Journal of Combinatorial Theory, Series A 116 (2009) 195–204

Contents lists available at ScienceDirect

Journal of Combinatorial Theory, Series A

www.elsevier.com/locate/jcta

Note

Optimality and uniqueness of the (4, 10, 1/6) spherical code

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ARTICLE INFO

Article history:
Received 28 August 2007
Available online 4 June 2008

Keywords:
Linear programming
Semidefinite programming
Spherical codes
Spherical designs
Petersen graph

ABSTRACT

Linear programming bounds provide an elegant method to prove optimality and uniqueness of an (n, N, t) spherical code. However, this method does not apply to the parameters $(4, 10, 1/6)$. We use semidefinite programming bounds instead to show that the Petersen code, which consists of the midpoints of the edges of the regular simplex in dimension 4, is the unique $(4, 10, 1/6)$ spherical code.

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1. Introduction

Let C be an N-element subset of the unit sphere $S^{n-1} \subseteq \mathbb{R}^n$. It is called an (n, N, t) *spherical code* if every two distinct points (c, c') of C have inner product $c \cdot c'$ at most t. An (n, N, t) spherical code is called *optimal* if there is no (n, N, t') spherical code with $t' < t$.

Only for a few parameters optimal spherical codes are known. The table [9, p. 115] lists all known cases in dimension $n = 3$. The tables [17, Table 9.1] and [11, Table 1] list all known cases in which optimality can be proven using linear programming bounds.

One source of optimal spherical codes are iterated kissing configurations coming from the E_8 root lattice in dimension 8 and the Leech lattice in dimension 24 (see [13]). Starting from the sphere packing defined by these lattices one fixes one sphere and considers all spheres in the packing touching the fixed one. The touching points, also called a *kissing configuration*, form $(8, 240, 1/2)$ and respectively $(24, 196560, 1/2)$ spherical codes. Then one views the kissing configuration as a packing in spherical geometry and repeats this construction. One gets $(7, 56, 1/3)$ and respectively $(23, 4600, 1/3)$ spherical codes.

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1 Supported by the Netherlands Organization for Scientific Research under grant NWO 639.032.203 and by the Deutsche Forschungsgemeinschaft (DFG) under grant SCHU 1503/4-2.

0097-3165/$ – see front matter © 2008 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcta.2008.05.001

More formally, one picks a point $x \in C$ from an $(n, M, 1/k)$ spherical code C in which x has M' points $N_x \subseteq C$ with inner product $1/k$. Then the points $(N_x - x/k)/\sqrt{1-1/k^2}$ form an $(n-1, M', 1/(k+1))$ spherical code.

In this way one gets sequences of spherical codes with parameters

$$(8, 240, 1/2), \quad (7, 56, 1/3), \quad (6, 27, 1/4), \quad (5, 16, 1/5), \quad (4, 10, 1/6), \quad (3, 6, 1/7),$$

and

$$(24, 196560, 1/2), \quad (23, 4600, 1/3), \quad (22, 891, 1/4), \quad (21, 336, 1/5), \quad (20, 170, 1/6).$$

By using linear programming bounds Levenshtein [17] proved that every sharp (see Section 3) spherical code is optimal. Levenshtein's theorem applies to all spherical codes above except to those with parameters $(4, 10, 1/6)$, $(3, 10, 1/7)$, $(21, 336, 1/5)$, $(20, 170, 1/6)$. In all optimal cases the spherical code is also unique up to orthogonal transformations. This was proved for the cases $(8, 240, 1/2)$, $(7, 56, 1/3)$, $(24, 196560, 1/2)$, $(23, 4600, 1/3)$ by Bannai and Sloane [5] and for $(22, 891, 1/4)$ by Cuypers [14] and independently by Cohn and Kumar [12] (who also corrected a minor error in the $(23, 4600, 1/3)$ case). For the cases $(6, 27, 1/4)$, $(5, 16, 1/5)$ see the discussion in [11, Appendix A]. One should point out that optimality does not imply uniqueness as one can see from the sharp $(q(q^3+1)/(q+1), (q+1)(q^3+1), 1/q^2)$ spherical codes from [10]. For some q there are two different spherical codes with these parameters.

