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

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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 $\phi$ is the set

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

We consider the problem of finding upper bounds of the size of a code $C$ contained in $\text{Cap}(e, \phi)$ with minimal angular distance $\theta$. 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:

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

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

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 $S^{n-1}$ ([8], [9], [11] and the survey [7, 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.

In this paper, we 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 [14].

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

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

where “$\succeq 0$” stands for “is positive semidefinite”.

We want to point out that one can consider other metric spaces $X$ with isometry
group in this framework. 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 $1 \times 1$. 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 numerical results. Section 4
translates the dual SDP into a statement on three variable polynomials, and contains
more material on orthogonality relations, positivity property and other classical
material which might be of independent interest.

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 $O(\mathbb{R}^n)$ acts homogeneously on the
unit sphere

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

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

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

(1)
where $\omega_n$ 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 $O(\mathbb{R}^n)$

\[ \text{Pol}_{\leq d}(S^{n-1}) = H^0_{n} \perp H^1_{n} \perp \ldots \perp H^d_{n}, \]

where $H^i_{n}$ is isomorphic to the $O(\mathbb{R}^n)$-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 $h^i_{n,k} := \dim(\text{Harm}_k^n)$.

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

\[ \text{Pol}_{\leq d}(S^{n-1}) = \mathcal{I}_0 \perp \mathcal{I}_1 \perp \ldots \perp \mathcal{I}_d, \]

where

\[ \mathcal{I}_k \simeq (d-k+1) \text{Harm}_{k,n}^{n-1}, \quad k = 0, \ldots, d. \]

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

\[ \mathcal{I}_k = H^i_{k,k} \perp \ldots \perp H^{i-1}_{k,k} \]

where, for $i \geq k$, $H^i_{k,k}$ is the unique subspace of $H^i_n$ isomorphic to Harm$_k^n$.

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

\[ Z^i_{k,n} : S^{n-1} \times S^{n-1} \to \mathbb{R}^{(d-k+1) \times (d-k+1)} \]

which is uniquely defined up to congruence. Let $(e^k_{s,1}, e^k_{s,2}, \ldots, e^k_{s,h_{n-1}})$ be an orthonormal basis of $H^i_{k,k+s}$. We assume that the basis $(e^k_{s,i})_{1 \leq i \leq h_{n-1}}$ is the image of $(e^k_{0,1}, e^k_{0,2}, \ldots, e^k_{0,h_{n-1}})$ by some $H$-isomorphism $\phi_s : H^i_{k,k} \to H^i_{k,k+s}$. Then, define

\[ E^i_{k,n}(x) := \frac{1}{h_{n-1}^i} \begin{pmatrix} e^k_{0,1}(x) & \cdots & e^k_{0,h_{n-1}}(x) \\ \vdots & & \vdots \\ e^k_{d-k,1}(x) & \cdots & e^k_{d-k,h_{n-1}}(x) \end{pmatrix}, \]

and

\[ Z^i_{k,n}(x, y) := E^i_{k,n}(x)E^i_{k,n}(y)^t \in \mathbb{R}^{(d-k+1) \times (d-k+1)}. \]

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

\[ Z^i_{k,n}(x, y) = Y^i_{k,n}(e \cdot x, e \cdot y, x \cdot y). \]

We denote the zonal polynomials of the unit sphere $S^{n-1}$ by $P^i_{k,n}$. In other words, if $n \geq 3$, then $P^i_{k,n}(t)$ is the Gegenbauer polynomial of degree $k$ with parameter $n/2 - 1$, normalized by the condition $P^0_{k,n}(1) = 1$. If $n = 2$, then $P^i_{k,n}(t)$ is the Chebyshev polynomial of the first kind with degree $k$. We give in [2, Theorem 3.2] the following explicit expressions for the coefficients of the matrices $Y^i_{k,n}$.
Theorem 2.1. We have, for all $0 \leq i, j \leq d - k$,
\begin{equation}
(Y^n_k)_{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),
\end{equation}
where
\[ Q_k^{n-1}(u, v, t) := \left( (1 - u^2)(1 - v^2) \right)^{k/2} P_k^{n-1}\left( \frac{t - uv}{\sqrt{(1 - u^2)(1 - v^2)}} \right), \]
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 $Y^n_k$ which underlies the semidefinite programming method:

