NEW UPPER BOUNDS FOR KISSING NUMBERS FROM SEMIDEFINITE PROGRAMMING

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ABSTRACT. Recently A. Schrijver derived new upper bounds for binary codes using semidefinite programming. In this paper we adapt this approach to codes on the unit sphere and we compute new upper bounds for the kissing number in several dimensions. In particular our computations give the (known) values for the cases $n = 3, 4, 8, 24$.

1. INTRODUCTION

In geometry, the kissing number problem asks for the maximum number τ_n of unit spheres that can simultaneously touch the unit sphere in n-dimensional Euclidean space without pairwise overlapping. The value of τ_n is only known for $n = 1, 2, 3, 4, 8, 24$. While its determination for $n = 1, 2$ is trivial, it is not the case for other values of n.

The case $n = 3$ was the object of a famous discussion between Isaac Newton and David Gregory in 1694. For a historical perspective of this discussion we refer to [6]. The first valid proof of the fact "$\tau_3 = 12$", like in the icosahedron configuration, was only given in 1953 by K. Schütte and B.L. van der Waerden in [22].

In the seventies, P. Delsarte developed a method, initially aimed at bounding codes on finite fields (see [8]), that yields an upper bound for τ_n as a solution of a linear program and more generally yields an upper bound for the size of spherical codes of given minimal distance. We shall refer to this method as the LP method. With this method, A.M. Odlyzko and N.J.A. Sloane ([15]), and independently V.I. Levenshtein ([13]), proved $\tau_8 = 240$ and $\tau_{24} = 196560$ which are respectively the number of shortest vectors in the root lattice E_8 and in the Leech lattice. For other values of n, the LP method gives in many cases the best known upper bounds. However, for $n = 3$ and $n = 4$ it only gives the upper bounds $\tau_3 \leq 13$ and $\tau_4 \leq 25$.

In 2003, O.R. Musin succeeded to prove the conjectured value $\tau_4 = 24$, which is the number of shortest vectors in the root lattice D_4, with a variation of the LP method (see [14] and the survey [18] of F. Pfender and G.M. Ziegler).

To complete the picture, let us discuss uniqueness of the optimal point configurations. For dimensions 8 and 24, uniqueness was proved by E. Bannai and N.J.A. Sloane ([3]). Their proof exploits the fact that the LP method obtains exactly the aimed value. For dimension 3, there are infinitely many possible configurations. In the regular icosahedron configuration, the angular distances between the contact points are strictly greater than the required $\pi/3$, hence these points can be moved around obtaining infinitely many new suitable configuration. This partially explains why the determination of τ_3 is difficult. On the contrary, uniqueness of the optimal configuration of points in dimension 4 is widely believed, but remains unproven.

The LP method, which was established by P. Delsarte, J.M. Goethals and J.J. Seidel in [9], handles the more general problem of the determination of a bound for the maximal number

$$A(n, \theta) = \max\{\mathrm{card}(C) : C \subset S^{n-1} \text{ with } c \cdot c' \leq \cos\theta \text{ for } c, c' \in C, c \neq c'\}$$

of points on the unit sphere with minimal angular distance θ. Such configurations of points, also called *spherical codes with minimal angular distance θ*, are of special interest in information theory. The kissing number problem is equivalent to the problem of finding $A(n, \pi/3)$.

In this paper, we define a semidefinite program (SDP for short) whose optimal solution gives an upper bound for $A(n, \theta)$ and strengthens the LP method. Computational results show that for several values of n this SDP method gives better upper bounds for τ_n than the LP method.

To be more precise, let us recall that the LP method relies on the existence of polynomials $P_k^n(t)$, satisfying the so-called positivity property:

$$(1) \qquad \text{for all finite } C \subset S^{n-1}, \quad \sum_{(c,c') \in C^2} P_k^n(c \cdot c') \geq 0.$$

These polynomials arise as zonal spherical polynomials on the sphere, i.e. the zonal polynomials associated to the decomposition of the space of polynomial functions under the action of the orthogonal group $\mathrm{O}(\mathbb{R}^n)$.

The consideration of the action restricted to a subgroup H of $\mathrm{O}(\mathbb{R}^n)$, chosen to be the stabilizer group of a fixed point $e \in S^{n-1}$, leads us to some symmetric matrices S_k^n whose coefficients are symmetric polynomials in three variables such that

$$(2) \qquad \text{for all finite } C \subset S^{n-1}, \quad \sum_{(c,c',c'') \in C^3} S_k^n(c \cdot c', c \cdot c'', c' \cdot c'') \succeq 0$$

where the sign "$\succeq 0$" stands for: "is positive semidefinite". The reason why we obtain matrices instead of functions comes from the fact that, in the decomposition of the space of polynomial functions on the sphere under the action of H, multiplicities greater than 1 appear. In fact these multiplicities are exactly the sizes of

the corresponding matrices. From (1) and (2) we derive an SDP whose solution gives an upper bound for $A(n, \theta)$.

Our approach adapts the method proposed by A. Schrijver in [21] to the unit sphere whereas he obtains new upper bounds for binary codes from an SDP. His work can also be interpreted in group theoretic terms, involving the isometry group of the Hamming space $\mathbb{F}_2^n$ and the subgroup stabilizing $(0, \ldots, 0)$ which is the group of permutations of the n positions. It is very likely that many other spaces of interest in coding theory can be treated likewise. The case of non-binary codes was considered by D.C. Gijswijt, A. Schrijver and H. Tanaka in [11].

The paper is organized as follows: Section 2 reviews on the LP method. Section 3 introduces and calculates the semidefinite zonal matrices associated to the action of H and leading to the matrices S_k^n. Section 4 defines the semidefinite program and its dual that establishes the desired bound. Section 5 discusses computational results.

