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The kissing number in four dimensions

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Abstract

The kissing number problem asks for the maximal number $k(n)$ of equal size nonoverlapping spheres in n-dimensional space that can touch another sphere of the same size. 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.

In this paper we present a solution of a long-standing problem about the kissing number in four dimensions. Namely, the equality $k(4) = 24$ is proved. The proof is based on a modification of Delsarte's method.

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 move 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. It is commonly said that Newton believed the answer was 12 balls, while Gregory thought that 13 might be possible. However, Casselman [8] found some puzzling features in this story.

The Newton-Gregory problem is often called the *thirteen spheres problem*. Hoppe [18] thought he had solved the problem in 1874. However, there was a mistake — an analysis of this mistake was published by Hales [17] in 1994. Finally, this problem was solved by Schütte and van der Waerden in 1953 [31].

A subsequent two-page sketch of a proof was given by Leech [22] in 1956. The thirteen spheres problem continues to be of interest, and several new proofs have been published in the last few years [20], [24], [6], [1], [26].

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.

Coxeter proposed upper bounds on $k(n)$ in 1963 [10]; 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. This conjecture was proved by Böröczky in 1978 [5].

The main progress in the kissing number problem in high dimensions was made at the end of the 1970s. In 1978: Kabatiansky and Levenshtein found an asymptotic upper bound $2^{0.401n(1+o(1))}$ for $k(n)$ [21]. (Currently known, the lower bound is $2^{0.2075n(1+o(1))}$ [32].) In 1979: Levenshtein [23], and independently Odlyzko and Sloane [27] (= [9, Chap.13]), using Delsarte's method, 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 [27] the Delsarte method was applied in dimensions up to 24 (see [9, 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 $k(3) \leq 13$ [10], [27].)

Improvements in the upper bounds on kissing numbers (for $n < 24$) were rather weak during the next years (see [9, Preface, Third Edition] for a brief review and references). Arestov and Babenko [2] proved that the bound $k(4) \leq 25$ cannot be improved using Delsarte's method. Hsiang [19] claims a proof of $k(4) = 24$. His work has not yet received 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 another 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 $\pi/3$?

This leads to an important generalization: a finite subset X of $\mathbf{S}^{n-1}$ is called a *spherical ψ-code* if for every pair (x, y) of X the inner product $x \cdot y \leq \cos\psi$; i.e., the minimal angular separation is at least ψ. Spherical 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 [9, Chap. 3].

Delsarte's method (also known in coding theory as Delsarte's linear programming method or Delsarte's scheme) is widely used for finding bounds for codes. This method is described in [9], [21] (see also [28] for a beautiful exposition).

In this paper we present an extension of the Delsarte method that allowed us to prove the bound $k(4) < 25$, i.e. $k(4) = 24$. This extension yields also a proof for $k(3) < 13$ [26].

The first version of these proofs used numerical solutions of some nonconvex constrained optimization problems [25] (see also [28]). Now, using a geometric approach, we reduced it to relatively simple computations.

The paper is organized as follows: Section 2 shows that the main theorem: $k(4) = 24$ easily follows from two lemmas: Lemma A and Lemma B. Section 3 reviews the Delsarte method and gives a proof of Lemma A. Section 4 extends Delsarte's bounds and reduces the upper bound problem for ψ-codes to some optimization problem. Section 5 reduces the dimension of the corresponding optimization problem. Section 6 develops a numerical method for a solution of this optimization problem and gives a proof of Lemma B.

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2. The main theorem

Let us introduce the following polynomial of degree nine:[1]

$$f_4(t) := \frac{1344}{25}\,t^9 - \frac{2688}{25}\,t^7 + \frac{1764}{25}\,t^5 + \frac{2048}{125}\,t^4 - \frac{1229}{125}\,t^3 - \frac{516}{125}\,t^2 - \frac{217}{500}\,t - \frac{2}{125}.$$

Lemma A. *Let $X = \{x_1, \dots, x_M\}$ be points in the unit sphere $\mathbf{S}^3$. Then*

$$S(X) = \sum_{i=1}^{M}\sum_{j=1}^{M} f_4(x_i \cdot x_j) \geq M^2.$$

We give a proof of Lemma A in the next section.

[1] The polynomial f_4 was found by the linear programming method (see details in the appendix). This method for $n = 4$, $z = 1/2$, $d = 9$, $N = 2000$, $t_0 = 0.6058$ gives $E \approx 24.7895$. For f_4, coefficients were changed to "better looking" ones with $E \approx 24.8644$.

Lemma B. *Suppose $X = \{x_1, \dots, x_M\}$ is a subset of $\mathbf{S}^3$ such that the angular separation between any two distinct points x_i, x_j is at least $\pi/3$. Then*

$$S(X) = \sum_{i=1}^{M}\sum_{j=1}^{M} f_4(x_i \cdot x_j) < 25M.$$

A proof of Lemma B is given at the end of Section 6.

Main theorem. $k(4) = 24$.

Proof. Let X be a spherical $\pi/3$-code in $\mathbf{S}^3$ with $M = k(4)$ points. Then X satisfies the assumptions in Lemmas A, B. Therefore, $M^2 \le S(X) < 25M$. From this $M < 25$ follows, i.e. $M \le 24$. From the other side we have $k(4) \ge 24$, showing that $M = k(4) = 24$. □

3. Delsarte's method

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 $\mathbf{R}^n$.

Let $X = \{x_1, x_2, \dots, x_M\}$ be any finite subset of the unit sphere $\mathbf{S}^{n-1} \subset \mathbf{R}^n$, $\mathbf{S}^{n-1} = \{x \colon x \in \mathbf{R}^n,\ x \cdot x = ||x||^2 = 1\}$. By $\phi_{i,j} = \operatorname{dist}(x_i, x_j)$ we denote the spherical (angular) distance between x_i, x_j. Clearly, $\cos\phi_{i,j} = x_i \cdot x_j$.

3-A. *Schoenberg's theorem.* Let $u_1, u_2, \dots, u_M$ be any real numbers. Then

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

or equivalently the Gram matrix $\Big(\cos\phi_{i,j}\Big)$ is positive semidefinite.

Schoenberg [29] extended this property to Gegenbauer polynomials $G_k^{(n)}$. He proved: *The matrix $\Big(G_k^{(n)}(\cos\phi_{i,j})\Big)$ is positive semidefinite for any finite $X \subset \mathbf{S}^{n-1}$.*

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 $\big(f(\cos\phi_{i,j})\big)$ is positive semidefinite, then $f(t)$ is a linear combination of $G_k^{(n)}(t)$ with nonnegative coefficients.*

3-B. *The Gegenbauer polynomials.* Let us recall definitions of Gegenbauer polynomials $C_k^{(n)}(t)$, which are defined by the expansion

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

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 $G_k^{(n)}(1) = 1$.) Also the Gegenbauer polynomials $G_k^{(n)}$ can be defined by the recurrence formula:

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

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 [7], [9], [15], [29]). 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, $U_0 = 1$, $U_1 = t$, $U_2 = (4t^2-1)/3$, $U_3 = 2t^3 - t$, $U_4 = (16t^4 - 12t^2 + 1)/5, \ \dots, \ U_9 = (256t^9 - 512t^7 + 336t^5 - 80t^3 + 5t)/5$.

