

THE KISSING NUMBER IN FOUR DIMENSIONS

Oleg R. Musin *

Abstract

The kissing number problem asks for the maximal number of equal size nonoverlapping spheres that can touch another sphere of the same size in n -dimensional space. This problem in dimension three was the subject of a famous discussion between Isaac Newton and David Gregory in 1694. In three dimensions the problem was finally solved only in 1953 by Schütte and van der Waerden. It was proved that the bounds given by Delsarte's method are not good enough to solve the problem in 4-dimensional space. In this paper we present a solution of the problem in dimension four, based on a modification of Delsarte's method.

Keywords: kissing number, contact number, spherical codes, Delsarte's method, Gegenbauer (ultraspherical) polynomials

1 Introduction

The *kissing number* $k(n)$ is the highest number of equal nonoverlapping spheres in \mathbf{R}^n that can touch another sphere of the same size. In three dimensions the kissing number problem is asking how many white billiard balls can *kiss* (touch) a black ball.

The most symmetrical configuration, 12 billiard balls around another, is if the 12 balls are placed at positions corresponding to the vertices of a regular icosahedron concentric with the central ball. However, these 12 outer balls do not kiss each other and may all moved freely. So perhaps if you moved all of them to one side a 13th ball would possibly fit in?

This problem was the subject of a famous discussion between Isaac Newton and David Gregory in 1694. (May 4, 1694; see [34] for details of this discussion.) It is commonly said that Newton believed the answer was 12 balls, while Gregory thought that 13 might be possible. However, Bill Casselman [9] found some puzzling features in this story.

The Newton-Gregory problem is often called the *thirteen spheres problem*. R. Hoppe [19] thought he had solved the problem in 1874. But, Thomas Hales

*Institute for Mathematical Study of Complex Systems, Moscow State University, Russia
omusin@gmail.com

[18] in 1994 published analysis of Hoppe's mistake (see also [33]). It appears that the first complete correct proof of this was published in 1953 by Schütte and van der Waerden [32]. A subsequent two-pages sketch of a proof was given by Leech [23] in 1956. (Leech's proof was presented in the first edition of the well known book by Aigner & Ziegler [1], the authors removed this chapter from the second edition because a complete proof includes too much spherical trigonometry.) The thirteen spheres problem continues to be of interest, new proofs have been published in the last few years by Wu-Yi Hsiang [21], Hiroshi Maehara [25], Károly Böröczky [7], and Kurt Anstreicher [2].

Note that $k(4) \geq 24$. Indeed, the unit sphere in \mathbf{R}^4 centered at $(0, 0, 0, 0)$ has 24 unit spheres around it, centered at the points $(\pm\sqrt{2}, \pm\sqrt{2}, 0, 0)$, with any choice of signs and any ordering of the coordinates. The convex hull of these 24 points yields a famous 4-dimensional regular polytope - the "24-cell". Its facets are 24 regular octahedra.

H.S.M. Coxeter proposed upper bounds on $k(n)$ in 1963 [11]; for $n = 4, 5, 6, 7$, and 8 these bounds were 26, 48, 85, 146, and 244, respectively. Coxeter's bounds are based on the conjecture that equal size spherical caps on a sphere can be packed no denser than packing where the Delaunay triangulation with vertices at the centers of caps consists of regular simplices. K. Böröczky proved this conjecture in 1978 [6].

The main progress in the kissing number problem in high dimensions was made in the end of 1970's. Vladimir Levenshtein [24], and independently Andrew Odlyzko and N.J.A. Sloane [28] (= [10, Chap.13]) using Delsarte's method in 1979 proved that $k(8) = 240$, and $k(24) = 196560$. This proof is surprisingly short, clean, and technically easier than all proofs in three dimensions.

However, $n = 8, 24$ are the only dimensions in which this method gives a precise result. For other dimensions (for instance, $n = 3, 4$) the upper bounds exceed the lower. In [28] the Delsarte method was applied in dimensions up to 24 (see [10, Table 1.5]). For comparison with the values of Coxeter's bounds on $k(n)$ for $n = 4, 5, 6, 7$, and 8 this method gives 25, 46, 82, 140, and 240, respectively. (For $n = 3$ Coxeter's and Delsarte's methods only gave $k(3) \leq 13$ [11, 28].) Kabatiansky and Levenshtein have found an asymptotic upper bound $2^{0.401n(1+o(1))}$ for $k(n)$ in 1978 [22]. The lower bound $2^{0.2075n(1+o(1))}$ was found in [35].

Improvements in the upper bounds on kissing numbers (for $n < 24$) were rather weak during next years ([10, Preface to Third Edition] gives a brief review and references). Arestov and Babenko [3] proved that the bound $k(4) \leq 25$ cannot be improved using Delsarte's method. Hsiang [20] claims a proof of $k(4) = 24$. His work has not received yet a positive peer review.

If M unit spheres kiss the unit sphere in \mathbf{R}^n , then the set of kissing points is an arrangement on the central sphere such that the (Euclidean) distance between any two points is at least 1. So the kissing number problem can be stated in other way: How many points can be placed on the surface of \mathbf{S}^{n-1} so that the angular separation between any two points is at least 60° ?

This leads to an important generalization: a finite subset X of \mathbf{S}^{n-1} is called a *spherical z -code* if for every pair (x, y) of X the scalar product $x \cdot y \leq z$. Spheri-

cal codes have many applications. The main application outside mathematics is in the design of signals for data transmission and storage. There are interesting applications to the numerical evaluation of n -dimensional integrals [10, Chap.3].

The Delsarte method (also known in coding theory as Delsarte's linear programming method, Delsarte's scheme, polynomial method) is described in [10, 22].¹ Let $f(t)$ be a real polynomial such that $f(t) \leq 0$ for $t \in [-1, z]$, the coefficients c_k 's in the expansion of $f(t)$ in terms of Gegenbauer polynomials $G_k^{(n)}$ are nonnegative, and $c_0 = 1$. Then the maximal number of points in a spherical z -code in \mathbf{S}^{n-1} is bounded by $f(1)$. Suitable coefficients c_k 's can be found by the linear programming method [10, Chapters 9,13].

In this paper we present an extension of the Delsarte method that allowed to prove the bound $k(4) < 25$, i.e. $k(4) = 24$. This extension yields also a proof for $k(3) < 13$ [27]. The first version of these proofs used a numerical solution of some nonconvex constrained optimization problems [26] (see also [29]). Now, using geometric approach, we reduced it to relatively simple computations.

2 Delsarte's method

Let $X = \{x_1, x_2, \dots, x_M\}$ be any finite subset of the unit sphere $\mathbf{S}^{n-1} \subset \mathbf{R}^n$, $\mathbf{S}^{n-1} = \{x : x \in \mathbf{R}^n, x \cdot x = \|x\|^2 = 1\}$. From here on we will speak of $x \in \mathbf{S}^{n-1}$ alternatively of points in \mathbf{S}^{n-1} or of vectors in \mathbf{R}^n .

By $\phi_{i,j}$ we denote the spherical (angular) distance between x_i, x_j . Note that for $X \subset \mathbf{S}^{n-1}$, $\cos \phi_{i,j} = x_i \cdot x_j$. It is clear that for any real numbers u_1, u_2, \dots, u_M the relation

$$\left\| \sum u_i x_i \right\|^2 = \sum_{i,j} \cos \phi_{i,j} u_i u_j \geq 0$$

holds, or equivalently the Gram matrix $\text{Gram}(X)$ is positive semidefinite, where $\text{Gram}(X) = (x_i \cdot x_j) = (\cos \phi_{i,j})$.

Schoenberg [30] extended this property to Gegenbauer polynomials $G_k^{(n)}$. He proved that if $g_{i,j} = G_k^{(n)}(\cos \phi_{i,j})$, then the matrix $(g_{i,j})$ is positive semidefinite. Schoenberg proved also that the converse holds: if $f(t)$ is a real polynomial and for any finite $X \subset \mathbf{S}^{n-1}$ the matrix $(f(\cos \phi_{i,j}))$ is positive semidefinite, then $f(t)$ is a linear combination of $G_k^{(n)}(t)$ with nonnegative coefficients.

Let us recall the definition of Gegenbauer polynomials. Suppose $C_k^{(n)}(t)$ be the polynomials defined by the expansion

$$(1 - 2rt + r^2)^{1-n/2} = \sum_{k=0}^{\infty} r^k C_k^{(n)}(t).$$

Then the polynomials $G_k^{(n)}(t) = C_k^{(n)}(t)/C_k^{(n)}(1)$ are called *Gegenbauer* or *ultraspherical* polynomials. (So the normalization of $G_k^{(n)}$ is determined by the condition $G_k^{(n)}(1) = 1$.)

¹See also Pfender & Ziegler [29] for a beautiful exposition.

Also the Gegenbauer polynomials $G_k^{(n)}$ can be defined by recurrence formula:

$$G_0^{(n)} = 1, \quad G_1^{(n)} = t, \quad \dots, \quad G_k^{(n)} = \frac{(2k+n-4)t G_{k-1}^{(n)} - (k-1) G_{k-2}^{(n)}}{k+n-3}$$

They are orthogonal on the interval $[-1, 1]$ with respect to the weight function $\rho(t) = (1-t^2)^{(n-3)/2}$ (see details in [8, 10, 16, 30]). In the case $n = 3$, $G_k^{(n)}$ are Legendre polynomials P_k , and $G_k^{(4)}$ are Chebyshev polynomials of the second kind (but with a different normalization than usual, $U_k(1) = 1$),

$$G_k^{(4)}(t) = U_k(t) = \frac{\sin((k+1)\phi)}{(k+1)\sin\phi}, \quad t = \cos\phi, \quad k = 0, 1, 2, \dots$$

For instance, $U_0 = 1$, $U_1 = t$, $U_2 = (4t^2 - 1)/3$, $U_3 = 2t^3 - t$, $U_4 = (16t^4 - 12t^2 + 1)/5$, \dots , $U_9 = (256t^9 - 512t^7 + 336t^5 - 80t^3 + 5t)/5$.

Let us now prove the bound of Delsarte's method. If a matrix $(g_{i,j})$ is positive semidefinite, then the sum of all its entries is nonnegative. Therefore, for $g_{i,j} = G_k^{(n)}(t_{i,j})$, $t_{i,j} := \cos\phi_{i,j}$, we have

$$\sum_{i=1}^M \sum_{j=1}^M G_k^{(n)}(t_{i,j}) \geq 0 \quad (2.1)$$

Suppose

$$f(t) = c_0 G_0^{(n)}(t) + \dots + c_d G_d^{(n)}(t), \quad \text{where } c_0 \geq 0, \dots, c_d \geq 0. \quad (2.2)$$

Let

$$S(X) = \sum_{i=1}^M \sum_{j=1}^M f(t_{i,j}).$$

Using (2.1), we get

$$S(X) = \sum_{k=0}^d \sum_{i=1}^M \sum_{j=1}^M c_k G_k^{(n)}(t_{i,j}) \geq \sum_{i=1}^M \sum_{j=1}^M c_0 G_0^{(n)}(t_{i,j}) = c_0 M^2. \quad (2.3)$$

Let $X = \{x_1, \dots, x_M\} \subset \mathbf{S}^{n-1}$ be a spherical z -code, i.e. for all $i \neq j$, $t_{i,j} = \cos\phi_{i,j} = x_i \cdot x_j \leq z$, i.e. $t_{i,j} \in [-1, z]$ (but $t_{i,i} = 1$). Suppose

$$f(t) \leq 0 \quad \text{for all } t \in [-1, z],$$

then $f(t_{i,j}) \leq 0$ for all $i \neq j$. That implies

$$S(X) = Mf(1) + 2f(t_{1,2}) + \dots + 2f(t_{M-1,M}) \leq Mf(1).$$

If we combine this with (2.3), then for $c_0 > 0$ we get

$$M \leq \frac{f(1)}{c_0} \quad (2.4)$$

The inequality (2.4) play a crucial role in the Delsarte method (see details in [3, 4, 5, 10, 14, 15, 22, 24, 28]). If $z = 1/2$ and $c_0 = 1$, then (2.4) implies

$$k(n) \leq f(1).$$

V.I. Levenshtein [24], and independently A.M. Odlyzko and N.J.A. Sloane [28] have found suitable polynomials $f(t)$ ($f(t) \leq 0$ for all $t \in [-1, 1/2]$), f satisfies (2.2), $c_0 = 1$) with

$$f(1) = 240 \text{ for } n = 8; \quad \text{and} \quad f(1) = 196560 \text{ for } n = 24.$$

Then

$$k(8) \leq 240, \quad k(24) \leq 196560.$$

For $n = 8, 24$ sphere packings: E_8 and Leech lattice give these kissing numbers. Thus $k(8) = 240$, and $k(24) = 196560$.