2. REVIEW OF THE LP METHOD ON THE UNIT SPHERE

We introduce the following notations. The standard inner product of the Euclidean space $\mathbb{R}^n$ is denoted by $x \cdot y$. The unit sphere

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

is homogeneous under the action of the orthogonal group $\mathrm{O}(\mathbb{R}^n) = \{O \in \mathbb{R}^{n \times n} : O^t O = I_n\}$, where I_n denotes the identity matrix. It is moreover two-point homogeneous, meaning that the orbits of $\mathrm{O}(\mathbb{R}^n)$ on pairs of points are characterized by the value of their inner product. 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

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

where $\omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}$ is the surface area of S^{n-1} for the standard measure $d\omega_n$. It is a well-known fact (see e.g. [23, Ch. 9.2]) that under the action of $\mathrm{O}(\mathbb{R}^n)$

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

where H_k^n is isomorphic to the $\mathrm{O}(\mathbb{R}^n)$-irreducible space

$$\mathrm{Harm}_k^n = \left\{ f \in \mathbb{R}[x_1, \ldots, x_n] : f \text{ homogeneous}, \deg f = k, \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} f = 0 \right\}$$

of harmonic polynomials in n variables which are homogeneous and have degree k. We set $h_k^n := \dim(\mathrm{Harm}_k^n) = \binom{n+k-1}{n-1} - \binom{n+k-3}{n-1}$.

A certain family of orthogonal polynomials is associated to the unit sphere. They will be denoted by P_k^n, with the convention that P_k^n has degree k and is normalized by $P_k^n(1) = 1$. For $n \geq 3$ these polynomials are up to multiplicative constants Gegenbauer polynomials C_k^λ with parameter $\lambda = n/2 - 1$. So they are given

by $P_k^n(t) = C_k^{n/2-1}(t)/C_k^{n/2-1}(1)$, and the Gegenbauer polynomials C_k^λ can be inductively defined by $C_0^\lambda(t) = 1$, $C_1^\lambda(t) = 2\lambda t$, and

$$kC_k^\lambda(t) = 2(k + \lambda - 1)tC_{k-1}^\lambda(t) - (k + 2\lambda - 2)C_{k-2}^\lambda(t), \quad \text{for } k \geq 2.$$

They are orthogonal with respect to the weight function $(1 - t^2)^{\lambda-1/2}$ on the interval $[-1, 1]$. For $n = 2$ the polynomials P_k^n coincide with the Chebyshev polynomials of the first kind T_k which can be inductively defined by $T_0(t) = 1$, $T_1(t) = t$, and

$$T_k(t) = -2tT_{k-1}(t) + T_{k-2}(t), \quad \text{for } k \geq 2,$$

and they are orthogonal with respect to the weight function $(1 - t^2)^{-1/2}$ on the interval $[-1, 1]$.

The polynomials $P_k^n(t)$ are related to the decomposition (3) by the so-called *addition formula* (see e.g. [1, Ch. 9.6]): for any orthonormal basis $(e_1, \ldots, e_{h_k^n})$ of H_k^n and for any pair of points $x, y \in S^{n-1}$ we have

$$(4) \qquad\qquad P_k^n(x \cdot y) = \frac{1}{h_k^n} \sum_{i=1}^{h_k^n} e_i(x)e_i(y).$$

From the addition formula (4), the positivity property (1) becomes obvious:

$$\sum_{(c,c') \in C^2} P_k^n(c \cdot c') = \sum_{(c,c') \in C^2} \frac{1}{h_k^n} \sum_{i=1}^{h_k^n} e_i(c)e_i(c')$$

$$= \frac{1}{h_k^n} \sum_{i=1}^{h_k^n} \sum_{(c,c') \in C^2} e_i(c)e_i(c') = \frac{1}{h_k^n} \sum_{i=1}^{h_k^n} \left(\sum_{c \in C} e_i(c) \right)^2 \geq 0.$$

Now we introduce the unknowns of the LP to be considered. For a spherical code C we define the two point distance distribution

$$x(u) := \frac{1}{\text{card}(C)} \, \text{card}\{(c, c') \in C^2 : c \cdot c' = u\},$$

where $u \in [-1, 1]$. Clearly, only a finite number of $x(u)$'s are not equal to zero, and the positivity property can be rewritten as a linear inequality in the $x(u)$'s:

$$(5) \qquad\qquad \sum_{u \in [-1,1]} x(u)P_k^n(u) \geq 0.$$

Moreover, the number of elements of C is given by $\text{card}(C) = \sum_{u \in [-1,1]} x(u)$. Noticing the obvious conditions $x(1) = 1$, $x(u) \geq 0$, and $x(u) = 0$ for $\cos\theta < u < 1$ if the minimal angular distance of C is θ, we are led to consider the following

linear program: For any $d \geq 1$, the optimal solution of the linear program

(6)
$$
\max \Big\{ \quad 1 + \sum_{u \in [-1, \cos \theta]} x(u) \quad :
$$
$$
x(u) = 0 \text{ for all but finitely many } u \in [-1, \cos \theta],
$$
$$
x(u) \geq 0 \text{ for all } u \in [-1, \cos \theta],
$$
$$
1 + \textstyle\sum_{u \in [-1, \cos \theta]} x(u) P_k^n(u) \geq 0 \text{ for all } k = 1, \ldots, d \Big\},
$$

gives an upper bound for $A(n, \theta)$. The dual linear problem is

(7)
$$
\min \Big\{ \quad 1 + \sum_{k=1}^{d} f_k \quad :
$$
$$
f_k \geq 0 \text{ for all } k = 1, \ldots, d,
$$
$$
\textstyle\sum_{k=1}^{d} f_k P_k^n(u) \leq -1 \text{ for all } u \in [-1, \cos \theta] \Big\}.
$$

By the duality theorem (cf. [10]) any feasible solution of (7) gives an upper bound for the optimal solution of (6). The dual linear program can be restated in the following way involving polynomials:

Theorem 2.1. *(see e.g. [9, Th. 4.3], [7, Ch. 9], [15])*
Let $F(t) = \sum_{k=0}^{d} f_k P_k^n(t)$ be a polynomial of degree at most d in $\mathbb{R}[t]$. If
  (a) $f_k \geq 0$ for all $k \geq 1$ and $f_0 > 0$ and
  (b) $F(u) \leq 0$ for all $u \in [-1, \cos \theta]$,
then
$$
A(n, \theta) \leq \frac{F(1)}{f_0}.
$$

3. SEMIDEFINITE ZONAL MATRICES

Now we fix a point $e \in S^{n-1}$, and let $H := \mathrm{Stab}(\mathrm{O}(\mathbb{R}^n), e)$ be the stabilizer of e in $\mathrm{O}(\mathbb{R}^n)$. Obviously, $H \simeq \mathrm{O}(\mathbb{R}^{n-1})$ since $\mathrm{O}(\mathbb{R}^{n-1})$ can be identified with the orthogonal group of the orthogonal complement of $\mathbb{R}e$.