Theorem 2.2. For any finite code $C \subset S^{n-1}$,
\begin{equation}
\sum_{(c, c') \in C^2} Y^n_k(e \cdot c, e \cdot c', c \cdot c') \succeq 0.
\end{equation}

Proof. We recall the straightforward argument:
\[ \sum_{(c, c') \in C^2} Z^n_k(c, c') = \left( \sum_{c \in C} E^n_k(c) \right) \left( \sum_{c \in C} E^n_k(c) \right)^t \succeq 0. \]

\[ \square \]

3. SEMIDEFINITE PROGRAMMING BOUND FOR CODES IN SPHERICAL CAPS

Let $C \subset \text{Cap}(e, \phi)$ be a code of minimal angular distance $\theta$. Define the domains $\Delta$ and $\Delta_0$ by
\[ \Delta := \{(u, v, t) : \cos \phi \leq u \leq v \leq 1, \]
\[ -1 \leq t \leq \cos \theta, \]
\[ 1 + 2uvt - u^2 - v^2 - t^2 \geq 0 \}, \]
and
\[ \Delta_0 := \{(u, u, 1) : \cos \phi \leq u \leq 1 \}. \]
The two-point distance distribution of $C$ is the map $y : \Delta \cup \Delta_0 \rightarrow \mathbb{R}$ given by
\[ y(u, v, t) = \frac{m(u, v)}{\text{card}(C)} \text{card}\{(c, c') \in C^2 : e \cdot c = u, e \cdot c' = v, c \cdot c' = t\}, \]
where
\[ m(u, v) = \begin{cases} 
2 & \text{if } u \neq v, \\
1 & \text{if } u = v. 
\end{cases} \]
We introduce the symmetric matrices $\overline{Y}^n_k(u, v, t)$ defined by
\[ \overline{Y}^n_k(u, v, t) := \frac{1}{2} \left( Y^n_k(u, v, t) + Y^n_k(v, u, t) \right). \]
Then, (9) is equivalent to the semidefinite condition
\[ \sum_{(u,v,t) \in \Delta \cup \Delta_0} y(u,v,t) Y^n_k(u,v,t) \succeq 0. \]
For any \( d \geq 0 \), the \( y(u,v,t) \)'s satisfy the following obvious properties:
- \( y(u,v,t) \geq 0 \) for all \( (u,v,t) \in \Delta \cup \Delta_0 \),
- \( y(u,v,t) = 0 \) for all but finitely many \( (u,v,t) \in \Delta \cup \Delta_0 \),
- \( \sum_{(u,u,1) \in \Delta_0} y(u,u,1) = 1 \),
- \( \sum_{(u,v,t) \in \Delta \cup \Delta_0} y(u,v,t) = \text{card}(C) \),
- \( \sum_{(u,v,t) \in \Delta \cup \Delta_0} y(u,v,t) Y^n_k(u,v,t) \succeq 0 \) for \( k = 0, \ldots, d \).

Hence a solution to the following semidefinite program is an upper bound for \( A(n, \theta, \phi) \).
\[
\text{max} \left\{ 1 + \sum_{(u,v,t) \in \Delta} y(u,v,t) : \begin{array}{l}
  y(u,v,t) \geq 0 \text{ for all } (u,v,t) \in \Delta \cup \Delta_0, \\
  y(u,v,t) = 0 \text{ for all but finitely many } (u,v,t) \in \Delta \cup \Delta_0, \\
  \sum_{(u,u,1) \in \Delta_0} y(u,u,1) = 1, \\
  \sum_{(u,v,t) \in \Delta \cup \Delta_0} y(u,v,t) Y^n_k(u,v,t) \succeq 0 \text{ for } k = 0, \ldots, d.
\end{array} \right\}
\]

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 \( \langle A, B \rangle = \text{Trace}(AB^t) \).

**Theorem 3.1.** Any feasible solution to the following semidefinite problem provides an upper bound on \( A(n, \theta, \phi) \).
\[
\text{min} \left\{ 1 + M : \begin{array}{l}
  F_k \succeq 0 \text{ for all } k = 0, \ldots, d, \\
  \sum_{k=0}^d \langle F_k, Y^n_k(u,u,1) \rangle \leq M \text{ for all } (u,u,1) \in \Delta_0, \\
  \sum_{k=0}^d \langle F_k, Y^n_k(u,v,t) \rangle \leq -1 \text{ for all } (u,v,t) \in \Delta.
\end{array} \right\}
\]

In order to make use of this theorem in computations we follow the same line as in [2, Section 5]. A theorem of M. Putinar ([17]) shows that the two last conditions
can be replaced by:
\[
\sum_{k=0}^{d} \langle F_k, Y_k^n(u, u, 1) \rangle = M - q_0(u) - p(u)q_1(u) - \sum_{i=1}^{4} p_i(u, v, t)r_i(u, v, t)
\]
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 given
in Table 1. For our computations we chose the parameter \(d = N = 10\).

