東 海 大 學 數 學 系 研 究 所

碩 士 論 文

指 導 教 授: 陳 文 豪 博 士

Kissing Number Problem and Its Applications

Kissing Number 問題及其應用

研究生: 張啓敏

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碩士學位口試委員審定書

本系碩士班 張啟敏 君

所提論文 Kissing Number 問題及其應用
(Kissing Number Problem and Its Applications)

合於碩士班資格水準，業經本委員會評審通過，特此證明。

口試委員：

指導教授： 陳文豪

所 長： 陳文豪

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- 摘　　要 -

Kissing number $k(n)$ 是一個討論在 n 維空間不重疊的單位球 S^{n-1} 能同時觸及中央單位球的最大數量。在本論文中我們討論了三維空間與四維空間的 Kissing number problem， 即討論給定一個單位球 S^2 (S^3)， 其周圍最多可以有幾個單位球能同時觸及中央單位球。 最後， 我們介紹了 Kissing number problem 在三維空間的應用， 其中包含了化學和晶體學。 Kissing number problem 爲著名問題 sphere packing problem 的基礎， sphere packing problem 爲考慮在給定的體積中可以找出相切球的最大數量， 利用 $k(3)$ 的結論推廣應用在較爲複雜的 sphere packing problem。

Abstract

Kissing number $k(n)$ is the highest number of equal nonoverlapping spheres in $\mathbb{R}^n$ that can touch another sphere of the same size. In this paper, we discussed the kissing number problem of dimension three and four. That is, we discussed how many unit balls can kiss a fixed ball.

Finally, we introduce applications of three dimension in chemistry and crystallography. The kissing number problem is the foundation of sphere packing problem. In mathematics, sphere packing problems concern arrangements of nonoverlapping identical spheres which fill a space. Using the conclusion of $k(3)$ and apply it to the complex sphere packing problem.

- 致 謝 辭 -

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- 目　　錄 -

第 1 章　Introduction

The kissing number $k(n)$ is the highest number of equal nonoverlapping spheres in $\mathbb{R}^n$ that can touch another sphere of the same size. In this paper, we discussed the kissing number problem of dimension three and four. In three dimension the kissing number is ask how many unit balls can kiss(touch) the center fixed ball. In four dimension, the kissing number can be stated in other way: How many points can be placed on the surface of S^3 so that the angular separation between any two points is at least $\frac{\pi}{3}$?

In chapter 2, we discussed the kissing number problem for three dimension, it is also called the thirteen spheres problem. This problem was a famous discussion between Isaac Newton and David Gregory in 1694. Newton believed the answer was 12, while Gregory thought that 13 might possible. The problem was solved until 1953. Actually, $k(3) = 12$. We use Fejes T**ó**th's lemma to estimate the area of spherical triangles and prove $k(3) = 12$.(Figure 1.0.1)

In chapter 3, we discussed the kissing number problem for $n = 4$. In section 3.1, we give a graph of outline of the main theorem $k(4) = 24$ and the main theorem proven by Lemma 3.3.1 and Lemma 3.3.2 . We show that Lemma 3.3.1 by Delsarte's method and inequality in section 3.3. Section 3.9 gives a proof of Lemma 3.3.2.

In chapter 4, we introduce applications of $k(3)$ in chemistry, crystallography and sphere packing problem. We give examples in chemistry and crystallography and intro-

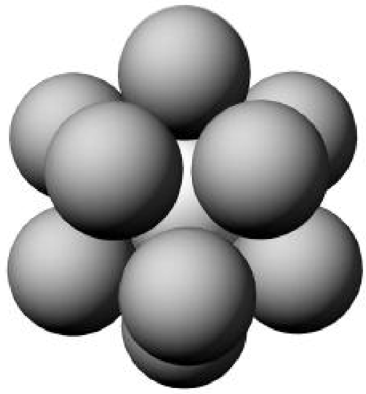

Figure 1.0.1: The graph of kissing number in three dimension.

duce the sphere packing problem.

第 2 章　Kissing Number Problem in Three Dimension

2.1　Basic Formulas and Lemmas

We introduce some basic formulas and key lemmas in this section.

Definition 2.1.1. The $\triangle(x, y, z)$ stands for a triangle with edge-length x, y, z and cap (ABC) stands for the cap enclosed by the circum-scribed circle of ABC and containing the triangle ABC.

Girard's formula 2.1.2.

$$|ABC| = \angle A + \angle B + \angle C - \pi,$$

where $|ABC|$ is the area of a triangle ABC.

Spherical cosine law 2.1.3. Let θ be the angle of $\triangle(x, y, z)$ opposite to the edge z. Then

$$\cos z = \cos x \cos y + \sin x \sin y \cos \theta.$$

Fejes Tóth's lemma 2.1.4. [9] Let d be the length of the shortest edge of a triangle ABC. If the angular radius of $cap(ABC)$ is less than d, then $|ABC| \geq |\triangle(d, d, d)|$.

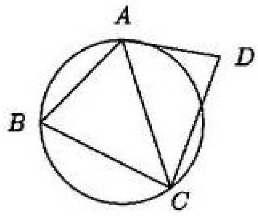

Figure 2.1.1: A proper diagonal AC of a quadrilateral $ABCD$

Suppose $ABCD$ is a quadrilateral. If D is not an interior point of $cap(ABC)$, then AC ia called a proper diagonal of $ABCD$.(Figure 2.1.1)

Proper diagonal lemma 2.1.5. [9] Let AC be a proper diagonal of a quadrilateral $ABCD$. If we deform $ABCD$ with keeping its edge lengths fixed so that the length of the diagonal AC decreases, then the area $|ABCD|$ decreases.

If a triangle ABC contains the center of $cap(ABC)$, then the triangle ABC is called a major triangle. Suppose ABC is a major triangle and triangle $AB'C$ is obtained by reflecting ABC with respect to the edge AC, then AC is a proper diagonal of the quadrilateral $ABCB'$. By Proper diagonal lemma, if x decreases in a major triangle $\triangle(x, y, z)$, $|\triangle(x, y, z)|$ decreases. And if P is the center of $cap(ABC)$, the intersection of the ray $\overrightarrow{OP}$ and the plane ABC is the circum-center of the planar triangle ABC. Therefore, if triangle ABC is a major triangle, the planar triangle ABC is an acute triangle or a right triangle. So we have the following

$$\text{(1) For every } x, y, z \in [\frac{\pi}{3}, \frac{\pi}{2}], \triangle(x, y, z) \text{ is a major triangle.} \tag{2.1.1}$$

$$\text{(2) For every } x, y \in [\frac{\pi}{3}, \frac{2\pi}{3}], \triangle(x, y, \frac{\pi}{2}) \text{ is a major triangle.} \tag{2.1.2}$$

2.2 The Main Theorem

Let X be a subset of S^2. If no two points of X are closer than $\frac{\pi}{3}$ in spherical distance, then X is called $\frac{\pi}{3}$-separated. So we have if n mutually nonoverlapping unit balls can simultaneously touch S^2 then there is a $\frac{\pi}{3}$-separated point set of cardinality n on S^2.

Theorem 2.2.1. [5] Every $\frac{\pi}{3}$-separated set on S^2 has at most 12 points.

Proof. Suppose $X \subset S^2$ be the maximal $\frac{\pi}{3}$ - separated point set, $|X| = n$, $\Gamma(X)$ is a convex hull of X and $\Gamma(X)$ contains the center of S^2. Now, we project the edge of $\Gamma(X)$ onto S^2 from the center of S^2 and divided S^2 into spherical polygons. By adding diagonals to these polygons, making a triangulation T of S^2. Then T satisfies the following

(1) By Euler's formula, T has $2n - 4$ triangles.

(2) Since the spherical triangle is projected by the vertex of $\Gamma(X)$ and adding diagonals. So the interior of the circum-scribed cap of each triangle in T contains no vertex of T.

(3) By(2), each edge of T is a proper diagonal of the quadrilateral obtained as the union of two triangles sharing the edge.

(4) If the radius of the circum-scribed cap of each triangle in T is greater than $\frac{\pi}{3}$, then we can add a point be a interior point of a triangle such that the edge of the triangle is decreases and the number of triangles is increases. So, the radius of the circum-scribed cap of each triangle in T is less than $\frac{\pi}{3}$.

By (4) and Fejes Tóth's lemma, the area of every triangle in T is greater or equal to $\delta = |\triangle(\frac{\pi}{3}, \frac{\pi}{3}, \frac{\pi}{3})|$. Hence, $2n - 4 \leq \frac{4\pi}{\delta} \approx 22.8$, $n \leq 13$. Now, we show that $n \neq 13$.

Lemma 2.2.2. [5] If n=13, then at most one edge of T has length greater than or equal to $\hat{a} = \arccos(\frac{1}{7}) \approx 1.427$.

Proof. Let $n = 13$, then T has $2n - 4 = 22$ triangles. Suppose the common edge AC of triangle ABC and triangle ACD is the longest edge of T. Let e denote the second longest edge. Now, we show $e < \hat{a}$.