When $n = 4$, a polynomial f of degree 9 with $f(1) \approx 25.5585$ was found in [28]. This implies $24 \leq k(4) \leq 25$.

3 An extension of Delsarte's method.

Let us now generalize the Delsarte bound $M \leq f(1)/c_0$.

Definition. Let $f(t)$ be a real function on the interval $[-1, 1]$. Consider on \mathbf{S}^{n-1} points y_0, y_1, \dots, y_m such that

$$y_i \cdot y_j \leq z \text{ for all } i \neq j, \quad f(y_0 \cdot y_i) > 0 \text{ for } 1 \leq i \leq m. \quad (3.1)$$

For fixed y_0 denote by $Q_m(y_0)$ the set of all $Y = \{y_1, \dots, y_m\}$ such that Y satisfies (3.1). Let $\mu = \mu(n, z, f)$ be the highest value of m with $Q_m(y_0) \neq \emptyset$, i.e. the constraints (3.1) define a non-empty set Y .

Suppose $0 \leq m \leq \mu$,

$$H(y_0; Y) = H(y_0; y_1, \dots, y_m) := f(1) + f(y_0 \cdot y_1) + \dots + f(y_0 \cdot y_m),$$

$$h_m = h_m(n, z, f) := \max_{Y \in Q_m(y_0)} \{H(y_0; Y)\},$$

$$h_{max} := \max \{h_0, h_1, \dots, h_\mu\}.$$

Theorem 1. Suppose $X \subset \mathbf{S}^{n-1}$ is a spherical z -code, $|X| = M$, and $f(t) = c_0 G_0^{(n)}(t) + \dots + c_d G_d^{(n)}(t)$ with $c_0 > 0$, $c_1 \geq 0, \dots, c_d \geq 0$. Then

$$M \leq \frac{h_{max}}{c_0} = \frac{1}{c_0} \max \{h_0, h_1, \dots, h_\mu\}.$$

Proof. By assumption f satisfies (2.2), then (2.3) yields $S(X) \geq c_0 M^2$.

Let $J(i) := \{j : f(x_i \cdot x_j) > 0, j \neq i\}$, and $X(i) = \{x_j : j \in J(i)\}$. Then

$$S_i(X) := \sum_{j=1}^M f(x_i \cdot x_j) \leq f(1) + \sum_{j \in J(i)} f(x_i \cdot x_j) = H(x_i; X(i)) \leq h_{max},$$

so then

$$S(X) = \sum_{i=1}^M S_i(X) \leq M h_{max}.$$

We have $c_0 M^2 \leq S(X) \leq M h_{max}$, i.e. $c_0 M \leq h_{max}$ as required. \square

Note that $h_0 = f(1)$. If $f(t) \leq 0$ for all $t \in [-1, z]$, then $\mu(n, z, f) = 0$, i.e. $h_{max} = h_0 = f(1)$. Therefore, this theorem yields the Delsarte bound $M \leq f(1)/c_0$.

The problem of evaluating of h_{max} in general case looks even more complicated than the upper bound problem for spherical z -codes. It is not clear how to find μ , what is an optimal arrangement for Y ?

Here we consider this problem only for a very restrictive class of functions

$$f(t) : f(t) \leq 0 \text{ for } t \in [-t_0, z], \quad 1 > t_0 > z \geq 0.$$

For these functions the assumption on f , $f(y_0 \cdot y_i) > 0$, for Y that satisfies (3.1), holds only if

$$\theta_i := \text{dist}(e_0, y_i) < \theta_0 = \arccos t_0,$$

where $e_0 = -y_0$ is the antipodal point to y_0 . In other words, Y lies in the spherical cap $C(e_0, \theta_0)$ of center e_0 and radius θ_0 . This assumption derives convexity condition for Y .

Theorem 2. *Suppose $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$ is a spherical z -code, Y belongs to the spherical cap $C(e_0, \theta_0)$, and $\theta_0 < \psi = \arccos z \leq 90^\circ$. Denote by Δ_m the convex hull of Y in \mathbf{S}^{n-1} . Then any y_k is a vertex of Δ_m , i.e. $\Delta_m^0 = Y$.*

(A subset of \mathbf{S}^{n-1} is called (spherical) *convex* if it contains, with every two nonantipodal points, the small arc of the great circle containing them. The closure of a convex set is convex and is the intersection of closed hemispheres (see details in [13]). If a subset Y of \mathbf{S}^{n-1} lies in a hemisphere, then the convex hull of Y is well defined, and is the intersection of all convex sets containing Y .)

Proof. In this paper we need the only one fact from spherical trigonometry, namely the *law of cosines*:

$$\cos \phi = \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos \varphi,$$

where for spherical triangle ABC the angular lengths of its sides are $\text{dist}(A, B) = \theta_1$, $\text{dist}(A, C) = \theta_2$, $\text{dist}(B, C) = \phi$, and $\angle BAC = \varphi$.

By assumption

$$\theta_k = \text{dist}(y_k, e_0) \leq \theta_0 < \psi, \quad 1 \leq k \leq m; \quad \phi_{k,j} := \text{dist}(y_k, y_j) \geq \psi, \quad k \neq j.$$

Let us prove that there are no y_k inside Δ_m . Assume the converse. Then consider the great $(n-2)$ -sphere Ω_k such that $y_k \in \Omega_k$, and Ω_k is orthogonal to the arc $e_0 y_k$. (Note that $\theta_k > 0$. Conversely, $y_k = e_0$ and $\phi_{k,j} = \theta_j \leq \theta_0 < \psi$.)

The great sphere Ω_k divides \mathbf{S}^{n-1} into two hemispheres: H_1 and H_2 . Suppose $e_0 \in H_1$, then at least one y_j belongs H_2 . Consider the triangle $e_0 y_k y_j$ and denote by $\gamma_{k,j}$ the angle $\angle e_0 y_k y_j$ in this triangle. The law of cosines yields

$$\cos \theta_j = \cos \theta_k \cos \phi_{kj} + \sin \theta_k \sin \phi_{k,j} \cos \gamma_{k,j}$$

Since $y_j \in H_2$, we have $\gamma_{k,j} > 90^\circ$, and $\cos \gamma_{k,j} < 0$ (Fig. 1). Therefore,

$$\cos \theta_j < \cos \phi_k \cos \phi_{k,j} < \cos \phi_{k,j} \leq \cos \psi,$$

then $\theta_j > \psi$ – a contradiction. \square

Now we show how to determine μ in our case. Denote by $A(n, \psi)$ the maximal size of a spherical n -dimensional z -code. (Here as above $\cos \psi = z$.) Note that $A(n, 60^\circ)$ is the kissing number $k(n)$.

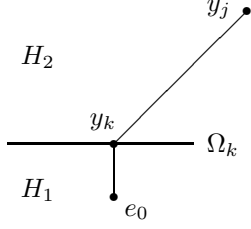


Fig. 1

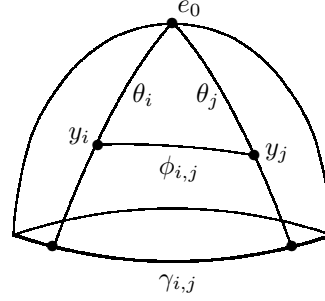


Fig. 2

Theorem 3. Suppose $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$ is a spherical z -code, $m \geq 2$, and Y lies in the spherical cap of center e_0 and radius θ_0 , where $t_0 = \cos \theta_0 \geq z$. Then

$$m \leq A\left(n-1, \arccos \frac{z - t_0^2}{1 - t_0^2}\right)$$

Proof. We have $\phi_{i,j} \geq \psi = \arccos z$, $i \neq j$; $\theta_i \leq \theta_0$, $1 \leq i \leq m$; and $\theta_0 \leq \psi$.

Let Π be the projection of Y onto equator \mathbf{S}^{n-2} from the pole e_0 . Denote by $\gamma_{i,j}$ the distances between points of Π in \mathbf{S}^{n-2} (Fig. 2). Then from the law of cosines and the inequality $\cos \phi_{i,j} \leq z$, we get

$$\cos \gamma_{i,j} = \frac{\cos \phi_{i,j} - \cos \theta_i \cos \theta_j}{\sin \theta_i \sin \theta_j} \leq \frac{z - \cos \theta_i \cos \theta_j}{\sin \theta_i \sin \theta_j}$$

$$\text{Let } Q(\alpha) = \frac{z - \cos \alpha \cos \beta}{\sin \alpha \sin \beta}, \text{ then } Q'(\alpha) = \frac{\cos \beta - z \cos \alpha}{\sin^2 \alpha \sin \beta}.$$

From this follows, if $0 < \alpha, \beta \leq \theta_0$, then $\cos \beta \geq z$ (because $\theta_0 \leq \psi$); so then $Q'(\alpha) \geq 0$, and $Q(\alpha) \leq Q(\theta_0)$. Therefore,

$$\cos \gamma_{i,j} \leq \frac{z - \cos \theta_i \cos \theta_j}{\sin \theta_i \sin \theta_j} \leq \frac{z - \cos^2 \theta_0}{\sin^2 \theta_0} = \frac{z - t_0^2}{1 - t_0^2}.$$

This completes the proof. \square

Corollary 1. *Suppose $f(t) \leq 0$ for $t \in [-t_0, z]$, $1 > t_0 \geq z \geq 0$. If $2t_0^2 \leq z + 1$, then*

$$\mu(n, z, f) \leq A\left(n - 1, \arccos \frac{z - t_0^2}{1 - t_0^2}\right),$$

otherwise $\mu(n, z, f) = 1$.

Proof. $2t_0^2 > z + 1$ if and only if $\psi > 2\theta_0$. Clearly that in this case the size of any z -code in the cap $C(e_0, \theta_0)$ is at most 1. In the other case $\mu \geq 2$ and it follows from Theorem 3. \square

Corollary 2. *Suppose $f(t) \leq 0$ for $t \in [-t_0, z]$, $1 > t_0 \geq z \geq 0$. Then*

$$\mu(3, z, f) \leq 5.$$

Proof. Note that

$$T = \frac{z - t_0^2}{1 - t_0^2} \leq \frac{z - z^2}{1 - z^2} = \frac{z}{1 + z} < \frac{1}{2}. \quad \text{Then } \delta = \arccos T > 60^\circ.$$

Thus $\mu(3, z, f) \leq A(2, \delta) \leq 360^\circ/\delta < 6$. \square

Corollary 3. *Suppose $f(t) \leq 0$ for $t \in [-t_0, z]$, $1 > t_0 > z \geq 0$.*

(i) *If $t_0 > \sqrt{z}$, then $\mu(4, z, f) \leq 4$.*

(ii) *If $z = 1/2$, $t_0 \geq 0.6058$, then $\mu(4, z, f) \leq 6$.*

Proof. Denote by $\varphi_k(M)$ the largest angular separation that can be attained in a spherical code on \mathbf{S}^{k-1} containing M points. In three dimensions the best codes and the values $\varphi_3(M)$ presently known for $M \leq 12$ and $M = 24$ (see [12, 17, 31]). Schütte and van der Waerden [31] proved that

$$\varphi_3(5) = \varphi_3(6) = 90^\circ, \quad \cos \varphi_3(7) = \cot 40^\circ \cot 80^\circ, \quad \varphi_3(7) \approx 77.86954^\circ.$$

(i) Since $z - t_0^2 < 0$, Corollary 1 yields: $\mu(4, z, f) \leq A(3, \delta)$, where $\delta > 90^\circ$. We have $\delta > \varphi_3(5)$. Thus $\mu < 5$.

