{R}_N^n to the set \mathcal{S} ; we will have to use functions in $\mathcal{R}_N^n(\alpha) \setminus \mathcal{R}_N^n$.

The following rather technical lemma will be helpful in our proofs.

Lemma 4.3. Let $0 \leq y \leq 1$ and let

$$\mathbf{M} = \begin{pmatrix} 1 & y & \dots & y & t \\ y & 1 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & y & t \\ y & \dots & y & 1 & t \\ t & \dots & t & t & 1 \end{pmatrix} \in \mathbb{R}^{(N+1) \times (N+1)}.$$

Then the following are equivalent.

- (i) $|t| \leq \sqrt{y + \frac{1-y}{N}}$.
- (ii) \mathbf{M} is positive semidefinite.
- (iii) There is a code $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in S^{N+1}$ with $\langle \mathbf{x}_0, \mathbf{x}_i \rangle = t$ and $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = y$ for $1 \leq i < j \leq N$.

(iv) *There is a code $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in S^{N+1}$ with $\sum_{i=1}^N \langle \mathbf{x}_0, \mathbf{x}_i \rangle = Nt$ and $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = y$ for $1 \leq i < j \leq N$.*

Proof. As noted before, (ii) and (iii) are equivalent, while (iii) \implies (iv) is clear. We will show that (i) \implies (iii) and that $\neg(\text{i}) \implies \neg(\text{iv})$.

If $|t| \leq \sqrt{y + \frac{1-y}{N}}$, let

$$\mathbf{x}_i = \sqrt{1-y} \mathbf{e}_i + \sqrt{y} \mathbf{e}_{N+1} \in S^{N+1}, \quad 1 \leq i \leq N,$$

and

$$\mathbf{x}_0 = \sum_{i=1}^N a \mathbf{e}_i + b \mathbf{e}_{N+1} + c \mathbf{e}_{N+2} \in S^{N+1},$$

where

$$a = \frac{t\sqrt{1-y}}{(N-1)y+1}, \quad b = \frac{Nt\sqrt{y}}{(N-1)y+1} \quad \text{and} \quad c = \sqrt{1 - \frac{Nt^2}{(N-1)y+1}}.$$

A straightforward calculation shows that this is a code as described in (iii).

Now suppose that $t > \sqrt{y + \frac{1-y}{N}}$. Let $\mathbf{x} = (1, \dots, 1, d)^\top \in \mathbb{R}^{N+1}$, where $d = -\sqrt{N^2y + N(1-y)}$, and let $\mathbf{M}' := \mathbf{X}^\top \mathbf{X}$ be the Gram matrix of the code from (iv), which looks like

$$\mathbf{M}' = \begin{pmatrix} 1 & y & \dots & y & t_1 \\ y & 1 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & y & t_{N-1} \\ y & \dots & y & 1 & t_N \\ t_1 & \dots & t_{N-1} & t_N & 1 \end{pmatrix} \in \mathbb{R}^{(N+1) \times (N+1)}.$$

with $\sum_{i=1}^N t_i = Nt$. Although \mathbf{M}' is positive semidefinite we get

$$\begin{aligned} \mathbf{x}^\top \mathbf{M}' \mathbf{x} &= N + N(N-1)y + d^2 + 2dNt \\ &< N + N(N-1)y + d^2 + 2dN\sqrt{y + \frac{1-y}{N}} = 0. \end{aligned}$$

The same argument with $d = \sqrt{N^2y + N(1-y)}$ yields a contradiction for $t < -\sqrt{y + \frac{1-y}{N}}$. \square

The following lemma gives lower bounds for functions in $\mathcal{R}(\alpha)$.

Lemma 4.4. *For $0 \leq \alpha \leq \frac{\pi}{2}$, let $f \in \mathcal{R}(\alpha)$, let $z = \cos \alpha$, and let*

$$g_\alpha(t) := \begin{cases} -\frac{1}{N} & \text{for } -\sqrt{z + \frac{1-z}{N}} \leq t < -\sqrt{z + \frac{1-z}{N+1}} \text{ for } N \in \mathbb{N} \\ 0 & \text{for } -\sqrt{z} \leq t < 1 \\ 1 & \text{for } t = 1 \end{cases}.$$

Then $f(t) \geq g_\alpha(t)$ for $-1 \leq t \leq z$.

For a plot of $g_{\frac{\pi}{3}}(t)$, see Figure 3 in Section 5.

Proof. First suppose that $f(t) < 0$ for some t with $-\sqrt{z} \leq t \leq z$. Choose N so that $f(t) < \frac{1}{N}$. By Lemma 4.3, there is a code $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in S^{N+1}$ with $\langle \mathbf{x}_0, \mathbf{x}_i \rangle = t$ and $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = z$ for $1 \leq i < j \leq N$. Since $f(t) < -\frac{1}{N}$, we have $\sum_{i=0}^N f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle) < 0$, and therefore $f \notin \mathcal{R}(\alpha)$, a contradiction.