(a) Suppose $e > \frac{\pi}{2}$. By the Proper diagonal lemma, if we deform the guadrilateral $ABCD$ with keeping its edge length so that the length of the diagonal AC becomes $\frac{\pi}{2}$, then $|ABCD|$ decreases. By (4), every edges has length less than $\frac{2\pi}{3}$, then triangles ABC and ACD become major triangle. If e is edge of $ABCD$, then

$$|ABCD| > |\triangle(\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{3})| + |\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})|$$

and

$$4\pi \geq (22-3)\delta + |\triangle(\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{3})| + |\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})| + |\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})|$$

$$\approx 19\delta + 1.047.0.679 + 0.679 = 12.874 > 4\pi,$$

it is a contradiction. On the other hand, if e is not an edge of $ABCD$, then $|ABCD| \geq 2|\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})|$, the area of two triangles sharing the edge e is greater than $2|\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})|$. So we have

$$4\pi \geq (22-4)\delta + 4|\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})|$$

$$\approx 18\delta + 4 \cdot 0.679 = 12.634 > 4\pi.$$

It is a contradiction.

(b) Suppose $\hat{a} \leq e \leq \frac{\pi}{2}$. By (2.1), triangles other than ABC, ACD are all major triangles. If e is an edge of $ABCD$, then

$$|ABCD| \geq |\triangle(\frac{\pi}{2}, \frac{\pi}{3}, \frac{\pi}{3})| + |\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})|$$

Consider triangle sharing edge e in common, the area of triangle is greater than $|\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})|$.

We have

$$4\pi \geq (22-3)\delta + |\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})| + |\triangle(\hat{a}, \hat{a}, \frac{\pi}{3})| + |\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})|$$

$$\approx 19\delta + 0.667 + 0.892 + 0.667 = 12.695 > 4\pi,$$

and it is a contradiction. If e is not an edge of $ABCD$, then $|ABCD| \geq 2|\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})|$ and area of two triangles sharing edge e in common is greater than $2|\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})|$.

We have

$$4\pi \geq (22-4)\delta + 4|\triangle(\hat{a}, \frac{\pi}{3}, \frac{\pi}{3})| \approx 12.59 > 4\pi.$$

It is a contradiction. Therefore, $e < \hat{a}$.

■

Lemma 2.2.3. [5] Let $\Theta = \Theta(x, y, z)$ be the angle of $\triangle(x, y, z)$ opposite to the edge z. If $\frac{\pi}{3} \leq x \leq y \leq \hat{a}$ and $\frac{\pi}{3} \leq z$, then $\Theta > \frac{\pi}{3}$.

Proof. By the Spherical cosine law, we have the angle Θ of $\triangle(x, y, z)$ opposite to z is monotone increasing on z, $\Theta(x, y, \frac{\pi}{3}) \leq \Theta(x, y, z)$ and $\cos z = \cos x \cos y + \sin x \sin y \cos \Theta$. Let

$$\cos \Theta = f(x, y, z) = \frac{\cos z - \cos x \cos y}{\sin x \sin y}$$

, we have

$$f_y(x, y, z) = \frac{\cos x - \cos y \cos z}{\sin^2 x \sin x} > 0$$

for $\frac{\pi}{3} \leq x \leq y \leq \hat{a}$. So y is increasing on $\frac{\pi}{3} \leq y \leq \hat{a}$ and

$$f_x(x, y, z) = \frac{\sin^2 x \cos y - \cos z \cos x + \cos^2 x \cos y}{\sin^2 x \sin x}$$

Consider

$$f_x(x, \hat{a}, \frac{\pi}{3}) = \frac{\sqrt{3}(2 - 7\cos x)}{24\sin^2 x},$$

$f_x(x, \hat{a}, \frac{\pi}{3})$ has maximal when $x = \frac{\pi}{3}$ or $x = \hat{a}$. Since $f(\frac{\pi}{3}, \hat{a}, \frac{\pi}{3}) = \frac{1}{2}$, $f(\hat{a}, \hat{a}, \frac{\pi}{3}) = \frac{47}{96}$, then $f(\frac{\pi}{3}, \hat{a}, \frac{\pi}{3}) > f(\hat{a}, \hat{a}, \frac{\pi}{3})$. We have $f(x, y, z) = \cos\Theta < f(\frac{\pi}{3}, \hat{a}, \frac{\pi}{3}) = \frac{1}{2}$. Hence, $\Theta > \frac{\pi}{3}$. ■

By Lemma 2.2.2, if $n = 13$, then at most one edge of T has length greater than or equal to $\hat{a}$. Let G be the graph obtained from T by eliminating the edges of length greater than or equal to $\hat{a}$. By Lemma 2.2.3, since $\Theta > \frac{\pi}{3}$, $2\pi \geq n\Theta \geq \frac{n\pi}{3}$, $n \leq 5$, each vertex of G has degree at most 5. If T has no edge of length greater than or equal to $\hat{a}$, then G has $\frac{(22\cdot 3)}{2} = 33$ edges and average degree of a vertex become $\frac{66}{13} > 5$. It is a contradiction. Therefore, by Lemma 2.2.2 and above, T must have exactly one edge of length at least $\hat{a}$. Now, consider the graph G, we have

(1) G is a planar graph having 32 edges, one quadrilateral and 20 triangles. And since every edge has two degree, G has 64 degree of vertices.

(2) G has one vertex of degree 4 and 12 vertices of degree 5.

(3) Every 3-cycle of G is the boundary of a triangular face.

Now, we consider case(a)and case(b)(Figure 2.2.1). Two cases are satisfy the above (1)(2)(3).

In the case(a): The four vertices of the quadrilateral are all of degree 5. In Figure 2.2.1 case(a), contain 12 vertices, every vertex has degree 5. Suppose the quadrilateral which the vertex's degree is 5. Therefore, it will be extending three edge from every vertex and it is difference. Beside, there is difference that every vertex connected is disjoint. Now, the sum of edges of Figure 2.2.1 is 36 and the degree of 13-th vertex at least 6, which is a contradiction.

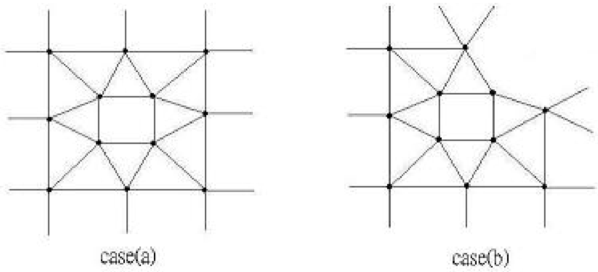

Figure 2.2.1: case(a) and case(b)

In the case(b): One vertex of the quadrilateral has degree 4. In Figure 2.2.1 case (b). Now, fixed the degree of vertex is 4 of quadrilateral and others degree is 5. So, it will be extending three edge from every vertex and it is difference. Beside, there is difference that every vertex connected is disjoint. Now, the sum of edges of Figure 2.2.1 is greater than 32. It is a contradiction. Hence, by case(a) and case(b) , $n \neq 13$. ■

第3章　Kissing Number Problem in Four Dimension

3.1 Outline of The Main Theorem $k(4) = 24$

We will introduce the step of the proof of $k(4) = 24$ in Figure 3.1.1.

1. Introduce the polynomial f_4.

f_4 made by Jacobi polynomial. As $n = 4$, Jacobi polynomial is the same as Chebyshev polynomial of the second kind. We use recurrence relation and mathematical induction to prove.

2. $k(4) = 24$.

Using lemma 3.3.1 and lemma 3.3.2 to prove $k_4 = 24$.

3. Introduce the Delsarte's method, inequality and Delsarte's bound.

We use Delsarte's method and inequality to prove lemma 3.3.1. And we get $k(4) \leq 25$ by Delsarte's bound.

4. (a) We extend Delsarte's bound to get theorem 3.5.2.

Theorem 3.5.2: $k(4) \leq \frac{h_{max}(n, \cos\frac{\pi}{3}, f)}{c_0} = \frac{1}{c_0}\max\{h_0, h_1, \cdots, h_m\}$, where $h_m := f(1) + f(y_0 \cdot y_1) + \ldots + f(y_0 \cdot y_m)$.

(b) We introduce the polynomial $\Phi(t_0, \frac{1}{2})$ and simplify the kissing number problem in dimension four to the sphere cap(e_0, θ_0). We calculate θ_0 and then get theorem 3.6.3.

Theorem 3.6.3: Let $Y = \{y_1, y_2, \cdots, y_m\} \subset S^{n-1}$ be the spherical $\frac{\pi}{3}$-code. Suppose $Y \subset cap(e_0, \theta_0)$ and $\frac{\pi}{2} \geq \frac{\pi}{3} > \theta_0 > 0$. Then any y_k is a vertex of Δ_m, where $\Delta_m = \Delta_m(Y)$ is the convex hull of Y.

(c) Consider the number of the vertices of cap(e_0, θ_0) on S^{n-1} and get theorem 3.7.1.

Theorem 3.7.1: Let $Y = \{y_1, y_2, \cdots, y_m\} \subset S^{n-1}$ be a spherical $\frac{\pi}{3}$-code. Suppose $Y \subset cap(e_0, \theta_0)$ and $0 < \frac{\pi}{6} \leq \theta_0 < \frac{\pi}{3} \leq \frac{\pi}{2}$. Then $m \leq A\big(n-1, \arccos \frac{\frac{1}{2} - \cos^2\theta_0}{\sin^2\theta_0}\big)$.

