SEMIDEFINITE PROGRAMMING, MULTIVARIATE ORTHOGONAL POLYNOMIALS, AND CODES IN SPHERICAL CAPS

CHRISTINE BACHOC AND FRANK VALLENTIN

ABSTRACT. In this paper we apply the semidefinite programming approach developed in [2] to obtain new upper bounds for codes in spherical caps. We compute new upper bounds for the one-sided kissing number in several dimensions where we in particular get a new tight bound in dimension 8. Furthermore we show how to use the SDP framework to get analytic bounds.

Dedicated to Eiichi Bannai in occasion of his 60th birthday

1. INTRODUCTION

Let S^{n-1} denote the unit sphere of the Euclidean space $\mathbb{R}^n$. The spherical cap with center $e \in S^{n-1}$ and angular radius ϕ is the set

$$\mathrm{Cap}(e, \phi) = \{x \in S^{n-1} : e \cdot x \geq \cos \phi\}.$$

Let us consider the problem to upper bound the size of a code C contained in $\mathrm{Cap}(e, \phi)$ with minimal angular distance θ. Following notations of [3], the maximal size of such a code is denoted by $A(n, \theta, \phi)$. Many reasons to consider this problem are exposed in [3], e.g. upper bounds for spherical codes can be derived from upper bounds for spherical cap codes through the following inequality:

$$\frac{A(n, \theta)}{\mathrm{vol}(S^{n-1})} \leq \frac{A(n, \theta, \phi)}{\mathrm{vol}(\mathrm{Cap}(e, \phi))}$$

where $A(n, \theta)$ stands as usual for the maximal size of a spherical code with minimal angular distance θ.

Moreover, it is a challenging problem, because the so-called linear programming method does not apply to this situation. In coding theory many of the best upper bounds are consequences of the so-called linear programming method due to P. Delsarte. This method gives upper bounds for codes from the solution of a certain linear program. It can be applied to symmetric spaces and has been successfully used to deal with two-point homogeneous spaces like the unit sphere S^{n-1} ([7], [8], [6, Chapter 9]), or with symmetric spaces which are not two-point homogeneous like Grassmannian spaces ([1]). However the method is not applicable to spaces which are not symmetric spaces like spherical caps.

Date: October 26, 2006.

The second author was supported by the Netherlands Organization for Scientific Research under grant NWO 639.032.203 and by the Deutsche Forschungsgemeinschaft (DFG) under grant SCHU 1503/4-1.

In this paper, we want to show that the approach developed in [2] based on semidefinite programming can be applied to the above problem. It turns out that it gives good numerical results. In particular we obtain improvements in the determination of the so-called one-sided kissing number, corresponding to $\phi = \pi/2$ and $\theta = \pi/3$, and denoted by $B(n)$ after [11].

Let us describe briefly the idea underlying our approach. The isometry group of $\mathrm{Cap}(e, \phi)$ is the group $H := \mathrm{Stab}(\mathrm{O}(\mathbb{R}^n), e)$ stabilizing the point e in $\mathrm{O}(\mathbb{R}^n)$. This group acts on the space $\mathrm{Pol}_{\leq d}(S^{n-1})$ of polynomial functions of degree at most d on the unit sphere. In the decomposition of this space into irreducible subspaces some irreducible subspaces occur with multiplicities. To each irreducible subspace with multiplicity m we can associate a $m \times m$ matrix Y whose coefficients are real polynomials in three variables (u, v, t) and have a very explicit expression in terms of Gegenbauer polynomials. Each matrix Y satisfies the positivity property:

$$\text{For all finite } C \subset S^{n-1}, \quad \sum_{(c,c') \in C^2} Y(e \cdot c, e \cdot c', c \cdot c') \succeq 0,$$

where "$\succeq 0$" stands for "is positive semidefinite".

We want to point out that the same framework can be developed for every metric space X with isometry group H. Only the expression of the matrices Y will depend on the specific situation. For a symmetric space X the multiplicities in the irreducible decomposition are equal to 1. Hence the matrices Y have size 1×1. So we recover the classical positivity property of zonal polynomials which underlies the linear programming method.

The paper is organized as follows: Section 2 recalls the needed notations and results of [2]. Section 3 states the semidefinite program (SDP for short) which obtains an upper bound for $A(n, \theta, \phi)$ and presents the numerical results. Section 4 translates the dual SDP into a statement on three variable polynomials, and states more material on orthogonality relations, positivity property and other classical material.

2. Review on the semidefinite zonal matrices

We start with some notations. The standard inner product of the Euclidean space $\mathbb{R}^n$ is denoted by $x \cdot y$. The orthogonal group $\mathrm{O}(\mathbb{R}^n)$ acts homogeneously on the unit sphere

$$S^{n-1} := \{x \in \mathbb{R}^n : x \cdot x = 1\}.$$

The space of real polynomial functions of degree at most d on S^{n-1} is denoted by $\mathrm{Pol}_{\leq d}(S^{n-1})$. It is endowed with the induced action of $\mathrm{O}(\mathbb{R}^n)$, and equipped with the standard $\mathrm{O}(\mathbb{R}^n)$-invariant inner product

$$(f, g) = \frac{1}{\omega_n} \int_{S^{n-1}} f(x) g(x) d\omega_n(x), \tag{1}$$

where ω_n is the surface area of S^{n-1} for the standard measure $d\omega_n$.