It is a classical result (see e.g. [23, Ch. 9.2]) that for the restricted action to H the decomposition of Harm_k^n into H-irreducible subspaces is given by:

$$
\mathrm{Harm}_k^n \simeq \bigoplus_{i=0}^{k} \mathrm{Harm}_i^{n-1}.
$$

Hence, each of the H_k^n in (3) decomposes likewise:

(8)
$$
H_k^n = H_{0,k}^{n-1} \perp H_{1,k}^{n-1} \perp \ldots \perp H_{k,k}^{n-1},
$$

where $H_{i,k}^{n-1} \simeq \mathrm{Harm}_i^{n-1}$. We give an explicit description of this decomposition in the proof of Theorem 3.2.

We summarize the situation in the following picture.

$$\begin{aligned}
\mathrm{Pol}_{\leq d}(S^{n-1}) &= & H_0^n & \perp & H_1^n & \perp & \ldots & \perp & H_d^n \\
&= & H_{0,0}^{n-1} & \perp & H_{0,1}^{n-1} & \perp & \ldots & \perp & H_{0,d}^{n-1} \\
& & & & \perp\; H_{1,1}^{n-1} & \perp & \ldots & \perp & H_{1,d}^{n-1} \\
& & & & & & \ldots\ldots & \ldots\ldots\ldots & \\
& & & & & & & \perp & H_{d,d}^{n-1}
\end{aligned}$$

The isotypic components of the H-decomposition of $\mathrm{Pol}_{\leq d}(S^{n-1})$ are

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

Now we show how to associate to each $\mathcal{I}_k$ a "zonal matrix" in view of an analogue of the addition formula (4).

Theorem 3.1. *Let $\mathcal{I} = R_0 \perp R_1 \perp \ldots \perp R_m \simeq (m+1)R$ be an isotypic component of $\mathrm{Pol}_{\leq d}(S^{n-1})$ under the action of H, with R an H-irreducible space of dimension h. Let $(e_{0,1},\ldots,e_{0,h})$ be an orthonormal basis of R_0 and let $\phi_i : R_0 \to R_i$ be H-isomorphisms preserving the inner product on $\mathrm{Pol}_{\leq d}(S^{n-1})$. Let $e_{i,j} = \phi_i(e_{0,j})$, so that $(e_{i,1},\ldots,e_{i,h})$ is an orthonormal basis of R_i. Define*

$$E(x) := \left(\frac{1}{\sqrt{h}} e_{i,j}(x)\right)_{\substack{0 \leq i \leq m \\ 1 \leq j \leq h}} = \frac{1}{\sqrt{h}} \begin{pmatrix} e_{0,1}(x) & \ldots & e_{0,h}(x) \\ \vdots & & \vdots \\ e_{m,1}(x) & \ldots & e_{m,h}(x) \end{pmatrix},$$

and

$$Z(x,y) := E(x)E(y)^t \in \mathbb{R}^{(m+1)\times(m+1)}.$$

Then the following properties hold for the matrix Z:

(a) $Z(x,y)$ does not depend on the choice of the orthonormal basis of R_0.

(b) The change of ϕ_i to $-\phi_i$ for some i or the choice of another decomposition of $\mathcal{I}$ as a sum of $m+1$ orthogonal H-submodules changes $Z(x,y)$ to some $OZ(x,y)O^t$ with $O \in \mathrm{O}(\mathbb{R}^{m+1})$.

(c) For all $g \in H$, $Z(g(x),g(y)) = Z(x,y)$.

(d) (Matrix-type positivity property)

(10) $\qquad\qquad$ *For all finite $C \subset S^{n-1}$, $\displaystyle\sum_{(c,c')\in C^2} Z(c,c') \succeq 0.$*

Proof. (a) If $(\epsilon_{0,1},\ldots,\epsilon_{0,h})$ is another orthonormal basis of R_0, then there is an orthogonal $h \times h$ matrix O with $(\epsilon_{0,1},\ldots,\epsilon_{0,h}) = (e_{0,1},\ldots,e_{0,h})O$. In this case the matrix $E(x)$ is changed to $E(x)O$ and, since $OO^t = I_h$, the matrix $Z(x,y)$ stays unchanged.

(b) By Schur's Lemma and by the irreducibility of R, there are only two possible choices for ϕ_i, namely ϕ_i and $-\phi_i$, once the subspaces R_i are fixed.

Let $\mathcal{I} = S_0 \perp \ldots \perp S_m$ be another decomposition of $\mathcal{I}$, together with H-isomorphisms $\psi_i : R_i \to S_i$ preserving the inner product on $\mathrm{Pol}_{\leq d}(S^{n-1})$. Then $\psi = (\psi_0,\ldots,\psi_m)$ defines an H-endomorphism of $\mathcal{I}$. Again by Schur's Lemma, for a suitable choice of basis in R_i and by permuting rows and columns, the matrix of ψ is block diagonal with h blocks of size $(m+1) \times (m+1)$ and with the same

$(m+1) \times (m+1)$ matrix $O \in \mathrm{O}(\mathbb{R}^{m+1})$ as blocks. This means that $E(x)$ changes to $OE(x)$ and so $Z(x, y)$ becomes $OZ(x, y)O^t$.