Using the conclusion of theorem 3.7.1 and we get corollary 3.7.4.

Corollary 3.7.4: If $t_0 \geq 0.6058$, then $m(4, \frac{1}{2}, f) \leq 6$.

(d) Introduce the optimal and irreducible sets.

Consider the set Y such that h_m attains its maximum and use the rotation of vertices of spherical cap. Then we get theorem 3.8.7.

Theorem 3.8.7: 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 length $\frac{\pi}{3}$.

(e) For $n = 4$, we get theorem 3.9.6.

Theorem 3.9.6: Let $Y \subset S^3$ be an irreducible set, $|Y| = 5$. Then Δ_m for $2 \leqslant m \leqslant 4$ is a regular simplex of edge length $\frac{\pi}{3}$ and Δ_5 is isometric to $p_5(\alpha)$ for some $\alpha \in [\frac{\pi}{3}, \frac{\pi}{2}]$.

(f) Consider $2 \leq m \leq 6$, we get theorem 3.10.3.

Theorem 3.10.3:

(1) $h_0 = f(1)$, $h_1 = f(1) + f(-1)$.

(2) $h_m \leq \lambda_m(\frac{\pi}{3}, \theta_0) \leq \lambda_m(N, \frac{\pi}{3}, \theta_0)$ for $2 \leq m \leq 5$.

(3) $h_6 \leq max\{f(-\cos\theta_0') + \lambda_5(\frac{\pi}{3}, \theta_0), f(-\frac{1}{\sqrt{2}}) + \lambda_5(\frac{\pi}{3}, \theta_0')\}$, $\theta_0' \in [\frac{\pi}{4}, \theta_0]$.

5. Using the step 4 to prove lemma 3.3.2.

Figure 3.1.1: Outline of $k_4 = 24$

3.2 Introduce The Polynomials

In this section, we introduce some polynomials. Consider the polynomial of degree nine :

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

f_4 is a monotone decreasing function on the interval $[-1, -t_0]$ and $f(t) \leqslant 0$ for $t \in [-t_0, \frac{1}{2}]$, $t_0 > \frac{1}{2} \geq 0$. The polynomial $f_4(t)$ was found by the linear programming method.

First, consider the finite set of inequalities at the points

$$t_j = -1 + 0.0015j, \quad \text{where} \quad 0 \leq j \leq 1000.$$

Next, choose a value of k and use linear programming to find $c_1, c_2, \cdots, c_k$ so as to minimize

$$\sum_{i=1}^{k} c_i p_i(t_j)$$

subject to the constrains

$$c_i \geq 0 \quad \text{for} \quad 1 \leq i \leq k, \text{and} \quad \sum_{i=1}^{k} c_i p_i(t_j) \leq -1 \quad \text{for} \quad 0 \leq j \leq 1000,$$

where $p_i(t)$ stands for the $Jacobi\ polynomial$ $p_i^{(\frac{1}{2},\frac{1}{2})}(t)$.

Definition 3.2.1. [2] The $Jacobi\ polynomial$

$$p_n^{(\alpha,\beta)}(x) := 2^{-n} \sum_{i=0}^{n} \binom{n+\alpha}{n-i} \binom{n+\beta}{i} (x-1)^i (x+1)^{n-i}, \quad x \in [-1, 1],$$

is a orthogonal with respect to the weight $(1-x)^\alpha(1+x)^\beta$ such that

$$\int_{-1}^{1} (1-x)^\alpha (1+x)^\beta p_n^{(\alpha,\beta)}(x) p_m^{(\alpha,\beta)}(x) = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)n!}\delta_{m,n}$$

where $\delta_{m,n} = \begin{cases} 1 & , m = n \\ 0 & , m \neq n \end{cases}$ and has the lead coefficient $2^{-n} \sum_{i=0}^{n} \binom{n+\alpha}{n-i} \binom{n+\beta}{i} = 2^{-n} \binom{2n+\alpha+\beta}{n}$.

Definition 3.2.2. ($Recurrence\ Relation$)[2]
The sequence $\{p_n^{(\alpha,\beta)}(x)\}_{n=1}^{\infty}$ satisfies

$$D_n p_{n+1}^{(\alpha,\beta)}(x) = (A_n + B_n) p_n^{(\alpha,\beta)}(x) - C_n p_{n-1}^{(\alpha,\beta)}(x)$$

where $\quad p_0^{(\alpha,\beta)}(x) = 1 \quad , \quad p_1^{(\alpha,\beta)}(x) = \frac{1}{2}[\alpha - \beta + (\alpha + \beta + 2)x] \quad and$

$$\begin{aligned} D_n &= 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta), \\ A_n &= (2n+\alpha+\beta+1)(\alpha^2 - \beta^2), \\ B_n &= (2n+\alpha+\beta+2)(2n+\alpha+\beta+1)(2n+\alpha+\beta), \\ C_n &= 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2). \end{aligned}$$

Definition 3.2.3. [1] [11] The $Gegenbauer\ polynomials$ $G_k^{(n)}(x)$ (Ultraspherical polynomials) can be defined by the recurrence formula:

$$G_0^{(k)}(x) = 1, \quad G_1^{(k)}(x) = x, \cdots, G_k^{(n)}(x) = \frac{(2k+n-4)xG_k^{(n-1)}(x) - (k-1)G_{k-2}^{(n)}(x)}{k+n-3}.$$

In the case n=4 are $Chebyshev\ polynomials\ of\ the\ second\ kind$, but with a different normalization than usual.

Now, we discuss the relation of Jacobi polynomial and Chebyshev polynomial.

Lemma 3.2.4. When $\alpha = \beta = \frac{1}{2}$, the $Jacobi\ polynomial$ are the $Chebyshev\ polynomial$ of the second kind $U_n(x)$, then

$$U_n(x) = 2^{2n} \binom{2n+1}{n+1}^{-1} p_n(x).$$

The $Chebyshev\ polynomial$ of the second kind satisfies the following recurrence relation

$$U_0(x) = 1 \quad , \quad U_1(x) = 2x \quad , \quad U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x), \quad n = 2, 3, \ldots.$$

Proof. For $n = 0$,

$$2^0 \binom{1}{1}^{-1} p_0(x) = p_0(x) = 1 = U_0(x).$$

when $n = 1$, we have

$$2^2 \binom{3}{2}^{-1} p_1(x) = 2^2 \frac{2!}{3!} p_1(x) = \frac{4}{3} p_1(x) 1 = 2x = U_1(x).$$

Suppose $n = k$ hold,

$$2^{2n} \binom{2n+1}{n+1}^{-1} p_n(x) = U_n(x).$$

Now consider n=k+1, then

$$\begin{aligned}
\text{left} &= 2^{2(k+1)} \binom{2(k+1)+1}{(k+1)+1}^{-1} p_{k+1}(x) \\
&= 2^{2(k+1)} \binom{2k+3}{k+2}^{-1} \left[\frac{x(2k+3)(2k+2)(2k+1)}{2(k+1)(k+2)(2k+1)} p_k - \frac{2(k+\frac{1}{2})(k+\frac{1}{2})(2k+3)}{2(k+1)(k+2)(2k+1)} p_{k-1} \right] \\
&= 2^{2(k+1)} \left[\frac{x}{2} \frac{(k+1)!k!}{(2k+1)!} p_k - \frac{(k+\frac{1}{2})^2(k+1)!k!}{(2k+2)!(2k+1)!} p_{k-1} \right] \\
&= 2^{2k+1} x \binom{2k+1}{k+1}^{-1} p_k - 2^{2k-2} 2^4 \frac{(2k+1)^2(k+1)!k!}{4(2k+2)!(2k+1)!} p_{k-1} \\
&= 2^{2k+1} x \binom{2k+1}{k+1}^{-1} p_k - 2^{2k-2} 2^2 \frac{(2k+1)(k+1)!k!}{(2k+2)!} p_{k-1} \\
&= 2^{2k+1} x \binom{2k+1}{k+1}^{-1} p_k - 2^{2k-2} \frac{k!(k-1)!}{(2k-1)!} p_{k-1} \\
&= 2^{2k+1} x \binom{2k+1}{k+1}^{-1} p_k - 2^{2k-2} \binom{2k-1}{k}^{-1} p_{k-1} \\
&= 2x \left[2^{2k} \binom{2k+1}{k+1}^{-1} p_k \right] - \left[2^{2(k-1)} \binom{2k-1}{k}^{-1} p_{k-1} \right] \\
&= 2xU_k - U_{k-1} = U_{k+1} = \text{right}.
\end{aligned}$$

■

3.3 The Main Theorem of Kissing Number and Lemmas

Lemma 3.3.1. [11] Let $X = \{x_1, x_2, \ldots, x_M\}$ be points in the unit sphere S^3. Then

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

Lemma 3.3.2. [11] Suppose $X = \{x_1, x_2, \ldots, x_M\}$ is a subset of S^3 such that the angular separation between any two points x_i, x_j is at least $\frac{\pi}{3}$, then

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

Theorem 3.3.3. [11]

$$k(4) = 24.$$

Proof. Let X be a spherical $\frac{\pi}{3}$-code on S^3, $M = K(4)$. Applying the Lemma 3.3.1 and Lemma 3.3.2, we obtain

$$M^2 \leq S(X) < 25M,$$

which implies $M < 25$. On the other hand, $M \geq 24$,[10] [12] [15] therefore $M = K(4) = 24$.