It is a classical result that under the action of $\mathrm{O}(\mathbb{R}^n)$

$$\mathrm{Pol}_{\leq d}(S^{n-1}) = H_0^n \perp H_1^n \perp \ldots \perp H_d^n, \tag{2}$$

where H_k^n is isomorphic to the $\mathrm{O}(\mathbb{R}^n)$-irreducible space of homogeneous, harmonic polynomials of degree k in n variables, denoted by Harm_k^n. For the dimension of these spaces we write $h_k^n := \dim(\mathrm{Harm}_k^n)$.

For the restricted action of the subgroup $H := \mathrm{Stab}(e, \mathrm{O}(\mathbb{R}^n))$, introduced above, we have the following decomposition into isotypic components:

$$\mathrm{Pol}_{\leq d}(S^{n-1}) = \mathcal{I}_0 \perp \mathcal{I}_1 \perp \ldots \perp \mathcal{I}_d, \tag{3}$$

where

$$\mathcal{I}_k \simeq (d-k+1)\,\mathrm{Harm}_k^{n-1}, \quad k = 0, \ldots, d.$$

More precisely, $\mathcal{I}_k$ decomposes as

$$\mathcal{I}_k = H_{k,k}^{n-1} \perp \ldots \perp H_{k,d}^{n-1}, \tag{4}$$

where, for $i \geq k$, $H_{k,i}^{n-1}$ is the unique subspace of H_i^n isomorphic to Harm_k^{n-1}.

The following construction associates to each $\mathcal{I}_k$ a matrix-valued function

$$Z_k^n : S^{n-1} \times S^{n-1} \to \mathbb{R}^{(d-k+1)\times(d-k+1)} \tag{5}$$

which is uniquely defined up to conjugation. Let $(e_{s,1}^k, e_{s,2}^k, \ldots, e_{s,h_k^{n-1}}^k)$ be an orthonormal basis of $H_{k,k+s}^{n-1}$, then define

$$E_k^n(x) := \frac{1}{\sqrt{h_k^{n-1}}} \begin{pmatrix} e_{0,1}^k(x) & \ldots & e_{0,h_k^{n-1}}^k(x) \\ \vdots & & \vdots \\ e_{d-k,1}^k(x) & \ldots & e_{d-k,h_k^{n-1}}^k(x) \end{pmatrix},$$

and

$$Z_k^n(x,y) := E_k^n(x) E_k^n(y)^t \in \mathbb{R}^{(d-k+1)\times(d-k+1)}. \tag{6}$$

Moreover, we assume that the basis $(e_{s,i}^k)_{1\leq i\leq h_k^{n-1}}$ is the image of $(e_{0,i}^k)_{1\leq i\leq h_k^{n-1}}$ by some H-isomorphism $\phi_s : H_{k,k}^{n-1} \to H_{k,k+s}^{n-1}$.

One can prove that, for all $g \in H$, $Z_k^n(g(x), g(y)) = Z_k^n(x,y)$. As a consequence, the coefficients of Z_k^n can be expressed as polynomials in the three variables $u = e \cdot x$, $v = e \cdot y$, $t = x \cdot y$. More precisely, let $Y_k^n(u,v,t)$ be the $(d-k+1) \times (d-k+1)$ matrix such that

$$Z_k^n(x,y) = Y_k^n(e \cdot x, e \cdot y, x \cdot y). \tag{7}$$

We denote the zonal polynomials of the unit sphere S^{n-1} by P_k^n. In other words, $P_k^n(t)$ is the Gegenbauer polynomial of degree k with parameter $n/2-1$, normalized by the condition $P_k^n(1) = 1$. We give in [2, Theorem 3.2] the following explicit expressions for the coefficients of the matrices Y_k^n:

Theorem 2.1. *We have, for all* $0 \le i, j \le d-k$,

$$\big(Y_k^n\big)_{i,j}(u,v,t) = \lambda_{i,j} P_i^{n+2k}(u) P_j^{n+2k}(v) Q_k^{n-1}(u,v,t), \tag{8}$$

where

$$Q_k^{n-1}(u,v,t) := \big((1-u^2)(1-v^2)\big)^{k/2} P_k^{n-1}\Big(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\Big),$$

and

$$\lambda_{i,j} = \frac{\omega_n}{\omega_{n-1}} \frac{\omega_{n+2k-1}}{\omega_{n+2k}} (h_i^{n+2k} h_j^{n+2k})^{1/2}.$$

We recall the matrix-type positivity property of the matrices Y_k^n which underlies the semidefinite programming method:

Theorem 2.2. *For any finite code* $C \subset S^{n-1}$,

$$\sum_{(c,c') \in C^2} Y_k^n(e \cdot c, e \cdot c', c \cdot c') \succeq 0. \tag{9}$$

Proof. We recall the straightforward argument:

$$\sum_{(c,c') \in C^2} Z_k^n(c,c') = \Big(\sum_{c \in C} E_k^n(c)\Big)\Big(\sum_{c \in C} E_k^n(c)\Big)^t \succeq 0.$$