Based on massive computer experiments Cohn et al. [6, Section 3.4] conjectured that the $(4, 10, 1/6)$ spherical code is optimal and unique. As we explain in Section 2 this spherical code is closely related to the Petersen graph and we call it the *Petersen code*. Whether the above spherical codes with parameters $(21, 336, 1/5)$ and $(20, 170, 1/6)$ are optimal and unique is currently unclear. At least in all these cases linear programming bounds cannot be used to show optimality. A $(3, 6, 1/7)$ spherical code is not optimal because the vertices of the regular octahedron form a $(3, 6, 0)$ spherical code which is a sharp spherical code.

The main result of this paper is the following theorem which proves the conjecture.

Theorem 1.1. *The Petersen code is an optimal* $(4, 10, 1/6)$ *spherical code. Up to orthogonal transformations it is the unique spherical code with these parameters.*

The proof is based on the semidefinite programming bounds for spherical codes developed in [2] and [3]. Currently this is the only new case we know where the semidefinite programming bound is tight and the linear programming bound is not. Another known case seems to be 8 points in S^2 which was solved by Schütte and van der Waerden in [19]. The linear programming bound gives 8.29 whereas our numerical calculations suggest that the semidefinite programming bound is tight.

We could not prove optimality of $(21, 336, 1/5)$ and $(20, 170, 1/6)$ spherical codes using semidefinite programming bounds. For the first case the linear programming bound equals 392 whereas our numerical calculations suggest that the semidefinite programming bound is approximately 363. However, we run into serious numerical problems here and at the moment we cannot definitely rule out that the semidefinite programming bound is sharp. For the second case the linear programming bound and the semidefinite programming bound coincide: They both give 206.25.

The structure of the paper is as follows: After giving some constructions and properties of the Petersen code in Section 2, which also reveal the origin of its name, we show in Section 3 that one *cannot* prove Theorem 1.1 using linear programming bounds. In Section 4 we recall the semidefinite programming bounds and in Section 5 we present a proof of Theorem 1.1 based on them.

2. Constructions and properties of the Petersen code

There are many possibilities to construct the Petersen code and we already gave one. Here we give two more.

The next construction justifies the name "Petersen code." The Petersen graph is a graph with 10 vertices and 15 edges. The vertices are given by the 2-element subsets of a 5-element set and they are adjacent whenever the corresponding 2-element subsets have empty intersection. Every point of the Petersen code corresponds to a vertex of the Petersen graph and the inner product between two points is $-2/3$ whenever the corresponding vertices are adjacent. The inner product is $1/6$ whenever the corresponding vertices are not adjacent. This defines a Gram matrix having rank 4 which is unique up to simultaneous permutation of rows and columns. The number of ordered pairs in the Petersen code with inner product $-2/3$ is 30 and those with inner product $1/6$ equals 60.

In the Petersen graph every vertex has three neighbors, every pair of adjacent vertices has no common neighbors and every pair of nonadjacent vertices has exactly one common neighbor. So it is a strongly regular graph with parameters $\nu = 10$, $k = 3$, $\lambda = 0$, $\mu = 1$. It is easy to see that it is uniquely defined by these parameters. For more information about strongly regular graphs see [4] and [8].

The next construction is geometric: After applying a suitable similarity transformation the midpoints of the edges of the regular simplex in dimension 4 form the Petersen code. Sometimes, this construction is also called the *second hypersimplex* $\Delta(2,5)$. The second hypersimplex is the 4-dimensional polytope defined as the convex hull of the points $e_i + e_j$ with $1 \leqslant i < j \leqslant 5$ where e_i is the ith standard unit vector in $\mathbb{R}^5$. For more information about second hypersimplices see [18].