3.4 Delsarte's Method , Inequality and Delsarte's Bound

Let $\phi_{i,j} = \text{dist}(x_i, x_j)$ be the spherical distance between x_i, x_j and $\cos\phi_{ij} = x_i \cdot x_j$. If $x_i \cdot x_j \leqslant \cos\frac{\pi}{3}$ for all $i \neq j$, then we called the set is a $\frac{\pi}{3}$-code.

Theorem 3.4.1. $(Schoenberg's\ Therem)$ [6]

Let $u_1, u_2, \cdots, u_M$ be any real numbers, then

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

or equivalently the $Gram\ matrix$ $\Big(\cos\phi_{ij}\Big)$ is a positive semidefinite.

Schoenberg extended this property to $Gegenbauer\ polynomial$.

Lemma 3.4.2. [6] $Gegenbauer\ polynomials$ $p_n^{(\lambda)}(\cos t)$, $n = 1, 2, \cdots$, $\lambda = \frac{1}{2}(k-1)$ are all $positive\ definite$ in S_k.

Proof. For $k = 1$, $p_n^{(\lambda)}(\cos t) = p_n^{(0)}(\cos t)$ is the Legendre polynomial and by the cosine addition formula, the statement is true. Assume $k = m-1$. $p_n^{(\lambda)}(\cos t)$ is $positive\ definite$ in S_{m-1} hold.

Consider $k = m$, $p_i \in S_m$ for $i = 1, 2, \cdots, N$ and associate with the points p_i and $p_{i'}$, on the equator S_{m-1} of equation $\Theta = \frac{1}{2}\pi$ such that the last $m-1$ polar coordinates $\theta_1, \cdots, \phi$ of both points p_i and $p_{i'}$ agree. We have

$$\cos p_i p_k = \cos\theta^i \cos\theta^k + \sin\theta^i \sin\theta^k \cos p_{i'} p_{k'}.$$

By the addition formula for Ultraspherical polynomials, we may write

$$p_n^{(\lambda)}(\cos p_i p_k) = \sum_{s=0}^{n} c_{n,\lambda,s} p_n^{\lambda,s}(\cos\theta^i) p_n^{\lambda,s}(\cos\theta^k) p_n^{\frac{1}{2}(m-2)}(\cos p_{i'} p_{k'}),$$

where $p_n^{\lambda,s}$ are the real polynomials associated to $p_n^{(\lambda)}$ and $c_{m,\lambda,s}$ are positive coefficients. Since $p_n^{\frac{1}{2}(m-2)}$ was assumed to be $positive\ definite$ in S_{m-1} then

$$\sum_{i=1}^{N}\sum_{j=1}^{N} p_n^{(\lambda)}(\cos p_i p_k)\xi_i\xi_k = \sum_{s=0}^{n} c_{n,\lambda,s} \sum_{i=1}^{N}\sum_{j=1}^{N} p_n^{\frac{1}{2}(m-2)}(\cos p_{i'} p_{k'})\eta_i\eta_k \geq 0,$$

where $\eta_i = p_n^{\lambda,s}(\cos\theta^i)\xi_i$. ∎

If a symmetric matrix M is positive semidefinite, then the sum of all its entries is nonnegative. Schoenberg's theorem implies that the matrix $\Big(G_k^{(n)}(t_{ij})\Big)$ is positive semidefinite, where $t_{i,j} := \cos\phi_{i,j}$. Then $\sum_{i=1}^{M}\sum_{j=1}^{M} G_k^{(n)}(t_{ij}) \geq 0$ $(*)$

Definition 3.4.3. [11] We denote by G_n^+ the set of continuous functions $f : [-1, 1] \to \mathbb{R}$ representable as series

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

whose coefficients satisfy the following conditions

$$c_0 > 0, \;\; c_k \geq 0 \;\text{ for }\; k = 1, 2, 3, \cdots \;\text{ and }\qquad f(1) = \sum_{k=0}^{\infty} c_k < \infty.$$

Suppose $f \in G_n^+$ and let

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

By $(*)$, we have

$$S(X) = \sum_{i=1}^{M} \sum_{j=1}^{M} \Big(\sum_{k=0}^{\infty} c_k G_k^{(n)}(t_{ij}) \Big) \geq \sum_{i=1}^{M} \sum_{j=1}^{M} \Big(c_0 G_0^{(n)}(t_{ij}) \Big) = c_0 M^2. \qquad (3.4.1)$$

Hence $S(X) \geq c_0 M^2$.

Next, using above definition, we will prove the Lemma 3.3.1.

Proof of lemma 3.3.1. f_4 can be written as

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

where $U_n(t)$ is $Chebyshev\ polynomial$ of the second kind, then $f_4 \in G_n^+$ and $c_0 = 1$, hence $S(X) \geq c_0 M^2 = M^2$. ■

Let $X = \{x_1, x_2, \ldots, x_M\} \subset S^{n-1}$ be a spherical $\frac{\pi}{3}$-code. Suppose $f \in G_n^+$ and $f(t) \leq 0$ for $t \in [-1, \frac{1}{2}]$, then $f(t_{ij}) \leq 0$ for all $i \neq j$. Then

$$S(X) := \sum_{i=1}^{M} \sum_{j=1}^{M} f(t_{ij}) = Mf(1) + 2f(t_{12}) + \cdots + 2f(t_{M-1,M}) \leq Mf(1).$$

By (3.4.1)

$$c_0 M^2 \leq S(X) \leq Mf(1),$$

then we obtain

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

Let $A(n, \frac{\pi}{3})$ be the maximal size of a $\frac{\pi}{3}$-code in S^{n-1}, then

$$A(n, \frac{\pi}{3}) \leq \frac{f(1)}{c_0}$$

If $n = 4$ and $c_0 = 1$, then

$$A(4, \frac{\pi}{3}) = k(4) \leq f(1),$$

$f_4(1) \approx 25.558$, hence $24 \leq k(4) \leq 25$.

3.5 An Extension of Delsarte's Bound

Let $f(t)$ be a function on the interval [-1,1]. For a given value $\frac{\pi}{3}$, consider points $y_0, y_1, \cdots, y_M$ on the sphere S^{n-1} such that $y_i \cdot y_j \leqslant \frac{1}{2} = \cos\frac{\pi}{3}$, $i \neq j$ and $f(y_0 \cdot y_i) > 0$ for $1 \leq i \leq M$. $(**)$

Definition 3.5.1. [11] For fixed $y_0 \in S^{n-1}$, $M \geq 0$ and $f(t)$, define the family $Q_M(y_0)$ of finite sets of pints from S^{n-1} by the formula

$$Q_M(y_0) := \begin{cases} \{y_0\} & , M = 0 \\ \{Y = \{y_1, y_2, \cdots, y_M\}\} \subset S^{n-1} : \{y_0\} \cup Y \;\; satisfies \;\; (**) & , M \geq 1. \end{cases}$$

Denote $m := \max\{M : Q_M(y_0) \neq \emptyset\}$. For $0 \leq M \leq m$, we define the function $H = H_f$ on the family $Q_M(y_0)$:

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

$$H(y_0; Y) = H(y_0; y_1, y_2, \cdots, y_m) := f(1) + f(y_0 \cdot y_1) + \cdots + f(y_0 \cdot y_m) \;\; \text{for} \;\; m \geq 1$$

Let

$$h_m := \sup_{Y \in Q_M(y_0)} \{H(y_0; Y)\} \;\; \text{and} \;\; h_{\max} := \max\{h_0, h_1, \cdots, h_m\}$$

Theorem 3.5.2. [11] Suppose $f \in G_n^+$. Then

$$A(n, \frac{\pi}{3}) \leq \frac{h_{max}(n, \cos\frac{\pi}{3}, f)}{c_0} = \frac{1}{c_0} \max\{h_0, h_1, \cdots, h_m\}.$$

Proof. Let $X = \{x_1, x_2, \cdots, x_M\} \subset S^{n-1}$ be a spherical $\frac{\pi}{3}$-code. Denote $J(i) := \{j \;;\; f(x_i \cdot x_j) > 0, i \neq j\}$, and $X(i) := \{x_j; j \in j(i)\}$. Then

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

Therefore

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

Since $f \in G_n^+$, $S(X) \geq c_0 M^2$ and by (3.1), we have

$$c_0 M^2 \leq S(X) \leq M h_{\text{max}},$$

which implies that

$$M \leq \frac{1}{c_0} h_{\text{max}} \tag{3.5.1}$$

■

3.6 The Class of Functions $\Phi(t_0, \frac{1}{2})$ and Δ_m

Definition 3.6.1. [11] Let real number t_0 satisfies $1 > t_0 > \frac{1}{2} \geq 0$. We denote by $\Phi(t_0, \frac{1}{2})$ the set of functions $f : [-1, 1] \to \mathbb{R}$ such that $f(t) \leq 0$ for $t \in [t_0, \frac{1}{2}]$.