□

3. Semidefinite programming bound for codes in spherical caps

Let $C \subset \mathrm{Cap}(e, \phi)$ be a code of minimal angular distance θ. Define the domains Δ and Δ_0 by

$$\begin{aligned} \Delta := \{(u,v,t) : \quad & \cos\phi \le u \le v \le 1, \\ & -1 \le t \le \cos\theta, \\ & 1 + 2uvt - u^2 - v^2 - t^2 \ge 0\}, \end{aligned}$$

and

$$\Delta_0 := \{(u,u,1) : \cos\phi \le u \le 1\}.$$

The two-point distance distribution of C is the map $y : \Delta \cup \Delta_0 \to \mathbb{R}$ given by

$$y(u,v,t) = \frac{m(u,v)}{\mathrm{card}(C)} \,\mathrm{card}\{(c,c') \in C^2 : e \cdot c = u, e \cdot c' = v, c \cdot c' = t\},$$

where

$$m(u,v) = \begin{cases} 2 & \text{if } u \ne v, \\ 1 & \text{if } u = v. \end{cases}$$

We introduce the symmetric matrices $\overline{Y}_k^n(u,v,t)$ defined by

$$\overline{Y}_k^n(u,v,t) := \frac{1}{2}\Big(Y_k^n(u,v,t) + Y_k^n(v,u,t)\Big).$$

Then, (9) is equivalent to the semidefinite condition

$$\sum_{(u,v,t)\in\Delta\cup\Delta_0} y(u,v,t)\overline{Y}_k^n(u,v,t) \succeq 0.$$

The $y(u,v,t)$'s satisfy the following obvious properties:

$$\begin{aligned}
&y(u,v,t) \geq 0 \text{ for all } (u,v,t) \in \Delta\cup\Delta_0,\\
&y(u,v,t) = 0 \text{ for almost all } (u,v,t) \in \Delta\cup\Delta_0,\\
&\sum_{(u,u,1)\in\Delta_0} y(u,u,1) = 1,\\
&\sum_{(u,v,t)\in\Delta\cup\Delta_0} y(u,v,t) = \mathrm{card}(C),\\
&\sum_{(u,v,t)\in\Delta\cup\Delta_0} y(u,v,t)\overline{Y}_k^n(u,v,t) \succeq 0 \text{ for all } k \geq 0.
\end{aligned}$$

Hence a solution to the following semidefinite program is an upper bound for $A(n,\theta,\phi)$.

$$\begin{aligned}
\sup\big\{\quad & 1 + \sum_{(u,v,t)\in\Delta} y(u,v,t) :\\
& y(u,v,t) \geq 0 \ \text{ for all } (u,v,t) \in \Delta\cup\Delta_0,\\
& y(u,v,t) = 0 \ \text{ for almost all } (u,v,t) \in \Delta\cup\Delta_0,\\
& \sum_{(u,u,1)\in\Delta_0} y(u,u,1) = 1,\\
& \sum_{(u,v,t)\in\Delta\cup\Delta_0} y(u,v,t)\overline{Y}_k^n(u,v,t) \succeq 0 \ \text{ for all } k \geq 0\big\}.
\end{aligned}$$

As usual, the dual problem is easier to handle. The duality theorem says that any feasible solution of the dual problem provides an upper bound for $A(n,\theta,\phi)$. For expressing the dual problem we use the standard notation $\langle A, B\rangle = \mathrm{Trace}(AB)$.

Theorem 3.1. *Any feasible solution to the following semidefinite problem provides an upper bound on* $A(n,\theta,\phi)$.

$$\begin{aligned}
\inf\big\{\quad & 1 + M :\\
& F_k \succeq 0 \ \textit{ for all } k \geq 0,\\
& F_k = 0 \textit{ for almost all } k \geq 0,\\
& \sum_{k\geq 0}\langle F_k, \overline{Y}_k^n(u,u,1)\rangle \leq M \quad \textit{for all } (u,u,1) \in \Delta_0,\\
& \sum_{k\geq 0}\langle F_k, \overline{Y}_k^n(u,v,t)\rangle \leq -1 \quad \textit{for all } (u,v,t) \in \Delta\big\}
\end{aligned} \tag{10}$$

In order to make use of this theorem in computations we follow the same line as in [2, Section 5]. A theorem of Putinar ([14]) shows that the two last conditions

n	best lower bound known	best upper bound previously known	SDP method
3	9	9 [9]	9
4	18	18 [11]	18
5	32	35 [12]	33
6	51	64 [12]	61
7	93	110 [12]	105
8	183	186 [12]	183
9		309 [12]	297
10			472

Table 1. Bounds on $B(n)$.

can be replaced by:

$$\sum_{k\geq 0} \langle F_k, \overline{Y}_k^n(u,u,1) = M - q_0(u) - p(u)q_1(u)$$

$$\sum_{k\geq 0} \langle F_k, \overline{Y}_k^n(u,v,t)\rangle = -1 - r_0(u,v,t) - \sum_{i=1}^{4} p_i(u,v,t)r_i(u,v,t)$$

where $p(u) = -(u-\cos\phi)(u-1)$, $p_1 = p(u)$, $p_2 = p(v)$, $p_3 = -(t+1)(t-\cos\theta)$, $p_4 = -(u^2+v^2+t^2) + 2uvt + 1$, and the polynomials $q_i(u)$, $0 \leq i \leq 1$ and $r_i(u,v,t)$, $0 \leq i \leq 4$ are sums of squares of polynomials. If we set the degree of those polynomials to be less than a given value N, and fix the parameter d, we relax (10) to a finite semidefinite program.

In the most interesting case $\cos\phi = 0$ and $\cos\theta = 1/2$, corresponding to the so-called one-sided kissing number $B(n)$, we obtain the computational results gathered in Table 1. For our computations we chose the parameter $d = N = 10$.