3-C. *Delsarte's inequality.* If a symmetric matrix is positive semidefinite, then the sum of all its entries is nonnegative. Schoenberg's theorem implies that the matrix $\left(G_k^{(n)}(t_{i,j})\right)$ is positive semidefinite, where $t_{i,j} := \cos\phi_{i,j}$, Then

$$\sum_{i=1}^{M}\sum_{j=1}^{M} G_k^{(n)}(t_{i,j}) \geq 0. \tag{3.1}$$

Definition 1. We denote by G_n^+ the set of continuous functions $f\colon [-1,1] \to \mathbf{R}$ representable as series

$$f(t) = \sum_{k=0}^{\infty} c_k G_k^{(n)}(t)$$

whose coefficients satisfy the following conditions:

$$c_0 > 0, \quad c_k \geq 0 \ \text{ for } k = 1,2,\dots, \quad f(1) = \sum_{k=0}^{\infty} c_k < \infty.$$

Suppose $f \in \mathsf{G}_n^+$ and let

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

Using (3.1), we get

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

Then

$$S(X) \geq c_0 M^2. \tag{3.2}$$

3-D. *Proof of Lemma* A. The expansion of f_4 in terms of $U_k = G_k^{(4)}$ is

$$f_4 = U_0 + 2\,U_1 + \frac{153}{25}\,U_2 + \frac{871}{250}\,U_3 + \frac{128}{25}\,U_4 + \frac{21}{20}\,U_9.$$

We see that $f_4 \in \mathsf{G}_4^+$ with $c_0 = 1$. So Lemma A follows from (3.2). □

3-E. *Delsarte's bound.* Let $X = \{x_1, \dots, x_M\} \subset \mathbf{S}^{n-1}$ be a spherical ψ-code, i.e. for all $i \neq j$, $t_{i,j} = \cos\phi_{i,j} = x_i \cdot x_j \leq z := \cos\psi$, i.e. $t_{i,j} \in [-1, z]$ (but $t_{i,i} = 1$).

Suppose $f \in \mathsf{G}_n^+$ and $f(t) \leq 0$ for all $t \in [-1, z]$; then $f(t_{i,j}) \leq 0$ for all $i \neq j$. That implies

$$S_f(X) = M f(1) + 2f(t_{1,2}) + \ldots + 2f(t_{M-1,M}) \leq M f(1).$$

If we combine this with (3.2), then we get $M \leq f(1)/c_0$.

Let $A(n, \psi)$ be the maximal size of a ψ-code in $\mathbf{S}^{n-1}$. Then we have:

$$A(n, \psi) \leq \frac{f(1)}{c_0}. \tag{3.3}$$

The inequality (3.3) plays a crucial role in the Delsarte method (see details in [2], [3],[4], [9], [13], [14], [21], [23], [27]). If $z = 1/2$ and $c_0 = 1$, then (3.3) implies

$$k(n) = A(n, \pi/3) \leq f(1).$$

Levenshtein [23], and independently Odlyzko and Sloane [27] for $n = 8, 24$ have found suitable polynomials $f(t)$: $f(t) \leq 0$ for all $t \in [-1, 1/2]$, $f \in \mathsf{G}_n^+$, $c_0 = 1$ 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 the minimal vectors in 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 [27]. This implies $24 \leq k(4) \leq 25$.

4. An extension of Delsarte's method

4-A. *An extension of Delsarte's bound.* Let $f(t)$ be any real function on the interval $[-1, 1]$. Let, for a given ψ, $z := \cos\psi$. Consider on the sphere $\mathbf{S}^{n-1}$ points $y_0, y_1, \dots, y_m$ such that

$$y_i \cdot y_j \leq z \text{ for all } i \neq j, \quad f(y_0 \cdot y_i) > 0 \text{ for } 1 \leq i \leq m. \tag{4.1}$$

Definition 2. For fixed $y_0 \in \mathbf{S}^{n-1}, m \geq 0, z,$ and $f(t)$ let us define the family $Q_m(y_0) = Q_m(y_0, n, f)$ of finite sets of points from $\mathbf{S}^{n-1}$ by the formula

$$Q_m(y_0) := \begin{cases} \{y_0\}, & m = 0, \\ \{Y = \{y_1, \ldots, y_m\} \subset \mathbf{S}^{n-1} \colon \{y_0\} \cup Y \text{ satisfies } (4.1)\}, & m \geq 1. \end{cases}$$

Denote $\mu = \mu(n, z, f) := \max\{m \colon Q_m(y_0) \neq \emptyset\}$.

For $0 \leq m \leq \mu$ we define the function $H = H_f$ on the family $Q_m(y_0)$:

$$H(y_0) := f(1) \quad \text{for} \quad m = 0,$$

$$H(y_0; Y) = H(y_0; y_1, \ldots, y_m) := f(1) + f(y_0 \cdot y_1) + \ldots + f(y_0 \cdot y_m) \text{ for } m \geq 1.$$

Let

$$h_m = h_m(n, z, f) := \sup_{Y \in Q_m(y_0)} \{H(y_0; Y)\}, \quad h_{\max} := \max\{h_0, h_1, \ldots, h_\mu\}.$$

THEOREM 1. *Suppose* $f \in \mathsf{G}_n^+$. *Then*

$$A(n, \psi) \leq \frac{h_{\max}(n, \cos\psi, f)}{c_0} = \frac{1}{c_0} \max\{h_0, h_1, \ldots, h_\mu\}.$$

Proof. Let $X = \{x_1, \ldots, x_M\} \subset \mathbf{S}^{n-1}$ be a spherical ψ-code. Since $f \in \mathsf{G}_n^+$, (3.2) yields: $S(X) \geq c_0 M^2$.

Denote $J(i) := \{j \colon f(x_i \cdot x_j) > 0,\ j \neq i\},\ X(i) := \{x_j : j \in J(i)\}$. 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 that

$$S(X) = \sum_{i=1}^{M} S_i(X) \leq M h_{\max}. \tag{4.2}$$

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

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 $M \leq f(1)/c_0$.

4-B. *The class of functions* $\Phi(t_0, z)$. The problem of evaluating $h_{\max}$ in the general case looks even more complicated than the upper bound problem for spherical ψ-codes. It is not clear how to find μ, which is an optimal arrangement for Y? Here we consider this problem only for a very restrictive class of functions $\Phi(t_0, z)$. For the bound given by Theorem 1 we need $f \in \mathsf{G}_n^+$. However, for evaluations of h_m we do not need this assumption. So we do not assume that $f \in \mathsf{G}_n^+$.

Definition 3. Let real numbers t_0, z satisfy $1 > t_0 > z \geq 0$. We denote by $\Phi(t_0, z)$ the set of functions $f\colon [-1,1] \to \mathbf{R}$ such that

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

Let $f \in \Phi(t_0, z)$, and let $Y \in Q_m(y_0, n, f)$. Denote

$$e_0 := -y_0, \quad \theta_0 := \arccos t_0, \quad \theta_i := \operatorname{dist}(e_0, y_i) \quad \text{for} \quad i = 1, \ldots, m.$$

(In other words, e_0 is the antipodal point to y_0.)

It is easy to see that $f(y_0 \cdot y_i) > 0$ only if $\theta_i < \theta_0$. Therefore, Y *is a spherical* ψ*-code in the open spherical cap* $\operatorname{Cap}(e_0, \theta_0)$ *of center* e_0 *and radius* θ_0 *with* $\pi/2 \geq \psi > \theta_0$. This assumption is quite restrictive and in particular derives the convexity property for Y. We use this property in the next section.

4-C. *Convexity property.* A subset of $\mathbf{S}^{n-1}$ is called *spherically 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 [12]).

Let $Y = \{y_1, \ldots, y_m\} \subset \operatorname{Cap}(e_0, \theta_0)$, $\theta_0 < \pi/2$. Then the convex hull of Y is well defined, and is the intersection of all convex sets containing Y. Denote the convex hull of Y by $\Delta_m = \Delta_m(Y)$.

Recall a definition of a vertex of a convex set: *A point* $y \in W$ *is called the vertex* (*extremal point*) *of a spherically convex closed set* W, *if the set* $W \setminus \{y\}$ *is spherically convex or*, *equivalently*, *there are no points* x, z *from* W *for which* y *is an interior point of the minor arc* $\widehat{xz}$ *of large radius connecting* x, z.

Theorem 2. *Let* $Y = \{y_1, \ldots, y_m\} \subset \mathbf{S}^{n-1}$ *be a spherical* ψ*-code. Suppose* $Y \subset \operatorname{Cap}(e_0, \theta_0)$, *and* $0 < \theta_0 < \psi \leq \pi/2$. *Then any* y_k *is a vertex of* Δ_m.

Proof. The cases $m = 1, 2$ are evident. For the case $m = 3$ the theorem can be easily proved by contradiction. Indeed, suppose that some point, for instance, y_2, is not a vertex of Δ_3. Then, firstly, the set Δ_3 is the arc $\widehat{y_1y_3}$, and, secondly, the point y_2 lies on the arc $\widehat{y_1y_3}$. From this it follows that $\operatorname{dist}(y_1, y_3) \geq 2\psi$, since Y is a ψ-code. On the other hand, according to the triangle inequality, we have

$$2\psi \leq \operatorname{dist}(y_1, y_3) \leq \operatorname{dist}(e_0, y_1) + \operatorname{dist}(e_0, y_3) < 2\theta_0.$$

We obtained the contradiction. It remains to prove the theorem for $m \geq 4$.