Let $f \in \Phi(t_0, \frac{1}{2})$ and $Y \in Q_M(y_0, n, f)$. Denote

$$e_0 := -y_0, \quad \theta_0 := \text{arccos}\, t_0, \quad \theta_i := \text{dist}(e_0, y_i) \quad \text{for} \quad i = 1, 2, \cdots, m,$$

where e_0 is the antipodal point to y_0

Lemma 3.6.2. If $\theta_i < \theta_0$, then $f(y_0 \cdot y_i) > 0$.

Proof. If $\theta_i < \theta_0$, then $\pi \geq \pi - \theta_i > \pi - \theta_0$, $\cos \pi \leq \cos(\pi - \theta_i) < \cos(\pi - \theta_0)$, which implies $-1 \leq \cos(\pi - \theta_i) < -t_0$, therefore $f(\cos(\phi_{0i})) > 0$ and conclude the proof. ■

From above lemma, Y is a spherical $\frac{\pi}{3}$-code in the open spherical $cap(e_0, \theta_0)$ of the center e_0 and radius θ_0 with $\frac{\pi}{2} \geq \frac{\pi}{3} > \theta_0$.

Theorem 3.6.3. [11] Let $Y = \{y_1, y_2, \cdots, y_m\} \subset S^{n-1}$ be the spherical $\frac{\pi}{3}$-code. Suppose $Y \subset cap(e_0, \theta_0)$ and $\frac{\pi}{2} \geq \frac{\pi}{3} > \theta_0 > 0$. Then any y_k is a vertex of Δ_m, where $\Delta_m = \Delta_m(Y)$ is the convex hull of Y.

Proof. The case $m = 1, 2$ are trivial. For $m = 3$, suppose y_2 is not a vertex of Δ_3.Then Δ_3 is the arc y_1y_3 and y_2 lies on the arc y_1y_3. Since Y is a $\frac{\pi}{3}$-code, then $\text{dist}(y_1, y_3) \geq \frac{2\pi}{3}$. According to the triangle inequality

$$\frac{2\pi}{3} \leq \text{dist}(y_1, y_3) \leq \text{dist}(y_1, e_0) + \text{dist}(y_3, e_0) < 2\theta_0$$

It is a contradiction. For $m = 4$. By the assumptions:

$\theta_k = \text{dist}(y_k, e_0) < \theta_0 < \frac{\pi}{3} \;\; for \;\; 1 \leq k \leq m, \quad \phi_{kj} := \text{dist}(y_k, y_j) \geq \frac{\pi}{3}, \;\; k \neq j.$

We assume that there exist a point y_k belonging both to the interior of Δ_m and relative interior of some facet of dimension d, $1 \leq d \leq dim\Delta_m$. Consider the great $(n-2)-sphere$ Ω_k such that $y_k \in \Omega_k$ and Ω_k is orthogonal to the arc e_0y_k. The great sphere Ω_k divides S^{n-1} into two closed hemisphere: H_1 and H_2. Suppose $e_0 \in H_1$, then at least one $y_j \in H_2$. Consider the triangle $e_0y_ky_j$ and denote by $\gamma_{k,j}$ the triangle $\angle e_0y_ky_j$ in this triangle. The law of cosines yield

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

Since $y_j \in H_2$, then $\gamma_{k,j} \geq \frac{\pi}{2}$ and $\cos\gamma_{k,j} \leq 0$.(Figure 3.6.1)

From the conditions of Theorem 3.6.3. We have

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

Using the law of cosines,

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

we have $0 < \cos\theta_j \leq \cos\theta_k \cos\phi_{k,j}$. Since $0 < \cos\phi_{k,j}$ and $\cos\theta_j < \cos\phi_{k,j} \leq \cos\phi$. Therefore, $\theta_j > \frac{\pi}{3}$, it is a contradiction. ■

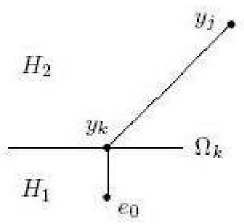

Figure 3.6.1:

3.7 The Bound m of an Extension of Delsarte's Method

We conclude the bound of m on S^{n-1}.

Theorem 3.7.1. [11] Let $Y = \{y_1, y_2, \cdots, y_m\} \subset S^{n-1}$ be a spherical $\frac{\pi}{3}$-code. Suppose $Y \subset cap(e_0, \theta_0)$ and $0 < \frac{\pi}{6} \le \theta_0 < \frac{\pi}{3} \le \frac{\pi}{2}$. Then

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

Proof. If $m \ge 2$, then $y_k \ne e_0$. Conversely, $\frac{\pi}{3} \le \text{dist}(y_i, y_j) = \text{dist}(e_0, y_i) < \theta_0$, it is a contradiction. The projection $\prod$ from the pole e_0 which sends $y_i \subset S^{n-1}$ along its meridian to the equator for all y_i. Denote $\gamma_{i,j} := \text{dist}(\prod(y_i), \prod(y_j))$.(Figure 3.7.1) By the law of cosines and $\cos\phi_{i,j} \le \cos\frac{\pi}{3} = \frac{1}{2}$. We have

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

Let $R(\alpha,\beta) = \frac{\frac{1}{2} - \cos\alpha\cos\beta}{\sin\alpha\sin\beta}$, then $\frac{\partial R(\alpha,\beta)}{\partial\alpha} = \frac{\cos\beta - z\cos\alpha}{\sin^2_\alpha\sin\beta}$. If $0 < \alpha, \beta < \theta_0$, then $\frac{\partial R(\alpha,\beta)}{\partial\alpha} > 0$. $R(\alpha,\beta)$ is a monotone increasing function in α. We obtain $R(\alpha,\beta) < R(\theta_0,\beta) < R(\theta_0,\theta_0)$. Therefore, $\cos\gamma_{i,j} = \frac{\cos\phi_{i,j} - \cos\theta_i\cos\theta_j}{\sin\theta_i\sin\theta_j} \le \frac{\frac{1}{2} - \cos^2\theta_0}{\sin^2\theta_0} = \cos\delta$, and $\prod(Y)$ is $\delta - code$ on the equator S^{n-2}. Thus, $m \le A(n-1, \delta)$.

■

Corollary 3.7.2. [11] Suppose $f \in \Phi(t_0, \frac{1}{2})$. If $2t_0^2 > \frac{3}{2}$, then $m(n, \frac{1}{2}, f) = 1$, otherwise $m(n, \frac{1}{2}, f) \le A(n-1, \arccos\frac{\frac{1}{2} - t_0^2}{1 - t_0^2})$.

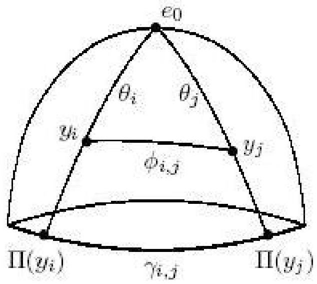

Figure 3.7.1:

Proof. Since $\cos\theta_0 = t_0$. $2t_0^2 > \frac{3}{2}$ if and only if $\frac{\pi}{3} > 2\theta_0$. In this case, any $\frac{\pi}{3}$-code in the $cap(e_0, \theta_0)$ have at most one point. Otherwise, $\frac{\pi}{3} \leq 2\theta_0$ and this corollary follows from Theorem 3.7.1. ■

Corollary 3.7.3. [11] Suppose $f \in \Phi(t_0, \frac{1}{2})$. Then $m(3, \frac{1}{2}, f) \leq 5$.

Proof. Since $\theta < \frac{\pi}{3}$ and $\cos\theta_0 = t_0$, then

$$T = \frac{\frac{1}{2} - t_0^2}{1 - t_0^2} \leq \frac{\frac{1}{1} - (\frac{1}{2})^2}{1 - (\frac{1}{2})^2} = \frac{\frac{1}{2}}{1 + \frac{1}{2}} < \frac{1}{2}.$$

we obtain $\delta = \arccos T > \frac{\pi}{3}$. Thus,$m(3, \frac{1}{2}, f) \leq A(2, \delta) \leq \frac{2\pi}{\delta} < 6$. ■

Corollary 3.7.4. [11] Suppose $f \in \Phi(t_0, \frac{1}{2})$. Then

(1) If $t_0 > \sqrt{\frac{1}{2}}$, then $m(4, \frac{1}{2}, f) \leq 4$.

(2) If $t_0 \geq 0.6058$, then $m(4, \frac{1}{2}, f) \leq 6$.

Proof. Denote by $\varphi_k(M)$ the largest angular separation that can be attained in a spherical code on S^{k-1} containing M points. *Schütte* and *van der waerden* proved that $\varphi_3(4) = \arccos(-\frac{1}{3}) \approx 109.47°$, $\varphi_3(5) = \varphi_3(6) = 90°$, $\cos\varphi_3(7) = \cot 40° \cot 80°$, $\varphi_3(7) \approx 77.86954°$. [8]

(1) Since $\frac{1}{2} - t_0^2 < 0$. By Corollary 3.7.2, $m(4, \frac{1}{2}, f) \leq A(3, \delta) = A(3, \text{arccos}\, \frac{\frac{1}{2}-t_0^2}{1-t_0^2})$, where $\delta > 90°$ We have $\delta > \varphi_3(5)$, thus $m < 5$.