The 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 (10). 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 (14). 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 (16), and independently to V.I. Levenshtein (13),
uniqueness is due to E. Bannai and N.J.A. Sloane (6). 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

\[
\begin{array}{|c|c|c|c|}
\hline
n & \text{best lower bound known} & \text{best upper bound previously known} & \text{SDP method} \\
\hline
3 & 9 & 9 \{10\} & 9 \\
4 & 18 & 18 \{14\} & 18 \\
5 & 32 & 35 \{15\} & 33 \\
6 & 51 & 64 \{15\} & 61 \\
7 & 93 & 110 \{15\} & 105 \\
8 & 183 & 186 \{15\} & 183 \\
9 & & 309 \{15\} & 297 \\
10 & & & 472 \\
\hline
\end{array}
\]
that it is a maximal 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 were not able to prove it.

4. POLYNOMIALS

4.1. Polynomial 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. [16]). 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 \( Y_n^k(u, v, t) \). 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
\[
F(u, v, t) = \sum_{k=0}^{d} \langle F_k, Y_k^n(u, v, t) \rangle.
\]

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

**Proof.** The polynomials \( Q_{n-1}^k(u, v, t) \) have degree \( k \) in the variable \( t \). Hence, \( F(u, v, t) \) has a unique expression of the form
\[
F(u, v, t) = \sum_{k=0}^{d} q_k(u, v) Q_{n-1}^k(u, v, t),
\]
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 \( \lambda_{i, j} P_i^{n+2k}(u) P_j^{n+2k}(v) \) for \( 0 \leq i, j \leq d - k \). Thus, there is a symmetric \((d - k + 1) \times (d - k + 1)\) matrix \( F_k \) so that
\[
q_k(u, v) = \sum_{0 \leq i, j \leq d - k} (F_k)_{i, j} \lambda_{i, j} P_i^{n+2k}(u) P_j^{n+2k}(v).
\]
Since one can write \( Y_k(u, v, t) \) as \( Q_{k-1}^{n-1}(u, v, t)(\lambda_{i, j} P_i^{n+2k}(u) P_j^{n+2k}(v)) \) we obtain decomposition (11). \( \square \)

**Remark 4.2.** The matrix coefficients of a polynomial \( F \) do only trivially 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 $P^n_k(t)$ are linear combinations of diagonal elements of the matrices $Y^n_k$ with non negative coefficients. As a consequence, the matrix coefficients of any polynomial $P(t) \in \mathbb{R}[t]$, are diagonal matrices. If $P(t) = \sum f_k P^n_k(t)$, 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 an analogue of the classical expression of the linear programming bound (see e.g. [7, 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. For a polynomial $F(u, v, t) \in \mathbb{R}^d$ let $(F_0, \ldots, F_d)$ be symmetric matrices such that

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

Suppose the following conditions hold:

(a) $F_k \succeq 0$ for all $0 \leq k \leq d$.
(b) $F_0 - f_0 E_0 \succeq 0$ for some $f_0 > 0$.
(c) $F(u, v, t) \leq 0$ for all $(u, v, t) \in \Delta$.
(d) $F(u, u, 1) \leq B$ for all $u \in [\cos \phi, 1]$.

Then, for any code $C$ in $\text{Cap}(e, \phi)$ with minimal angular distance at least $\theta$, $\text{card}(C) \leq \frac{B}{f_0}$.