(ii) Note that for $t_0 \geq 0.6058$,

$$\arccos \frac{1/2 - t_0^2}{1 - t_0^2} > 77.87^\circ.$$

So Corollary 1 implies $\mu(4, 1/2, f) \leq A(3, 77.87^\circ)$. Since $77.87^\circ > \varphi_3(7)$, we have $A(3, 77.87^\circ) < 7$, i.e. $\mu \leq 6$. \square

Corollary 1 shows that if t_0 is close enough to 1, then μ is small enough. Then one gets relatively small - dimensional optimization problems for computation of numbers h_m for small n . If additionally $f(t)$ is a monotone decreasing function on $[-1, -t_0]$, then these problems can be reduced to low-dimensional optimization problems of a type that can be easily treated numerically.

4 Optimal and irreducible sets

In this section we consider $f(t)$ that satisfies the monotonicity assumption:

$f(t)$ is a monotone decreasing function on the interval $[-1, -t_0]$,

$$f(t) \leq 0 \text{ for } t \in [-t_0, z], \quad 1 > t_0 > z \geq 0 \quad (*)$$

Consider a spherical z -code $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$ such that Y lies in a spherical cap $C(e_0, \theta_0)$ of center e_0 and radius θ_0 with $\theta_0 < \psi = \arccos z \leq 90^\circ$. As above, $\theta_k = \text{dist}(y_k, e_0)$, $\phi_{i,j} = \text{dist}(y_i, y_j)$, Δ_m is the convex hull of Y in \mathbf{S}^{n-1} , $\cos \theta_0 = t_0$, and $y_0 = -e_0$. Then $H(y_0; Y)$ is represented in the form:

$$F(\theta_1, \dots, \theta_m) := H(y_0; Y) = f(1) + f(-\cos \theta_1) + \dots + f(-\cos \theta_m). \quad (4.1)$$

Since Y is a z -code, we have the constraint $\phi_{i,j} \geq \psi$ for all $i \neq j$. Denote by $\Gamma_\psi(Y)$ the graph with the set of vertices Y and the set of edges $y_i y_j$ such that $\phi_{i,j} = \psi$.

Definition. We say that a spherical z -code Y , $|Y| = m$, in a spherical cap $C(e_0, \theta_0) \subset \mathbf{S}^{n-1}$, $\theta_0 < \psi \leq 90^\circ$, is *optimal for f* if $H(y_0; Y) = h_m$. If optimal Y is not unique up to isometry, then we call Y as optimal if the graph $\Gamma_\psi(Y)$ has the maximal number of edges.

Let us call a spherical z -code Y in a cap $C(e_0, \theta_0) \subset \mathbf{S}^{n-1}$ as *irreducible* if there are no points $y_i \in Y$ can be shifted towards e_0 (i.e. this shift decreases θ_i) such that Y' , what is obtained after this shifting, is also a z -code. As above, in the case when irreducible Y is not defined uniquely up to isometry by θ_i , we say that Y is irreducible if the graph $\Gamma_\psi(Y)$ has the maximal number of edges.

Proposition 1. *Suppose $f(t)$ satisfies the monotonicity assumption (*). If Y is optimal for f , then Y is irreducible.*

Proof. Since (4.1), we have that the function $F(\theta_1, \dots, \theta_m)$ increases whenever θ_k decreases. From this follows that no y_k can be shifted towards e_0 . In the converse case, $H(y_0; Y)$ increases whenever y_k tends to e_0 . It contradicts the optimality of the initial set Y . \square

Lemma 1. *If Y is irreducible, then*

- (i) $e_0 \in \Delta_m = \text{conv } Y$;
- (ii) If $m > 1$, then $\deg y_i > 0$ for all $y_i \in Y$, where by $\deg y_i$ denoted the degree of the vertex y_i in the graph $\Gamma_\psi(Y)$.

Proof. (i) Otherwise whole Y can be shifted to e_0 .

- (ii) Indeed, if $\phi_{i,j} > \psi$ for all $j \neq i$, then y_i can be shifted towards e_0 . \square

For $m = 1$ from this follows that $e_0 = y_1$. Thus

$$h_1 = f(1) + f(-1). \quad (4.2)$$

For $m = 2$, Lemma 1 implies that $\phi_{1,2} = \psi$, i.e. $\Delta_2 = y_1y_2$ is an arc of length ψ .

Consider $\Delta_m \subset \mathbf{S}^{n-1}$ of dimension k , $\dim \Delta_m = k$. Since Δ_m is a convex set, there exists the great k -dimensional sphere \mathbf{S}^k in \mathbf{S}^{n-1} containing Δ_m .

Note that if $\dim \Delta_m = 1$, then $m = 2$. Indeed, since $\dim \Delta_m = 1$, it follows that Y belongs to the great circle \mathbf{S}^1 . It is clear that in this case $m = 2$. (For instance, $m > 2$ contradicts Theorem 2 for $n = 2$.)

To prove our main results in this section for $n = 3, 4$ we need the following fact. (For $n = 3$, when Δ is an arc, a proof of this claim is trivial.)

Lemma 2. *Consider in \mathbf{S}^{n-1} an arc ω and a regular simplex Δ , both are with edge lengths ψ , $\psi \leq 90^\circ$. Suppose the intersection of ω and Δ is not empty. Then at least one of the distances between vertices of ω and Δ is less than ψ .*

Proof. We have $\omega = u_1u_2$, $\Delta = v_1v_2 \dots v_k$, $\text{dist}(u_1, u_2) = \text{dist}(v_i, v_j) = \psi$.

Assume the converse. Then $\text{dist}(u_i, v_j) \geq \psi$ for all i, j . By U denote the union of the spherical caps of centers v_i , $i = 1, \dots, k$, and radius ψ . Let B be the boundary of U . Note that u_1 and u_2 don't lie inside U . If $\{u'_1, u'_2\} = \omega \cap B$, then $\psi = \text{dist}(u_1, u_2) \geq \text{dist}(u'_1, u'_2)$, and $\omega' \cap \Delta \neq \emptyset$, where $\omega' = u'_1u'_2$.

We have the following optimization problem: to find an arc w_1w_2 of minimal length subject to the constraints $w_1, w_2 \in B$, and $w_1w_2 \cap \Delta \neq \emptyset$? It is not hard to prove that $\text{dist}(w_1, w_2)$ attains its minimum when w_1 and w_2 are at the distance of ψ from all v_i , i.e. $w_1v_1 \dots v_k$ and $w_2v_1 \dots v_k$ are regular simplices with the common facet Δ . Using this, it can be shown by direct calculation that

$$\cos \alpha = \frac{2kz^2 - (k-1)z - 1}{1 + (k-1)z}, \quad \alpha = \min \text{dist}(w_1, w_2), \quad z = \cos \psi \quad (4.3)$$

We have $\alpha \leq \psi$. From (4.3) follows that $\cos \alpha \geq z$ if and only if $z \geq 1$ or $(k+1)z + 1 \leq 0$. It contradicts the assumption $0 \leq z < 1$. \square

Now we consider irreducible sets in three dimensions. In this case $\dim \Delta_m \leq 2$.

Theorem 4. *Suppose Y is irreducible and $\dim(\Delta_m) = 2$.*

Then $3 \leq m \leq 5$, and Δ_m is a spherical regular triangle, rhomb, or equilateral pentagon with edge lengths ψ .

Proof. From Corollary 2 follows that $m \leq 5$. On the other hand, $m > 2$. Then $m = 3, 4, 5$. Theorem 2 implies that Δ_m is a convex polygon. From Lemma 1 it follows that $e_0 \in \Delta_m$, and $\deg y_i \geq 1$.

First let us prove that if $\deg y_i \geq 2$ for all i , then Δ_m is equilateral m -gon with edge lengths ψ . Indeed, it is clear for $m = 3$.

Lemma 2 implies that two diagonals of Δ_m of lengths ψ do not intersect each other. That yields the proof for $m = 4$. When $m = 5$, it remains to consider the case where Δ_5 consists of two regular non overlapping triangles

with a common vertex (Fig. 3). This case contradicts the convexity of Δ_5 . Indeed, $\angle y_i y_1 y_j > 60^\circ$ (see the proof of Corollary 2), then

$$180^\circ \geq \angle y_2 y_1 y_5 = \angle y_2 y_1 y_3 + \angle y_3 y_1 y_4 + \angle y_4 y_1 y_5 > 180^\circ$$

- a contradiction.

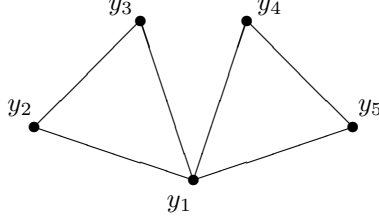


Fig. 3

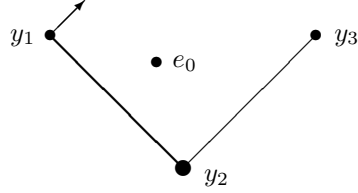


Fig. 4

Now we prove that $\deg y_i \geq 2$. Suppose $\deg y_1 = 1$, i.e. $\phi_{1,2} = \psi$, $\phi_{1,i} > \psi$ for $i = 3, \dots, m$. If $e_0 \notin y_1 y_2$, then after sufficiently small turn of y_1 round y_2 to e_0 (Fig. 4) the distance θ_1 decreases - a contradiction. (This turn will be considered in Lemma 3 with more details.)

It remains to consider the case: $e_0 \in y_1 y_2$. If $\phi_{i,j} = \psi$ where $i > 2$ or $j > 2$, then $e_0 \notin y_i y_j$. Indeed, in the converse case, we have two intersecting diagonals of lengths ψ . Therefore, $\deg y_i \geq 2$ for $2 < i \leq m$. For $m = 3, 4$ it implies the proof. For $m = 5$ there is the case where $Q_3 = y_3 y_4 y_5$ is a regular triangle of side length ψ . Note that $y_1 y_2$ cannot intersect Q_3 (otherwise we again have intersecting diagonals of lengths ψ), then $y_1 y_2$ is a side of Δ_5 . In this case, as above, after sufficiently small turn of Q_3 round y_2 to e_0 the distance θ_i , $i = 3, 4, 5$, decreases - a contradiction. \square

Now we extend these results to four dimensions.²

Let us consider a rotation $R(\varphi, \Omega)$ on \mathbf{S}^{n-1} about an $(n-3)$ - dimensional great sphere Ω in \mathbf{S}^{n-1} . Without loss of generality, we may assume that

$$\Omega = \{\vec{u} = (u_1, \dots, u_n) \in \mathbf{R}^n : u_1 = u_2 = 0, u_1^2 + \dots + u_n^2 = 1\}.$$

²In the first version of this paper for $m \geq n$ has been claimed that any vertex of $\Gamma_\psi(Y)$ has degree at least $n-1$. However, E. Bannai, M. Tagami, and referees of this paper found some gaps in our exposition. Most of them are related to “degenerated” configurations. In this paper we need only the case $n = 4, m < 6$. For this case E. Bannai and M. Tagami verified each step of our proof, considered all “degenerated” configurations, and finally gave clean and detailed proof (see E. Bannai and M. Tagami: On optimal sets in Musin’s paper “The kissing number in four dimensions” in the Proceedings of the COE Workshop on Sphere Packings, November 1-5, 2004, in Fukuoka Japan). I wish to thank Eiichi Bannai, Makoto Tagami, and anonymous referees for helpful and useful comments. Now this claim in general case can be considered only as conjecture.