In this table, the values in the column of the best lower bounds known correspond to the number of points in an hemisphere from the best known kissing configurations, given by the root systems D_3, D_4, D_5, E_6, E_7, E_8.

Our method gives a tight upper bound in three cases. In dimension 3 we get with parameters $d = N = 4$ the bound $B(3) \leq 9.6685$ and hence we recover the exact values $B(3) = 9$ first proved by G. Fejes Tóth ([9]). In dimension 4 we get with parameters $d = N = 6$ the bound $B(4) \leq 18.5085$ and hence we recover the exact value $B(4) = 18$ first proved by O.R. Musin ([11]). In dimension 8 we find a new tight upper bound. The famous configuration of 240 points of S^7 given by the root system E_8 is well known to be an optimal spherical code of minimal angular distance $\pi/3$, which is moreover unique up to isometry. Optimality is due to A.M. Odlyzko and N.J.A. Sloane ([13]), and independently to V.I. Levenshtein ([10]), uniqueness is due to E. Bannai and N.J.A. Sloane ([5]). From these 240 points we get a code of the hemisphere as follows: Take e among these points, then the subset of those points lying in the hemisphere with center e consists in 183 points. We obtain a bound of 183.012 with $d = N = 8$ in our computation. Hence, it proves

that it is an optimal code of the hemisphere, in other words that

$$B(8) = 183.$$

It is reasonable to believe that the configuration of 183 points of E_8 is unique up to isometry. Unfortunately we cannot prove it.

4. POLYNOMIALS

4.1. **A restatement of the SDP bound for codes in spherical caps.** We want to give an equivalent expression of the bound provided by Theorem 3.1 in terms of polynomials. Such an expression will be useful to prove analytic bounds without the use of software for solving semidefinite programs, just like in the case of the linear programming (LP) bound (see e.g. [13]). Moreover, we aim at setting bounds in the form of explicit functions of $\cos\theta$ and $\cos\phi$. We start with a lemma which shows that any polynomial in the variables u, v, t can be expressed in terms of the matrix coefficients of the $Y_k^n(u, v, t)$. In our situation it suffices to restrict to polynomials which are symmetric in u, v. We introduce the following notation:

$$R_d := \{F \in \mathbb{R}[u, v, t] : F(u, v, t) = F(v, u, t), \deg_{(u,t)}(F) \leq d, \deg_t(F) \leq d\}$$

where $\deg_{(u,t)}$ stands for the total degree in the variables u, t.

Lemma 4.1. *Let $F(u, v, t) \in R_d$. There exists a unique sequence of $d + 1$ real symmetric matrices $(F_0, F_1, \ldots, F_d)$ such that F_k is a $(d - k + 1) \times (d - k + 1)$ matrix and*

$$F(u, v, t) = \sum_{k=0}^{d} \langle F_k, \overline{Y}_k^n(u, v, t)\rangle. \tag{11}$$

We shall say that $(F_0, \ldots, F_d)$ are the matrix coefficients of F.

Proof. The polynomials $Q_k^{n-1}(u, v, t)$ have degree k in the variable t, so that $F(u, v, t)$ has a unique expression of the form $F(u, v, t) = \sum_{k=0}^{d} q_k(u, v)Q_k^{n-1}(u, v, t)$, where $q_k(u, v)$ is symmetric in u, v and has degree in u at most $d - k$. Since $P_i^{n+2k}(u)$ has degree i, q_k has a unique expression as a linear combination of the products $P_i^{n+2k}(u)P_j^{n+2k}(v)$ for $0 \leq i, j \leq d - k$. Thus, $q_k = \langle A_k, P_k\rangle$ with $(P_k)_{i,j} = P_i^{n+2k}(u)P_j^{n+2k}(v)$ and a symmetric matrix A_k. Since $Q_k^{n-1}(u, v, t)$ factor out from Y_k^n, we obtain the announced decomposition with $F_k = A_k$ put to a conjugation. □

Remark 4.2. *The matrix coefficients of a polynomial F do not really depend on the choice of d. The matrix coefficients associated to $d' \geq d$ will simply be the ones associated to d, enlarged by sufficiently many rows and columns of zeros.*

Remark 4.3. *From* [2, Proposition 3.5]*, the polynomials $P_k^n(t)$ are linear combinations of diagonal elements of the matrices $\overline{Y}_k^n$ with non negative coefficients. As a consequence, the matrix coefficients of any polynomial $P(t) \in \mathbb{R}[t]$, are diagonal matrices. If $P(t) = \sum f_k P_k^n(t)$, with all $f_k \geq 0$, then the matrix coefficients F_k of P are also non negative, and, moreover, the top left corner of F_0 equals f_0.*

The following reformulation of Theorem 3.1 is closer to the classical expression of the linear programming bound (see e.g. [6, Chapter 9, Theorem 4]).