Proof. The statement follows immediately from Theorem 3.1 because the matrices $G_0 = F_0/f_0 - E_0$ and $G_k = F_k/f_0$ for $1 \leq k \leq d$ 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 $Y^n_k$’s:

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

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

$$S \geq \langle f_0 E_0, \sum_{(c, c') \in C^2} Y^n_0(e \cdot c, e \cdot c', c \cdot c') \rangle$$

$$= f_0 \sum_{(c, c') \in C^2} \langle Y^n_0(e \cdot c, e \cdot c', c \cdot c') \rangle = f_0 \text{card}(C)^2.$$
On the other hand, if we split the sum $S$ into diagonal terms belonging to pairs $(c, c)$ and into cross terms belonging to pairs $(c, c')$ with $c \neq c'$, we obtain from condition (c) and (d)

$$S = \sum_{c \in \mathbb{C}} F(e \cdot c, e \cdot c, 1) + \sum_{(c, c') \in \mathbb{C}^2, c \neq c'} F(e \cdot c, e \cdot c', c \cdot c')$$

(13)

$$\leq B \text{card}(C) + 0,$$

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 \text{card}(C) \leq B/f_0. \quad \square

**Remark 4.5.** Like in the LP method, the above proof gives additional information on the case of equality. Namely, if for a given code $C$ and a given polynomial $F$, we have \text{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 $(c, c') \in \mathbb{C}^2$, 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 $\lambda_{ij}$ from the coefficients of $Y_k$, so that polynomials with rational coefficients have rational matrix coefficients. It changes the above defined $F_k$ to congruence, 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.** ($d = 1$)

We consider the polynomial $F = t - \cos \theta - uv + \cos^2 \phi$. The matrices of the decomposition (11) are: $F_0 = \left( \begin{array}{cc} a & 0 \\ 0 & 0 \end{array} \right)$ 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 $B = 1 - \cos \theta$ because $F(u, u, 1) = 1 - \cos \theta - u^2 + \cos^2 \phi$. We obtain:

If $\cos \phi \geq 0$ and $\cos \theta < \cos^2 \phi$, then $A(n, \theta, \phi) \leq \frac{1 - \cos \theta}{\cos^2 \phi - \cos \theta}$.

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 $F_0 = \left( \begin{array}{cc} c^2 & -c \\ -c & 1 \end{array} \right)$ with $c = \cos \phi$, $f_0 = a$, $B = 1 - \cos \theta$.

The above bound is already proved in [3, Theorem 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 $A(n - 1, w(\theta, \phi))$ is also a bound for $A(n, \theta, \phi)$. More generally, LP bounds for $A(n - 1, w(\theta, \phi))$ are also bounds for $A(n, \theta, \phi)$: Let $f(x)$ be a polynomial of degree $d$ that realizes an LP bound on $S^{n-2}$ for the angle $w(\theta, \phi)$. We can take polynomial approximations of the function

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

obtained by the truncated developments of the powers $((1 - u^2)(1 - v^2))^{k/2}$ around $u = \cos \phi, v = \cos \phi$. 
Example 2. \((d = 2)\)
We consider the polynomial \(F = (t + 1)(t - \cos \theta) + a((u - \cos \phi)(u - 1) + (v - \cos \phi)(v - 1)).\) 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 if we expand it in terms of the basis \(P_k(t)\) whenever \(\cos \theta \leq 1/n.\) More precisely its constant coefficient equals \((1/n - \cos \theta)\) while the two others are positive. So we only need to make sure that \(F_0\) is positive semidefinite. We find that:

\[
F_0 = \begin{pmatrix}
2a(1/n + \cos \phi) + 1/n - \cos \theta & -a(1 + \cos \phi) & a(1 - 1/n) \\
-a(1 + \cos \phi) & (1 - \cos \theta) & 0 \\
a(1 - 1/n) & 0 & (1 - 1/n)
\end{pmatrix}
\]

Let

\[
f_0(a) := -a^2\left(\frac{(1 + \cos \phi)^2}{1 - \cos \theta} + (1 - \frac{1}{n})\right) + 2a\left(\frac{1}{n} + \cos \phi\right) + \frac{1}{n} - \cos \theta.
\]

Then, an easy calculation shows that \(F_0 \geq 0\) iff \(f_0(a) \geq 0,\) and that \(F_0 - f_0E_0 \geq 0\) iff \(f_0 \leq f_0(a).\) The best bound is obtained when \(f_0 = f_0(a)\) attains the maximal value

\[
(f_0)_{\max} = \left(\frac{1}{n} - \cos \theta\right) + \frac{(1/n + \cos \phi)^2}{(1 + \cos \phi)^2 + 1 - \frac{1}{n}}.
\]

The final bound equals

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

and is valid as long as \((f_0)_{\max} > 0\) and \((\frac{1}{n} + \cos \phi) > 0\) (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 \(A(n, \theta),\) obtained from the polynomial \((t + 1)(t - \cos \theta),\) which is

\[
\frac{2(1 - \cos \theta)}{(\frac{1}{n} - \cos \theta)}
\]

For example, when \(\cos \phi = \cos \theta = 0,\) we recover the exact bound of \(2n - 1\) (see also \([12]\)).