In this paper we need only one fact from spherical trigonometry, namely the *law of cosines* (or the *cosine theorem*):

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

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

By the assumptions:

$$\theta_k = \mathrm{dist}(y_k, e_0) < \theta_0 < \psi \ \text{ for } \ 1 \le k \le m; \quad \phi_{k,j} := \mathrm{dist}(y_k, y_j) \ge \psi, \ k \ne j.$$

Let us prove that there is no point y_k belonging both to the interior of Δ_m and relative interior of some facet of dimension d, $1 \le d \le \dim \Delta_m$. 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 $\phi_{k,j} = \theta_j \le \theta_0 < \psi$.)

The great sphere Ω_k divides $\mathbf{S}^{n-1}$ into two closed hemispheres: H_1 and H_2. Suppose e_0 lies in the interior of H_1, then at least one y_j belongs to 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 $\gamma_{k,j} \ge 90°$, and $\cos\gamma_{k,j} \le 0$ (Fig. 1). From the conditions of Theorem 2 there follow the inequalities

$$\sin\theta_k > 0, \quad \sin\phi_{k,j} > 0, \quad \cos\theta_k > 0, \quad \cos\theta_j > 0.$$

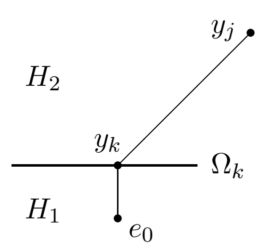


Figure 1

Hence, using the cosine theorem we obtain

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

$$0 < \cos\theta_j \le \cos\theta_k \cos\phi_{k,j}.$$

From these inequalities and $0 < \cos\theta_k < 1$ it follows that, firstly,

$$0 < \cos\phi_{k,j} \quad \Big(\text{i.e. } \psi \le \phi_{k,j} < \pi/2\Big),$$

and, secondly, the inequalities

$$\cos\theta_j < \cos\phi_{k,j} \le \cos\psi.$$

Therefore, $\theta_j > \psi$. This contradiction completes the proof of Theorem 2. □

4-D. *Bounds on μ.*

THEOREM 3. *Let $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$ be a spherical ψ-code. Suppose $Y \subset \overline{\text{Cap}}(e_0, \theta_0)$, and $0 < \psi/2 \le \theta_0 < \psi \le \pi/2$. Then*

$$m \le A\left(n-1, \arccos\frac{\cos\psi - \cos^2\theta_0}{\sin^2\theta_0}\right).$$

Proof. It is easy to see that the assumption $0 < \psi/2 \le \theta_0 < \psi \le \pi/2$ guarantees, firstly, that the right side of the inequality in Theorem 3 is well defined, secondly, that there is Y with $m \ge 2$.

If $m \ge 2$, then $y_i \ne e_0$. Conversely, $\psi \le \text{dist}(y_i, y_j) = \text{dist}(e_0, y_j) = \theta_j < \theta_0$, a contradiction. Therefore, the projection Π from the pole e_0 which sends $x \in \mathbf{S}^{n-1}$ along its meridian to the equator of the sphere is defined for all y_i.

Denote $\gamma_{i,j} := \text{dist}\,(\Pi(y_i), \Pi(y_j))$ (see Fig. 2). Then from the law of cosines and the inequality $\cos\phi_{i,j} \le z = \cos\psi$, we get

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

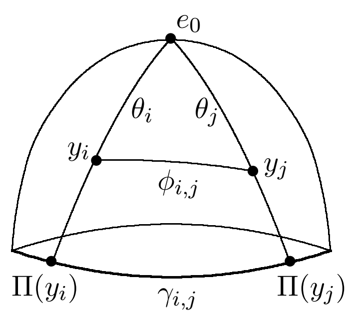


Figure 2

Let

$$R(\alpha,\beta) = \frac{z - \cos\alpha\cos\beta}{\sin\alpha\sin\beta}, \quad \text{then} \quad \frac{\partial R(\alpha,\beta)}{\partial\alpha} = \frac{\cos\beta - z\cos\alpha}{\sin^2\alpha\sin\beta}.$$

We have $\theta_0 < \psi$. Therefore, if $0 < \alpha, \beta < \theta_0$, then $\cos\beta > z$. That yields: $\partial R(\alpha,\beta)/\partial\alpha > 0$; i.e., $R(\alpha,\beta)$ is a monotone increasing function in α. We obtain $R(\alpha,\beta) < R(\theta_0,\beta) = R(\beta,\theta_0) < R(\theta_0,\theta_0)$.

Therefore,

$$\cos\gamma_{i,j} \le \frac{z - \cos\theta_i\cos\theta_j}{\sin\theta_i\sin\theta_j} < \frac{z - \cos^2\theta_0}{\sin^2\theta_0} = \cos\delta.$$

Thus $\Pi(Y)$ is a δ-code on the equator $\mathbf{S}^{n-2}$. That yields $m \le A(n-1,\delta)$. $\square$

Corollary 1. *Suppose* $f \in \Phi(t_0, z)$. *If* $2t_0^2 > z+1$, *then* $\mu(n,z,f) \le 1$; *otherwise*

$$\mu(n,z,f) \le A\Big(n-1, \arccos\frac{z-t_0^2}{1-t_0^2}\Big).$$

Proof. Let $\cos\psi = z$, $\cos\theta_0 = t_0$. Then $2t_0^2 > z+1$ if and only if $\psi > 2\theta_0$. Clearly in this case the size of any ψ-code in the cap $\mathrm{Cap}(e_0, \theta_0)$ is at most 1. Otherwise, $\psi \le 2\theta_0$ and this corollary follows from Theorem 3. $\square$

Corollary 2. *Suppose* $f \in \Phi(t_0, z)$. *Then*

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

Proof. Note that

$$T = \frac{z-t_0^2}{1-t_0^2} \le \frac{z-z^2}{1-z^2} = \frac{z}{1+z} < \frac{1}{2}. \quad \text{Then } \ \delta = \arccos T > \pi/3.$$

Thus $\mu(3,z,f) \le A(2,\delta) \le 2\pi/\delta < 6$. $\square$

Corollary 3. *Suppose* $f \in \Phi(t_0, z)$.

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

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

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 $M \le 12$ and $M = 24$ (see [11], [16], [30]). It is well known [16], [30] that $\varphi_3(5) = \varphi_3(6) = 90°$. It has been proved by Schütte and van der Waerden [30] that

$$\cos\varphi_3(7) = \cot 40° \cot 80°, \quad \varphi_3(7) \approx 77.86954°.$$

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

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

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

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

4-E. *Optimization problem.* Let

$$t_0 := \cos\theta_0, \quad z := \cos\psi, \quad \cos\delta := \frac{z-t_0^2}{1-t_0^2}, \quad \mu^* := A(n-1,\delta).$$

For given $n, \psi, \theta_0, f \in \Phi(t_0, z), e_0 \in \mathbf{S}^{n-1}$, and $m \le \mu^*$, the value $h_m(n, z, f)$ is the solution of the following optimization problem on $\mathbf{S}^{n-1}$:

$$\text{maximize } \ f(1) + f(-e_0 \cdot y_1) + \ldots + f(-e_0 \cdot y_m)$$

subject to the constraints

$$y_i \in \mathbf{S}^{n-1}, \ i = 1, \ldots, m, \quad \operatorname{dist}(e_0, y_i) \le \theta_0, \quad \operatorname{dist}(y_i, y_j) \ge \psi, \ i \ne j.$$

The dimension of this problem is $(n-1)m \le (n-1)\mu^*$. If μ^* is small enough, then for small n it gets relatively small dimensional optimization problems for computation of values h_m. If additionally $f(t)$ is a monotone decreasing function on $[-1, -t_0]$, then in some cases this problem can be reduced to $(n-1)$-dimensional optimization problem of a type that can be treated numerically.