For $t < -\sqrt{z}$ choose N such that $-\sqrt{z + \frac{1-z}{N}} \leq t < -\sqrt{z + \frac{1-z}{N+1}}$, and let $y \leq z$ such that $-\sqrt{y + \frac{1-y}{N}} = t$. By Lemma 4.3, there is a code $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in S^{N+1}$ with $\langle \mathbf{x}_0, \mathbf{x}_i \rangle = t$ and $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = y$ for $1 \leq i < j \leq N$. If $f(t) < -\frac{1}{N}$, then $\sum_{i=0}^N f(\langle \mathbf{x}_0, \mathbf{x}_i \rangle) < 0$, and therefore $f \notin \mathcal{R}(\alpha)$, a contradiction. \square

Observe that $g_\alpha \notin \mathcal{R}(\alpha)$. A simple example of vectors showing this is

$$\mathbf{x}_1 = \begin{pmatrix} \sqrt{1-z} \\ 0 \\ \sqrt{z} \end{pmatrix}, \mathbf{x}_2 = \begin{pmatrix} 0 \\ \sqrt{1-z} \\ \sqrt{z} \end{pmatrix}, \mathbf{x}_0 = -\frac{(1+\varepsilon)\mathbf{x}_1 + \mathbf{x}_2}{\|(1+\varepsilon)\mathbf{x}_1 + \mathbf{x}_2\|} \in S^2.$$

Here, $1 + g_\alpha(\langle \mathbf{x}_0, \mathbf{x}_1 \rangle) + g_\alpha(\langle \mathbf{x}_0, \mathbf{x}_2 \rangle) = 1 - 1 - \frac{1}{2} < 0$.

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

Lemma 4.5. *Let $z = \cos \alpha$, let $\theta_0 < -\sqrt{z}$, and let $f : [-1, \theta_0] \rightarrow \mathbb{R}$. Let $n > N$ and let $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in S^{n-1}$ 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 $\mathbf{x}_i = (x_i^1, x_i^2, \dots, x_i^n)^\top$. We rotate/reflect the set $\{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N\}$ (not changing any of the scalar products) such that $\mathbf{x}_0 = \mathbf{e}_1$, $x_i^j = 0$ for $j > i+1$ and $x_i^{i+1} \geq 0$ for all i . By (ii), $x_i^1 < -\sqrt{z}$, and thus, $x_i^1 \cdot x_j^1 > z$. 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 $x_{i-1}^i > 0$ and $x_i^j < 0$ for all $1 \leq j \leq i \leq N$ (and $\{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{N-1}\}$ is

linearly independent).

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

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 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 proving the lemma. \square

From this we get the following proposition, showing that Lemma 4.4 is sharp in some sense.

Proposition 4.6. *Let $z = \cos \alpha$, let $k \in \mathbb{N}$, and let*

$$h_\alpha^k(t) := \begin{cases} -\frac{1}{k} & \text{for } -1 \leq t < -\sqrt{z + \frac{1-z}{k+1}} \\ 0 & \text{for } -\sqrt{z + \frac{1-z}{k+1}} \leq t < 1 \\ 1 & \text{for } t = 1 \end{cases}.$$

Then $h_\alpha^k \in \mathcal{R}(\alpha)$.

Proof. Suppose for the sake of contradiction that $h_\alpha^k \notin \mathcal{R}(\alpha)$. Then there is a set of points $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{k+1} \in S^{n-1}$ for some $n > N + 1$ such that $\langle \mathbf{x}_i, \mathbf{x}_j \rangle \leq z$ and $\langle \mathbf{x}_0, \mathbf{x}_j \rangle < -\sqrt{z + \frac{1-z}{k+1}}$ for $0 \leq i < j \leq k + 1$. By Lemma 4.5, we may assume that in fact $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = z$ for $1 \leq i < j \leq k + 1$. But this is a contradiction to Lemma 4.3. \square

5. THE MAIN RESULT

One can add the functions from Proposition 4.6 to the set of Gegenbauer polynomials in some dimension n , and this will give a larger set \mathcal{S} . But in most cases, this does not give an improvement to the known bounds on N and α . This is different for the following function. With the inclusion of this function in the set \mathcal{S} , numerous improvements are possible.

Proposition 5.1. *Let $0 \leq z = \cos \alpha < 1$ and*

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

Then $f_\alpha \in \mathcal{R}(\alpha)$.