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 \((t + 1)(t - \cos \theta),\) by 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 this subsection, we calculate the scalar product induced on \(\mathbb{R}[u, v, t]\) by the natural scalar product on \(\text{Pol}(S^{n-1})\) defined by \([1].\)

Proposition 4.8. Let \(P \in \mathbb{R}[u, v, t]\) be a polynomial. We have

\[
\frac{1}{\omega_n^2} \int_{S^{n-1}} P(e \cdot x, e \cdot y, x \cdot y)d\omega_n(x)d\omega_n(y) = \int_{\Omega} P(u, v, t)k(u, v, t)dudvdt
\]
where
\[ k(u, v, t) = \frac{\omega_{n-1} \omega_{n-2}}{\omega_n^2} (1 - u^2 - v^2 - t^2 + 2uvt)^{\frac{n-2}{2}} \]
and
\[ \Omega = \{(u, v, t) : -1 \leq u, v, t \leq 1, 1 + 2uvt - u^2 - v^2 - t^2 \geq 0 \}. \]

**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
\[ d\omega_n(x) = (1 - u^2)^{\frac{n-3}{2}} dud\omega_n - (1 - u^2)^{\frac{n-3}{2}} (\zeta \cdot \xi) \]
with \( y = ve + (1 - v^2)^{\frac{1}{2}} \xi \), we have
\[ \int_{S^{n-1}} P(e \cdot x, e \cdot y, x \cdot y) d\omega_n(x) \]
\[ = \int_{S^{n-2}} \int_{-1}^{1} P(u, v, uv + ((1 - u^2)(1 - v^2))^{\frac{1}{2}} \zeta \cdot \xi)(1 - u^2)^{\frac{n-3}{2}} dud\omega_n - (1 - u^2)^{\frac{n-3}{2}} d\omega_n, \]
where \( t := uv + ((1 - u^2)(1 - v^2))^{\frac{1}{2}} \alpha \). With this change of variables having Jacobian \( ((1 - u^2)(1 - v^2))^{\frac{1}{2}} \) we obtain
\[ \int_{S^{n-1}} P(e \cdot x, e \cdot y, x \cdot y) d\omega_n(x) \]
\[ = \omega_{n-2} \int_{\Omega(v)} P(u, v, t)(1 - u^2 - v^2 - t^2 + 2uvt)^{\frac{n-4}{2}} (1 - u^2)^{-\frac{n-4}{2}} dudt, \]
where
\[ \Omega(v) = \{(u, t) : -1 \leq u, t \leq 1, 1 + 2uvt - u^2 - v^2 - t^2 \geq 0 \}. \]

Hence
\[ \int_{(S^{n-1})^2} P(e \cdot x, e \cdot y, x \cdot y) d\omega_n(x) d\omega_n(y) \]
\[ = \omega_{n-1} \omega_{n-2} \int_{\Omega} P(u, v, t)(1 - u^2 - v^2 - t^2 + 2uvt)^{\frac{n-4}{2}} dudvdt \]

**Definition 4.9.** With the notations of Proposition 4.8, the following expression defines a scalar product on \( \mathbb{R}[u, v, t] \):
\[ [F, G] = \int_{\Omega} F(u, v, t)G(u, v, t)k(u, v, t)dudvdt. \]

From Proposition 4.8 it is the scalar product induced by the standard scalar product (1) on \( \text{Pol}(S^{n-1}) \).
The subspaces $H^i_{k,j}$ 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 $k, k'$ and all $i, j, i', j'$ we have

\[(Y^n_k)_{i,j}, (Y^n_{k'})_{i',j'}] = \frac{\delta_{i,j,k} \delta_{i',j',k'}}{h_k^{n-1}}.\]  \hspace{1cm} (15)

(b) For all symmetric matrices $A, B$ and all $k, k'$ we have

\[\langle A, Y^n_k \rangle, \langle B, Y^n_{k'} \rangle] = \frac{\delta_{k,k'} \langle A, B \rangle}{h_k^{n-1}}.\]  \hspace{1cm} (16)

**Proof.** Obvious. \hfill \Box

4.3. **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) of Theorem 4.4.