By [15, Theorem 5.5] the Petersen code forms a spherical 2-design: A spherical code $C \subseteq S^{n-1}$ forms a *spherical M-design* if for every polynomial function $f : \mathbb{R}^n \to \mathbb{R}$ of degree at most M, the average over C equals the average over the sphere S^{n-1}.

3. Linear programming bounds

Linear programming bounds provide an elegant method to prove optimality and uniqueness of an (n, N, t) spherical code. In particular a theorem of Levenshtein [17, Theorem 1.2], which covers many cases in a unified way is based on them. Before we prove that linear programming bounds cannot prove the optimality of the $(4, 10, 1/6)$ spherical code we briefly review the underlying notions (see also e.g. [15, Theorem 4.3], [16], [13, Chapter 9], [2, Theorem 2.1]).

The positivity property of the Gegenbauer polynomials $C_k^{n/2-1}$ (see [1, Chapter 6.4]), which are normalized by $C_k^{n/2-1}(1) = 1$, underlies the linear programming bounds for spherical codes in S^{n-1}: For every degree $k = 0, 1, \ldots$ and every finite subset C of S^{n-1} we have

$$\sum_{(c,c') \in C^2} C_k^{n/2-1}(c \cdot c') \geqslant 0. \tag{1}$$

One formulation of the linear programming bounds is as follows.

Theorem 3.1. *Let $F(x)$ be a polynomial with expansion*

$$F(x) = \sum_{k=0}^{d} f_k C_k^{n/2-1}(x) \tag{2}$$

in terms of Gegenbauer polynomials $C_k^{n/2-1}$. Suppose that

(a) *all coefficients f_k are nonnegative,*
(b) $f_0 > 0$,
(c) $F(x) \leqslant 0$ *for all* $x \in [-1, t]$.

Then an (n, N, t) spherical code satisfies

$$N \leqslant \frac{F(1)}{f_0}. \tag{3}$$

Proof. For an (n, N, t) spherical code C we have the inequalities

$$NF(1) \geqslant \sum_{(c,c)\in C^2} F(1) + \sum_{\substack{(c,c')\in C^2 \\ c\neq c'}} F(c\cdot c') = \sum_{(c,c')\in C^2} F(c\cdot c') \geqslant N^2 f_0, \tag{4}$$

where the first inequality is due to (c) and the second due to (a) and the positivity property (1). This together with (b) implies (3). □

If there exists an (n, N, t) spherical code C so that $N = \lfloor F(1)/f_0 \rfloor$ in (3), then, of course, C is a maximal (n, N, t) spherical code, i.e. N is the maximal number of points one can place on the sphere S^{n-1} so that distinct points have inner product at most t. If furthermore $N = F(1)/f_0$, then C is an optimal (n, N, t) spherical code. This can be seen as follows. If (3) is tight it follows from the proof that for an (n, N, t) spherical code C one has $F(c\cdot c') = 0$ for distinct $c, c' \in C$. Suppose C' is an (n, N, t') spherical code with $t' < t$. Then, $F(c\cdot c') = 0$ for all distinct $c, c' \in C'$. Now we perturb C' continuously to another (n, N, t'') spherical code C'' with $t' < t'' < t$. Still we would have that $c\cdot c'$ is a root of the polynomial F for all distinct $c, c' \in C''$ yielding a contradiction.

Levenshtein's theorem says that for every sharp spherical code there is a polynomial satisfying the assumptions of Theorem 3.1 for which (3) is tight. A spherical code C is called *sharp* if it is a spherical M-design and the number m of different inner products between distinct points satisfies $M \geqslant 2m - 1$. The Petersen code is a spherical 2-design and there are 2 different inner products between distinct points. Thus, Levenshtein's theorem does not apply to it.