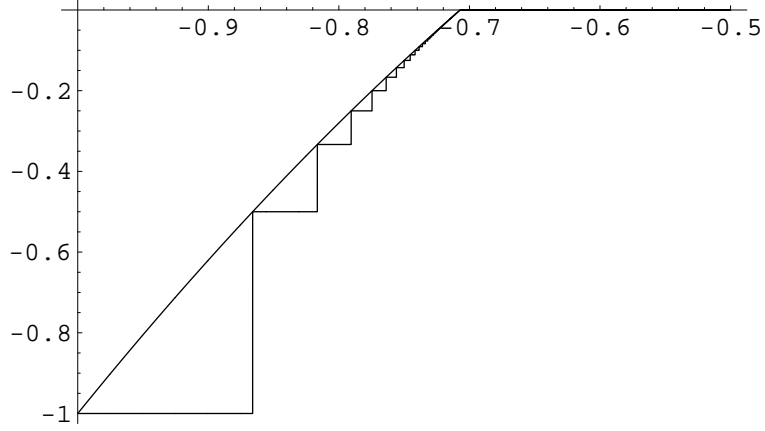


FIGURE 3. A plot of $f_{\frac{\pi}{3}}(t)$ and $g_{\frac{\pi}{3}}(t)$

Proof. Suppose that $f_\alpha \notin \mathcal{R}(\alpha)$, then $f_\alpha \notin \mathcal{R}_{N+1}^n(\alpha)$ for some minimal N . Further we may assume that $n > N$ since $\mathcal{R}_{N+1}^{n+1}(\alpha) \subseteq \mathcal{R}_{N+1}^n(\alpha)$ for all n . Let $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N, \mathbf{x}_0) \in \mathbb{R}^{n \times (N+1)}$ such that $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ is a spherical (n, N, α) -code and so that $S = \sum_{i=1}^N f_\alpha(\langle \mathbf{x}_0, \mathbf{x}_i \rangle)$ is minimal. As $f_\alpha \notin \mathcal{R}_{N+1}^n(\alpha)$, we have $S < 0$. Due to the minimality of N , we have $\langle \mathbf{x}_0, \mathbf{x}_i \rangle < -\sqrt{z}$ for $1 \leq i \leq N$.

By Lemma 4.5, 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 $\mathbf{x}_0 = (x_0^1, x_0^2, \dots, x_0^n)^\top$. 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} . We will show that we can choose \mathbf{x}_0 such that $x_0^i = x_0^j$ for all $i, j \leq N$. This implies that $\mathbf{M} = \mathbf{X}^\top \mathbf{X}$ is of the form of Lemma 4.3 and thus

$$\langle x_0, x_i \rangle = x_0^i \sqrt{1-z} \geq -\sqrt{z + \frac{1-z}{N}}$$

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

$$S = \sum_{i=0}^N f(\langle x_0, x_i \rangle) \geq 1 + N f\left(-\sqrt{z + \frac{1-z}{N}}\right) = 0,$$

a contradiction proving the proposition.

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

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

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 , establishing the proposition. \square

The function f_α shares the following property with the h_α^k :

For every (n, N, α) -code \mathbf{X} , the matrix $(f_\alpha(x_{ij}))$ is positive semidefinite.

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 [12]). For other $n \leq 30$, the best currently known bounds were not improved.

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 [11]).

6. POSSIBLE IMPROVEMENTS

Let us consider how we might improve our bounds by further exploring $\mathcal{R}^n(\alpha)$. Lemma 4.4 gives a lower bound for functions in $\mathcal{R}(\alpha)$ using regular simplices as the extremal configurations. But in S^{n-1} , there can be at most n points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ such that $\langle \mathbf{x}_0, \mathbf{x}_i \rangle = \langle \mathbf{x}_0, \mathbf{x}_j \rangle$ and

| 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 | 278082 |
| 26 | 196848 | 396974 | 396444 |

* : 379 and 12215 with some extra inequalities

TABLE 1. New upper bounds for the kissing number

| n | N | lower bound | Delsarte bound | new upper bound |
|-----|-----|-------------|----------------|-----------------|
| 3 | 13 | 57.13 | 60.42 | 60.35 |
| 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 | 64.38 |
| 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 | 83.15 |
| 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 α in (n, N, α) -codes

$\langle \mathbf{x}_i, \mathbf{x}_j \rangle = z = \cos \alpha$. Thus, there may be functions $f \in \mathcal{R}^n(\alpha)$ for which $-\frac{1}{n} \leq f(t) < g_\alpha(t)$ for some $t \geq -\sqrt{z + \frac{1-z}{n+1}}$. The analysis gets much more complicated, though, as one has to consider configurations which are not regular simplices.