Denote by $R(\varphi, \Omega)$ the rotation in the plane $\{u_i = 0, i = 3, \dots, n\}$ through an angle φ about the origin Ω :

$$u'_1 = u_1 \cos \varphi - u_2 \sin \varphi, \quad u'_2 = u_1 \sin \varphi + u_2 \cos \varphi, \quad u'_i = u_i, \quad i = 3, \dots, n.$$

Let

$$H_+ = \{\vec{u} \in \mathbf{S}^{n-1} : u_2 \geq 0\}, \quad H_- = \{\vec{u} \in \mathbf{S}^{n-1} : u_2 \leq 0\},$$

$$Q = \{\vec{u} \in \mathbf{S}^{n-1} : u_2 = 0, u_1 > 0\}, \quad \bar{Q} = \{\vec{u} \in \mathbf{S}^{n-1} : u_2 = 0, u_1 \geq 0\}.$$

Note that H_- and H_+ are closed hemispheres of \mathbf{S}^{n-1} , $\bar{Q} = Q \cup \Omega$, and \bar{Q} is a hemisphere of the unit sphere $\Omega_2 = \{\vec{u} \in \mathbf{S}^{n-1} : u_2 = 0\}$ bounded by Ω .

Lemma 3. *Consider two points y and e_0 in \mathbf{S}^{n-1} . Suppose $y \in Q$ and $e_0 \notin \bar{Q}$. If $e_0 \in H_+$, then any rotation $R(\varphi, \Omega)$ of y with sufficiently small positive φ decreases the distance between y and e_0 . If $e_0 \in H_-$, then any rotation $R(\varphi, \Omega)$ of y with sufficiently small negative φ decreases the distance between y and e_0 .*

Proof. Let y be rotated into the point $y(\varphi)$. If the coordinate expressions of y and e_0 are

$$y = (u_1, 0, u_3, \dots, u_n), \quad u_1 > 0; \quad e_0 = (v_1, v_2, \dots, v_n), \quad \text{then}$$

$$r(\varphi) := y(\varphi) \cdot e_0 = u_1 v_1 \cos \varphi + u_1 v_2 \sin \varphi + u_3 v_3 + \dots + u_n v_n.$$

Therefore, $r'(\varphi) = -u_1 v_1 \sin \varphi + u_1 v_2 \cos \varphi$, i.e. $r'(0) = u_1 v_2$. Then

$$r'(0) > 0 \quad \text{iff} \quad v_2 > 0, \quad \text{i.e.} \quad e_0 \in H_+;$$

$$r'(0) < 0 \quad \text{iff} \quad v_2 < 0 \quad \text{i.e.} \quad e_0 \in H_-.$$

That proves the lemma for $v_2 \neq 0$. In the case $v_2 = 0$, by assumption ($e_0 \notin \bar{Q}$) we have $v_1 < 0$. In this case $r'(0) = 0$, and $r''(0) = -u_1 v_1 > 0$, i.e. $\varphi = 0$ is a minimum point. This completes the proof. \square

Proposition 2. *Let Y be irreducible and $m = |Y| \geq n$. Suppose there are no closed great hemispheres \bar{Q} in \mathbf{S}^{n-1} such that \bar{Q} contains $n - 1$ points from Y and e_0 . Then any vertex of $\Gamma_\psi(Y)$ has degree at least $n - 1$.*

Proof. Without loss of generality, we may assume that

$$\phi_{1,i} = \psi, \quad i = 2, \dots, \deg y_1 + 1; \quad \phi_{1,i} > \psi, \quad i = \deg y_1 + 2, \dots, m.$$

Suppose $\deg y_1 < n - 1$. Then $\phi_{1,i} > \psi$ for $i = n, \dots, m$. Let us consider the great $(n - 3)$ -dimensional sphere Ω in \mathbf{S}^{n-1} that contains the points y_2, \dots, y_{n-1} . Then Lemma 3 implies that a rotation $R(\varphi, \Omega)$ of y_1 with sufficiently small φ decreases θ_1 . It contradicts the irreducibility of Y . \square

Proposition 3. *If Y is irreducible, $|Y| = n$, $\dim \Delta_n = n - 1$, then $\deg y_i = n - 1$ for all $i = 1, \dots, n$. In other words, Δ_n is a regular simplex of edge lengths ψ .*

Proof. Clearly, Δ_n is a spherical simplex. Denote by F_i its facets,

$$F_i := \text{conv} \{y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_n\}.$$

Let for $\sigma \subset I_m := \{1, \dots, m\}$

$$F_\sigma := \bigcap_{i \in \sigma} F_i.$$

We claim for $i \neq j$ that:

$$\text{If } e_0 \notin F_{\{i,j\}}, \text{ then } \phi_{i,j} = \psi. \quad (4.4)$$

Conversely, from Lemma 3 follows that there exists a rotation $R(\varphi, \Omega_{ij})$ of y_i (or y_j if $e_0 \in F_i$) decreases θ_i (respectively, θ_j), where Ω_{ij} is the great $(n-3)$ -dimensional sphere contains $F_{\{i,j\}}$. It contradicts the irreducibility assumption for Y .

This yields, if there is no pair $\{i, j\}$ such that $e_0 \in F_{\{i,j\}}$, then $\phi_{i,j} = \psi$ for all i, j from I_m .

Suppose $e_0 \in F_\sigma$, where σ has maximal size and $|\sigma| > 1$. Let $\bar{\sigma} = I_m \setminus \sigma$. From (4.4) follows that $\phi_{i,j} = \psi$ if $i \in \bar{\sigma}$ or $j \in \bar{\sigma}$. It remains to prove that $\phi_{i,j} = \psi$ for $i, j \in \sigma$.

Let Λ be the intersection of the spheres of centers y_i , $i \in \bar{\sigma}$, and radius ψ . Then Λ is a sphere in \mathbf{S}^{n-1} of dimension $|\sigma| - 1$. Note that all y_i , $i \in \sigma$, lie on Λ at the same distance from e_0 . It is clear that Y is irreducible if and only if y_i , $i \in \sigma$, on Λ are vertices of a regular simplex of edge length ψ .

Finally, we have that all edges of Δ_n are of lengths ψ as required. \square

Corollary 4. *If $n > 3$, then Δ_4 is a regular tetrahedron of edge lengths ψ .*

Proof. Let us show that $\dim \Delta_4 = 3$. In the converse case, $\dim \Delta_4 = 2$, and from Theorem 4 follows that Δ_4 is a rhomb. Suppose $y_1 y_3$ is the minimal length diagonal of Δ_4 . Then $\phi_{2,4} > \psi$ (see Lemma 2). Let us consider a sufficiently small turn of the facet $y_1 y_2 y_3$ round $y_1 y_3$. If $e_0 \notin y_1 y_3$, then this turn decreases either θ_4 (if $e_0 \in y_1 y_2 y_3$) or θ_2 , a contradiction. In the case $e_0 \in y_1 y_3$ any turn of y_2 round $y_1 y_3$ decreases $\phi_{2,4}$ and doesn't change θ_2 . Obviously, there is a turn such that $\phi_{2,4}$ becomes is equal to ψ . That contradicts the irreducibility of Y also. \square

Lemma 4. *If $Y \subset \mathbf{S}^3$ is irreducible, $|Y| = 5$, then $\deg y_i \geq 3$ for all i .*

Proof. (1) Let us show that $\dim \Delta_5 = 3$. In the converse case, $\dim \Delta_5 = 2$, and from Theorem 4 follows that Δ_5 is a convex equilateral pentagon. Suppose $y_1 y_3$ is the minimal length diagonal of Δ_5 . We have $\phi_{2,k} > \psi$ for $k > 3$. Suppose $e_0 \notin y_1 y_3$. If $e_0 \in y_1 y_2 y_3$ then any sufficiently small turn of the facet $y_1 y_2 y_3$ round $y_1 y_3$ decreases θ_4 and θ_5 , otherwise it decreases θ_2 , a contradiction. In the case $e_0 \in y_1 y_3$ any turn of y_2 round $y_1 y_3$ decreases $\phi_{2,k}$ for $k = 4, 5$, and

doesn't change θ_i . It can be shown in the elementary way that there is a turn such that $\phi_{2,4}$ or $\phi_{2,5}$ becomes is equal to ψ , a contradiction.

In three dimensions there exist only two combinatorial types of convex polytopes with 5 vertices: (A) and (B) (see Fig. 5). In the case (A) the arc y_3y_5 lies inside Δ_5 , and for (B): $y_2y_3y_4y_5$ is a facet of Δ_5 .

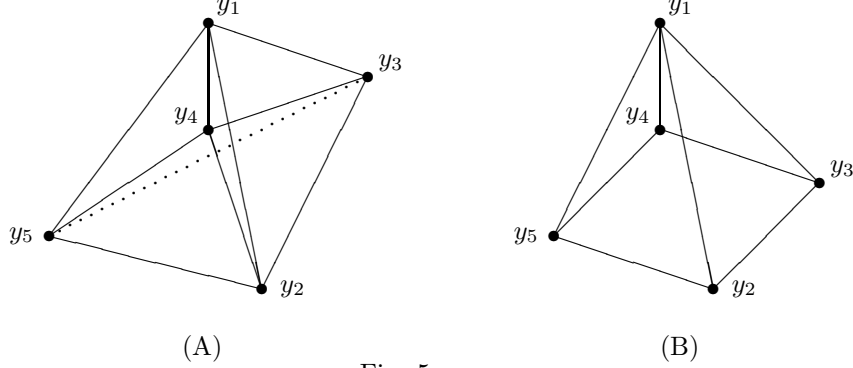


Fig. 5

(2) By s_{ij} we denote the arc y_iy_j , and by s_{ijk} denote the triangle $y_iy_jy_k$. Let \tilde{s}_{ijk} be the intersection of the great 2-hemisphere Q_{ijk} and Δ_5 , where Q_{ijk} contains y_i, y_j, y_k and bounded by the great circle passes through y_i, y_j . Proposition 2 yields: if there are no i, j, k such that $e_0 \in \tilde{s}_{ijk}$, then $\deg y_i \geq 3$ for all i .

It remains to consider all cases $e_0 \in \tilde{s}_{ijk}$. Note that for (A) $\tilde{s}_{ijk} \neq s_{ijk}$ only for three cases: $i = 1, 2, 4$; where $j = 3, k = 5$, or $j = 5, k = 3$ ($\tilde{s}_{i35} = \tilde{s}_{i53}$).

(3) Lemma 1 yields that $\deg y_k > 0$. Now we consider the cases $\deg y_k = 1, 2$.

If $\deg y_k = 1$, $\phi_{k,\ell} = \psi$, then $e_0 \in s_{k\ell}$.

Indeed, otherwise there exists the great circle Ω in \mathbf{S}^3 such that Ω contains y_ℓ , and the great sphere passes through Ω and y_k doesn't pass through e_0 . Then Lemma 3 implies that a rotation $R(\varphi, \Omega)$ of y_k with sufficiently small φ decreases θ_k - a contradiction.

Since $\theta_0 < \psi$, e_0 can not be a vertex of Δ_5 . Therefore, e_0 lies inside $s_{k\ell}$. From this follows if s_{ij} for any j doesn't intersect $s_{k\ell}$, then $\deg y_i \geq 2$.

Arguing as above it is easy to prove that

If $\deg y_k = 2$, $\phi_{k,i} = \phi_{k,j} = \psi$, then $e_0 \in \tilde{s}_{ijk}$.