(c) Since $e_{i,j}(g^{-1}(x)) = (ge_{i,j})(x)$, the computation of $Z(g^{-1}(x), g^{-1}(y))$ amounts to replace in the definition of $Z(x, y)$ the $e_{i,j}$ by $ge_{i,j}$. Since R_i is H-stable, $\epsilon_{i,j} := ge_{i,j}$, with $j = 1, \ldots, h$, is another orthonormal basis of R_i, and

$$\phi_i(\epsilon_{1,j}) = \phi_i(ge_{1,j}) = g\phi_i(e_{1,j}) = ge_{i,j} = \epsilon_{i,j}.$$

Hence from (a) we conclude $Z(g^{-1}(x), g^{-1}(y)) = Z(x, y)$.

(d) We have $\displaystyle\sum_{(c,c')\in C^2} Z(c, c') = \Big(\sum_{c\in C} E(c)\Big)\Big(\sum_{c\in C} E(c)\Big)^t \succeq 0.$ $\hfill \square$

The orbits of H on pairs of points on the unit sphere $x, y \in S^{n-1}$ are characterized by the values of the three inner products $e \cdot x$, $e \cdot y$, and $x \cdot y$. By definition the coefficients $Z_{i,j}(x, y)$ of $Z(x, y)$ are polynomials in the variables $x_1, \ldots, x_n, y_1, \ldots, y_n$. Then, property (c) of Theorem 3.1 implies that they can be expressed as polynomials in the three variables $u = e \cdot x$, $v = e \cdot y$, and $t = x \cdot y$.

By Z_k^n, for $0 \le k \le d$, let us denote the matrix associated to $\mathcal{I}_k$ as defined above, and more precisely to the decomposition (9) of $\mathcal{I}_k$. Now we shall calculate the matrix $Y_k^n(u, v, t)$ with

(11) $$Z_k^n(x, y) = Y_k^n(e \cdot x, e \cdot y, x \cdot y).$$

Theorem 3.2. *With the above notations, we have, for all $0 \le i, j \le d - k$,*

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

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

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

Proof. We explicitly use an orthonormal basis of $H_{k,k+i}^{n-1}$ to calculate $Y_k^n(u, v, t)$. Such a basis is constructed in [1, Ch. 9.8]. Let us recall the construction. For $x \in S^{n-1}$, let

$$x = ue + \sqrt{1 - u^2}\zeta,$$

where $u = x \cdot e$ and ζ belongs to the unit sphere S^{n-2} of $(\mathbb{R}e)^\perp$. With $f \in H_k^{n-1} \subset \mathrm{Pol}_{\le k}(S^{n-2})$ we associate $\varphi(f) \in \mathrm{Pol}_{\le k}(S^{n-1})$ defined by:

$$\varphi(f)(x) = (1 - u^2)^{k/2} f(\zeta).$$

Note that the multiplication by $(1-u^2)^{k/2}$ forces $\varphi(f)$ to be a polynomial function in the coordinates of x. Clearly φ commutes with the action of H. Hence $\varphi(H_k^{n-1})$ is a subspace of $\mathrm{Pol}_{\le k}(S^{n-1})$ which is isomorphic to Harm_k^{n-1}. More generally, the set $\{\varphi(f)P(u) : f \in \mathrm{Harm}_k^{n-1}, \deg P \le i\}$ is a subspace of $\mathrm{Pol}_{\le k+i}(S^{n-1})$ which is isomorphic to $i + 1$ copies of Harm_k^{n-1}. By induction on k and i there

exist polynomials $P_i(u)$ of degree i such that $\varphi(H_k^{n-1})P_i(u) = H_{k,k+i}^{n-1}$. Note that this construction could be used to derive decomposition (8) explicitly.

We can exploit the fact that the subspaces $H_{k,l}^{n-1}$ are pairwise orthogonal to prove an orthogonality relation between the polynomials P_i. Then this orthogonality relation will enable us to identify the polynomials P_i as multiples of Gegenbauer polynomials. Let us recall that the measures on S^{n-1} and on S^{n-2} are related by:

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

Whenever $i \neq j$ we have for all $f \in H_k^{n-1}$

$$
\begin{aligned}
0 &= \frac{1}{\omega_n} \int_{S^{n-1}} \varphi(f) P_i(u) \varphi(f) P_j(u) d\omega_n(x) \\
&= \frac{1}{\omega_n} \int_{S^{n-1}} f(\zeta)^2 (1-u^2)^k P_i(u) P_j(u) d\omega_n(x) \\
&= \frac{1}{\omega_n} \int_{S^{n-2}} f(\zeta)^2 d\omega_{n-1}(\zeta) \int_{-1}^{1} (1-u^2)^{k+(n-3)/2} P_i(u) P_j(u) du,
\end{aligned}
$$

from which we derive that

$$\int_{-1}^{1} (1-u^2)^{k+(n-3)/2} P_i(u) P_j(u) du = 0;$$

hence the polynomials $P_i(u)$ are proportional to $P_i^{n+2k}(u)$. We obtain an orthonormal basis of $H_{k,k+i}^{n-1}$ from an orthonormal basis $(f_1, \ldots, f_h)$ of H_k^{n-1} by taking $e_{i,j} = \lambda_i \varphi(f_j) P_i^{n+2k}(u)$ for a suitable normalizing factor λ_i. We compute λ_i in a similar way as above:

$$
\begin{aligned}
1 &= \frac{1}{\omega_n} \int_{S^{n-1}} \left(\lambda_i \varphi(f_j) P_i^{n+2k}(u)\right)^2 d\omega_n(x) \\
&= \frac{1}{\omega_n} \int_{S^{n-2}} \left(f_j(\zeta)\right)^2 d\omega_{n-1}(\zeta) \int_{-1}^{1} \lambda_i^2 (1-u^2)^{k+(n-3)/2} \left(P_i^{n+2k}(u)\right)^2 du \\
&= \frac{\omega_{n-1}}{\omega_n} \int_{-1}^{1} \lambda_i^2 (1-u^2)^{k+(n-3)/2} \left(P_i^{n+2k}(u)\right)^2 du.
\end{aligned}
$$