Theorem 4.4. *Let E_0 be the matrix whose only non zero entry is the top left corner which contains 1. Let $F(u,v,t) \in R_d$. Let $(F_0,\dots,F_d)$ be symmetric matrices such that*

$$F(u,v,t) = \sum_{k=0}^{d} \langle F_k, \overline{Y}_k^n(u,v,t)\rangle.$$

Suppose the following conditions hold:

(a) *For all $0 \le k \le d$, $F_k \succeq 0$.*
(b) *$\tilde{F}_0 \succeq 0$ where $\tilde{F}_0 = F_0 - f_0 E_0$ for some $f_0 > 0$.*
(c) *$F(u,v,t) \le 0$ for all $(u,v,t) \in \Delta$.*
(d) *$F(u,u,1) \le B$ for all $u \in [\cos\phi, 1]$.*

Then, for any code in $\mathrm{Cap}(e,\phi)$ with minimal angular distance at least equal to θ,

$$\mathrm{card}(C) \le \frac{B}{f_0}.$$

Proof. It follows from Theorem 3.1 because the matrices $G_0 = F_0/f_0 - E_0$ and $G_k = F_k/f_0$ for $1 \le k \le d$ are a feasible solution to the SDP (10) with $M = B/f_0 - 1$.

We also give a direct proof, which has the additional feature to give information about the case when the obtained bound coincides with the size of a certain code. Let

$$S := \sum_{(c,c')\in C^2} F(e\cdot c, e\cdot c', c\cdot c').$$

We expand F in the $\overline{Y}_k^n$'s:

$$S = \sum_{k=0}^{d} \langle F_k, \sum_{(c,c')\in C^2} \overline{Y}_k^n(e\cdot c, e\cdot c', c\cdot c')\rangle.$$

On one hand, from property (9) together with the fact that $\langle A, B\rangle \ge 0$ for two positive semidefinite matrices A, B we obtain

$$\begin{aligned} S &\ge \langle f_0 E_0, \sum_{(c,c')\in C^2} \overline{Y}_0^n(e\cdot c, e\cdot c', c\cdot c')\rangle \\ &= f_0 \sum_{(c,c')\in C^2} \big(\overline{Y}_0^n\big)_{0,0}(e\cdot c, e\cdot c', c\cdot c') \;=\; f_0\,\mathrm{card}(C)^2. \end{aligned} \tag{12}$$

On the other hand, if we separate in S the pairs (c,c') with $c = c'$, we obtain from condition (c) and (d)

$$\begin{aligned} S &= \underbrace{\sum_{c\in C} F(e\cdot c, e\cdot c, 1)}_{B\,\mathrm{card}(C)} + \underbrace{\sum_{(c,c')\in C^2, c\ne c'} F(e\cdot c, e\cdot c', c\cdot c')}_{0,} \\ &\le \end{aligned} \tag{13}$$

because $(e\cdot c, e\cdot c, 1)\in\Delta_0$ and $(e\cdot c, e\cdot c', c\cdot c')\in\Delta$ if $c\neq c'$. Now (12) and (13) together give the inequality $\mathrm{card}(C)\leq B/f_0$. □

Remark 4.5. *Like in the LP method, the above proof gives a hint on the case of equality. Namely, if for a given code C and a given polynomial F, we have $\mathrm{card}(C)=B/f_0$, the inequality* (13) *must be an equality. So, $F(u,v,t)=0$ for all (u,v,t) running through the set of triples $(e\cdot c, e\cdot c', c\cdot c')$ with $c\neq c'$ and $(c,c')\in C^2$, and $F(u,u,1)=B$ for all $u=e\cdot c$ with $c\in C$.*

Remark 4.6. *In view of explicit computations, it is more convenient to remove the factor $\lambda_{i,j}$ from the coefficients of Y_k^n, so that polynomials with rational coefficients have rational matrix coefficients. It changes the above defined F_k to conjugates, hence does not affect the property to be positive semidefinite. These are the matrix coefficients we discuss about in the next two examples.*

Example 1. ($d=1$)
Let $F=t-\cos\theta-uv+\cos^2\phi$. The matrices of the decomposition (11) are: $F_0=\left(\begin{smallmatrix}a&0\\0&0\end{smallmatrix}\right)$ with $a=cos^2\phi-\cos\theta$ and $F_1=(1)$. Condition (a) of Theorem 4.4 is fulfilled if $a\geq 0$. Condition (b) holds for $f_0=a$. Obviously (c) holds if $\cos\phi\geq 0$ and, since $F(u,u,1)=1-\cos\theta-u^2+\cos^2\phi$, $B=1-\cos\theta$. We obtain:

$$\text{If } \cos\phi\geq 0 \text{ and } \cos\theta<\cos^2\phi, \mathrm{card}(C)\leq\frac{1-\cos\theta}{\cos^2\phi-\cos\theta}.$$

It is worth to point out that the polynomial $G=(t-\cos\theta)-\cos\phi(u+v-2\cos\phi)$ leads to exactly the same bound. This time $F_0=\left(\begin{smallmatrix}c+a&-c\\-c&1\end{smallmatrix}\right)$ with $c=\cos\phi$, $f_0=a$, $B=1-\cos\theta$.

The above bound is already proved in [3, Th 5.2]. Indeed with the notations of [3], let $w(\theta,\phi)$ be defined by $\cos w(\theta,\phi)=(\cos\theta-\cos^2\phi)/(\sin^2\phi)$; we have just proved that the Rankin bound for $A(n-1,w(\theta,\phi))$ applies to $\mathrm{card}(C)$. More generally, we recover the LP bounds for $A(n-1,w(\theta,\phi))$ by the following : let $f(x)$ be a polynomial of degree d that realizes the best LP bound on S^{n-2} for the angle $w(\theta,\phi)$. We can take polynomial approximations of the function

$$F(u,v,t)=\big((1-u^2)(1-v^2)\big)^{d/2}f\Big(\frac{t-uv}{\big((1-u^2)(1-v^2)\big)^{1/2}}\Big)$$

obtained by the truncated developments of the powers $\big((1-u^2)(1-v^2)\big)^{k/2}$ around $u=\cos\phi$, $v=\cos\phi$.