5. Optimal and irreducible sets

5-A. *The monotonicity assumption and optimal sets.*

Definition 4. We denote by $\Phi^*(z)$ the set of all functions $f \in \bigcup\limits_{\tau_0 > z} \Phi(\tau_0, z)$ such that $f(t)$ is a monotone decreasing function on the interval $[-1, -\tau_0]$, and $f(-1) > 0 > f(-\tau_0)$.

For any $f \in \Phi^*(z)$, denote $t_0 = t_0(f) := \sup\{t \in [\tau_0, 1] \colon f(-t) < 0\}$.

Clearly, if $f \in \Phi^*(z)$, then $f \in \Phi(t_0, z)$, i.e. $f(t) \le 0$ for $t \in [-t_0, z]$. Moreover, if $f(t)$ is a continious function on $[-1, -z]$, then $f(-t_0) = 0$.

Consider a spherical ψ-code $Y = \{y_1, \ldots, y_m\} \subset \operatorname{Cap}(e_0, \theta_0) \subset \mathbf{S}^{n-1}$. Then we have the constraint: $\phi_{i,j} := \operatorname{dist}(y_i, y_j) \ge \psi$ for all $i \ne j$. Denote by $\Gamma_\psi(Y)$ the graph with the set of vertices Y and the set of edges $y_i y_j$ with $\phi_{i,j} = \psi$.

Definition 5. Let $f \in \Phi^*(z), \ \psi = \arccos(z), \ \theta_0 = \arccos(t_0)$. We say that a spherical ψ-code $Y = \{y_1, \ldots, y_m\} \subset \operatorname{Cap}(e_0, \theta_0) \subset \mathbf{S}^{n-1}$ is optimal for f if $H_f(-e_0; Y) = h_m(n, z, f)$.

If optimal Y is not unique up to isometry, then we call Y optimal if the graph $\Gamma_\psi(Y)$ has the maximal number of edges.

Let $\theta_k := \operatorname{dist}(y_k, e_0)$. Then $H(-e_0; Y)$ can be represented in the form:

$$F_f(\theta_1, \ldots, \theta_m) := H_f(-e_0; Y) = f(1) + f(-\cos\theta_1) + \ldots + f(-\cos\theta_m).$$

We call $F(\theta_1, \ldots, \theta_m) = F_f(\theta_1, \ldots, \theta_m)$ *the efficient function.* Clearly, if $f \in \Phi^*(z)$, then the efficient function is *a monotone decreasing function in the interval* $[0, \theta_0]$ *for any variable* θ_k.

5-B. *Irreducible sets.*

Definition 6. Let $0 < \theta_0 < \psi \leq \pi/2$. We say that a spherical ψ-code $Y = \{y_1, \dots, y_m\} \subset \mathrm{Cap}(e_0, \theta_0) \subset \mathbf{S}^{n-1}$ is *irreducible* (or jammed) if any y_k cannot be shifted towards e_0 (i.e. this shift decreases θ_k) such that Y', which is obtained after this shifting, is also a ψ-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. *Let $f \in \Phi^*(z)$. Suppose $Y \subset \mathrm{Cap}(e_0, \theta_0) \subset \mathbf{S}^{n-1}$ is optimal for f. Then Y is irreducible.*

Proof. The efficient function $F(\theta_1, \dots, \theta_m)$ increases whenever θ_k decreases. From this it follows that y_k cannot be shifted towards e_0. In the converse case, $H(-e_0; Y) = F(\theta_1, \dots, \theta_m)$ increases whenever y_k tends to e_0. This contradicts the optimality of the initial set Y. □

LEMMA 1. *If $Y = \{y_1, \dots, y_m\}$ is irreducible, then*

(i) *$e_0 \in \Delta_m$ =convex hull of Y;*

(ii) *If $m > 1$, then $\deg y_i > 0$ for all $y_i \in Y$, where $\deg y_i$ denotes the degree of the vertex y_i in the graph $\Gamma_\psi(Y)$.*

Proof. (i) Otherwise whole Y can be shifted towards e_0.
(ii) Clearly, if $\phi_{i,j} > \psi$ for all $j \neq i$, then y_i can be shifted towards e_0. □

For $m = 1$, it follows that $e_0 = y_1$; i.e., $h_1 = \sup\{F(\theta_1)\} = F(0)$. Thus

$$h_1 = f(1) + f(-1). \tag{5.1}$$

For $m = 2$, Lemma 1 implies that $\mathrm{dist}\,(y_1, y_2) = \psi$, i.e.

$$\Delta_2 = y_1 y_2 \textit{ is an arc of length } \psi. \tag{5.2}$$

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 with edge lengths ψ, $\psi \leq \pi/2$. 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 $\omega = u_1u_2,\ \Delta = v_1v_2\dots v_k, \mathrm{dist}(u_1,u_2) = \mathrm{dist}(v_i,v_j) = \psi$. Assume the converse. Then $\mathrm{dist}(u_i,v_j) \ge \psi$ 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 do not lie inside U. If $\{u_1',u_2'\} = \omega \bigcap B$, then $\psi = \mathrm{dist}(u_1,u_2) \ge \mathrm{dist}(u_1',u_2')$, and $\omega' \bigcap \Delta \ne \emptyset$, where $\omega' = u_1'u_2'$.

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 $w_1w_2 \bigcap \Delta \ne \emptyset$. It is not hard to prove that $\mathrm{dist}(w_1,w_2)$ attains its minimum when w_1 and w_2 are at distance 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, we show by direct calculation that

$$\cos\alpha = \frac{2kz^2-(k-1)z-1}{1+(k-1)z}, \quad \alpha = \min \mathrm{dist}(w_1,w_2),\ z = \cos\psi. \tag{5.3}$$

We have $\alpha \le \psi$. From (5.3), it follows that $\cos\alpha \ge z$ if and only if $z \ge 1$ or $(k+1)z+1 \le 0$. This contradicts the assumption $0 \le z < 1$. □

5-C. *Irreducible sets in* $\mathbf{S}^2$. Now we consider irreducible sets for $n = 3$. In this case $\dim\Delta_m \le 2$.

THEOREM 4. *Suppose Y is irreducible and* $\dim(\Delta_m) = 2$. *Then* $3 \le m \le 5$, *and Δ_m is a spherical regular triangle, rhomb, or equilateral pentagon with edge lengths ψ.*

Proof. From Corollary 2 it follows that $m \le 5$. On the other hand, $m > 2$. Then $m = 3$, 4, 5. Theorem 2 implies that Δ_m is a convex polygon with vertices $y_1,\dots,y_m$. From Lemma 1 it follows that $e_0 \in \Delta_m$, and $\deg y_i \geqslant 1$.

First let us prove that if $\deg y_i \ge 2$ for all i, then Δ_m is an 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 nonoverlapping triangles with a common vertex (Fig. 3). This case contradicts the convexity of Δ_5. Indeed, since the angular sum in a spherical triangle is strictly greater than $180°$ and a larger side of a spherical triangle subtends the opposite large angle, we have $\angle y_iy_1y_j > 60°$. Then

$$180° \ge \angle y_2y_1y_5 = \angle y_2y_1y_3 + \angle y_3y_1y_4 + \angle y_4y_1y_5 > 180°$$

— a contradiction.

Now we prove that $\deg y_i \ge 2$. Suppose $\deg y_1 = 1$, i.e. $\phi_{1,2} = \psi,\ \phi_{1,i} > \psi$ for $i = 3,\dots,m$. (Recall that $\phi_{i,j} = \mathrm{dist}(y_i,y_j)$.) If $e_0 \notin y_1y_2$, then after a sufficiently small turn of y_1 around 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.)