From the addition formula (4) applied to $\left(P_i^{n+2k}(u)\right)^2$ one easily shows that

$$\int_{-1}^{1} (1-u^2)^{k+(n-3)/2} \left(P_i^{n+2k}(u)\right)^2 du = \frac{\omega_{n+2k}}{\omega_{n+2k-1} h_i^{n+2k}},$$

so we obtain

$$\lambda_i^2 = \frac{\omega_n}{\omega_{n-1}} \frac{\omega_{n+2k-1}}{\omega_{n+2k}} h_i^{n+2k}.$$

Now we are in the situation of Theorem 3.1 with

$$R_0 = H_{k,k}^{n-1}, R_1 = H_{k,k+1}^{n-1}, \ldots, R_{d-k} = H_{k,d}^{n-1}$$

and their orthonormal basis $(e_{0,1}, \ldots, e_{0,h}), \ldots, (e_{d-k,1}, \ldots, e_{d-k,h})$. The isomorphisms ϕ_i are the multiplications by $(\lambda_i/\lambda_1) P_i^{n+2k}(u)$.

Then, the coefficient (i,j), with $0 \leq i, j \leq d-k$, of Z_k^n is given by:

$$\left(Z_k^n\right)_{i,j}(x,y)$$

$$= \quad \frac{1}{h}\sum_{s=1}^{h} e_{i,s}(x)e_{j,s}(y)$$

$$= \quad \frac{1}{h}\sum_{s=1}^{h} \lambda_i(1-u^2)^{k/2}f_s(\zeta)P_i^{n+2k}(u)\lambda_j(1-v^2)^{k/2}f_s(\xi)P_j^{n+2k}(v)$$

$$= \quad \lambda_i\lambda_j P_i^{n+2k}(u)P_j^{n+2k}(v)\big((1-u^2)(1-v^2)\big)^{k/2}\frac{1}{h}\sum_{s=1}^{h} f_s(\zeta)f_s(\xi)$$

$$= \quad \lambda_i\lambda_j P_i^{n+2k}(u)P_j^{n+2k}(v)\big((1-u^2)(1-v^2)\big)^{k/2}P_k^{n-1}(\zeta\cdot\xi),$$

where we have written $y = ve + \sqrt{1-v^2}\xi$ and where we applied the addition formula (4) to get the last equality. Now we define $\lambda_{i,j} = \lambda_i\lambda_j$ and since

$$\zeta\cdot\xi = (t-uv)/\sqrt{(1-u^2)(1-v^2)},$$

we have completed the proof. $\qquad\qquad\square$

Remark 3.3. *We would like to point out that the role of the number d is only to cut Y_k^n to a matrix of finite size. Indeed, d does not enter in the expression of $\left(Y_k^n\right)_{i,j}(u,v,t)$. It is better to view the matrices Y_k^n as matrices of infinite size with all finite principal minors having the matrix-type positivity property.*

Remark 3.4. *For the semidefinite programming bounds in Section 4 we only use the matrix-type positivity property of the matrices Y_k^n. This property is preserved if one replaces Y_k^n by $AY_k^n A^t$ with an invertible matrix A. So, e.g. one could replace the expression of $\left(Y_k^n\right)_{i,j}(u,v,t)$ in (12) by the simpler $u^iv^jQ_k^{n-1}(u,v,t)$.*

Due to the specific choice of the unit vector e defining the subgroup H, the coefficients of Y_k^n are not symmetric polynomials. We introduce the symmetrization S_k^n of Y_k^n and state the announced property (2).

Corollary 3.5. *For all $d \geq 0$, for all $k \geq 0$, let Y_k^n be the matrix in Theorem 3.2 and let S_k^n be defined by*

$$(13) \qquad\qquad S_k^n = \frac{1}{6}\sum_{\sigma}\sigma Y_k^n,$$

where σ runs through the group of all permutations of the variables u,v,t which acts on matrix coefficients in the obvious way. Then the matrices S_k^n are symmetric and have symmetric polynomials as coefficients. We have:

$$(14) \qquad \textit{For all finite } C \subset S^{n-1}, \sum_{(c,c')\in C^2} Y_k^n(e\cdot c, e\cdot c', c\cdot c') \succeq 0,$$

and

$$(15) \qquad \textit{for all finite } C \subset S^{n-1}, \sum_{(c,c',c'')\in C^3} S_k^n(c\cdot c', c\cdot c'', c'\cdot c'') \succeq 0.$$

Proof. Note that $\left(Y_k^n\right)_{j,i}(u,v,t) = \left(Y_k^n\right)_{i,j}(v,u,t)$ which gives the desired properties of S_k^n. Property (10) rephrases to (14) and property (15) is obtained from (14) by taking $e = c'' \in C$ and summing over all $c'' \in C$.   □

To end this section we show that the positivity property (1) is actually a consequence of the matrix-type positivity property (2). As shown in the following proposition one can express the polynomials P_k^n as a linear combination of diagonal elements of the matrices Y_k^n with non-negative coefficients.

Proposition 3.6. *We have the following expression for the polynomials $P_k^n(t)$ in terms of matrix coefficients of $Y_k^n(u,v,t)$:*

$$(16) \qquad P_k^n(t) = \sum_{s=0}^{k} \frac{h_s^{n-1}}{h_k^n} \left(Y_s^n\right)_{k-s,k-s}(u,v,t).$$

Consequently, property (14) *or property* (2) *implies* (1).