Example 2. ($d=2$)
Let $F=(t+1)(t-\cos\theta)+a\big((u-\cos\phi)(u-1)+(v-\cos\phi)(v-1)\big)$. The parameter $a>0$ will be chosen later to optimize the bound. Condition (c) is obviously fulfilled and condition (d) holds with $B=2(1-\cos\theta)$. The polynomial $(t+1)(t-\cos\theta)$ has non negative coefficients on the P_k^n under the condition $\cos\theta\leq 1/n$. More precisely its constant coefficient equals$\big(\frac{1}{n}-\cos\theta\big)$ while the two others are positive. So we only need to make sure that F_0 is positive

semidefinite. We find that:

$$F_0 = \begin{pmatrix} 2a(\frac{1}{n}+\cos\phi)+\frac{1}{n}-\cos\theta & -a(1+\cos\phi) & a(1-\frac{1}{n}) \\ & (1-\cos\theta) & 0 \\ & & (1-\frac{1}{n}) \end{pmatrix}.$$

Let

$$f_0(a) := -a^2\Big(\frac{(1+\cos\phi)^2}{1-\cos\theta}+(1-\frac{1}{n})\Big)+2a\big(\frac{1}{n}+\cos\phi\big)+\frac{1}{n}-\cos\theta.$$

Then, an easy calculation shows that $F_0 \succeq 0$ iff $f_0(a) \geq 0$, and that $\tilde{F}_0 = F_0 - f_0 E_0 \succeq 0$ iff $f_0 \leq f_0(a)$. The best bound is obtained when $f_0 = f_0(a)$ attains the maximal value

$$(f_0)_{\max} = \big(\frac{1}{n}-\cos\theta\big)+\frac{\big(\frac{1}{n}+\cos\phi\big)^2}{\Big(\frac{(1+\cos\phi)^2}{1-\cos\theta}+1-\frac{1}{n}\Big)}.$$

The final bound equals

$$\frac{2(1-\cos\theta)}{(f_0)_{\max}}.$$

and is valid as long as $(f_0)_{\max} > 0$ and $\big(\frac{1}{n}+\cos\phi\big) > 0$ (this last condition holds because $(f_0)_{\max}$ must be attained at a positive a).

It is worth noticing that the resulting bound is smaller than the LP bound for the entire sphere, obtained from the polynomial $(t+1)(t-\cos\theta)$, which is

$$\frac{2(1-\cos\theta)}{\big(\frac{1}{n}-\cos\theta\big)}.$$

For example, when $\cos\phi = \cos\theta = 0$, we recover the exact bound of $2n-1$.

Remark 4.7. *We can interpret the two examples treated above as follows: in both cases, we have perturbed the optimal polynomial for the LP method, respectively $t-\cos\theta$ and $(t+1)(t-\cos\theta)$, with a polynomial in the variables u, v, which affects the first matrix coefficient F_0 and increases the value of the constant coefficient f_0. However it seems difficult to generalize this approach.*

4.2. **Orthogonality relations in $\mathbb{R}[u,v,t]$.** In this subsection, we calculate the scalar product induced on $\mathbb{R}[u,v,t]$ by the natural scalar product on $\mathrm{Pol}(S^{n-1})$ defined by (1).

Proposition 4.8. *Let $P \in \mathbb{R}[u,v,t]$. We have*

$$\frac{1}{\omega_n^2}\int_{(S^{n-1})^2} P(e\cdot x, e\cdot y, x\cdot y)d\omega_n(x)d\omega_n(y) = \int_\Omega P(u,v,t)k(u,v,t)dudvdt$$

where

$$k(u,v,t) = \frac{\omega_{n-1}\omega_{n-2}}{\omega_n^2}(1-u^2-v^2-t^2+2uvt)^{\frac{n-4}{2}}$$

and

$$\Omega = \{(u,v,t): \quad -1 \leq u,v,t \leq 1, \\ 1+2uvt-u^2-v^2-t^2 \geq 0\}.$$

Proof. If $u = e \cdot x$ and $\zeta \in S^{n-2}$ is defined by $x = ue + (1-u^2)^{\frac{1}{2}}\zeta$, we have

$$d\omega_n(x) = (1-u^2)^{\frac{n-3}{2}} du d\omega_{n-1}(\zeta).$$

With $y = ve + (1-v^2)^{\frac{1}{2}}\xi$, we have

$$\begin{aligned}
&\int_{S^{n-1}} P(e\cdot x, e\cdot y, x\cdot y) d\omega_n(x) \\
&= \int_{S^{n-2}} \int_{-1}^{1} P(u, v, uv + \big((1-u^2)(1-v^2)\big)^{\frac{1}{2}} \zeta\cdot\xi)(1-u^2)^{\frac{n-3}{2}} du d\omega_{n-1}(\zeta) \\
&= \omega_{n-2} \int_{-1}^{1}\int_{-1}^{1} P(u,v,t)(1-\alpha^2)^{\frac{n-4}{2}}(1-u^2)^{\frac{n-3}{2}} d\alpha du,
\end{aligned}$$