To keep the analysis manageable, we will require that $f(t) \geq 0$ for $t \geq -z$ and that f is monotone increasing. This way, one has to consider only configurations such that $\mathbf{x}_1, \dots, \mathbf{x}_N$ are the vertices of a spherical polytope, and $-\mathbf{x}_0$ is inside this polytope. We get a new lower bound for such

functions:

$$f(t) \geq g_\alpha^n(t) := \begin{cases} -\frac{1}{N} & \text{for } -\sqrt{z + \frac{1-z}{N}} \leq t < -\sqrt{z + \frac{1-z}{N+1}}, N < n \\ \frac{1}{n} & \text{for } -\sqrt{z + \frac{1-z}{n}} \leq t < -z \\ 0 & \text{for } -z \leq t < 1 \\ 1 & \text{for } t = 1 \end{cases}$$

The proof is the same as the one of Lemma 4.4, but only using configurations with up to n vertices other than \mathbf{x}_0 . Observe that $g_\alpha^n \notin \mathcal{R}^n(\alpha)$. But we can use g_α^n in our linear program to find out the limitations of this approach towards improvements of the kissing number bounds—thus we get lower bounds to the upper bounds achievable with this method. The results up to dimension 16 are given in Table 3.

| n | lower bound | Delsarte bound | bd. using $f_{\frac{\pi}{3}}$ | hypothetical bd. using $g_{\frac{\pi}{3}}^n$ |
|-----|-------------|----------------|-------------------------------|---|
| 3 | 12 | 13 | 13 | 12 |
| 4 | 24 | 25 | 25 | 24 |
| 6 | 72 | 82 | 82 | 80 |
| 7 | 126 | 140 | 140 | 135 |
| 9 | 306 | 380 | 379 | 366 |
| 10 | 500 | 595 | 594 | 561 |
| 11 | 582 | 915 | 915 | 877 |
| 12 | 840 | 1416 | 1416 | 1370 |
| 13 | 1130 | 2233 | 2233 | 2132 |
| 14 | 1582 | 3492 | 3492 | 3268 |
| 15 | 2564 | 5430 | 5430 | 5262 |
| 16 | 4320 | 8313 | 8312 | 8159 |

TABLE 3. Lower bounds for upper bounds on $k(n)$

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

For dimensions three and four, using $f_{\frac{\pi}{3}}$ alone gives marginal improvements to the bounds on the kissing numbers achieved with the Delsarte method—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 [10]. For dimension four, only recently a proof for $k(4) = 24$ was found by Musin [7]. The same techniques also yield the arguably simplest proof for dimension three [8].

Our techniques give a new framework for Musin's proofs. We will give a short sketch of this reformulation for dimension four. Similarly to $g^4_{\frac{\pi}{3}}$, define the function

$$g(t) := \begin{cases} -\frac{1}{N} & \text{for } -\sqrt{\frac{N+1}{2N}} \leq t < -\sqrt{\frac{N+2}{2N+2}}, N < 4 \\ \frac{1}{4} & \text{for } -\sqrt{\frac{5}{8}} \leq t < -0.6058 \\ 0 & \text{for } -0.6058 \leq t < 1 \\ 1 & \text{for } t = 1 \end{cases}.$$

Run the linear program using $\mathcal{S} = \{g, G_1^4, G_2^4, \dots, G_9^4\}$, finding a linear combination with non-negative coefficients

$$f = c + c_0 g + \sum_{i=1}^9 c_i G_i^4,$$

maximizing c while maintaining $f(x) \leq 0$ for $x \leq \frac{1}{2}$ and $f(1) \leq 1$. The function f is not necessarily in $\mathcal{P}^4(\frac{\pi}{3})$ as $g \notin \mathcal{R}^4(\frac{\pi}{3})$. To avoid this problem, let

$$h(t) = \begin{cases} \min \left\{ -\frac{f(t) - c_0 g(t)}{1 - c_0}, 0 \right\} & \text{for } t \leq \frac{1}{2} \\ 1 & \text{for } t > \frac{1}{2} \end{cases}.$$

If we can show that $h \in \mathcal{R}^4(\frac{\pi}{3})$, then this will prove that

$$k(4) \leq \frac{1}{c} \approx 24.79 < 25,$$

as

$$\tilde{f} = c + c_0 h + \sum_{i=1}^9 c_i G_i^4$$

is a function with $\tilde{f}(x) \leq 0$ for $x \leq \frac{1}{2}$ and $\tilde{f}(1) \leq 1$.

Comparing h to the ninth degree polynomial used in Musin's proof in [7], one sees that they are identical up to a constant factor on $[-1, -0.6058]$. Since $h(x) \geq 0$ for $x \geq -0.6058$, Musin shows that one only needs to consider configurations $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N$ with $N \leq 6$. Musin's further analysis can be directly translated into a proof that $h \in \mathcal{R}^4(\frac{\pi}{3})$.

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