(4) Now we prove that $\deg y_k \geq 2$ for all k . Conversely, $\deg y_k = 1$, $e_0 \in s_{k\ell}$.

a). First we consider the case when $s_{k\ell}$ is an "external" edge of Δ_5 . For the type (A) that means $s_{k\ell}$ differs from s_{35} , and for (B) it is not s_{35} or s_{24} . Since Δ_5 is convex, there exists the great 2-sphere Ω_2 passes through y_k, y_ℓ such that 3 other points y_i, y_j, y_q lie inside the hemisphere H_+ bounded by Ω_2 . Let Ω be the great circle in Ω_2 that contains y_ℓ and is orthogonal to the arc $s_{k\ell}$. Then (Lemma 3) there exists a small turn of y_i, y_j, y_q round Ω that simultaneously decreases $\theta_i, \theta_j, \theta_q$ - a contradiction.

b). For the type (A) when $\deg y_3 = 1$, $\phi_{3,5} = \psi$, $e_0 \in s_{35}$; we claim that s_{124} is a regular triangle with side length ψ . Indeed, from (3) follows that $\deg y_i \geq 2$ for $i = 1, 2, 4$. Moreover, if $\deg y_i = 2$, then $e_0 = s_{35} \cap s_{124}$. Therefore, in any case, $\phi_{1,2} = \phi_{1,4} = \phi_{2,4} = \psi$. We have the arc s_{35} and the regular triangle s_{124} , both are with edge lengths ψ . Then from Lemma 2 follows that some $\phi_{i,j} < \psi$ - a contradiction.

c). Now for the type (B) consider the case: $\deg y_3 = 1$, $\phi_{3,5} = \psi$, $e_0 \in s_{35}$. Then for y_2 we have: $\deg y_2 = 1$ only if $\phi_{2,4} = \psi$, $e_0 = s_{24} \cap s_{35}$; $\deg y_2 = 2$ only if $\phi_{2,4} = \phi_{2,5} = \psi$; and $\phi_{2,4} = \phi_{1,2} = \phi_{2,5} = \psi$ if $\deg y_2 = 3$. Thus, in any case, $\phi_{2,4} = \psi$. We have two intersecting diagonals s_{24}, s_{35} of lengths ψ . Then Lemma 2 contradicts the assumption that Y is a z -code. This contradiction concludes the proof that $\deg y_k \geq 2$ for all k .

(5) Finally let us prove that $\deg y_k \geq 3$ for all k . Assume the converse. Then $\deg y_k = 2$, $e_0 \in \tilde{s}_{ijk}$, where $\phi_{k,i} = \phi_{k,j} = \psi$.

Case facet: Let s_{ijk} be a facet of Δ_5 , and $e_0 \notin s_{ij}$. By the same argument as in (4a), where Ω_2 be the great sphere contains s_{ijk} , and Ω be the great circle passes through y_i, y_j , we can prove that there exists a shift decreases θ_ℓ, θ_q for two other points y_ℓ, y_q from Y , a contradiction.

If $e_0 \in s_{ij}$, then any turn of $s_{\ell q}$ round Ω doesn't change θ_ℓ and θ_q . However, if this turn is in a positive direction, then it decreases $\phi_{k,\ell}$ and $\phi_{k,q}$. Clearly, there exists a turn when $\phi_{k,\ell}$ or $\phi_{k,q}$ is equal to ψ - a contradiction.

It remains to consider all cases where s_{ijk} is not a facet. Namely, there are the following cases: s_{124}, s_{135} (type (A)), s_{234} (type (B)).

Case s_{124} : We have $\deg y_1 = 2$, $\phi_{1,2} = \phi_{1,4} = \psi$, $e_0 \in s_{124}$. Consider a small turn of y_3 round s_{24} towards y_1 . If $e_0 \notin s_{24}$, then this turn decreases θ_3 . Therefore, the irreducibility yields $\phi_{3,5} = \psi$. In the case $e_0 \in s_{24}$, $\theta'_3 = \theta_3$, but $\phi_{1,3}$ decreases. It again implies $\phi_{3,5} = \psi$. Since s_{35} cannot intersects a regular triangle s_{124} [see Lemma 2, (4b)], $\phi_{2,4} > \psi$. Then $\deg y_2 = \deg y_4 = 3$. (Since $e_0 \in s_{124}$, $\deg y_2 = 2$ only if $\phi_{2,4} = \psi$.) Thus we have three isosceles triangles $s_{243}, s_{241}, s_{245}$. Using this and $\phi_{3,5} = \psi$, we obviously have $\phi_{1,i} < \psi$ for $i = 3, 5$, - a contradiction.

Case s_{135} (type (A)): This case has two subcases: $\tilde{s}_{135}, \tilde{s}_{315}$.

In the subcase \tilde{s}_{135} we have $\deg y_1 = 2$, $\phi_{1,3} = \phi_{1,5} = \psi$, $e_0 \in \tilde{s}_{135}$. If $e_0 \notin s_{135}$, then any turn of y_1 round s_{35} decreases θ_1 (Lemma 3). Then $e_0 \in s_{135}$. Clearly, any small turn of y_2 round s_{35} increases $\phi_{2,4}$. On the other hand, this turn decreases θ_2 (if $e_0 \notin s_{35}$) and $\phi_{1,2}$. Arguing as above, we get a contradiction. The subcase \tilde{s}_{315} , where $\phi_{3,5} = \psi$, can be proven by the same arguments as Case s_{124} .

Case s_{234} (type (B)): This case has two subcases: $\tilde{s}_{234}, \tilde{s}_{324}$.

In fact, \tilde{s}_{234} is the same as Case facet, and \tilde{s}_{324} can be proven in the same way as subcase \tilde{s}_{135} . This concludes the proof. \square

Lemma 4 yields that the degree of any vertex of $\Gamma_\psi(Y)$ is not less than 3. This implies that at least one vertex of $\Gamma_\psi(Y)$ has degree 4. Indeed, if all vertices of $\Gamma_\psi(Y)$ are of degree 3, then the sum of the degrees equals 15, i.e. is

not an even number. There exists only one type of $\Gamma_\psi(Y)$ with these conditions (Fig. 6). The lengths of all edges of Δ_5 except y_2y_4 , y_3y_5 are equal to ψ . For fixed $\phi_{2,4} = \alpha$, Δ_5 is uniquely defined up to isometry. Therefore, we have the 1-parametric family $P_5(\alpha)$ on \mathbf{S}^3 . If $\phi_{3,5} \geq \phi_{2,4}$, then $z \geq \cos \alpha \geq 2z - 1$.

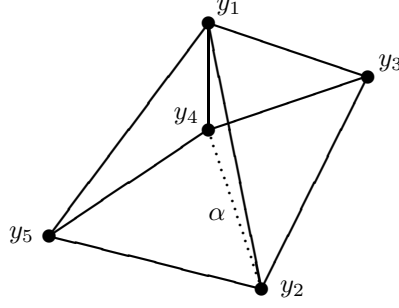


Fig. 6: $P_5(\alpha)$

These results can be summarized as follows.

Theorem 5. *Let $Y \subset \mathbf{S}^3$ be an irreducible set, $|Y| = m \leq 5$. Then Δ_m for $2 \leq m \leq 4$ is a regular simplex of edge lengths ψ , and Δ_5 is isometric to $P_5(\alpha)$ for some $\alpha \in [\psi, \arccos(2z - 1)]$.*

5 On calculations of h_m

In this technical section we explain how to find an upper bound on h_m for $n = 4$, $m \leq 6$. Note that Theorem 5 gets for computation of h_m a low-dimensional optimization problem (see (5.3)). Our first approach for this problem was to apply numerical methods [26]. However, that is a nonconvex constrained optimization problem. In this case, the Nelder-Mead simplex method and other local improvements methods cannot guarantee finding a global optimum. It's possible (using estimations of derivatives) to organize computational process in such way that it gives a global optimum. However, such solutions are very hard to verify and some mathematicians don't accept that kind of proofs. Fortunately, using geometric approach, estimations of h_m can be reduced to relatively simple computations.

First consider the case $m = 2$. Suppose f satisfies the monotonicity assumption (*), and Y is optimal. Then $\tilde{f}(\theta) := f(-\cos \theta)$ is a monotone decreasing function in θ , $\Delta_2 = y_1y_2$ is an arc of length ψ , $e_0 \in \Delta_2$, and $\theta_1 + \theta_2 = \psi$, where $\theta_i \leq \theta_0$. Since (4.1), $F(\theta_1, \theta_2)$ is a symmetric function in θ_1, θ_2 . We can assume that $\theta_1 \leq \theta_2$, then $\theta_1 \in [\psi - \theta_0, \psi/2]$. Since $\Theta_2(\theta_1) := \psi - \theta_1$ is a monotone decreasing function, $\tilde{f}(\Theta_2(\theta_1))$ is a monotone increasing function in θ_1 . Thus for any $\theta_1 \in [\zeta, \xi] \subset [\psi - \theta_0, \psi/2]$:

$$F(\theta_1, \theta_2) \leq \Phi_2([\zeta, \xi]) := f(1) + \tilde{f}(\zeta) + \tilde{f}(\psi - \xi).$$

Let $a_1 = \psi - \theta_0$, a_2, \dots, a_N , $a_{N+1} = \psi/2$ be points in $[\psi - \theta_0, \psi/2]$ such that $a_{i+1} = a_i + \varepsilon$, where $\varepsilon = (\theta_0 - \psi/2)/N$. If $\theta_1 \in [a_i, a_{i+1}]$, then $h_2 = H(y_0; Y) = F(\theta_1, \theta_2) \leq \Phi_2([a_i, a_{i+1}])$. Thus

$$h_2 \leq \lambda_2(N, \psi, \theta_0) := \max_{1 \leq i \leq N} \{\Phi_2(c_i)\}, \text{ where } c_i := [a_i, a_{i+1}].$$

Clearly, $\lambda_2(N, \psi, \theta_0)$ tends to h_2 as $N \rightarrow \infty$ ($\varepsilon \rightarrow 0$).

That implies a very simple method for calculations of h_2 . Now we extend this approach to higher m .

Suppose we know what optimal $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$ is up to isometry. Let us assume that $\dim \Delta_m = n - 1$, and $V := y_1 \dots y_{n-1}$ is a facet of Δ_m . Then $\text{rank}\{y_1, \dots, y_{n-1}\} = n - 1$, and Y belongs to the hemisphere H_+ , where H_+ contains Y and bounded by the great sphere \tilde{S} passes through V .

Let us show that any $y \in H_+$ is uniquely determined by the set of distances $\theta_i = \text{dist}(y, y_i)$, $i = 1, \dots, n - 1$. Indeed, there are at most two solutions: $y_+ \in H_+$ and $y_- \in H_-$ of the quadratic equation

$$y \cdot y = 1, \text{ where } y \cdot y_i = \cos \theta_i, \ i = 1, \dots, n - 1. \quad (5.1)$$

Note that $y_+ = y_-$ if and only if $y \in \tilde{S}$.

This implies that θ_k , $k \geq n$, is determined by θ_i , $i = 1, \dots, n - 1$;

$$\theta_k = \Theta_k(\theta_1, \dots, \theta_{n-1}).$$

It is not hard to solve (5.1) and, therefore, to give an explicit expression for Θ_k .