where $t := uv + \big((1-u^2)(1-v^2)\big)^{\frac{1}{2}}\alpha$. With this change of variables having Jacobian $\big((1-u^2)(1-v^2)\big)^{\frac{1}{2}}$ we obtain

$$\begin{aligned}
&\int_{S^{n-1}} P(e\cdot x, e\cdot y, x\cdot y) d\omega_n(x) \\
= \quad & \omega_{n-2} \int_{\Omega(v)} P(u,v,t) k(u,v,t) (1-v^2)^{-\frac{n-3}{2}} du dt,
\end{aligned}$$

where

$$\begin{aligned}
\Omega(v) = \{(u,t): \quad & -1 \le u, t \le 1, \\
& 1 + 2uvt - u^2 - v^2 - t^2 \ge 0\}.
\end{aligned}$$

Hence

$$\begin{aligned}
&\int_{(S^{n-1})^2} P(e\cdot x, e\cdot y, x\cdot y) d\omega_n(x) d\omega_n(y) \\
= \quad & \omega_{n-1}\omega_{n-2} \int_{\Omega} P(u,v,t) k(u,v,t) du dv dt
\end{aligned}$$

□

Definition 4.9. *With the notations of Proposition 4.8, the following expression defines a scalar product on* $\mathbb{R}[u,v,t]$*:*

$$[F,G] = \int_{\Omega} F(u,v,t) G(u,v,t) k(u,v,t) du dv dt. \tag{14}$$

From Proposition 4.8, it is the scalar product induced by the standard scalar product (1) *on* $\mathrm{Pol}(S^{n-1})$.

The subspaces $H^{n-1}_{k,i}$ are pairwise orthogonal. Consequently the matrix coefficients of $Y^n_k(u,v,t)$ are pairwise orthogonal for $[\cdot,\cdot]$. Their norm is also easy to compute, and we obtain the following useful formulas:

Proposition 4.10.

(a) *For all k and all i, j we have*

$$[\big(Y_k^n\big)_{i,j}, \big(Y_{k'}^n\big)_{i',j'}] = \frac{\delta_{(i,j,k),(i',j',k')}}{h_k^{n-1}}. \tag{15}$$

(b) *For all symmetric matrices A, B,*

$$[\langle A, \overline{Y}_k^n\rangle, \langle B, \overline{Y}_{k'}^n\rangle] = \frac{\delta_{k,k'}\langle A, B\rangle}{h_k^{n-1}}. \tag{16}$$

Proof. Obvious. □

4.3. **A characterization of the positive definite polynomials.** In view of Theorem 4.4, we are concerned with the construction of polynomials satisfying condition (a). We prove in this subsection that this property is stable under multiplication. We start with a characterization of the set of polynomials satisfying (a).

Definition 4.11. *We say that the polynomial $F(u, v, t) \in \mathbb{R}[u, v, t]$ is* positive definite *if, for all finite $C \subset S^{n-1}$, for all function $\alpha : C \to \mathbb{R}$,*

$$\sum_{(c,c')\in C^2} \alpha(c)\alpha(c')F(e \cdot c, e \cdot c', c \cdot c') \geq 0. \tag{17}$$

The polynomials $F(u, v, t)$ of the form

$$F(u, v, t) = \sum_{k=0}^{d} \langle F_k, \overline{Y}_k^n(u, v, t)\rangle$$

with $F_k \succeq$ for all $0 \leq k \leq d$ are positive definite in the above sense. Note that it is slightly stronger than the positivity property of the matrices Y_k^n proved in Theorem 2.2; the argument is essentially the same, it follows from the equality

$$\sum_{(c,c')\in C^2} \alpha(c)\alpha(c')Z_k^n(c, c') = \Big(\sum_{c\in C} \alpha(c)E_k^n(c)\Big)\Big(\sum_{c\in C} \alpha(c)E_k^n(c)\Big)^t \succeq 0.$$

Our goal now is to prove that all positive definite polynomials in R_d arise in this way.

Proposition 4.12. *Let $F(u, v, t) \in R_d$. Let $(F_0, \ldots, F_d)$ be symmetric matrices such that*

$$F(u, v, t) = \sum_{k=0}^{d} \langle F_k, \overline{Y}_k^n(u, v, t)\rangle.$$

If F is positive definite, then $F_k \succeq 0$ for all $0 \leq k \leq d$.

Proof. Let $\tilde{F}(x, y) = F(e \cdot x, e \cdot y, x \cdot y)$. By compactness, F is positive definite if and only if for all $f \in \mathrm{Pol}(S^{n-1})$,

$$\int_{\left(S^{n-1}\right)^2} f(x)f(y)\tilde{F}(x, y)d\omega_n(x)d\omega_n(y) \geq 0.$$

As a consequence, if $Q(x)$ is any matrix,

$$\int_{\left(S^{n-1}\right)^2} \langle Q(x), Q(y)\rangle \tilde{F}(x,y) d\omega_n(x) d\omega_n(y) \geq 0.$$

Let us fix $k \in \{0, \ldots, d\}$ and let A be a $(d-k+1)\times(d-k+1)$ symmetric, positive semidefinite matrix. Because of expression (6) of Z_k^n, we can write $AZ_k^n(x,y)$ in the form $Q(x)Q(y)^t$. Hence,

$$\int_{\left(S^{n-1}\right)^2} \langle A, Z_k^n(x,y)^t\rangle \tilde{F}(x,y) d\omega_n(x) d\omega_n(y) \geq 0.$$