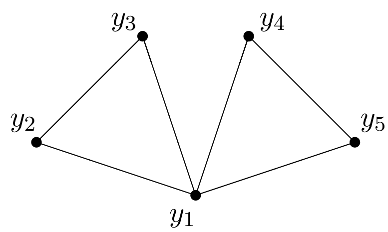


Figure 3

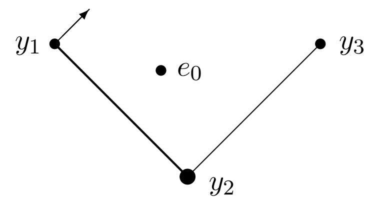


Figure 4

It remains to consider the case: $e_0 \in y_1y_2$. If $\phi_{i,j} = \psi$ where $i > 2$ or $j > 2$, then $e_0 \notin y_iy_j$. 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 $m = 3, 4$ this implies the proof. For $m = 5$ there is the case where $Q_3 = y_3y_4y_5$ is a regular triangle of side length ψ. Note that y_1y_2 cannot intersect Q_3 (otherwise we again have intersecting diagonals of lengths ψ), and so y_1y_2 is a side of Δ_5. In this case, as above, after a sufficiently small turn of Q_3 around y_2 to e_0 the distance $\theta_i,\ i = 3, 4, 5$, decreases – a contradiction. $\square$

5-D. *Rotations and irreducible sets in n dimensions.* Now we extend these results to n 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

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

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

$$u_1' = u_1 \cos\varphi - u_2 \sin\varphi, \quad u_2' = u_1 \sin\varphi + u_2 \cos\varphi, \quad u_i' = u_i,\ i = 3, \ldots, n.$$

Let

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

[2]In the first version of this paper for $m \geq n$ it 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 Bannai and 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). Now this claim for all n can be considered only as conjecture. In **5-D** we prove the claim when $\{y_i\}$ are in "general position". I wish to thank Eiichi Bannai, Makoto Tagami, and anonymous referees for helpful and useful comments.

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

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

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

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

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

$$r'(0) < 0 \text{ iff } \quad v_2 < 0, \quad \text{i.e.} \quad e_0 \in \overset{\circ}{H}_-\,.$$

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. □

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

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

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. This contradicts the irreducibility of Y. □

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,

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

Let for $\sigma \subset I_n := \{1, \dots, n\}$

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

We claim for $i \neq j$ that:

$$\text{(5.4)} \qquad \textit{If } e_0 \notin F_{\{i,j\}}, \textit{ then } \phi_{i,j} = \psi.$$

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

Now, 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_n.

Suppose $e_0 \in F_\sigma$, where σ has maximal size and $|\sigma| > 1$. Let $\bar{\sigma} = I_n \setminus \sigma$. From (5.4) it 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 $F_\sigma =$ convex hull of $\{y_i\colon\ \in \bar{\sigma}\}$, and for any fixed point x from F_σ (in particular for $x = e_0$) the distance $\operatorname{dist}(x, y)$ possesses the same value (depending only on x) on the entire set $y \in \Lambda$. Then y_i, $i \in \sigma$, lie in Λ at the same distance from e_0. It is clear that Y is irreducible if and only if y_i, $i \in \sigma$, in Λ are vertices of a regular simplex of edge length ψ.

Finally, all edges of Δ_n are of lengths ψ as required. □

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 it follows that Δ_4 is a rhomb. Suppose y_1y_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 $y_1y_2y_3$ around y_1y_3. If $e_0 \notin y_1y_3$, then this turn decreases either θ_4 (if $e_0 \in y_1y_2y_3$) or θ_2, a contradiction. In the case $e_0 \in y_1y_3$ any turn of y_2 around y_1y_3 decreases $\phi_{2,4}$ and does not change θ_2. Obviously, there is a turn such that $\phi_{2,4}$ becomes equal to ψ. That contradicts the irreducibility of Y also. □

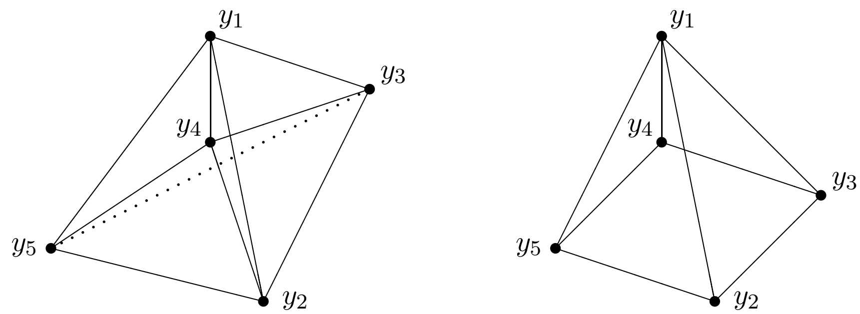
5-E. *Irreducible sets in $\mathbf{S}^3$.*

Lemma 4. *If $Y \subset \mathbf{S}^3$ is irreducible and $|Y| = 5$, 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 it follows that Δ_5 is a convex equilateral pentagon. Suppose y_1y_3 is the minimal length diagonal of Δ_5. We have $\phi_{2,k} > \psi$ for $k > 3$. Suppose $e_0 \notin y_1y_3$. If $e_0 \in y_1y_2y_3$ then any sufficiently small turn of the facet $y_1y_3y_4y_5$ around y_1y_3 decreases θ_4 and θ_5; otherwise it decreases θ_2, a contradiction. In the case $e_0 \in y_1y_3$ any turn of y_2 around y_1y_3 decreases $\phi_{2,k}$

for $k = 4, 5$, and does not change θ_i. It can be shown in an elementary way that there is a turn such that $\phi_{2,4}$ or $\phi_{2,5}$ becomes equal to ψ, a contradiction.

In three dimensions there exist only two combinatorial types of convex polytopes with five 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.



(A) (B)

Figure 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 is bounded by the great circle passing 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 $\deg y_k = 1, 2$.

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

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 does not 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 cannot be a vertex of Δ_5. Therefore, e_0 lies inside $s_{k\ell}$. From this we have: If s_{ij} for any j does not intersect $s_{k\ell}$, then $\deg y_i \geq 2$.

Arguing as above, we can prove that

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

(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 type (A) this 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 three 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 around Ω that simultaneously decreases $\theta_i, \theta_j, \theta_q$ — a contradiction.

b) For 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 a) it follows that $\deg y_i \geq 2$ for $i = 1, 2, 4$. Moreover, if $\deg y_i = 2$, then $e_0 = s_{35} \bigcap s_{124}$. 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 it follows that some $\phi_{i,j} < \psi$ — a contradiction.

c) Now for 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 $\phi_{2,4} = \psi,\ e_0 = s_{24} \bigcap s_{35}$; $\deg y_2 = 2$ 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 ψ-code. This contradiction concludes the proof that $\deg y_k \geq 2$ for all k.

(5) Finally we 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 (**4**a), where Ω_2 the great sphere contains s_{ijk}, and Ω the great circle passes through y_i, y_j, we can prove that there exist 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 $s_{\ell q}$ around Ω does not 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. These are: $s_{124},\ s_{135}$ (type (A) and type (B)), 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 around 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. This again implies $\phi_{3,5} = \psi$. Since s_{35} cannot intersects a regular triangle s_{124} [see Lemma 2, (**4**b)], $\phi_{2,4} > \psi$. 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 (B)) is equivalent to the Case s_{124}.

Case s_{135} (*type* (A)). This case has two subcases: $\tilde{s}_{351},\ \tilde{s}_{153}$. 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 around s_{35} decreases θ_1 (Lemma 3). Then $e_0 \in s_{135}$. Clearly, any small turn of y_2 around 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: $\tilde{s}_{243}$, $\tilde{s}_{234}$. It is not hard to see that $\tilde{s}_{243}$ follows from Case facet, and $\tilde{s}_{234}$ 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 $z \geq \cos\alpha \geq 2z - 1$.

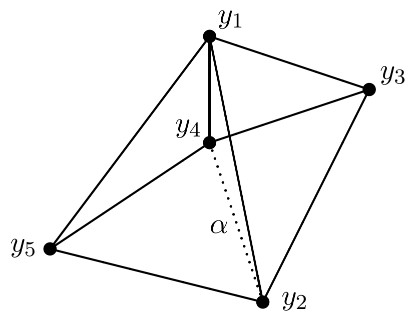


Figure 6: $P_5(\alpha)$

Thus Theorem 4, Corollary 4 and Lemma 4 for $n = 4$ yield:

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-F. *Optimization problem.* We see that if Y is optimal, then for some cases Y can be determined up to isometry. For fixed $y_i \in \mathbf{S}^{n-1}$, $i = 1, \ldots, m$, the function H depends only on a position $y = -y_0 = e_0 \in \mathbf{S}^{n-1}$. Now,

$$H_m(y) := f(1) + f(-y \cdot y_1) + \ldots + f(-y \cdot y_m);$$

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

Thus for h_m we have the following $(n-1)$-dimensional optimization problem:

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

subject to the constraint

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

We present an efficient numerical method for solving this problem in the next section.