Now we show that it is not possible to prove the optimality of the Petersen code with help of Theorem 3.1. Suppose that the polynomial $F(x) = 1 + \sum_{k=1}^{d} f_k C_k^1(x)$ satisfies $f_k \geqslant 0$ for $k = 1, \ldots, d$, and $F(x) \leqslant 0$ for all $x \in [-1, 1/6]$. If F would prove that the Petersen code is optimal, then the inequalities in (4) are equalities, so we would have that

$$10 = F(1) = 1 + \sum_{k=1}^{d} f_k, \tag{5}$$

and that

$$0 = F(-2/3) = F(1/6), \tag{6}$$

and furthermore that for all k with $f_k > 0$,

$$0 = \sum_{(c,c')\in C^2} C_k^1(c\cdot c') = 10 + 30C_k^1(-2/3) + 60C_k^1(1/6). \tag{7}$$

We shall show that (7) only holds for $k = 1$ and $k = 2$: By [1, (6.4.11)] we have the following expression:

$$C_k^1(\cos\theta) = \frac{1}{k+1}\sum_{j=0}^{k} \cos\bigl((k-2j)\theta\bigr). \tag{8}$$

Hence,

$$\lim_{k\to\infty} C_k^1(-2/3) = \lim_{k\to\infty} C_k^1(1/6) = 0, \tag{9}$$

so that for sufficiently large k, (7) cannot hold true. Checking the remaining cases it follows that (7) is only valid for $k = 1, 2$. Hence, F is of degree 2, but then F cannot satisfy the conditions (5) and (6) and $F(x) \leqslant 0$ for $x \in [-1, 1/6]$.

This argument gives rather pessimistic estimates. In fact, numerical computations suggest that for all $d \geqslant 3$ the optimal polynomial is

$$F(x) = 1 + \frac{2270}{680}x + \frac{2775}{680}\left(\frac{4}{3}x^2 - \frac{1}{3}\right) + \frac{1500}{680}\bigl(2x^3 - x\bigr), \tag{10}$$

and so the best upper bound one can probably prove using Theorem 3.1 is 10.625. We checked this for all $d \leqslant 40$ by computer.

4. Semidefinite programming bounds

As we have seen above the positivity property of the polynomials $C_k^{n/2-1}$ plays a crucial role for the linear programming bounds. For the semidefinite programming bounds this is replaced by the positivity property of the matrices S_k^n. From [2] we recall the matrices S_k^n and their positivity property. First we define the entry (i, j) with $i, j \geqslant 0$ of the (infinite) matrix Y_k^n containing polynomials in x, y, z by

$$\big(Y_k^n\big)_{i,j}(x, y, z) = x^i y^j \cdot \big((1-x^2)(1-y^2)\big)^{k/2} C_k^{n/2-3/2}\bigg(\frac{z-xy}{\sqrt{(1-x^2)(1-y^2)}}\bigg), \tag{11}$$

and then we get S_k^n by symmetrization:

$$S_k^n = \frac{1}{6}\sum_\sigma \sigma Y_k^n, \tag{12}$$

where σ runs through all permutations of the variables x, y, z which acts on the matrix coefficients in the obvious way. The matrices S_k^n satisfy the positivity property:

$$\text{for all finite } C \subseteq S^{n-1}, \quad \sum_{(c,c',c'')\in C^3} S_k^n(c\cdot c', c\cdot c'', c'\cdot c'') \succcurlyeq 0, \tag{13}$$

where "$\succcurlyeq 0$" stands for "is positive semidefinite" where we mean that every finite minor is positive semidefinite. Note that the difference between (11) and the original [2, (12)] is due to a change of basis which does not affect the positivity property.

The interval $[-1, t]$ of the linear programming bounds is supplemented by the domain

$$D = \big\{(x, y, z)\colon\ -1 \leqslant x, y, z \leqslant t,\ 1 + 2xyz - x^2 - y^2 - z^2 \geqslant 0\big\}. \tag{14}$$

We need some more notation. The space of (finite) symmetric matrices is a Euclidean space with inner product $\langle F, G\rangle = \operatorname{trace}(FG)$. The cone of positive semidefinite matrices is self dual, i.e. one has $\langle F, G\rangle \geqslant 0$ for all positive semidefinite G if and only if F is positive semidefinite. If F is a symmetric matrix with m rows and m columns, then we interpret $\langle F, S_k^n\rangle$ as the inner product of F with the principal minor of S_k^n of appropriate size.