(2) $t_0 \geq 0.6058$. $\delta = \text{arccos}\, \frac{\frac{1}{2}-t_0^2}{1-t_0^2} > 77.87°$. Since $77.87° = \delta > \varphi_3(7)$ and by Corollary 3.7.2 $\mu(4, \frac{1}{2}, f) \leq A(3, 77.87°)$, we have $A(3, 77.87°) < 7$

■

Hence, we consider the set Y, $|Y| \leq 6$ on S^3.

3.8 Optimal and Irreducible Sets

Definition 3.8.1. [11] We denote by $\Phi^*(\frac{1}{2})$ the set of all functions $f \in \bigcup_{\tau_0 > \frac{1}{2}} \Phi(\tau, \frac{1}{2})$ such that $f(t)$ is monotone decreasing function on the interval $[-1. - \tau_0]$ and $f(-1) > 0 > f(-\tau)$.

For any $f \in \Phi^*(\frac{1}{2})$, denote $t_0 = t_0(f) := \text{sup}\{t \in [\tau_0, 1] : f(-t) < 0\}$. Consider a spherical $\frac{\pi}{3}$-code $Y = \{y_1, y_2, \ldots, y_m\} \subset cap(e_0, \theta_0) \subset S^{n-1}$, then denote by $\Gamma_{\frac{\pi}{3}}(Y)$ the graph with the set of vertices Y and the set of edges $y_i y_j$ with $\phi_{ij} = \frac{\pi}{3}$.

Definition 3.8.2. [11] Let $f \in \Phi^*(\frac{1}{2})$, $\theta_0 = \text{arccos}(t_0)$. If $H_f(-e_0; Y) = h_m(n, z, f)$, then spherical $\frac{\pi}{3}$-code $Y = \{y_1, y_2, \ldots, y_m\} \subset cap(e_0, \theta_0) \subset S^{n-1}$ is called optimal.

Definition 3.8.3. [11] Let $0 < \theta_0 < \frac{\pi}{3} \leq \frac{\pi}{2}$. We say that a spherical $\frac{\pi}{3}$-code $Y = \{y_1, y_2, \ldots, y_m\} \subset cap(e_0, \theta_0) \subset S^{n-1}$ is irreducible if any y_k can not be shifted toward e_0 such that Y' which is obtained after this shifting, is also a $\frac{\pi}{3}$-code.

Proposition 3.8.4. [11] Let $f \in \Phi^*(\frac{1}{2})$. Suppose $Y \subset cap(e_0, \theta_0) \subset S^{n-1}$ is optimal for f. Then Y is irreducible.

Proof. Let $F_f(\theta_1, \ldots, \theta_m) := H_f(-e_0; Y) = F(1) + f(-\cos\theta_1) + \cdots + f(-\cos\theta_m)$, where $\theta_k := \text{dist}(y_k, e_0)$. $F_f(\theta_1, \ldots, \theta_m)$ is increasing when θ_k decreases. If y_k shifted toward e_0, then $F_f(\theta_1, \ldots, \theta_m)$ is increasing. It is contradicts with the optimality of the initial set Y. ■

Lemma 3.8.5. [11] If $Y = \{y_1, y_2, \ldots, y_m\}$ is irreducible, then

(1) $e_0 \in \Delta_m$= convex hull of Y.

(2) 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 $\Gamma_{\frac{\pi}{3}}(Y)$.

Lemma 3.8.5 plays an important role in the following sections.

Lemma 3.8.6. [11] Consider in S^{n-1} an arc ω and a regular simplex Δ ,both are with edge $\frac{\pi}{3}$. Suppose the intersection of ω and Δ is not empty, then at least one the distance between vertices of ω and Δ is less than $\frac{\pi}{3}$.

Proof. Let $w = u_1u_2$, $\Delta = v_1v_2 \ldots v_k$, dist$(u_1, u_2)$ = dist$(v_i, v_j) = \frac{\pi}{3}$ for $i \neq j$. Suppose not. Let dist$(u_i, v_j) \geqslant \frac{\pi}{3}$ for all i, j, U be the union of the $cap(v_i, \frac{\pi}{3})$, where $\frac{\pi}{3}$ is the radius and v_i is the center for $i = 1, 2, \ldots, k$ and B is the boundary of U. Since dist$(u_i, v_j) \geqslant \frac{\pi}{3}$, then u_1 and u_2 don't lie inside U. If $\{u'_1, u'_2\}$ $=w \bigcap B$, then $\frac{\pi}{3}$ = dist$(u_1, u_2) \geqslant$ dist(u'_1, u'_2) and $w' \bigcap \Delta \neq \emptyset$, where $w' = u'_1u'_2$. Now we find the minimal length of an arc w_1w_2 such that $w_1, w_2 \in B$ and $w_1w_2 \bigcap B \neq \emptyset$. Then dist$(w_1, w_2)$ attains its minimum when dist(w_1, v_i) = dist$(w_2, v_j) = \frac{\pi}{3}$. Using this and $\cos\alpha = \frac{2kz^2-(k-1)z-1}{1+(k-1)z}$, α= min dist(w_1, w_2), $z = \cos\frac{\pi}{3} = \frac{1}{2}$. Then we have $\cos\alpha \geq z$ if and only if $z \geq 1$ or $(k+1)z + 1 \leq 0$. It is a contradiction. ■

Consider $\Delta_m \subset S^{n-1}$ of dimension k, dim$(\Delta_m) = k$. Since Δ_m is a convex set, there exists the great k-dimensional S^k in S^{n-1} containing Δ_m. If $dim(\Delta_m) = 1$, then $m = 2$. Conversely, it is contradicts Theorem 3.6.3.

Theorem 3.8.7. [11] 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 length $\frac{\pi}{3}$.

Proof. By corollary 3.7.3 and $m > 2$, then m=3, 4, 5. Δ_m is a convex polygon with vertices $y_1, y_2, \ldots, y_m$ and $e_0 \in \Delta_m$, deg $y_i \geq 1$ by Lemma 3.8.5. We claim if deg $y_i \geq 2$ for all i, then Δ_m is an equilateral m-gon with length $\frac{\pi}{3}$. Lemma 3.8.6 implies that two diagonals of Δ_m of length $\frac{\pi}{3}$ do not intersect each other. That yield 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 common vertex.(Figure 3.8.1) Since the angular sum in spherical triangle is strictly greater than $180°$, we have $\angle y_i y_1 y_j > 60°$. Then $180° > \angle y_2 y_1 y_5 = \angle y_2 y_1 y_3 + \angle y_3 y_1 y_4 + \angle y_4 y_1 y_5 > 180°$. It is a contraction.

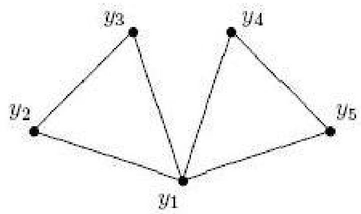

Figure 3.8.1:

Now, we prove that deg $y_i \geq 2$ for all i. Suppose deg $y_1 = 1$. We consider two cases, case(1): $e_0 \notin y_1y_2$ and case(2): $e_0 \in y_1y_2$. In the case(1), $e_0 \notin y_1y_2$.Then turn y_1 round y_2 to e_0 the θ_1 decreases, it is a contradiction. In the case(2), if $\phi_{ij} = \frac{\pi}{3}$ where $i > 2$ or $j > 2$ then $e_0 \notin y_iy_j$. Conversely, we have two intersecting diagonals of length $\frac{\pi}{3}$. Therefore deg $y_i \geqslant 2$ for $2 < i \leqslant m$. It implies the proof for $m = 3$ and $m = 4$. For $m = 5$, there is the case where $Q_3 = y_3y_4y_5$ is a regular triangle of side length $\frac{\pi}{3}$. By Lemma 3.8.6, arc y_1y_2 can not intersect Q_3, then arc y_1y_2 is a side of Δ_5. In this case, as above sufficiently small turn of Q_3 round y_2 to e_0 the distance θ_i, $i = 3, 4, 5$ decreases. It is a contradiction. ■

3.9 Rotations and Irreducible Sets in 4-Dimension

Consider a rotation $R(\varphi, \Omega)$ on S^3 about an 1-dimensional great sphere Ω in S^3. We may assume that $\Omega = \{\vec{u} = (u_1, u_2, u_3, u_4) \in R^4 : u_1 = u_2 = 0, u_1^2 + u_2^2 + u_3^2 + u_4^2 = 1\}$. Denote by $R(\varphi, \Omega)$ the rotation in the plane $\{u_i = 0,\ i = 3, 4\}$ through an angle φ about the origin Ω: $u_1' = u_1 \cos\varphi - u_2 \sin\varphi$, $u_2' = u_1 \sin\varphi + u_2 \cos\varphi$, $u_i' = u_i$ for $i = 3, 4$. Let $H_+ = \{\vec{u} \in S^3 : u_2 \geq 0\}$, $H_- = \{\vec{u} \in S^3 : u_2 \leq 0\}$, $Q = \{\vec{u} \in S^3 : u_2 = 0, u_1 > 0\}$, $\bar{Q} = \{\vec{u} \in S^3 : u_2 = 0, u_1 \geq 0\}$.