6. On calculations of h_m

In this technical section we explain how to find an upper bound on h_m for $n = 4,\ m \le 6$. Note that Theorem 5 gives for computation of h_m a low-dimensional optimization problem (see **5-F**). Our first approach for this problem was to apply numerical methods [25]. However, that is a nonconvex constrained optimization problem. In this case, the Nelder-Mead simplex method and other local improvements cannot guarantee finding a global optimum. It is possible (using estimations of derivatives) to organize the computational process in such way that it gives a global optimum. However, such solutions are very hard to verify and some mathematicians do not accept that kind of proof. Fortunately, using a geometric approach, estimations of h_m can be reduced to relatively simple computations.

Throughout this section we use the function $\tilde f(\theta)$ defined for $f \in \Phi^*(z)$ by

$$\tilde f(\theta) := \begin{cases} f(-\cos\theta) & 0 \le \theta \le \theta_0 = \arccos t_0 \ \text{ (see Definition 4)} \\ -\infty & \theta > \theta_0. \end{cases}$$

Since $f \in \Phi^*(z)$, $\tilde f(\theta)$ is a monotone decreasing function in θ on $[0, \theta_0]$.

6-A. *The case* $m = 2$. Suppose $m = 2$ and Y is optimal for $f \in \Phi^*(z)$. Then $\Delta_2 = y_1y_2$ is an arc of length ψ, $e_0 \in \Delta_2$, and $\theta_1 + \theta_2 = \psi$, where $\theta_i \le \theta_0$ (see Lemma 1 and (5.2)). The efficient function $F(\theta_1, \theta_2) = f(1) + \tilde f(\theta_1) + \tilde f(\theta_2)$ is a symmetric function in θ_1, θ_2.

We can assume that $\theta_1 \le \theta_2$, and 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 $\theta_1 \in [u, v] \subset [\psi - \theta_0, \psi/2]$ we have

$$F(\theta_1, \theta_2) \le \Phi_2([u, v]) := f(1) + \tilde f(u) + \tilde f(\psi - v).$$

Let $u_1 = \psi - \theta_0,\ u_2, \dots, u_N,\ u_{N+1} = \psi/2$ be points in $[\psi - \theta_0, \psi/2]$ such that $u_{i+1} = u_i + \varepsilon$, where $\varepsilon = (\theta_0 - \psi/2)/N$. If $\theta_1 \in [u_i, u_{i+1}]$, then $h_2 = H(y_0; Y) = F(\theta_1, \theta_2) \le \Phi_2([u_i, u_{i+1}])$. Thus

$$h_2 \le \lambda_2(N, \psi, \theta_0) := \max_{1 \le i \le N} \{\Phi_2(s_i)\}, \quad \text{where } \ s_i := [u_i, u_{i+1}].$$

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

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

6-B. *The function* Θ_k. Suppose we know that (up to isometry) optimal $Y = \{y_1, \dots, y_m\} \subset \mathbf{S}^{n-1}$. Let us assume that $\dim \Delta_m = n - 1$, and $V :=$ convex hull of $\{y_1 \dots y_{n-1}\}$ is a facet of Δ_m. Then $\operatorname{rank}\{y_1, \dots, y_{n-1}\} = n-1$, and Y belongs to the hemisphere H_+, where H_+ contains Y and is bounded by the great sphere $\tilde{S}$ passing through V.

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

$$y \cdot y = 1 \ \text{ with } \ y \cdot y_i = \cos\theta_i,\ i = 1, \dots, n-1. \tag{6.1}$$

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

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

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

It is not hard to solve (6.1) and, therefore, to give an explicit expression for Θ_k.

For instance, let Δ_n be a regular simplex of edge lengths $\pi/3$. (We need this case for $n = 3, 4$.) Then[3]

$$\begin{aligned}\cos\theta_3 &= \cos\Theta_3(\theta_1, \theta_2)\\ &= \frac{1}{3}\left(\cos\theta_1 + \cos\theta_2 + \sqrt{6 - 8[\cos\theta_1\cos\theta_2 + (\cos\theta_2 - \cos\theta_1)^2]}\right);\end{aligned}$$

$$\cos\theta_4 = \cos\Theta_4(\theta_1, \theta_2, \theta_3) = \frac{1}{4}\Bigg(\cos\theta_1 + \cos\theta_2 + \cos\theta_3$$

$$+\sqrt{10}\sqrt{1 + \cos\theta_1\cos\theta_2 + \cos\theta_1\cos\theta_3 + \cos\theta_2\cos\theta_3 - \tfrac{3}{2}(\cos^2\theta_1 + \cos^2\theta_2 + \cos^2\theta_3)}\Bigg).$$

6-C. *Extremal points of* Θ_k *on* D. Let $\mathbf{a} = (a_1, \dots, a_{n-1})$, where $0 < a_i \leq \theta_0 < \psi$. (Recall that $\phi_{i,j} = \mathrm{dist}(y_i, y_j)$; $\cos\psi = z$; $\cos\theta_0 = t_0$.) Now we consider a domain $D(\mathbf{a})$ in H_+, where

$$D(\mathbf{a}) = \{y \in H_+ :\ \mathrm{dist}(y, y_i) \leq a_i,\ 1 \leq i \leq n-1\}.$$

In other words, $D(\mathbf{a})$ is the intersection of the closed caps $\mathrm{Cap}(y_i, a_i)$ in H_+:

$$D(\mathbf{a}) = \bigcap_{i=1}^{n-1} \mathrm{Cap}(y_i, a_i) \bigcap H_+.$$

Suppose $\dim D(\mathbf{a}) = n-1$. Then $D(\mathbf{a})$ has "vertices", "edges", and "k-faces" for $k \leq n-1$. Indeed, let

$$\begin{aligned}\sigma \subset I &:= \{1, \dots, n-1\}, \quad 0 < |\sigma| \leq n-1;\\ \tilde{F}_\sigma &:= \{y \in D(\mathbf{a}) :\ \mathrm{dist}(y, y_i) = a_i\ \forall\, i \in \sigma\}.\end{aligned}$$

It is easy to prove that $\dim \tilde{F}_\sigma = n - 1 - |\sigma|$; $\tilde{F}_\sigma$ belongs to the boundary B of $D(\mathbf{a})$; and if $\sigma \subset \sigma'$, then $\tilde{F}_{\sigma'} \subset \tilde{F}_\sigma$.

[3] I am very grateful to referees for these explicit formulas.

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

$$\operatorname{dist}(y_k, p_k(\mathbf{a})) = \operatorname{dist}(y_k, D(\mathbf{a})).$$

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

$$p_k(\mathbf{a}) \in \tilde{F}_\sigma. \tag{6.2}$$

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

Let $\sigma_k(\mathbf{a})$ denote $\sigma \subset I$ of the maximal size such that σ satisfies (6.2). Then for $\sigma_k(\mathbf{a}) = I$, $p_k(\mathbf{a}) = p_*(\mathbf{a})$, and for $|\sigma_k(\mathbf{a})| < n-1$, $p_k(\mathbf{a})$ belongs to the open part of $\tilde{F}_{\sigma_k(\mathbf{a})}$.

Consider $n = 3$. There are two cases for $p_k(\mathbf{a})$ (see Fig. 7): $p_3(\mathbf{a}) = p_*(\mathbf{a}) = \tilde{F}_{\{1,2\}}$, and $p_4(\mathbf{a})$ is the intersection in H_+ of the great circle passing through y_1, y_4, and the circle $\tilde{S}(y_1, a_1)$ of center y_1 and radius a_1 ($\tilde{F}_{\{1\}} \subset \tilde{S}(y_1, a_1)$). The same holds for all dimensions.