Proof. The addition formula (4) holds for any orthonormal basis of H_k^n. We take an orthonormal basis of H_k^n obtained by concatenation of orthormal basis of the spaces $H_{0,k}^{n-1}, H_{1,k}^{n-1}, \ldots, H_{k,k}^{n-1}$. If $(e_{s,1}^k, e_{s,2}^k, \ldots, e_{s,h_s^{n-1}}^k)$ denotes an orthonormal basis of $H_{s,k}^{n-1}$, we have from Theorem 3.1

$$\left(Y_s^n\right)_{k-s,k-s}(e \cdot x, e \cdot y, x \cdot y) = \frac{1}{h_s^{n-1}} \sum_{i=1}^{h_s^{n-1}} e_{s,i}^k(x) e_{s,i}^k(y).$$

By the addition formula (4)

$$P_k^n(x \cdot y) = \frac{1}{h_k^n} \sum_{s=0}^{k} \sum_{i=1}^{h_s^{n-1}} e_{s,i}^k(x) e_{s,i}^k(y)$$

$$= \sum_{s=0}^{k} \frac{h_s^{n-1}}{h_k^n} \left(Y_s^n\right)_{k-s,k-s}(e \cdot x, e \cdot y, x \cdot y),$$

and hence

$$P_k^n(t) = \sum_{s=0}^{k} \frac{h_s^{n-1}}{h_k^n} \left(Y_s^n\right)_{k-s,k-s}(u,v,t).$$

Since the coefficients h_s^{n-1}/h_k^n are non-negative, and since the diagonal elements of a semidefinite matrix are non-negative, (1) is a consequence of (14).

With the action of the permutation group of the variables u, v, t

$$\frac{1}{3}\left(P_k^n(u) + P_k^n(v) + P_k^n(t)\right) = \sum_{s=0}^{k} \frac{h_s^{n-1}}{h_k^n} \left(S_s^n\right)_{k-s,k-s}(u,v,t).$$

Replacing $u = c \cdot c'$, $v = c \cdot c''$, $t = c' \cdot c''$ and summing over $(c, c', c'') \in C^3$ for a code C, we obtain (1) from (2).

□

4. THE SEMIDEFINITE PROGRAMMING BOUND

In this section we set up an SDP whose optimum gives an upper bound for $A(n, \theta)$ which is at least as good as the LP method.

For a spherical code C we define the three points distance distribution

$$x(u, v, t) := \frac{1}{\text{card}(C)} \, \text{card}\{(c, c', c'') \in C^3 : c \cdot c' = u, c \cdot c'' = v, c' \cdot c'' = t\},$$

where $u, v, t \in [-1, 1]$ and the matrix

$$\begin{pmatrix} 1 & u & v \\ u & 1 & t \\ v & t & 1 \end{pmatrix},$$

being the Gram matrix of three vectors on a unit sphere, is positive semidefinite.

The last condition together with the first is equivalent to the fact that the determinant of the Gram matrix is non-negative, hence

(17)
$$1 + 2uvt - u^2 - v^2 - t^2 \geq 0.$$

The two point distance distribution $x(u)$ as defined in Section 2 and the three point distance distribution $x(u, v, t)$ are related by $x(u, u, 1) = x(u)$. The three point distance distribution satisfies the following obvious properties:

$$x(u, v, t) \geq 0,$$
$$x(1, 1, 1) = 1,$$
$$x(\sigma(u), \sigma(v), \sigma(t)) = x(u, v, t) \ \text{ for all permutations } \sigma,$$
$$\sum_{u,v,t} x(u, v, t) = \text{card}(C)^2,$$
$$\sum_{u} x(u, u, 1) = \text{card}(C).$$

Furthermore, from the positivity properties (5) and (15), we have for any $d \geq 0$:

$$\sum_{u} x(u, u, 1) P_k^n(u) \geq 0 \ \text{ for } k = 1, \ldots, d,$$
$$\sum_{u,v,t} x(u, v, t) S_k^n(u, v, t) \succeq 0 \ \text{ for } k = 0, \ldots, d,$$

where the matrix S_k^n has size $(d - k + 1) \times (d - k + 1)$. If the minimal angular distance of C is θ, we have moreover

$$x(u, v, t) = 0 \ \text{ whenever } u, v, t \notin [-1, \cos \theta] \cup \{1\}.$$

To factor out the action of the permutations of the variables u, v, t we introduce the domains

$$D = \{(u, v, t) : -1 \leq u \leq v \leq t \leq \cos \theta \text{ and } 1 + 2uvt - u^2 - v^2 - t^2 \geq 0\},$$

$$D_0 = \{(u, u, 1) : -1 \leq u \leq \cos \theta\}, \qquad I = [-1, \cos \theta],$$

and $m(u, v, t)$ with

$$m(u, v, t) = \begin{cases} 6 & \text{if } u \neq v \neq t, \\ 3 & \text{if } u = v \neq t \text{ or } u \neq v = t \text{ or } u = t \neq v, \\ 1 & \text{if } u = v = t. \end{cases}$$

From the discussion above, a solution to the following semidefinite program in the variables $x'(u, v, t) = m(u, v, t)x(u, v, t)$ is an upper bound for $A(n, \theta)$:

$$1 + \max \left\{ \frac{1}{3} \sum_{u \in I} x'(u, u, 1) : \right.$$

$$x'(u, v, t) = 0 \text{ for all but finitely many } (u, v, t) \in D \cup D_0,$$

$$x'(u, v, t) \geq 0 \text{ for all } (u, v, t) \in D \cup D_0,$$

$$\left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix} \right) + \frac{1}{3} \sum_{u \in I} x'(u, u, 1) \left(\begin{smallmatrix} 0 & 1 \\ 1 & 1 \end{smallmatrix} \right) + \sum_{(u,v,t) \in D} x'(u, v, t) \left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix} \right) \succeq 0,$$

$$3 + \sum_{u \in I} x'(u, u, 1) P_k^n(u) \geq 0 \text{ for } k = 1, \dots, d,$$

$$\left. S_k^n(1, 1, 1) + \sum_{(u,v,t) \in D \cup D_0} x'(u, v, t) S_k^n(u, v, t) \succeq 0 \text{ for } k = 0, \dots, d \right\}.$$

The third constraint deserves some further explanation. We have already noticed that

$$\mathrm{card}(C)^2 = 1 + \sum_{(u,v,t) \in D \cup D_0} x'(u, v, t) = \left(1 + \sum_{u \in I} x(u, u, 1) \right)^2,$$

which implies

$$\sum_{(u,v,t) \in D} x'(u, v, t) + \frac{1}{3} \sum_{u \in I} x'(u, u, 1) - \left(\frac{1}{3} \sum_{u \in I} x'(u, u, 1) \right)^2 \geq 0,$$

and this is equivalent to the semidefinite condition:

$$\begin{pmatrix} 1 & \dfrac{1}{3} \sum_{u \in I} x'(u, u, 1) \\ \dfrac{1}{3} \sum_{u \in I} x'(u, u, 1) & \sum_{(u,v,t) \in D} x'(u, v, t) + \dfrac{1}{3} \sum_{u \in I} x'(u, u, 1) \end{pmatrix} \succeq 0.$$