Lemma 3.9.1. Consider two points y and e_0 in S^3. 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 $y(\varphi)$, $y = (u_1, 0, u_3, u_4), u_1 > 0$ and $e_0 = (v_1, v_2, v_3, v_4)$. Then

$$\begin{aligned}
\gamma(\varphi) &:= y(\varphi) \cdot e_0 \\
&= (u_1(\varphi), u_2(\varphi), u_3(\varphi), u_4(\varphi)) \cdot e_0 \\
&= (u_1 \cos\varphi - u_2 \sin\varphi, u_1 \sin\varphi + u_2 \cos\varphi, u_3, u_4) \cdot e_0 \\
&= u_1 v_1 \cos\varphi - u_2 v_1 \sin\varphi + u_1 v_2 \sin\varphi + u_2 v_2 \cos\varphi + u_3 v_3 + u_4 v_4 \\
&= u_1 v_1 \cos\varphi + u_1 v_2 \sin\varphi + u_3 v_3 + u_4 v_4
\end{aligned}$$

Thus $\gamma'(\varphi) = -u_1 v_1 \sin\varphi + u_1 v_2 \cos\varphi$ and $\gamma'(0) = u_1 v_2$, where $u_1 > 0$. So we have $\gamma'(0) > 0$ iff $v_2 > 0$, $\gamma'(0) < 0$ iff $v_2 < 0$ and if $v_2 = 0$, by assumption $e_0 \notin \bar{Q}$, then $v_1 < 0$. Since $\gamma'(0) = 0$ and $\gamma''(0) = -u_1 v_1 > 0$. Therefore, $\varphi = 0$ is a minimum point.

■

Proposition 3.9.2. Let Y be irreducible and $|Y| = m \geq 4$. Suppose there are no closed great hemisphere $\bar{Q}$ in S^3 such that $\bar{Q}$ contains 3 points from Y and e_0. Then any vertex of $\Gamma_{\frac{\pi}{3}}(Y)$ has degree at least 3.

Proof. Suppose deg $y_1 < 3$, then $\phi_{1,i} > \frac{\pi}{3}$ for $i = 4, 5, \ldots, m$. Consider the great 1-dim sphere Ω in S^3 that contains the points y_2, y_3. By Lemma 3.9.1, a rotation $R(\varphi, \Omega)$ of y_1 with sufficiently small φ decreases the distance between y_1 and e_0, it is a contradiction. ■

Proposition 3.9.3. [11] If Y is irreducible, $|Y| = n$ and $dim\Delta_n = n - 1$, then deg $y_i = n - 1$ for all $i = 1, 2, \ldots, n$. In other words,Δ_n is a regular simplex of edge length $\frac{\pi}{3}$.

Proof. Δ_n is a spherical simplex. Denote by F_i its facet, $F_i := conv\{y_1, y_2, \ldots, y_{i-1}, y_{i+1}, \ldots, y_n\}$ and $F_\sigma := \bigcap_{i \in \sigma} F_i$ for $\sigma \subset I_n := \{1, 2, \ldots, n\}$. We claim that:

$$\text{if} \quad e_0 \notin F\{i,j\}, \text{then} \quad \phi_{i,j} = \frac{\pi}{3} \quad \text{for all} \quad i \neq j. \tag{3.9.1}$$

Conversely, there exist a rotation $R(\varphi, \Omega_{i,j})$ of y_i decreases θ_i, where $\Omega_{i,j}$ is the great $(n-3) - dim$ sphere contains $F_{\{i,j\}}$. It contradicts the irreducibility assumption for Y. So we have if there is no pair $\{i, j\}$ such that $e_0 \in F_{\{i,j\}}$, then $\phi_{i,j} = \frac{\pi}{3}$ for all i, j. Suppose $e_0 \in F_\sigma$, where σ has maximal size and $|\sigma| > 1$. Let $\bar{\sigma} = I_n\ \sigma$, from (3.9.1), we have if $i \in \sigma$ or $j \in \sigma$, then $\phi_{i,j} = \frac{\pi}{3}$. It remains to prove $\phi_{i,j} = \frac{\pi}{3}$ for all $i, j \in \sigma$. Let Λ be the intersection of the sphere of centers y_i, $i \in \sigma$ and radius $\frac{\pi}{3}$. Then Λ is a sphere in S^{n-1} of dimension $|\sigma| - 1$. Since F_σ=convex hull of $\{y_i, i \in \bar{\sigma}\}$ and all the distance dist(x, y) are the same for $x \in F_\sigma$ and $y \in \Lambda$. Then $y_i, i \in \sigma$ lie in Λ at the same distance from e_0. Thus, Y is irreducible if and only if $y_i, i \in \sigma$, in Λ are vertices of a regular simplex of edge length $\frac{\pi}{3}$.

■

Proposition 3.9.4. [11] If $n > 3$, then Δ_4 is a regular tetrahedron of edge length $\frac{\pi}{3}$.

Proof. We show that dim$\Delta_4 = 3$. Suppose dim$\Delta_4 = 2$ and Δ_4 is a rhomb by Theorem 3.8.7. Let y_1y_3 is the minimal length of Δ_4 and the sum of the lengths of any two sides of a triangle is larger than that of the third side on sphere, then $\phi_{2,4} > \frac{\pi}{3}$. Consider a sufficiently small turn of the facet $y_1y_2y_4$ round y_1y_3. If $e_0 \notin y_1y_3$, then decreases either θ_2 or θ_4. If $e_0 \in y_1y_3$ any turn of y_2 round y_1y_3 decreases $\phi_{2,4}$ and doesn't change θ_2. Then there exist a turn of y_2 such that $\phi_{2,4}$ is become to $\frac{\pi}{3}$,it is a contradiction. Therefore, dim$\Delta_4 = 3$ and Δ_4 is a regular tetrahedron of edge length $\frac{\pi}{3}$ by Proposition 3.9.3. ■

Now we consider the irreducible sets $|Y| = 5$ on S^3 and prove that deg $y_k \geq 3$ for all y_k in the irreducible sets. The proof step are following:

Show that dim Δ_5=3

↓

Introduce the $\tilde{S}_{ijk}$

↓

Show if deg $y_k = 1, \phi_{kl} = \frac{\pi}{3}$, then $e_0 \in s_{kl}$

↓

Show that deg $y_k = 1$ is wrong for all k

↓

Show deg $y_k \geq 3$ for all k

Lemma 3.9.5. [11] If $Y \subset S^3$ is irreducible and $|Y| = 5$, then deg $y_k \geq 3$ for all k.

The detail of proof step as following.

Proof. Step1: Show that dim$\Delta_5 = 3$. Conversely, suppose dim$\Delta_5 = 2$ and Δ_5 is a convex equilateral pentagon by Theorem 3.8.7. Let y_1y_3 be the minimal length diagonal of Δ_5. We have $\phi_{2,4} > \frac{\pi}{3}$ and $\phi_{2,5} > \frac{\pi}{3}$. Suppose $e_0 \notin y_1y_3$. If $e_0 \in y_1y_2y_3$, then any sufficiently small turn of the facet $y_1y_3y_4y_5$ round y_1y_3 decreases θ_4 and θ_5 , otherwise it decreases θ_2, it is a contradiction. If $e_0 \in y_1y_3$, then any turn of y_2 round y_1y_3 decreases $\phi_{2,i}$, $i > 3$ and does not change θ_i. Then there is a turn such that $\phi_{2,4}$ or $\phi_{2,5}$ becomes is equal to $\frac{\pi}{3}$, it is a contradiction. Thus, dim$\Delta_5 = 3$. There exist two combinatorial of Δ_5: (A) and (B). In the case(A), the arc y_3y_5 lies inside Δ_5 and case (B) $y_2y_3y_4y_5$ is a facet of Δ_5.(Figure 3.9.1)

step2: Introduce the $\tilde{S}_{ijk}$. We denoted by s_{ij} the arc y_iy_j and denote by $s_{i,j,k}$ the triangle $y_iy_jy_k$. Let $\tilde{S}_{ijk}$ be the intersection of great 2-hemisphere $Q_{i,j,k}$ and Δ_5, where $Q_{i,j,k}$ contains $y_iy_jy_k$ and bounded by the great circle passes through y_iy_j. By proposition 3.9.2, we have if there are no i, j, k such that $e_0 \in \tilde{S}_{ijk}$, then deg $y_i \geq 3$ for all i. Now, we consider the case $e_0 \in \tilde{S}_{ijk}$. $S_{ijk} \neq \tilde{S}_{ijk}$ for the case(A), $i = 1, 2, 4$; $j = 3, k = 5$ or $j = 5, k = 3$.

step3: Show if deg $y_k = 1, \phi_{k,l} = \frac{\pi}{3}$, then $e_0 \in s_{kl}$. By Lemma 3.8.5, we have deg $y_k > 0$ for all k. If deg $y_k = 1, \phi_{k,l} = \frac{\pi}{3}$, then $e_0 \in s_{kl}$. Otherwise, there exists a rotation $R(\varphi, \Omega)$ of y_k in S^3 with sufficient small φ decreases θ_k, where Ω is the great circle in S^3 and contains y_l does not pass through e_0, it is a contradiction.

step4: Show deg $y_k = 1$ is wrong for all k. Suppose deg $y_k = 1$, $e_0 \in s_{kl}$.