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

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

Denote by $s(\sigma, k)$ the intersection of $S_\sigma(k)$ and $\tilde{S}_\sigma$ in $D(\mathbf{a})$,

$$s(\sigma, k) = S_\sigma(k) \bigcap \tilde{S}_\sigma \bigcap D(\mathbf{a}).$$

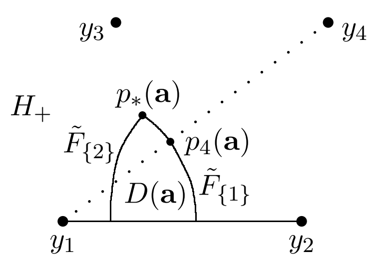


Figure 7

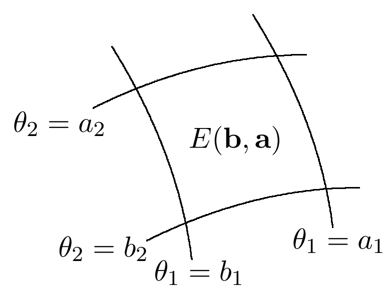


Figure 8

LEMMA 5. *Suppose* $D(\mathbf{a}) \neq \emptyset$, $0 < a_i \leq \theta_0$ *for all* i, *and* $k \geq n$. *Then*

(i) $p_k(\mathbf{a}) \in s(\sigma_k(\mathbf{a}), k)$,

(ii) *if* $s(\sigma, k) \neq \emptyset$, $|\sigma| < n-1$, *then* $s(\sigma, k)$ *consists of the one point* $p_k(\mathbf{a})$.

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

(ii) Note that $s(\sigma, k)$ belongs to the intersection in $D(\mathbf{a}) \subset H_+$ of the spheres $S(y_i, a_i)$, $i \in \sigma$, 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 $\tilde{S}(y_k, \mathrm{dist}(y_k, p))$ touches $\tilde{S}_{\sigma'}$ at p. Thus $p = p_k(\mathbf{a})$. □

Lemma 5 implies a simple method for calculations of the minimum of Θ_k on $D(\mathbf{a})$. For this we can consider $s(\sigma, k)$, $\sigma \subset I$, and if $s(\sigma, k) \neq \emptyset$, then $s(\sigma, k) = \{p_k(\mathbf{a})\}$, 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 a very simple method.

Corollary 5. *Suppose $|Y| = n$, $0 < a_i \leq \theta_0$ for all i, and $D(\mathbf{a})$ lies inside Δ_n. Then*

$$\theta_n \geq \Theta_n(a_1, \ldots, a_{n-1}) \ \textit{for all} \ y \in D(\mathbf{a}).$$

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

6-D. *Upper bounds on H_m.* Suppose $\dim \Delta_m = n - 1$, and $y_1 \ldots y_{n-1}$ is a facet of Δ_m. Then (see **5-F** for the definitions of H_m and $T(Y, \theta_0)$)

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

where

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

Lemma 6. *Suppose $f \in \Phi^*(z)$, $|Y| = m$, $\dim \Delta_m = n - 1$, $y_1 \ldots y_{n-1}$ is a facet of Δ_m, $\mathrm{dist}(y_i, y_j) \geq \psi > \theta_0$ for $i \neq j$, $0 \leq b_i < a_i \leq \theta_0$ for $i = 1, \ldots, n-1$; and $\Theta_k(\mathbf{a}) \leq \theta_0$ for all $k \geq n$. If $D(\mathbf{a}) \neq \emptyset$, then*

$$H_m(y) \leq \Phi_Y(\mathbf{b}, \mathbf{a}) \quad \textit{for any} \quad y \in E(\mathbf{b}, \mathbf{a}) := D(\mathbf{a}) \setminus U(\mathbf{b}),$$

where

$$\Phi_Y(\mathbf{b},\mathbf{a}) := f(1) + \tilde{f}(b_1) + \ldots + \tilde{f}(b_{n-1}) + \tilde{f}(\Theta_n(p_n(\mathbf{a}))) + \ldots + \tilde{f}(\Theta_m(p_m(\mathbf{a}))),$$

$$U(\mathbf{b}) := \bigcup_{i=1}^{n-1} \mathrm{Cap}(y_i, b_i).$$

Proof. We have for $1 \le i \le n-1$ and $y \in E(\mathbf{b},\mathbf{a})$, $\theta_i \ge b_i$ (Fig. 8). By the monotonicity assumption this implies $\tilde{f}(\theta_i) \le \tilde{f}(b_i)$. On the other hand, $y \in D(\mathbf{a})$. Then Lemma 5 yields $\tilde{f}(\theta_k) \le \tilde{f}(\Theta_k(p_k(\mathbf{a})))$ for $k \ge n$. □

From Corollary 5 and Lemma 6 we obtain

COROLLARY 6. *Let* $|Y| = n$. *Suppose* f, $\mathbf{a}$, $\mathbf{b}$, *and* Y *satisfy the assumptions of Lemma* 6 *and Corollary* 5. *Then for any* $y \in E(\mathbf{b},\mathbf{a})$:

$$H_m(y) \le f(1) + \tilde{f}(b_1) + \ldots + \tilde{f}(b_{n-1}) + \tilde{f}(\Theta_n(\mathbf{a})).$$

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 a given positive integer N. Then the grid (tessellation) $L(N)$ consists of N^{n-1} cells, any cell $c \in L(N)$ $(\theta_1, \ldots, \theta_{n-1})$ in c we have

$$b_i(c) \le \theta_i \le a_i(c), \quad a_i(c) = b_i(c) + \varepsilon, \quad i = 1, \ldots, n-1.$$

Let $\tilde{L}(N)$ be the subset of cells c in $L(N)$ such that $D(\mathbf{a}(c)) \ne \emptyset$. There exists $c \in L(N)$ such that H_m attains its maximum on $T(Y,\theta_0)$ at some point in $E(\mathbf{b}(c),\mathbf{a}(c))$. 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* $\mathrm{dist}(y, y_i) \le \theta_0$ *for all* i. *Then*

$$H_m(y) \le \max_{c \in \tilde{L}(N)} \{\Phi_Y(\mathbf{b}(c), \mathbf{a}(c))\}.$$

6-E. *Upper bounds on* h_m. Suppose Δ_m is a regular simplex of edge length ψ. Then the efficient function F is a symmetric function in the variables $\theta_1, \ldots, \theta_m$. Consider this problem only on the domain

$$\Lambda := \{y \in \Delta_m : \ \psi - \theta_0 \le \theta_1 \le \theta_2 \le \ldots \le \theta_m \le \theta_0\}.$$

Let $L_\Lambda(N)$ be the subset of cells c in $\tilde{L}(N)$ such that $E(\mathbf{b}(c),\mathbf{a}(c)) \bigcap \Lambda \ne \emptyset$. Then we have an explicit expression for $\Phi_m(c) := \Phi_Y(\mathbf{b}(c),\mathbf{a}(c))$ (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,

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

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 $\theta_4(\alpha) := \mathrm{dist}(y, y_4(\alpha))$ 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 that

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

Combining this with Lemma 7, we get

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

$$R_{1,2,3}(c) = \tilde f(b_1(c)) + \tilde f(b_2(c)) + \tilde f(b_3(c)),$$

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

where $p_k(\mathbf{a}, \alpha) = p_k(\mathbf{a})$ with $y_k = y_k(\alpha)$.

Clearly, $\lambda_m(2N, \psi, \theta_0) \le \lambda_m(N, \psi, \theta_0)$. It is not hard to show that

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

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

LEMMA 8. *Let* $n = 4,\ f \in \Phi^*(z),\ \sqrt{z} > t_0 > z,\ \theta_0' \in [\arccos\sqrt{z}, \theta_0]$. *Then*

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

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 $\theta_1 \le \theta_2 \le \ldots \le \theta_6$. Then from Corollary 3(i) we obtain that

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

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

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

$$H(y_0; y_1, \dots, y_5) \le h_5 = \lambda_5(\psi, \theta_0), \qquad \tilde f(\theta_6) \le \tilde f(\theta_0').$$

Then $h_6 \le \tilde f(\theta_0') + \lambda_5(\psi, \theta_0)$.