**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 $C \subset S^n$, for all functions $\alpha : C \rightarrow \mathbb{R}$,

\[\sum_{(c,c') \in C^2} \alpha(c)\alpha(c')F(e \cdot c, e \cdot c', c \cdot c') \geq 0.\]  \hspace{1cm} (17)

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

\[F(u,v,t) = \sum_{k=0}^d \langle F_k, Y^n_k(u,v,t) \rangle\]

with $F_k \succeq 0$ for all $0 \leq k \leq d$ are positive definite in the above sense. Note that (17) is slightly stronger than the positivity property of the matrices $Y^n_k$ proved in Theorem 2.2; the argument is essentially the same, as it follows from the equality

\[\sum_{(c,c') \in C^2} \alpha(c)\alpha(c')Z^n_k(c,c') = \left( \sum_{c \in C} \alpha(c)E^n_k(c) \right) \left( \sum_{c \in C} \alpha(c)E^n_k(c) \right)^t \succeq 0.\]

We prove with next proposition 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

\[F(u,v,t) = \sum_{k=0}^d \langle F_k, Y^n_k(u,v,t) \rangle.\]

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 $f \in \text{Pol}(S^{n-1})$,
\[
\int_{(S^{n-1})}^2 f(x)f(y)\tilde{F}(x, y)d\omega_n(x)d\omega_n(y) \geq 0.
\]

As a consequence, if $Q(x)$ is any matrix,
\[
\int_{(S^{n-1})}^2 \langle Q(x), Q(y) \rangle \tilde{F}(x, y)d\omega_n(x)d\omega_n(y) \geq 0.
\]

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 $Z^n_k$, we can write $\langle A, Z^n_k(x, y)^t \rangle$ in the form $\langle Q(x), Q(y) \rangle$. Hence,
\[
\int_{(S^{n-1})}^2 \langle A, Z^n_k(x, y)^t \rangle \tilde{F}(x, y)d\omega_n(x)d\omega_n(y) \geq 0.
\]

In terms of the scalar product $[\cdot, \cdot]$ this is equivalent to
\[
\langle [A, \overline{Y}^n_k], F \rangle \geq 0.
\]

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

Remark 4.13. This characterization of positive definite functions is in fact already proved in [4, Section III] in a more general context: for compact spaces which are homogeneous under the action of their automorphism group, but not necessarily two-point homogeneous. The assumption that the group acts transitively is however not needed in the proof.

Corollary 4.14. 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 $F = \langle A, \overline{Y}^n_k \rangle, G = \langle B, \overline{Y}^n_l \rangle$, where $A$ and $B$ are positive semidefinite matrices. Again, we write $\langle A, Z^n_k(x, y)^t \rangle = \langle Q(x), Q(y) \rangle$ and $\langle B, Z^n_l(x, y)^t \rangle = \langle T(x), T(y) \rangle$. 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
\[
\sum_{(c, c') \in \mathbb{C}^2} \alpha(c)\alpha(c') \tilde{F}(c, c') \tilde{G}(c, c')
\]
\[
= \sum_{(c, c') \in \mathbb{C}^2} \alpha(c)\alpha(c') \langle Q(c), Q(c') \rangle \langle T(c), T(c') \rangle
\]
\[
= \sum_{(c, c') \in \mathbb{C}^2} \langle \alpha(c) Q(c) \otimes T(c), \alpha(c') Q(c') \otimes T(c') \rangle
\]
\[
= \langle U_C, U_C \rangle \geq 0
\]
with
\[ U_C = \sum_{c \in C} \alpha(c) Q(c) \otimes T(c). \]

4.4. **Reproducing kernels.** We define the kernel \( K_d : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R} \) by
\[
K_d((u, v, t), (u', v', t')) := \sum_{k=0}^n h_k^{n-1} \langle \overline{Y}_k(u, v, t), \overline{Y}_k(u', v', t') \rangle.
\]

**Proposition 4.15.** The kernel \( K_d \) is the reproducing kernel of the space \( R_d \), i.e., for all \( F \in R_d \) and all \( (u', v', t') \in \mathbb{R}^3 \) we have
\[
[K_d(\cdot, (u', v', t')), F] = F(u', v', t').
\]

**Proof.** It is straightforward from (16).

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