Now we can state the semidefinite programming bounds. The following polynomial formulation can be deduced from [2, Theorem 4.2]. We provide an independent proof which has the additional feature that it gives information in the case when the theorem provides tight results.

Theorem 4.1. *Let $F(x, y, z)$ be a symmetric polynomial with expansion*

$$F(x, y, z) = \sum_{k=0}^{d} \big\langle F_k, S_k^n(x, y, z)\big\rangle, \tag{15}$$

in terms of the matrices S_k^n. Suppose that

(a) *all F_k are positive semidefinite,*
(b) *$F_0 - f_0 E_0 \succcurlyeq 0$ for some $f_0 > 0$ (E_0 is the matrix whose only nonzero entry is the top left corner which contains 1),*
(c) *$F(x, y, z) \leqslant 0$ for all $(x, y, z) \in D$,*
(d) *$F(x, x, 1) \leqslant B$ for all $x \in [-1, t]$.*

Then an (n, N, t) spherical code satisfies

$$N \leqslant \frac{3B + \sqrt{9B^2 + 4f_0(F(1,1,1) - 3B)}}{2f_0}. \tag{16}$$

Proof. Let C be an (n, N, t) spherical code. Define

$$S = \sum_{(c,c',c'')\in C^3} F(c \cdot c', c \cdot c'', c' \cdot c''). \tag{17}$$

Split this sum into three parts according to the indices $C_1, C_2, C_3 \subseteq C^3$ where C_i contains all triples with i pairwise different elements. The contribution of C_1 to S is $NF(1,1,1)$, the one of C_2 at most $3N(N-1)B$ and the one of C_3 is at most zero. Together,

$$S \leqslant NF(1,1,1) + 3N(N-1)B. \tag{18}$$

On the other hand,

$$\begin{aligned} S &= \sum_{k=0}^{d} \left\langle F_k, \sum_{(c,c',c'')\in C^3} S_k^n(c \cdot c', c \cdot c'', c' \cdot c'') \right\rangle && (19)\\ &\geqslant \left\langle f_0 E_0, \sum_{(c,c',c'')\in C^3} S_k^n(c \cdot c', c \cdot c'', c' \cdot c'') \right\rangle && (20)\\ &= N^3 f_0, && (21)\end{aligned}$$

yielding the statement of the theorem. □

A few remarks about the theorem and its proof are in order.

If the bound (16) is tight, then all inequalities in the proof must be equalities. In particular, the univariate polynomial $F(x,x,1) - B$ has roots at the inner products $c \cdot c'$ for distinct $c, c' \in C$. So we can argue in the same way as in the case of the linear programming bounds that tightness implies optimality.

If the bound (16) is tight, we have the following identities: Let C be an (n, N, t) spherical code with

$$\begin{aligned} D(C) &= \{(c \cdot c', c \cdot c'', c' \cdot c''):\ (c,c',c'') \in C^3\},\\ I(C) &= \{c \cdot c':\ (c,c') \in C^2,\ c \neq c'\}. \end{aligned} \tag{22}$$

Let F be a polynomial satisfying the hypothesis of Theorem 4.1 with constants B and f_0 and proving the tight bound $(3B + \sqrt{9B^2 + 4f_0(F(1,1,1) - 3B)})/2f_0$. Then

(i) $N^2 f_0 - F(1,1,1) - 3(N-1)B = 0$,
(ii) $F(x,y,z) = 0$ for all $(x,y,z) \in D(C)$,
(iii) $F(x,x,1) = B$ for all $x \in I(C)$,
(iv) $\langle F_k, \sum_{(c,c',c'')\in C^3} S_k^n(c \cdot c', c \cdot c'', c' \cdot c'')\rangle = 0$ for all $k = 1, \dots, d$,
(v) $\langle F_0, \sum_{(c,c',c'')\in C^3} S_0^n(c \cdot c', c \cdot c'', c' \cdot c'')\rangle = N^3 f_0$.