Let $\bar{\xi} = (\xi_1, \dots, \xi_{n-1})$, where $0 < \xi_i \leq \theta_0 < \psi$. (Recall that $\phi_{i,j} = \text{dist}(y_i, y_j)$; $\cos \psi = z$; $\cos \theta_0 = t_0$.) Now we consider a domain $D(\bar{\xi})$ in H_+ , where

$$D(\bar{\xi}) = \{y \in H_+ : \text{dist}(y, y_i) \leq \xi_i, \ 1 \leq i \leq n - 1\}.$$

In other words, $D(\bar{\xi})$ is the intersection of the spherical caps $C(y_i, \xi_i)$ in H_+ :

$$D(\bar{\xi}) = \bigcap_{i=1}^{n-1} C(y_i, \xi_i) \cap H_+.$$

Suppose $\dim D(\bar{\xi}) = n - 1$. Then $D(\bar{\xi})$ has “vertices”, “edges”, and “ k -faces” for $k \leq n - 1$. Indeed, let

$$\sigma \subset I := \{1, \dots, n - 1\}, \quad 0 < |\sigma| \leq n - 1;$$

$$\tilde{F}_\sigma := \{y \in D(\bar{\xi}) : \text{dist}(y, y_i) = \xi_i \ \forall i \in \sigma\}.$$

It is easy to prove that $\dim \tilde{F}_\sigma = n - 1 - |\sigma|$; \tilde{F}_σ belongs to the boundary B of $D(\bar{\xi})$; and if $\sigma \subset \sigma'$, then $\tilde{F}_{\sigma'} \subset \tilde{F}_\sigma$. Actually, $D(\bar{\xi})$ is combinatorially equivalent to an $(n - 1)$ -dimensional simplex.

Now we consider the minimum of $\Theta_k(\theta_1, \dots, \theta_{n-1})$ on $D(\bar{\xi})$ for $k \geq n$. In other words, we are looking for a point $p_k(\bar{\xi}) \in D(\bar{\xi})$ such that

$$\text{dist}(y_k, p_k(\bar{\xi})) = \text{dist}(y_k, D(\bar{\xi})).$$

Since $\phi_{i,k} \geq \psi > \theta_0$, all y_k lie outside $D(\xi)$. Clearly, Θ_k achieves its minimum at some point in B . Therefore, there is $\sigma \subset I$ such that

$$p_k(\bar{\xi}) \in \tilde{F}_\sigma \quad (5.2)$$

Suppose $\sigma = I$, then F_σ is a vertex of $D(\xi)$. Let us denote this point by $p_*(\xi)$. Note that the function Θ_k at the point $p_*(\xi)$ is equal to $\Theta_k(\xi)$.

Let $\sigma_k(\xi)$ be $\sigma \subset I$ of maximal size such that σ satisfies (5.2). Then for $\sigma_k(\bar{\xi}) = I$, $p_k(\bar{\xi}) = p_*(\bar{\xi})$, and for $|\sigma_k(\bar{\xi})| < n - 1$, $p_k(\bar{\xi})$ belongs to the open part of $\tilde{F}_{\sigma_k(\bar{\xi})}$.

Consider $n = 3$. There are two cases for $p_k(\xi)$ (see Fig. 7): $p_3(\xi) = p_*(\xi) = \tilde{F}_{\{1,2\}}$, $p_4(\xi)$ is the intersection in H_+ of the great circle passes through y_1 , y_4 , and the circle $\tilde{S}(y_1, \xi_1)$ of center y_1 and radius ξ_1 ($\tilde{F}_{\{1\}} \subset \tilde{S}(y_1, \xi_1)$). The same holds for all dimensions.

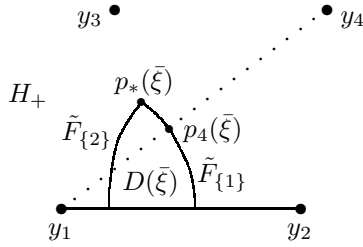


Fig. 7

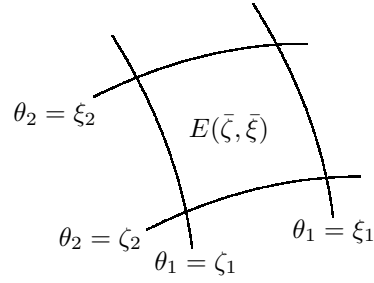


Fig. 8

Denote by $S_\sigma(k)$ the great $|\sigma|$ -dimensional sphere passes through y_i , $i \in \sigma$, and y_k . Let $\tilde{S}(y_i, \xi_i)$ be the sphere of center y_i and radius ξ_i ; and for $\sigma \subset I$

$$\tilde{S}_\sigma := \bigcap_{i \in \sigma} \tilde{S}(y_i, \xi_i).$$

Denote by $s(\sigma, k)$ the intersection of $S_\sigma(k)$ and \tilde{S}_σ in H_+ ,

$$s(\sigma, k) = S_\sigma(k) \bigcap \tilde{S}_\sigma \bigcap H_+$$

Lemma 5. *Suppose $D(\bar{\xi}) \neq \emptyset$, $0 < \xi_i \leq \theta_0$ for all i , and $k \geq n$. Then*

- (i) $p_k(\tilde{\xi}) \in s(\sigma_k(\tilde{\xi}), k)$,
(ii) if $s(\sigma, k) \neq \emptyset$, $|\sigma| < n - 1$, then $s(\sigma, k)$ consists of the one point $p_k(\bar{\xi})$.

Proof. (i) Let $\theta_k^* := \Theta_k(p_k(\tilde{\xi})) = \text{dist}(y_k, p_k(\tilde{\xi}))$. Since Θ_k achieves its minimum at $p_k(\tilde{\xi})$, the sphere $\tilde{S}(y_k, \theta_k^*)$ touches the sphere $\tilde{S}_{\sigma(\tilde{\xi})}$ at $p_k(\tilde{\xi})$. If some sphere touches the intersections of spheres, then the touching point belongs to the great sphere passes through the centers of these spheres. Thus $p_k(\tilde{\xi}) \in S_{\sigma(\tilde{\xi})}(k)$.

(ii) Note that $s(\sigma, k)$ belongs to the intersection in H_+ of the spheres $S(y_i, \xi_i)$, $i \in \sigma$, and $S_\sigma(k)$. Any intersection of spheres is also a sphere. Since

$$\dim S_\sigma(k) + \dim \tilde{S}_\sigma = n - 1,$$

this intersection is empty, or is a 0-dimensional sphere (i.e. 2-points set). In the last case, one point lies in H_+ , and another one in H_- . Therefore, $s(\sigma, k) = \emptyset$, or $s(\sigma, k) = \{p\}$. Denote by σ' the maximal size $\sigma' \supset \sigma$ such that $s(\sigma', k) = \{p\}$. It is not hard to see that $\tilde{S}(y_k, \text{dist}(y_k, p))$ touches $\tilde{S}_{\sigma'}$ at p . Thus $p = p_k(\bar{\xi})$. \square

Lemma 5 implies a simple method for calculations of the minimum of Θ_k on $D(\bar{\xi})$. For this we can consider $s(\sigma, k)$, $\sigma \subset I$, and if $s(\sigma, k) \neq \emptyset$, then $s(\sigma, k) = \{p_k(\bar{\xi})\}$, so then Θ_k attains its minimum at this point. In the case when Δ_n is a simplex we can find the minimum by very simple method.

Corollary 5. *Suppose $|Y| = n$, $\bar{\xi}$ satisfies the assumptions of Lemma 5, and $D(\bar{\xi})$ lies inside Δ_n . Then*

$$\theta_n \geq \Theta_n(\xi_1, \dots, \xi_{n-1}) \text{ for all } y \in D(\bar{\xi}).$$

Proof. Clearly, Δ_n is a simplex. Since $D(\bar{\xi})$ lies inside Δ_n , for $|\sigma| < n - 1$ the intersection of \tilde{S}_σ and $S_\sigma(k)$ is empty. Thus $p_n(\bar{\xi}) = p_*(\bar{\xi})$. \square

For fixed $y_i \in \mathbf{S}^{n-1}$, $i = 1, \dots, m$; the function H depends only on a position $y = -y_0 = e_0 \in \mathbf{S}^{n-1}$. Let

$$H_m(y) := f(1) + f(-y \cdot y_1) + \dots + f(-y \cdot y_m),$$

i.e. $H_m(y) = H(-y; Y)$. Then

$$h_m = \max_y \{H_m(y)\}$$

subjects to the constraint

$$y \in T(Y, \theta_0) := \{y \in \Delta_m \subset \mathbf{S}^{n-1} : y \cdot y_i \geq t_0, i = 1, \dots, m\}; \quad (5.3)$$

where $y_i \cdot y_j \leq z$ for $i \neq j$, and $1 > t_0 > z \geq 0$.

Suppose $\dim \Delta_m = n - 1$, and $y_1 \dots y_{n-1}$ is a facet of Δ_m . Then (4.1) yields

$$H_m(y) = F(\theta_1, \dots, \theta_{n-1}, \Theta_n, \dots, \Theta_m) = \tilde{F}_m(\theta_1, \dots, \theta_{n-1}),$$

where

$$\begin{aligned} \tilde{F}_m(\theta_1, \dots, \theta_{n-1}) &:= f(1) + \tilde{f}(\theta_1) + \dots + \tilde{f}(\theta_{n-1}) + \tilde{f}(\Theta_n(\theta_1, \dots, \theta_{n-1})) + \dots \\ &+ \tilde{f}(\Theta_m(\theta_1, \dots, \theta_{n-1})), \end{aligned}$$

$$\tilde{f}(\theta) := \begin{cases} f(-\cos \theta) & 0 \leq \theta \leq \theta_0 \\ -\infty & \theta > \theta_0 \end{cases}$$

Lemma 6. Suppose f satisfies $(*)$, $|Y| = m$, $\dim \Delta_m = n - 1$, $y_1 \dots y_{n-1}$ is a facet of Δ_m , $\text{dist}(y_i, y_j) \geq \psi > \theta_0$ for $i \neq j$, $0 \leq \zeta_i < \xi_i \leq \theta_0$ for $i = 1, \dots, n - 1$; and $\Theta_k(\xi) \leq \theta_0$ for all $k \geq n$. If $D(\xi) \neq \emptyset$, then

$$H_m(y) \leq \Phi_Y(\bar{\zeta}, \bar{\xi}) \quad \text{for any } y \in E(\bar{\zeta}, \bar{\xi}) := D(\bar{\xi}) \setminus U(\bar{\zeta}),$$

where

$$\Phi_Y(\bar{\zeta}, \bar{\xi}) := f(1) + \tilde{f}(\zeta_1) + \dots + \tilde{f}(\zeta_{n-1}) + \tilde{f}(\Theta_n(p_n(\bar{\xi}))) + \dots + \tilde{f}(\Theta_m(p_m(\bar{\xi}))),$$

$$U(\bar{\zeta}) := \bigcup_{i=1}^{n-1} C(y_i, \zeta_i).$$

Proof. We have for $1 \leq i \leq n - 1$ and $y \in E(\bar{\zeta}, \bar{\xi})$: $\theta_i \geq \zeta_i$ (Fig. 8). By the monotonicity assumption $(*)$ this implies $\tilde{f}(\theta_i) \leq \tilde{f}(\zeta_i)$. On the other hand, $y \in D(\bar{\xi})$. Then Lemma 5 yields $\tilde{f}(\theta_k) \leq \tilde{f}(\Theta_k(p_k(\bar{\xi})))$ for $k \geq n$. \square

From Corollary 5 and Lemma 6 follow

Corollary 6. Let $|Y| = n$. Suppose f , ξ , ζ , and Y satisfy the assumptions of Lemma 6 and Corollary 5. Then for any $y \in E(\bar{\zeta}, \bar{\xi})$:

$$H_m(y) \leq f(1) + \tilde{f}(\zeta_1) + \dots + \tilde{f}(\zeta_{n-1}) + \tilde{f}(\Theta_n(\bar{\xi})).$$

Let $K(n, \theta_0) := [0, \theta_0]^{n-1}$, i.e. $K(n, \theta_0)$ is an $(n - 1)$ -dimensional cube of side length θ_0 . Consider for $K(n, \theta_0)$ the cubic grid $L(N)$ of sidelength ε , where $\varepsilon = \theta_0/N$ for given positive integer N . Then the grid (tessellation) $L(N)$ consists of N^{n-1} cells, any cell $c \in L(N)$ is an $(n - 1)$ -dimensional cube of sidelength ε , and for any point $(\theta_1, \dots, \theta_{n-1})$ in c we have

$$\zeta_i(c) \leq \theta_i \leq \xi_i(c), \quad \xi_i(c) = \zeta_i(c) + \varepsilon, \quad i = 1, \dots, n - 1.$$