Remark 4.1. *We want to point out that, despite of the fact that* (2) *implies* (1)*, as is proved in Proposition 3.6, the inequalities* $3 + \sum_{u \in I} x'(u, u, 1) P_k^n(u) \geq 0$ *should not be removed from our SDP. Indeed, the last inequalities do not imply them for an arbitrary set of numbers* $x'(u, v, t)$*, unless these numbers satisfy the additional equalities:*

$$\sum_{u,v} x(u, v, t) = \left(\sum_u x(u, u, 1) \right) x(t, t, 1) \quad \text{for all } t.$$

These equalities do hold for codes, but they are not semidefinite conditions. It can be noticed that the third constraint in the maximization problem above is a weaker consequence of them.

Just like in the LP method, the main problem with the above SDP, is that the unknowns $x(u, v, t)$ are indexed by a continuous domain of $\mathbb{R}^3$. We cannot exploit the information that only a finite number of them are not equal to zero, because we don't know to which values of (u, v, t) they correspond. We solve this problem by applying duality theory.

Before we derive the SDP dual to the above one we recall the principle of weak duality. We use the standard notation for the inner product of symmetric matrices: $\langle A, B \rangle = \text{Trace}(AB)$. Let J be a (possible infinite) set of indices, let $S_j \in \mathbb{R}^{m \times m}$ be symmetric matrices with $j \in J$, let $C \in \mathbb{R}^{m \times m}$ be a symmetric matrix, and let $c_j \in \mathbb{R}$ be real numbers. Suppose that the real numbers $x_j \in \mathbb{R}$ are a feasible solution of the primal problem, i.e. $x_j = 0$ for all but finitely many $j \in J$, and $C - \sum_{j \in J} x_j S_j \succeq 0$. Furthermore, suppose that the symmetric matrix $F \in \mathbb{R}^{m \times m}$ is a feasible solution of the dual problem, i.e. $\langle F, S_j \rangle = c_j$ for all $j \in J$, and $F \succeq 0$. Then, we have $\sum_{j \in J} c_j x_j = \langle \sum_{j \in J} x_j S_j, F \rangle \leq \langle C, F \rangle$.

In our case this specializes as follows: The set of indices is $J = D_0 \cup D$. The matrices $S_{(u,v,t)}$ are block matrices with four blocks of different type. We get one block for each positivity constraint in the above SDP. So F is also a block matrix with four blocks of different type. In this case it can be simplified to three blocks. The first block of F consists of the matrix $\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$. The second block of F is the diagonal matrix with coefficients $a_1, \ldots, a_d$ The third block of F is again a block matrix with blocks $F_0, \ldots, F_d$ which have the same size as the matrices S_k^n. The matrix C is a block matrix as well. The first block of C contains the matrix $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. The first entry of the second block is 3, the other entries in this block are zero. The third block of C consists of the matrices $S_k^n(1, 1, 1)$. The real numbers $c_{(u,v,t)}$ are zero if $(u, v, t) \in D$ and equal to $1/3$ if $(u, v, t) \in D_0$. In the following theorem we give the SDP dual to the above one. Furthermore we apply the simplification $S_k^n(1, 1, 1) = 0$ for $k \geq 1$.

Theorem 4.2. *Any feasible solution of the following semidefinite problem gives an upper bound on $A(n, \theta)$:*

$$1 + \min \left\{ \; \sum_{k=1}^{d} a_k + b_{11} + \langle F_0, S_0^n(1, 1, 1) \rangle : \right.$$

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix} \succeq 0,$$

$$a_k \geq 0 \; \text{for } k = 1, \ldots, d,$$

$$F_k \succeq 0 \; \text{for } k = 0, \ldots, d,$$

$$\sum_{k=1}^{d} a_k P_k^n(u) + 2b_{12} + b_{22} + 3 \sum_{k=0}^{d} \langle F_k, S_k^n(u, u, 1) \rangle \leq -1,$$

$$\left. b_{22} + \sum_{k=0}^{d} \langle F_k, S_k^n(u, v, t) \rangle \leq 0 \right\},$$

where the last inequality holds for all $(u, v, t) \in D$ and the second to last inequality holds for all $u \in I$.

Note that if the last inequality holds for all $(u, v, t) \in D$, then it also holds for the larger domain

$$D' := \{(u, v, t) : -1 \leq u, v, t \leq \cos \theta \text{ and } 1 + 2uvt - u^2 - v^2 - t^2 \geq 0\},$$

because the coefficients in S_k^n are symmetric polynomials.

5. COMPUTATIONAL RESULTS

In this section, we describe one possible strategy to derive explicit upper bounds for τ_n from Theorem 4.2. Thereby we make use of techniques form polynomial optimization introduced e.g. in [12] and [16] which we shall briefly recall here.

We consider the polynomials

$$p(u) = -(u + 1/4)^2 + 9/16,$$

$$p_1(u, v, t) = p(u), \quad p_2(u, v, t) = p(v), \quad p_3(u, v, t) = p(t),$$

$$p_4(u, v, t) = 1 + 2uvt - u^2 - v^2 - t^2,$$

and we obviously have

$$
\begin{aligned}
I &= \{u \in \mathbb{R} : p(u) \geq 0\}, \\
D' &= \{(u, v, t) \in \mathbb{R}^3 : p_i(u, v, t) \geq 0, \ i = 1, \ldots, 4\}.
\end{aligned}
$$

We say that a polynomial $f \in \mathbb{R}[x_1, \ldots, x_n]$ is a *sum of squares* if it can be written as $f = \sum_{i=1}^{k} g_i^2$, for $k \in \mathbb{N}$ and $g_i \in \mathbb{R}[x_1, \ldots, x_n]$. A polynomial $p(x_1, \ldots, x_n)$ of degree $2m$ is a sum of squares if and only if there is a positive semidefinite matrix Q so that $p(x_1, \ldots, x_n) = z^t Q z$ where z is the vector of monomials $z = (1, x_1, \ldots, x_n, x_1 x_2, \ldots, x_{n-1} x_n, \ldots, x_n^m)$. So assuring that a polynomial is a sum of squares is a semidefinite condition.