Semidefinite programming bounds are at least as strong as linear programming bounds: If $G = \sum_{k=0}^{d} g_k C_k^{n/2-1}(x)$ is a polynomial which satisfies the hypothesis of Theorem 3.1, then the polynomial $F(x,y,z) = (G(x) + G(y) + G(z))/3$ satisfies the hypothesis of Theorem 4.1 with $B = G(1)/3$ and $f_0 = g_0$. This is because one sets $F_0 = g_0 E_0$ and from [2, Proposition 3.6] it follows that one can express G with semidefinite matrix coefficients.

From [3, Lemma 4.1] it follows that one can express every symmetric polynomial in the form (15). However, this expansion is not unique, e.g.

$$\begin{aligned} x + y + z &= \left\langle \begin{pmatrix} 0 & 3/2 \\ 3/2 & 0 \end{pmatrix}, S_0^n \right\rangle + \langle (0), S_1^n \rangle \\ &= \left\langle \begin{pmatrix} 0 & 0 \\ 0 & 3 \end{pmatrix}, S_0^n \right\rangle + \langle (3), S_1^n \rangle, \end{aligned} \tag{23}$$

where only the second expansion involves semidefinite matrices and where

$$S_0^n = \begin{pmatrix} 1 & (x+y+z)/3 \\ (x+y+z)/3 & (xy+xz+yz)/3 \end{pmatrix}, \qquad S_1^n = \big((x+y+z)/3 - (xy+xz+yz)/3\big). \tag{24}$$

5. Proof of optimality and uniqueness

In this section we prove Theorem 1.1 with the help of Theorem 4.1. Although we can present a proof which one can verify essentially without using computer we relied heavily on computer assistance to find it.

To show that the Petersen code is the unique $(4, 10, 1/6)$ spherical code we use the matrices $F_0 \in \mathbb{R}^{4\times 4}$, $F_1 \in \mathbb{R}^{3\times 3}$, $F_2 \in \mathbb{R}^{1\times 1}$ given by

$$F_0 = \begin{pmatrix} 2882/3 & 114 & -2500 & 0 \\ 114 & 324 & 216 & 0 \\ -2500 & 216 & 8716 & 1296 \\ 0 & 0 & 1296 & 11664 \end{pmatrix},$$

$$F_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 3588 & -4536 \\ 0 & -4536 & 11664 \end{pmatrix}, \qquad F_2 = (\,2000\,). \tag{25}$$

Let

$$m_{ijk} = \frac{1}{6}\sum_{\sigma} \sigma\big(x^i y^j z^k\big), \quad 0 \leqslant i \leqslant j \leqslant k, \tag{26}$$

where σ runs through all permutations of the variables x, y, z, be the polynomial which one gets by symmetrizing $x^i y^j z^k$. Then,

$$\begin{aligned} F(x,y,z) = {} & 11664 m_{320} + 11664 m_{221} + 7128 m_{220} - 9072 m_{211} \\ & + 432 m_{210} - 2412 m_{111} + 324 m_{110} + 228 m_{100} - 118/3, \end{aligned} \tag{27}$$

and

$$F(x,x,1) - B = \frac{1}{3888}\left(x + \frac{2}{3}\right)^2 \left(x - \frac{1}{6}\right)\left(x^2 + \frac{4}{9}x + \frac{20}{27}\right). \tag{28}$$

It is a straightforward computation that F satisfies the condition of Theorem 4.1 with $F(1,1,1) = 59750/3$, $B = 250$, $f_0 = 800/3$ so that it shows $N \leqslant 10$ for a $(4, N, 1/6)$ spherical code. This finishes the proof of the optimality.