Let $\tilde{L}(N)$ be the subset of cells c in $L(N)$ such that $D(\bar{\xi}(c)) \neq \emptyset$. There exists $c \in L(N)$ such that H_m attains its maximum on $T(Y, \theta_0)$ at some point in $E(\bar{\zeta}(c), \bar{\xi}(c))$. Therefore, Lemma 6 yields

Lemma 7. Suppose f and Y satisfy the assumptions of Lemma 6, N is a positive integer, and $y \in \Delta_m$ is such that $\text{dist}(y, y_i) \leq \theta_0$ for all i . Then

$$H_m(y) \leq \max_{c \in \tilde{L}(N)} \{\Phi_Y(\bar{\zeta}(c), \bar{\xi}(c))\}$$

Now we apply these results for computations of h_m . Suppose Δ_m is a regular simplex of edge length ψ . Since (4.1), F is a symmetric function in the variables $\theta_1, \dots, \theta_m$. Then we can consider this problem only on the domain

$$\Lambda := \{y \in \Delta_n : \psi - \theta_0 \leq \theta_1 \leq \theta_2 \leq \dots \leq \theta_m \leq \theta_0\}.$$

Let $L_\Lambda(N)$ be the subset of cells c in $\tilde{L}(N)$ such that $c \cap \Lambda \neq \emptyset$. If $c \in L_\Lambda(N)$ lies inside Δ_m ,³ then we have an explicit expression for $\Phi_m(c) := \Phi_Y(\bar{\zeta}(c), \bar{\xi}(c))$

³Clearly, it holds for all $c \in L_\Lambda(N)$ if N is sufficiently large.

(see Corollary 6). For $n = 4$, Theorem 5 implies that Δ_m is a regular simplex, where $m = 2, 3, 4$. Thus from Lemma 7 follows

$$h_m \leq \lambda_m(N, \psi, \theta_0) := \max_{c \in L_\Lambda(N)} \{\Phi_m(c)\}.$$

Now we consider the case $n = 4$, $m = 5$. Theorem 5 yields: Δ_5 is isometric to $P_5(\alpha)$ for some $\alpha \in [\psi, \psi' := \arccos(2z - 1)]$ (see Fig. 6). Let the vertices y_1, y_2, y_3 of $P_5(\alpha)$ be fixed. Then the vertices $y_4(\alpha)$, $y_5(\alpha)$ are uniquely determined by α .

Note that for any $y \in D(\theta_0, \theta_0, \theta_0)$ the distance $\theta_4(\alpha) := \text{dist}(y, y_4(\alpha))$ increases, and $\theta_5(\alpha)$ decreases whenever α increases. Let $\alpha_1 = \psi$, $\alpha_2, \dots, \alpha_N$, $\alpha_{N+1} = \psi'$ be points in $[\psi, \psi']$ such that $\alpha_{i+1} = \alpha_i + \epsilon$, where $\epsilon = (\psi' - \psi)/N$. Then

$$\theta_4(\alpha_i) < \theta_4(\alpha_{i+1}), \quad \theta_5(\alpha_i) > \theta_5(\alpha_{i+1}),$$

so then

$$\tilde{f}(\theta_4(\alpha_i)) > \tilde{f}(\theta_4(\alpha_{i+1})), \quad \tilde{f}(\theta_5(\alpha_i)) < \tilde{f}(\theta_5(\alpha_{i+1})).$$

Combining this with Lemma 7, we get

$$h_5 \leq \lambda_5(N, \psi, \theta_0) := f(1) + \max_{c \in L(N)} \{R_{1,2,3}(c) + \max_{1 \leq i \leq N} \{R_{4,5}(c, i)\}\},$$

$$R_{1,2,3}(c) = \tilde{f}(\zeta_1(c)) + \tilde{f}(\zeta_2(c)) + \tilde{f}(\zeta_3(c)),$$

$$R_{4,5}(c, i) = \tilde{f}(\Theta_4(p_4(\bar{\xi}(c), \alpha_i))) + \tilde{f}(\Theta_5(p_5(\bar{\xi}(c), \alpha_{i+1}))),$$

where $p_k(\bar{\xi}, \alpha) = p_k(\bar{\xi})$ with $y_k = y_k(\alpha)$.

Clearly, $\lambda_m(N + 1, \psi, \theta_0) \leq \lambda_m(N, \psi, \theta_0)$. It's not hard to show that

$$h_m = \lambda_m(\psi, \theta_0) := \lim_{N \rightarrow \infty} \lambda_m(N, \psi, \theta_0).$$

Finally let us consider the case: $n = 4$, $m = 6$. In this case, we give an upper bound on h_6 by separate argument.

Lemma 8. *Let $n = 4$, f satisfies $(*)$, $\sqrt{z} > t_0 > z$, $\theta'_0 \in [\arccos \sqrt{z}, \theta_0]$. Then*

$$h_6 \leq \max \{ \tilde{f}(\theta'_0) + \lambda_5(\psi, \theta_0), f(-\sqrt{z}) + \lambda_5(\psi, \theta'_0) \}.$$

Proof. Let $Y = \{y_1, \dots, y_6\} \subset C(e_0, \theta_0) \subset \mathbf{S}^3$, where Y is an optimal z -code. We may assume that $\theta_1 \leq \theta_2 \leq \dots \leq \theta_6$. Then from Corollary 3(i) follows that

$$\theta_0 \geq \theta_6 \geq \theta_5 \geq \arccos \sqrt{z}.$$

Let us consider two cases: (a) $\theta_0 \geq \theta_6 \geq \theta'_0$, (b) $\theta'_0 \geq \theta_6 \geq \arccos \sqrt{z}$.

(a) We have $h_6 = H(y_0; y_1, \dots, y_6) = H(y_0; y_1, \dots, y_5) + \tilde{f}(\theta_6)$,

$$H(y_0; y_1, \dots, y_5) \leq h_5 = \lambda_5(\psi, \theta_0), \quad \tilde{f}(\theta_6) \leq \tilde{f}(\theta'_0).$$

Then $h_6 \leq \tilde{f}(\theta'_0) + \lambda_5(\psi, \theta_0)$.

(b) In this case all $\theta_i \leq \theta'_0$, i.e. $Y \subset C(e_0, \theta'_0)$. Since

$$H(y_0; y_1, \dots, y_5) \leq \lambda_5(\psi, \theta'_0), \quad \tilde{f}(\theta_6) \leq f(-\sqrt{z}),$$

it follows that $h_6 \leq f(-\sqrt{z}) + \lambda_5(\psi, \theta'_0)$. \square

We have proved the following theorem.

Theorem 6. *Suppose $n = 4$, f satisfies $(*)$, $\sqrt{z} > t_0 > z > 0$, and N is a positive integer. Then*

- (i) $h_0 = f(1), \quad h_1 = f(1) + f(-1);$
- (ii) $h_m = \lambda_m(\psi, \theta_0) \leq \lambda_m(N, \psi, \theta_0)$ for $2 \leq m \leq 5;$
- (iii) $h_6 \leq \max \{ \tilde{f}(\theta'_0) + \lambda_5(\psi, \theta_0), f(-\sqrt{z}) + \lambda_5(\psi, \theta'_0) \} \quad \forall \theta'_0 \in [\arccos \sqrt{z}, \theta_0].$

6 $k(4) = 24$

For $n = 4$, $z = \cos 60^\circ = 1/2$ we apply this extension of Delsarte's method with

$$f(t) = 53.76t^9 - 107.52t^7 + 70.56t^5 + 16.384t^4 - 9.832t^3 - 4.128t^2 - 0.434t - 0.016$$

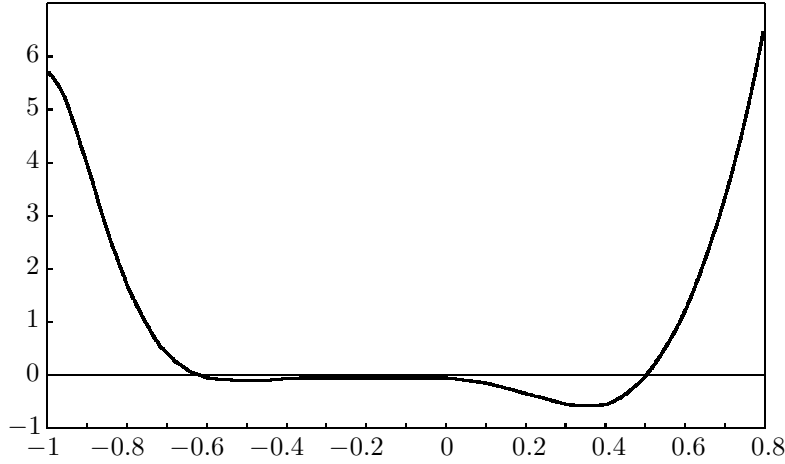


Fig. 9. The graph of the function $f(t)$

The expansion of f in terms of $U_k = G_k^{(4)}$ is

$$f = U_0 + 2U_1 + 6.12U_2 + 3.484U_3 + 5.12U_4 + 1.05U_9$$

The polynomial f has two roots on $[-1, 1]$: $t_1 = -t_0$, $t_0 \approx 0.60794$, $t_2 = 1/2$, $f(t) \leq 0$ for $t \in [-t_0, 1/2]$, and f is a monotone decreasing function on the interval $[-1, -t_0]$. The last property holds because there are no zeros of the derivative $f'(t)$ on $[-1, -t_0]$. Therefore, f satisfies $(*)$ for $z = 1/2$.

Remark. The polynomial f was found by using the algorithm in Appendix. This algorithm for $n = 4$, $z = 1/2$, $d = 9$, $N = 2000$, $t_0 = 0.6058$ gives $E \approx 24.7895$. For the polynomial f the coefficients c_k were changed to “better looking” ones with $E \approx 24.8644$.

We have $t_0 > 0.6058$. Then Corollary 3(ii) gives $\mu \leq 6$. Let us apply Theorem 6 with $\psi = \arccos z = 60^\circ$, $\theta_0 = \arccos t_0 \approx 52.5588^\circ$ for calculations of h_m . We get

$$h_0 = f(1) = 18.774, \quad h_1 = f(1) + f(-1) = 24.48,$$

$$h_2 \approx 24.8644, \quad h_3 \approx 24.8345, \quad h_4 \approx 24.818, \quad h_5 \approx 24.6856.$$

Let $\theta'_0 = 50^\circ$. We have $\tilde{f}(50^\circ) \approx 0.0906$, $\arccos \sqrt{z} = 45^\circ$, $\tilde{f}(45^\circ) \approx 0.4533$,

$$\lambda_5(60^\circ, \theta_0) = h_5 \approx 24.6856, \quad \lambda_5(60^\circ, 50^\circ) \approx 23.9181,$$

$$h_6 \leq \max \{ \tilde{f}(50^\circ) + h_5, \tilde{f}(45^\circ) + \lambda_5(60^\circ, 50^\circ) \} \approx 24.7762 < h_2.$$

Thus $h_{max} = h_2 < 25$.

Theorem 7. $k(4) = 24$

Proof. Let X be a spherical $1/2$ -code in \mathbf{S}^3 with $M = k(4)$ points. The polynomial f is such that $c_0 = 1$, $h_{max} < 25$. Theorem 1 yields: $k(4) \leq h_{max} < 25$. Recall that $k(4) \geq 24$. Consequently, $k(4) = 24$. \square

7 Concluding remarks

This extension of Delsarte’s method can be applied to other dimensions and spherical z -codes.

The most interesting application is a new proof for the Newton-Gregory problem, $k(3) < 13$. In dimension three computations of h_m are technically easier than for $n = 4$. This proof needs from mathematics just basic calculus and simple spherical geometry (see details in [27]).