It is easy to see that the last two conditions of the semidefinite program in Theorem 4.2 are satisfied if the following two equalities hold:

$$-1 - \sum_{k=1}^{d} a_k P_k^n(u) - 2b_{12} - b_{22} - 3 \sum_{k=0}^{d} \langle F_k, S_k^n(u, u, 1) \rangle = q(u) + p(u)q_1(u),$$

$$-b_{22} - \sum_{k=0}^{d} \langle F_k, S_k^n(u, v, t) \rangle = r(u, v, t) + \sum_{i=1}^{4} p_i(u, v, t) r_i(u, v, t)$$

where q, q_1 and $r, r_1, \ldots, r_4$ are sums of squares.

It is not apriori clear that the relaxation of using this specific sum of squares representation is strong enough. The following theorem of M. Putinar justifies our approach.

Theorem 5.1. *([19]) Let $K = \{x \in \mathbb{R}^n : p_1(x) \geq 0, \ldots, p_s(x) \geq 0\}$ be a compact semialgebraic set. Suppose that there is a polynomial P of the form $P = q + p_1 q_1 + \cdots + p_s q_s$, where q and all q_i's are sums of squares, so that the set $\{x \in \mathbb{R}^n : P(x) \geq 0\}$ is compact. Then, every polynomial p which is positive on*

K can be written as $p = r + p_1 r_1 + \cdots + p_s r_s$, where r and all r_i's are sums of squares.

Now we use these considerations to formulate a finite-dimensional semidefinite program which gives an upper bound on the kissing number τ_n: We fix d and restrict the polynomials $q, q_1, r, r_1, \ldots, r_4$ to polynomials having degree at most N, with $N \geq d$. Then we can use the computer to find a feasible solution of this finite-dimensional semidefinite program. A feasible solution of it is at the time a feasible solution of the SDP in Theorem 4.2. So it gives an upper bound on the kissing number τ_n.

We implemented this approach and give our results in Table 5.1.

n	best lower bound known	best upper bound previously known		LP method	SDP method
3	12	12	(Schütte, v.d. Waerden [22])	13	12
4	24	24	(Musin [14])	25	24
5	40	46	(Odlyzko, Sloane [15])	46	45
6	72	82	(O., S. [15])	82	78
7	126	140	(O., S. [15])	140	135
8	240	240	(O., S. [15], Levenshtein [12])	240	240
9	306	379	(Rzhevskii, Vsemirnov [20])	380	366
10	500	594	(Pfender [17])	595	567

Table 5.1. Bounds on τ_n.

The values of the last column were found by solving the above semidefinite program for the values $d = 10$ and $N = 10$. The values of the third column were obtained by Odlyzko and Sloane by Theorem 2.1 using the value $d = 30$. They pointed out that even $d = 11$ would suffice for $n \leq 10$. Our calculations were performed by the program `csdp` (Version 5.0) of B. Borchers ([2]) which is available on the Internet (http://infohost.nmt.edu/~borchers/csdp.html). After solving the SDP with `csdp` we checked independently whether the solution satisfies the desired constraints. This can be done using rational arithmetic only. So our computations give rigorous proofs of the stated upper bounds. Due to numerical instabilities we were not able to perform this calculation for larger n and/or larger d, N. The smallest values of d and N which solve the kissing number problem in dimension 3 is $d = N = 5$. Then, we obtain by the SDP method $\tau_3 \leq 12.8721$. For the kissing number problem in dimension 4 it is $d = N = 7$, and the SDP method gives $\tau_4 \leq 24.5797$.

For the lower bounds in the first column we refer to the Catalogue of Lattices of G. Nebe and N.J.A. Sloane (http://www.research.att.com/~njas/lattices/kiss.html).

Using the polynomial $p(u) = -(u + 1/3)^2 + 4/9$ we computed upper bounds for $A(n, \cos^{-1} 1/3)$. Hereby we improved several entries of the Table 9.2 of [7] where all best upper bounds previously known were obtained by the LP method. We give our results in Table 5.2. Again we used the values $d = 10$ and $N = 10$ to obtain the last column.

n	best lower bound known	best upper bound previously known	SDP method
3	9	9	9
4	14	15	15
5	20	24	23
6	32	37	35
7	56	56	56
8	64	78	74
9	96	107	99
10		146	135

Table 5.2. Bounds on $A(n, \cos^{-1} 1/3)$.

We were also able to improve the best known upper bounds for the so-called Tammes problem with N spheres: What is the largest minimal angle $\theta(N)$ that can be obtained by a spherical code of S^2 with cardinality N. Let us recall that the answer is only known for $N \leq 12$ and for $N = 24$ (see [7, Ch. 1]). For $N = 13$, the best known lower bound is $0.997223593 \approx 57.1367031°$ whereas the best-known upper bound is $1.02746114 \lesssim 58.8691870°$ due to K. Böröczky and L. Szabo [4]. We obtained $A(3, \cos^{-1}(0.5225)) \leq 12.99$ using $d = N = 10$, giving the new upper bound of $1.02101593 \lesssim 58.4999037°$. Other values are collected in Table 5.3; the lower bounds are taken from the homepage of N.J.A. Sloane (http://www.research.att.com/~njas/packings/). The upper bounds for $N \geq 14$ where established in [5].

N	best lower bound known	best upper bound previously known	SDP method
13	57.13	58.87	58.50
14	55.67	58.00	56.58
15	53.65	55.84	55.03
16	52.24	53.92	53.27
17	51.09	52.11	51.69

Table 5.3. Bounds on $\theta(N)$ (given in degrees).

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