Before showing uniqueness, let us describe how we derived F_0, F_1, F_2. We have

$$S_0^4(x,y,z) = \begin{pmatrix} 1 & m_{100} & m_{200} & m_{300} \\ m_{100} & m_{110} & m_{210} & m_{310} \\ m_{200} & m_{210} & m_{220} & m_{320} \\ m_{300} & m_{310} & m_{320} & m_{330} \end{pmatrix},$$

$$S_1^4(x,y,z) = \begin{pmatrix} m_{100} - m_{110} & m_{110} - m_{210} & m_{210} - m_{310} \\ m_{110} - m_{210} & m_{111} - m_{220} & m_{211} - m_{320} \\ m_{210} - m_{310} & m_{211} - m_{320} & m_{221} - m_{330} \end{pmatrix},$$

$$S_2^4(x,y,z) = (\,-\tfrac{1}{2} + \tfrac{5}{2} m_{200} - 3 m_{111} + m_{220}\,). \tag{29}$$

Then $0 = \sum_{k=0}^{2} \langle K_{i,k}, S_k^4 \rangle$ for

$$K_{1,0} = \begin{pmatrix} 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad K_{1,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad K_{1,2} = (0),$$
$$K_{2,0} = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{5}{4} & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{5}{4} & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad K_{2,1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad K_{2,2} = (1),$$
$$K_{3,0} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad K_{3,1} = \begin{pmatrix} 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad K_{3,2} = (0),$$
$$K_{4,0} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}, \qquad K_{4,1} = \begin{pmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 \end{pmatrix}, \qquad K_{4,2} = (0), \tag{30}$$

i.e. the matrices $K_{i,k}$ form a basis of the kernel of the linear map which assigns symmetric polynomials to the matrix coefficients. From the discussion following the proof of Theorem 4.1 we know that the matrix entries have to satisfy the equalities (i)–(v) where

$$\sum_{(c,c',c'')\in C^3} S_0^4(c\cdot c', c\cdot c'', c'\cdot c'') = \begin{pmatrix} 1000 & 0 & 250 & \frac{125}{9} \\ 0 & 0 & 0 & 0 \\ 250 & 0 & \frac{125}{2} & \frac{125}{36} \\ \frac{125}{9} & 0 & \frac{125}{36} & \frac{125}{648} \end{pmatrix},$$
$$\sum_{(c,c',c'')\in C^3} S_1^4(c\cdot c', c\cdot c'', c'\cdot c'') = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$\sum_{(c,c',c'')\in C^3} S_2^4(c\cdot c', c\cdot c'', c'\cdot c'') = (0). \tag{31}$$

We restrict our search to polynomials F satisfying

$$\frac{\partial F}{\partial x}\left(-\frac{2}{3}, -\frac{2}{3}, \frac{1}{6}\right) = 0, \qquad \frac{\partial F}{\partial x}\left(-\frac{2}{3}, \frac{1}{6}, \frac{1}{6}\right) = 0, \qquad \frac{\partial F}{\partial x}\left(-\frac{2}{3}, -\frac{2}{3}, 1\right) = 0. \tag{32}$$

Furthermore, we restrict our search to those polynomials lying in the subspace of dimension 9 spanned by

$$m_{320}, \quad m_{221}, \quad m_{220}, \quad m_{211}, \quad m_{210}, \quad m_{111}, \quad m_{110}, \quad m_{100}, \quad 1. \tag{33}$$

The one-dimensional affine subspace

$$\begin{aligned} F_\gamma(x,y,z) = {} & (11664m_{320} + 9720m_{220} - 1296m_{210} - 6480m_{111} + 2268m_{110} - 108m_{100} - 18) \\ & + \gamma(34992m_{221} - 7776m_{220} - 27216m_{211} + 5184m_{210} + 12204m_{111} \\ & - 5832m_{110} + 1008m_{100} - 64), \quad \gamma \in \mathbb{R}, \end{aligned} \tag{34}$$

satisfies all these linear equalities. We have

$$F_\gamma(x,y,z) = \sum_{k=0}^{2} \langle A_k, S_k^4\rangle + \gamma\langle B_k, S_k^4\rangle \tag{35}$$

with

$$A_0 = \begin{pmatrix} -18 & -54 & 0 & 0 \\ -54 & 2268 & -648 & 0 \\ 0 & -648 & 3240 & 5832 \\ 0 & 0 & 5832 & 0 \end{pmatrix},$$
$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -6480 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad A_2 = (0), \tag{36}$$

and

$$B_0 = \begin{pmatrix} -64 & 504 & 0 & 0 \\ 504 & -5832 & 2592 & 0 \\ 0 & 2592 & 4428 & -13608 \\ 0 & 0 & -13608 & 34992 \end{pmatrix},$$
$$B_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 12204 & -13608 \\ 0 & -13608 & 34992 \end{pmatrix}, \qquad B_2 = (0). \tag{37}$$