(b) In this case all $\theta_i \le \theta_0'$; i.e. $Y \subset C(e_0, \theta_0')$. Since

$$H(y_0; y_1, \dots, y_5) \le \lambda_5(\psi, \theta_0'), \qquad \tilde f(\theta_6) \le f(-\sqrt{z}),$$

it follows that $h_6 \le f(-\sqrt{z}) + \lambda_5(\psi, \theta_0')$. $\square$

We have proved the following theorem.

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

(i) $h_0 = f(1), \quad h_1 = f(1) + f(-1)$;

(ii) $h_m \le \lambda_m(\psi, \theta_0) \le \lambda_m(N, \psi, \theta_0)$ *for* $2 \le m \le 5$;

(iii) $h_6 \le \max\{\tilde{f}(\theta_0') + \lambda_5(\psi, \theta_0),\ f(-\sqrt{z}) + \lambda_5(\psi, \theta_0')\}\ \forall\ \theta_0' \in [\arccos\sqrt{z}, \theta_0]$.

6-F. *Proof of Lemma* B. First we show that $f_4 \in \Phi^*(1/2)$ (see Fig. 9). Indeed, the polynomial f_4 has two roots on $[-1, 1]$: $t_1 = -t_0$, $t_0 \approx 0.60794$, $t_2 = 1/2$; $f_4(t) \le 0$ for $t \in [-t_0, 1/2]$, and f_4 is a monotone decreasing function on the interval $[-1, -t_0]$. The last property holds because there are no zeros of the derivative $f_4'(t)$ on $[-1, -t_0]$. Thus, $f_4 \in \Phi^*(1/2)$.

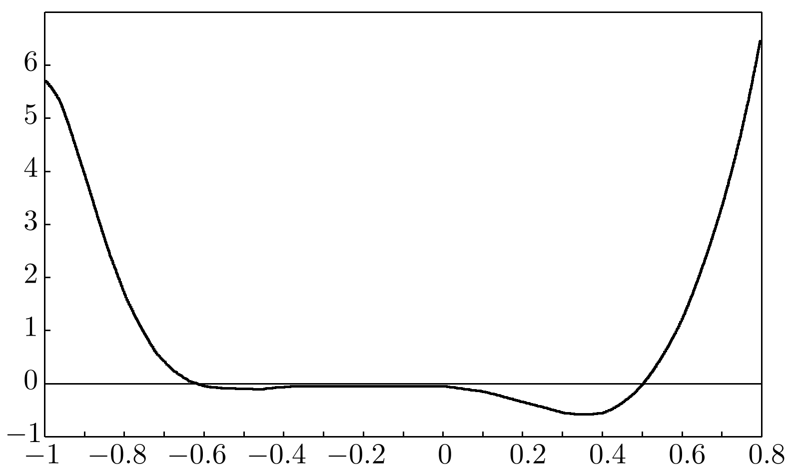


Figure 9. The graph of the function $f_4(t)$

We have $t_0 > 0.6058$. Then Corollary 3(*ii*) gives $\mu \le 6$. For calculations of h_m let us apply Theorem 6 with $\psi = \arccos z = 60°$, $\theta_0 = \arccos t_0 \approx 52.5588°$. We get

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

H_2 achieves its maximum at $\theta_1 = 30°$. Then

$$h_2 = f(1) + 2f(-\cos 30°) \approx 24.8644.$$

For $m = 3$ we have

$$h_3 = \lambda_3(60°, \theta_0) \approx 24.8345$$

at $\theta_3 = \theta_0$, $\theta_1 = \theta_2 \approx 30.0715°$.

The polynomial H_4 attains its maximum

$$h_4 \approx 24.818$$

at the point with $\theta_1=\theta_2\approx 30.2310^\circ,\ \ \theta_3=\theta_4\approx 51.6765^\circ$, and

$$h_5\approx 24.6856$$

at $\alpha=60^\circ,\ \theta_1\approx 42.1569^\circ,\ \theta_2=\theta_4=32.3025^\circ,\ \theta_3=\theta_5=\theta_0$.

Let $\theta_0'=50^\circ$. We have $\tilde f(50^\circ)\approx 0.0906$, $\arccos\sqrt{z}=45^\circ$, $\tilde f(45^\circ)\approx 0.4533$,

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

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

Thus $h_{\max}=h_2<25$. By (4.2), we have $S(X)<25M$.

7. Concluding remarks

This extension of the Delsarte method can be applied to other dimensions and spherical ψ-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 much easier than for $n=4$ (see [26]).

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 $f\in\Phi^*(1/2),\ t_0\approx 0.5907,\ \mu(3,1/2,f)=4$, 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 $c_0=1,\ c_i\ge 0$, we have $k(3)\le h_{\max}=12.88<13$.

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 [9, Table 1.5]. ("Presumably" because the equality $h_{\max}=E$ is not proven yet.)

In 9 and 10 dimensions Table 1.5 gives:

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

Our method gives:

$$n=9: \qquad \deg f=11,\ E=h_1=366.7822,\ t_0=0.54;$$
$$n=10: \qquad \deg f=11,\ E=h_1=570.5240,\ t_0=0.586.$$

For these dimensions there is a good chance to prove that $k(9)\le 366$, $k(10)\le 570$.

From the equality $k(3)=12$, it follows that $\varphi_3(13)<60^\circ$. The method gives $\varphi_3(13)<59.4^\circ$ ($\deg f=11$). The lower bound on $\varphi_3(13)$ is 57.1367° [16]. Therefore, we have $57.1367^\circ\le\varphi_3(13)<59.4^\circ$.

By our approach it can be proven that $\varphi_4(25) < 59.81°$, $\varphi_4(24) < 60.5°$. that can be proven by the same method as Theorem 4.) This improve the bounds:

$$\varphi_4(25) < 60.79°, \ \ \varphi_4(24) < 61.65° \text{ [23] (cf. [4]);} \ \ \varphi_4(24) < 61.47° \text{ [4];}$$

$$\varphi_4(25) < 60.5°, \quad \varphi_4(24) < 61.41° \text{ [3].}$$

Now in these cases we have

$$57.4988° \ < \varphi_4(25) < 59.81°, \quad 60° \le \varphi_4(24) < 60.5°.$$ [4]

However, for $n = 5, 6, 7$ direct use of this extension of the Delsarte method does not give better upper bounds on $k(n)$ than Odlyzko-Sloane's bounds [27]. It is an interesting challange to find better methods.

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

In this appendix we present an algorithm for computation "optimal"[5] polynomials f such that $f(t)$ is a monotone decreasing function on the interval $[-1, -t_0]$, and $f(t) \le 0$ for $t \in [-t_0, z]$, $t_0 > z \ge 0$. This algorithm is 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 a method was employed by Odlyzko and Sloane [27] for the same purpose.

We have a polynomial f represented in the form $f(t) = 1 + \sum\limits_{k=1}^{d} c_k G_k^{(n)}(t)$ and the following constraints for f:

(C1) $c_k \ge 0$, $1 \le k \le d$;

(C2) $f(a) > f(b)$ for $-1 \le a < b \le -t_0$;

(C3) $f(t) \le 0$ for $-t_0 \le t \le z$.

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

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

When $m = 2n-2$, Δ_m presumably is a regular $(n-1)$-dimensional cross-polytope.[6] In this case $\cos\rho_m = \sqrt{z}$.

Let $I_n = \{1, \ldots, n\} \bigcup \{2n-2\}$, $m \in I_n$, $b_m = -\cos\rho_m$. Then $H_m(y_c) = f(1) + mf(b_m)$. If F_0 is such that $H(y_0; Y) \le E = F_0 + f(1)$, then

[4] The long-standinding conjecture: The maximal kissing arrangment in four dimensions is unique up to isometry (in other words, is the "24-cell"), and $\varphi_4(24) = 60°$.

[5] Open problem: Is it true that for given t_0, d this algorithm defines f with minimal $h_{\max}$?

[6] This is also an open problem.

(C4) $f(b_m) \le F_0/m$, $m \in I_n$.

Note that $E = F_0 + 1 + c_1 + \ldots + c_d = F_0 + f(1)$ 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: $c_1, \ldots, c_d,\ F_0,\ E.$

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

Second: Use linear programming to find $F_0, c_1, \ldots, c_d$ so as to minimize $E - 1 = F_0 + \sum\limits_{k=1}^{d} c_k$, subject to the constraints

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

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

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

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