In terms of the scalar product $[\cdot,\cdot]$ it is equivalent to

$$[\langle A, \overline{Y}_k^n\rangle, F] \geq 0.$$

Since from (16) $[\langle A, \overline{Y}_k^n\rangle, F] = \left(h_k^{n-1}\right)^{-1}\langle A, F_k\rangle$, we have proved that $\langle A, F_k\rangle \geq 0$ for all $A \succeq 0$, and so $F_k \succeq 0$. □

Corollary 4.13. *Let $F, G \in R_d$. If F and G are positive definite, then the product FG is also positive definite.*

Proof. From Proposition 4.12 it suffices to consider the case $F = \langle A, \overline{Y}_k^n\rangle$, $G = \langle B, \overline{Y}_l^n\rangle$, where A and B are positive semidefinite matrices. Like we did before, we write $AZ_k^n(x,y) = Q(x)Q(y)^t$ and $BZ_l^n(x,y) = T(x)T(y)^t$. With the formula

$$\langle Q(x), Q(y)\rangle\langle T(x), T(y)\rangle = \langle Q(x)\otimes T(x), Q(y)\otimes T(y)\rangle$$

we have

$$\begin{aligned}
\sum_{(c,c')\in C^2} &\alpha(c)\alpha(c')\tilde{F}(c,c')\tilde{G}(c,c') \\
&= \sum_{(c,c')\in C^2} \alpha(c)\alpha(c')\langle Q(c), Q(c')\rangle\langle T(c), T(c')\rangle \\
&= \sum_{(c,c')\in C^2} \langle \alpha(c)Q(c)\otimes T(c), \alpha(c')Q(c')\otimes T(c'))\rangle \\
&= \langle U_C, U_C\rangle \geq 0
\end{aligned}$$

with

$$U_C = \sum_{c\in C} \alpha(c) Q(c)\otimes T(c).$$

□

4.4. **The reproducing kernels.** We introduce the following notation: we let $X := (u,v,t)$ be as before the variables of the polynomial ring $\mathbb{R}[u,v,t]$, and we let $X' := (u',v',t') \in \mathbb{R}^3$. Moreover, we define:

$$K_d(X,X') := \sum_{k=0}^{n} h_k^{n-1}\langle \overline{Y}_k^n(X), \overline{Y}_k^n(X')\rangle. \tag{18}$$

Proposition 4.14. *$K_d(X, X')$ is the* reproducing kernel *of the space R_d, i.e., for all $F \in R_d$,*

$$[K_d(X, X'), F] = F(X'). \tag{19}$$

Proof. It is straightforward from (16). □

REFERENCES

[1] C. Bachoc, *Linear programming bounds for codes in Grassmannian spaces*, IEEE Trans. Inf. Th. **52-5** (2006), 2111–2125.

[2] C. Bachoc, F. Vallentin, *New upper bounds for kissing numbers from semidefinite programming*, preprint, October 2006, arXiv:math.MG/0608426.

[3] A. Barg, O.R. Musin, *Codes in spherical caps*, preprint, June 2006, arXiv:math.MG/0606734.

[4] B. Borchers, *CSDP, A C library for semidefinite programming*, Optimization Methods and Software **11** (1999) 613–623.

[5] E. Bannai and N.J.A. Sloane, *Uniqueness of certain spherical codes*, Canad J. Math. **33** (1981), 437–449.

[6] J.H. Conway and N.J.A. Sloane, *Sphere Packings, Lattices and Groups*, Springer-Verlag, 1988.

[7] P. Delsarte, *An algebraic approach to the association schemes of coding theory*, Philips Res. Rep. Suppl. (1973), vi+97.

[8] P. Delsarte, J.M. Goethals and J.J. Seidel, *Spherical codes and designs*, Geom. Dedicata **6** (1977), 363–388.

[9] G. Fejes Tóth, *Ten-neighbor packing of equal balls*, Periodica Math. Hungar. **12** (1981), 125–127.

[10] V.I. Levenshtein, *On bounds for packing in n-dimensional Euclidean space*, Soviet Math. Dokl. **20** (1979), 417–421.

[11] O.R. Musin, *The one-sided kissing number in four dimensions*, preprint, August 2006, arXiv:math.MG/0511071.

[12] O.R. Musin, *Bounds for codes by semidefinite programming*, preprint, September 2006, arXiv:math.MG/0609155.

[13] A.M. Odlyzko and N.J.A. Sloane, *New bounds on the number of unit spheres that can touch a unit sphere in n dimensions*, J. Combin. Theory Ser. A **26** (1979), 210–214.

[14] M. Putinar, *Positive polynomials on compact semi-algebraic sets*, Ind. Univ. Math. J. **42** (1993), 969–984.

C. BACHOC, LABORATOIRE A2X, UNIVERSITÉ BORDEAUX I, 351, COURS DE LA LIBÉRATION, 33405 TALENCE FRANCE

E-mail address: bachoc@math.u-bordeaux1.fr

F. VALLENTIN, CENTRUM VOOR WISKUNDE EN INFORMATICA (CWI), KRUISLAAN 413, 1098 SJ AMSTERDAM, THE NETHERLANDS

E-mail address: f.vallentin@cwi.nl