In this affine subspace we want to find a polynomial which satisfies the inequalities (c) and (d) from Theorem 4.1 and which at the same time has a representation of the form (15) with positive semidefinite matrices F_k. Hence, we are left with the problem of finding a matrix in the intersection of an affine subspace with the cone of positive semidefinite matrices which is a basic task in semidefinite programming. Since this problem is not known to be in NP—in fact it is the major open problem in the theory of semidefinite programming—it is not a priori clear that a solution exists which one can nicely describe.

We solved these two semidefinite programming problems separately and we used the numerical software `csdp` [7] for this task: If $0.28 \lessapprox \gamma \lessapprox 0.68$, then F_γ satisfies (c). If $0.18 \lessapprox \gamma \lessapprox 0.38$, then F_γ has a representation of the form (15) with positive semidefinite matrices. We make the Ansatz $\gamma = \frac{1}{3}$ and try to find a nice representation. For this we solve the semidefinite feasibility problem

$$A_k + \frac{1}{3} B_k + \beta_1 K_{1,k} + \beta_2 K_{2,k} + \beta_3 K_{3,k} + \beta_4 K_{4,k} \succcurlyeq 0, \quad k = 0, 1, 2, \tag{38}$$

which luckily happens to have the solution $\beta_1 = \beta_3 = \beta_4 = 0$ and $\beta_2 = 2000$.

To show uniqueness we first derive the three points distance distribution α of a $(4, 10, 1/6)$ spherical code C which is defined by

$$\alpha(x, y, z) = \frac{1}{|C|} \left| \left\{ (c, c', c'') \in C^3 \colon\ c \cdot c' = x,\ c \cdot c'' = y,\ c' \cdot c'' = z \right\} \right|. \tag{39}$$

Since $-2/3$ and $1/6$ are the only roots of the polynomial $F(x, x, 1) - B$, these are the only inner products which can occur among distinct points in C. This enables us to use (iv) and (v) together with the relations

$$\begin{aligned} &\alpha(x, y, z) = \alpha\big(\sigma(x, y, z)\big) \quad \text{for all permutations } \sigma \text{ of } x, y, z, \\ &\alpha(1, 1, 1) = 1, \\ &\sum_{(x,y,z) \in D} \alpha(x, y, z) = 100, \\ &\sum_{x \in [-1,1]} \alpha(x, x, 1) = 10, \end{aligned} \tag{40}$$

to determine α by solving a system of linear equations: It is

$$\begin{aligned}
&\alpha(-2/3,-2/3,1/6)=6, \qquad \alpha(-2/3,-2/3,1)=3,\\
&\alpha(-2/3,1/6,1/6)=12, \qquad \alpha(1/6,1/6,1/6)=18,\\
&\alpha(1/6,1/6,1)=6, \qquad \alpha(1,1,1)=1. \qquad (41)
\end{aligned}$$

Now by [15, Theorem 5.5] C is a spherical 2-design. By [15, Theorem 7.4] it carries a 2-class association scheme whose valencies and intersection numbers are uniquely determined. In fact it is a strongly regular graph with parameters $v=10$, $k=3$, $\lambda=0$, $\mu=1$. This uniquely defines the Petersen graph which finishes the proof of the uniqueness.

Acknowledgments

We thank Henry Cohn for communicating this problem at the Oberwolfach seminar "Sphere Packings: Exceptional Geometric Structures and Connections to other Fields" in November 2005 and for further helpful discussions. We thank the two anonymous referees for useful suggestions.

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