Let

$$f(t) = \frac{2431}{80}t^9 - \frac{1287}{20}t^7 + \frac{18333}{400}t^5 + \frac{343}{40}t^4 - \frac{83}{10}t^3 - \frac{213}{100}t^2 + \frac{t}{10} - \frac{1}{200}.$$

Then f satisfies $(*)$, $t_0 \approx 0.5907$, $\mu(3, 1/2, f) = 4$, and $h_{max} = h_1 = 12.88$. The expansion of f in terms of Legendre polynomials $P_k = G_k^{(3)}$ is

$$f = P_0 + 1.6P_1 + 3.48P_2 + 1.65P_3 + 1.96P_4 + 0.1P_5 + 0.32P_9.$$

Since $c_0 = 1$, $c_i \geq 0$, $k(3) \leq h_{max} = 12.88 < 13$.

Direct application of the method developed in this paper, presumably could lead to some improvements in the upper bounds on kissing numbers in dimensions 9, 10, 16, 17, 18 given in [10, Table 1.5]. (“Presumably” because the equality $h_{max} = E$ is not proven yet.)

In 9 and 10 dimensions Table 1.5 gives:

$$306 \leq k(9) \leq 380, \quad 500 \leq k(10) \leq 595.$$

The algorithm gives:

$$n = 9 : \deg f = 11, E = h_1 = 366.7822, t_0 = 0.54;$$

$$n = 10 : \deg f = 11, E = h_1 = 570.5240, t_0 = 0.586.$$

For these dimensions there is a good chance to prove that

$$k(9) \leq 366, \quad k(10) \leq 570.$$

From the equality $k(3) = 12$ follows $\varphi_3(13) < 60^\circ$. The method gives $\varphi_3(13) < 59.4^\circ$ ($\deg f = 11$). The lower bound on $\varphi_3(13)$ is 57.1367° [17]. Therefore, we have $57.1367^\circ \leq \varphi_3(13) < 59.4^\circ$.

Using our approach it can be proven that $\varphi_4(25) < 59.81^\circ$, $\varphi_4(24) < 60.5^\circ$. That improve the bounds:

$$\varphi_4(25) < 60.79^\circ, \quad \varphi_4(24) < 61.65^\circ [24] \text{ (cf. [5]); } \varphi_4(24) < 61.47^\circ [5];$$

$$\varphi_4(25) < 60.5^\circ, \quad \varphi_4(24) < 61.41^\circ [4].$$

Now in these cases we have

$$57.4988^\circ < \varphi_4(25) < 59.81^\circ, \quad 60^\circ \leq \varphi_4(24) < 60.5^\circ.$$

However, for $n = 5, 6, 7$ direct use of this extension of the Delsarte method doesn't give better upper bounds on $k(n)$ than the Delsarte method. It is an interesting problem to find better methods.

Appendix. An algorithm for computation suitable polynomials $f(t)$

In this Appendix is presented an algorithm for computation “optimal”⁴ polynomials f such that $f(t)$ is a monotone decreasing function on the interval $[-1, -t_0]$, and $f(t) \leq 0$ for $t \in [-t_0, z]$, $t_0 > z \geq 0$. This algorithm based on our knowledge about optimal arrangement of points y_i for given m . Coefficients c_k can be found via discretization and linear programming; such method had been employed already by Odlyzko and Sloane [28] for the same purpose.

Let us have a polynomial f represented in the form $f(t) = 1 + \sum_{k=1}^d c_k G_k^{(n)}(t)$.

We have the following constraints for f : (C1) $c_k \geq 0$, $1 \leq k \leq d$;
(C2) $f(a) > f(b)$ for $-1 \leq a < b \leq -t_0$; (C3) $f(t) \leq 0$ for $-t_0 \leq t \leq z$.

We do not know e_0 where H_m attains its maximum, so for evaluation of h_m let us use $e_0 = y_c$, where y_c is the center of Δ_m . All vertices y_k of Δ_m are at the distance of ρ_m from y_c , where

$$\cos \rho_m = \sqrt{(1 + (m-1)z)/m}.$$

⁴Open problem: is it true that for given t_0, d this algorithm defines f with minimal h_{max} ?

When $m = 2n - 2$, Δ_m presumably is a regular $(n - 1)$ -dimensional cross-polytope.⁵ In this case $\cos \rho_m = \sqrt{2}$.

Let $I_n = \{1, \dots, n\} \cup \{2n - 2\}$, $m \in I_n$, $b_m = -\cos \rho_m$, then $H_m(y_c) = f(1) + mf(b_m)$. If F_0 is such that $H(y_0; Y) \leq E = F_0 + f(1)$, then (C4) $f(b_m) \leq F_0/m$, $m \in I_n$. Note that $E = F_0 + 1 + c_1 + \dots + c_d = F_0 + f(1)$ is a lower estimate of h_{max} . A polynomial f that satisfies (C1-C4) and gives the minimal E can be found by the following

Algorithm.

Input: n, z, t_0, d, N .

Output: c_1, \dots, c_d, F_0, E .

First replace (C2) and (C3) by a finite set of inequalities at the points $a_j = -1 + \epsilon j$, $0 \leq j \leq N$, $\epsilon = (1 + z)/N$:

Second use linear programming to find F_0, c_1, \dots, c_d so as to minimize

$$E - 1 = F_0 + \sum_{k=1}^d c_k \quad \text{subject to the constraints}$$

$$c_k \geq 0, \quad 1 \leq k \leq d; \quad \sum_{k=1}^d c_k G_k^{(n)}(a_j) \geq \sum_{k=1}^d c_k G_k^{(n)}(a_{j+1}), \quad a_j \in [-1, -t_0];$$

$$1 + \sum_{k=1}^d c_k G_k^{(n)}(a_j) \leq 0, \quad a_j \in [-t_0, z]; \quad 1 + \sum_{k=1}^d c_k G_k^{(n)}(b_m) \leq F_0/m, \quad m \in I_n.$$

Let us note again that $E \leq h_{max}$, and $E = h_{max}$ only if $h_{max} = H_{m_0}(y_c)$ for some $m_0 \in I_n$.

Acknowledgment. I wish to thank Eiichi Bannai, Dmitry Leshchiner, Sergei Ovchinnikov, Makoto Tagami and Günter Ziegler for helpful discussions and useful comments on this paper.

I am very grateful to Ivan Dynnikov who pointed out a gap in arguments on earlier draft of [26].

References

- [1] M. Aigner and G.M. Ziegler, Proofs from THE BOOK, Springer, 1998 (first ed.) and 2002 (second ed.)
- [2] K. Anstreicher, The thirteen spheres: A new proof, Discrete and Computational Geometry, **31**(2004), 613-625.
- [3] V.V. Arestov and A.G. Babenko, On Delsarte scheme of estimating the contact numbers, Proc. of the Steklov Inst. of Math. **219** (1997), 36-65.

⁵It is also an open problem.

- [4] V.V. Arestov and A.G. Babenko, Estimates for the maximal value of the angular code distance for 24 and 25 points on the unit sphere in \mathbf{R}^4 , Math. Notes, **68** (2000), 419-435.
- [5] P.G. Boyvalenkov, D.P. Danev and S.P. Bumova, Upper bounds on the minimum distance of spherical codes, IEEE Trans. Inform. Theory, **42**(5), 1996, 1576-1581.
- [6] K. Böröczky, Packing of spheres in spaces of constant curvature, Acta Math. Acad. Sci. Hung. **32** (1978), 243-261.
- [7] K. Böröczky, The Newton-Gregory problem revisited, Proc. Discrete Geometry, Marcel Dekker, 2003, 103-110.
- [8] B.C. Carlson, Special functions of applied mathematics, Academic Press, 1977.
- [9] B. Casselman, The difficulties of kissing in three dimensions, Notices Amer. Math. Soc., **51**(2004), 884-885.
- [10] J.H. Conway and N.J.A. Sloane, Sphere Packings, Lattices, and Groups, New York, Springer-Verlag, 1999 (Third Edition).
- [11] H.S.M. Coxeter, An upper bound for the number of equal nonoverlapping spheres that can touch another of the same size, Proc. of Symp. in Pure Math. AMS, **7** (1963), 53-71 = Chap. 9 of H.S.M. Coxeter, Twelve Geometric Essays, Southern Illinois Press, Carbondale Il, 1968.
- [12] L. Danzer, Finite point-sets on \mathbf{S}^2 with minimum distance as large as possible, Discr. Math., **60** (1986), 3-66.
- [13] L. Danzer, B. Grünbaum, and V. Klee. Helly's theorem and its relatives. Proc. Sympos. Pure Math., vol. 7, AMS, Providence, RI, 1963, pp. 101-180.
- [14] Ph. Delsarte, Bounds for unrestricted codes by linear programming, Philips Res. Rep., **27**, 1972, 272-289.
- [15] Ph. Delsarte, J.M. Goethals and J.J. Seidel, Spherical codes and designs, Geom. Dedic., **6**, 1977, 363-388.
- [16] A. Erdélyi, editor, Higher Transcendental Function, McGraw-Hill, NY, 3 vols, 1953, Vol. II, Chap. XI.
- [17] L. Fejes Tóth, Lagerungen in der Ebene, auf der Kugel und in Raum, Springer-Verlag, 1953; Russian translation, Moscow, 1958.
- [18] T. Hales, The status of the Kepler conjecture, Mathematical Intelligencer **16**(1994), 47-58.
- [19] R. Hoppe, Bemerkung der Redaction, Archiv Math. Physik (Grunet) **56** (1874), 307-312.

- [20] W.-Y. Hsiang, The geometry of spheres, in Differential Geometry (Shanghai, 1991), Word Scientific, River Edge, NJ, 1993, pp. 92-107.
- [21] W.-Y. Hsiang, Least Action Principle of Crystal Formation of Dense Packing Type and Kepler's Conjecture, World Scientific, 2001.
- [22] G.A. Kabatiansky and V.I. Levenshtein, Bounds for packings on a sphere and in space, Problems of Information Transmission, **14**(1), 1978, 1-17.
- [23] J. Leech, The problem of the thirteen spheres, Math. Gazette **41** (1956), 22-23.
- [24] V.I. Levenshtein, On bounds for packing in n -dimensional Euclidean space, Sov. Math. Dokl. **20**(2), 1979, 417-421.
- [25] H. Maehara, Isoperimetric theorem for spherical polygons and the problem of 13 spheres, Ryukyu Math. J., **14** (2001), 41-57.
- [26] O.R. Musin, The problem of the twenty-five spheres, Russian Math. Surveys, **58**(2003), 794-795.
- [27] O.R. Musin, The kissing problem in three dimensions, preprint, October 2004, math. MG/0410324.
- [28] 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. of Combinatorial Theory A26(1979), 210-214.
- [29] F. Pfender and G.M. Ziegler, Kissing numbers, sphere packings, and some unexpected proofs, Notices Amer. Math. Soc., **51**(2004), 873-883.
- [30] I.J. Schoenberg, Positive definite functions on spheres, Duke Math. J., **9** (1942), 96-107.
- [31] K. Schütte and B.L. van der Waerden, Auf welcher Kugel haben 5,6,7,8 oder 9 Punkte mit Mindestabstand 1 Platz? Math. Ann. **123** (1951), 96-124.
- [32] K. Schütte and B.L. van der Waerden, Das Problem der dreizehn Kugeln, Math. Ann. **125** (1953), 325-334.
- [33] G.G. Szpiro, Kepler's conjecture, Wiley, 2002.
- [34] G.G. Szpiro, Newton and the kissing problem, <http://plus.maths.org/issue23/features/kissing/>
- [35] A.D. Wyner, Capabilities of bounded discrepancy decoding, Bell Sys. Tech. J. **44** (1965), 1061-1122.