(a) First, we consider the s_{kl} is an external edge of Δ_5. For the case(A), it is not s_{35} and for case(B) it is not s_{35} or s_{24}. Then there exists a great 2-hemisphere Ω_2 pass through y_k, y_l such that other points y_i, y_j, y_m lie inside the hemisphere H_+ bounded by Ω_2. Let Ω be the great circle in Ω_2 that contains y_l and it orthogonal to s_{kl}. By Lemma 3.9.1, there exists a rotation $R(\varphi, \Omega)$ such that the distance $\theta_j, \theta_j, \theta_m$ decreases, it is a contradiction. Therefore, deg $y_k = 1$, $e_0 \in s_{kl}$ is wrong for the s_{kl} is an external edge of Δ_5.

(b) Next, consider the case(A). Suppose deg $y_3 = 1, \phi_{3,5} = \frac{\pi}{3}$, $e_0 \in s_{35}$. By(a), we claim s_{124} is a regular triangle with side length $\frac{\pi}{3}$. If deg $y_i = 2$ for $i = 1, 2, 4$, then $e_0 \in s_{124} \cap s_{35}$. Since $\phi_{24} = \phi_{14} = \phi_{12} = \phi_{35} = \frac{\pi}{3}$, by Lemma 3.8.6, we have at least

one distance $\phi_{i,j}$ less than $\frac{\pi}{3}$, it is a contradiction. Therefore, $\phi_{35} > \frac{\pi}{3}$.
(c) For the case(B). Suppose deg $y_3 = 1, \phi_{3,5} = \frac{\pi}{3}$, $e_0 \in s_{35}$. Then for the point y_2, deg $y_2 = 1$ only if $\phi_{24} = \frac{\pi}{3}$ and $e_0 \in s_{24} \cap s_{35}$; deg $y_2 = 2$ only if $\phi_{24} = \frac{\pi}{3}$ and $\phi_{25} = \frac{\pi}{3}$; deg $y_2 = 3$ only if $\phi_{24} = \frac{\pi}{3}$, $\phi_{25} = \frac{\pi}{3}$ and $\phi_{12} = \frac{\pi}{3}$. In any case, $\phi_{24} = \frac{\pi}{3}$ and we have two intersection diagonal s_{24} and s_{35} of length $\frac{\pi}{3}$, it is a contradiction by Lemma 3.8.6. Hence deg $y_i \geqslant 2$ for all i.
step5: Finally, we show deg $y_k \geq 3$ for all k. Suppose deg $y_k = 2, \phi_{k,i} = \phi_{k,j} = \frac{\pi}{3}$, then $e_0 \in \tilde{S}_{ijk}$. We consider the s_{ijk} be the facet of Δ_5 and $e_0 \notin s_{ik}$. By the same argument as in 4(a), there exists a rotation $R(\varphi, \Omega)$, where Ω_2 contains S_{kij} and Ω be the great circle passes through y_k, y_i, then decreases θ_l, θ_q for two other point y_l, y_q, it is a contradiction. Next, consider s_{ijk} is not a facet of Δ_5. There are the following cases: s_{124}, s_{135} (case(A) and case(B)), s_{234} (case(B)). In s_{124}. Suppose deg $y_1 = 2, \phi_{1,2} = \phi_{1,4} = \frac{\pi}{3}$, $e_0 \in s_{124}$. Consider a small turn of y_3 round s_{24} toward y_1. If $e_0 \notin s_{24}$, then decreases θ_3. Since Y is irreducible, then $\phi_{3,5} = \frac{\pi}{3}$. If $e_0 \in s_{24}$ and doesn't change θ_3, but $\phi_{1,3}$ decreases. It implies $\phi_{3,5} = \frac{\pi}{3}$. By Lemma 3.8.6, a regular triangle s_{124} can't intersects s_{35}, then $\phi_{2,4} > \frac{\pi}{3}$. So deg $y_2 = degy_4 = 3$. Thus we have three isosceles triangle s_{243}, s_{241} and s_{245}. Using this and $\phi_{3,5} = \frac{\pi}{3}$, then $\phi_{1,i} < \frac{\pi}{3}$ for $i = 3, 5$, it is a contradiction. s_{135}(case(B)) is equivalent to the s_{124}. In the s_{135}(case (A)), this case has two subcases: $\tilde{S}_{351}, \tilde{S}_{135}$. Suppose deg $y_1 = 2$, $\phi_{1,3} = \phi_{1,5} = \frac{\pi}{3}$, $e_0 \in s_{135}$. If $e_0 \notin s_{135}$, then any small turn of y_1 round s_{35} decreases θ_1 by Lemma 3.8.5. Thus, $e_0 \in s_{135}$. Consider a small turn of y_2 round s_{35} decreases θ_2 and $\phi_{1,2}$, it is a contradiction. The subcase $\tilde{S}_{351}$, where $\phi_{3,5} = \frac{\pi}{3}$, is equivalent to the case s_{124}. In the s_{234}(case(B)), this case also has two subcases: $\tilde{S}_{243}, \tilde{S}_{234}$. The subcase $\tilde{S}_{243}$ can be prove in the same way as the case facet and $\tilde{S}_{234}$ is equivalent to the $\tilde{S}_{135}$. This concludes the proof. ■

By Lemma 3.9.5, we have the degree of any vertex of $\Gamma_{\frac{\pi}{3}}(Y)$ is at least 3. If all vertices of $\Gamma_{\frac{\pi}{3}}(Y)$ are of degree 3, then the sum of the degree equals 15. Thus, at

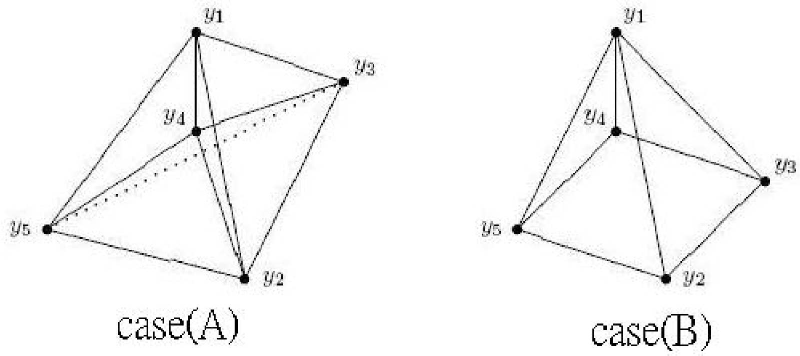

Figure 3.9.1: case(A) and case(B)

least one vertex has degree 4. Now, consider the Δ_5, by Lemma 3.9.5, we have the length of all edges of Δ_5 are equal to $\frac{\pi}{3}$ except y_2y_4, y_3y_5. We fixed $\phi_{2,4} = \alpha$ and if $2\theta_0 \geqslant \phi_{3,5} \geqslant \phi_{2,4} \geqslant \frac{\pi}{3}$, $t_0 \geqslant \frac{1}{2}$, then $0 \leqslant \cos\alpha \leqslant \frac{1}{2}$. Therefore, Δ_5 is a 1-parametric family $p_5(\alpha)$ on S^3.(Figure 3.9.2) Thus from Proposition 3.9.4 and Lemma 3.9.5 for

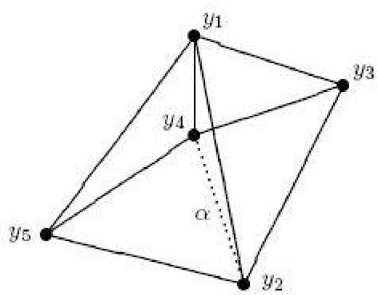

Figure 3.9.2: $p_5(\alpha)$

$n = 4$, we have the following theorem.

Theorem 3.9.6. [11] Let $Y \subset S^3$ be an irreducible set, $|Y| = 5$. Then Δ_m for $2 \leqslant m \leqslant 4$ is a regular simplex of edge length $\frac{\pi}{3}$ and Δ_5 is isometric to $p_5(\alpha)$ for some $\alpha \in [\frac{\pi}{3}, \frac{\pi}{2}]$.

3.10 On Calculations of h_m for $2 \le m \le 6$

We consider h_m for $2 \le m \le 6$.

Lemma 3.10.1. Let $n = 4$, $f \in \Phi^*(\frac{1}{2})$, Y is a optimal set on S^3 and $|Y| = m$ for $2 \le m \le 5$. Then $h_m \le \lambda_m(N, \frac{\pi}{3}, \theta_0)$, where N is a positive integer and θ_0 is the radius of the spherical cap.

Proof. For $m = 2$. Suppose $m = 2$ and $\Delta_2 = y_1y_2$ is an arc with length $\frac{\pi}{3}$, $e_0 \in \Delta_2$ and $\theta_1 + \theta_2 = \frac{\pi}{3}$. Then $h_2 = f(1) + f(-\cos\theta_1) + f(-\cos\theta_2)$. Assume $\theta_1 \le \theta_2$, $\theta_1 \in [\frac{\pi}{3} - \theta_0, \frac{\pi}{6}]$. Since $\theta_2 = \frac{\pi}{3} - \theta_1$ is a monotone decreasing function, $f(-\cos\theta_2)$ is a monotone increasing function in θ_1. For $\theta_1 \in [u, v] \subset [\frac{\pi}{3} - \theta_0, \frac{\pi}{6}]$, then

$$h_2 \le \Phi_2([u, v]) := f(1) + f(-\cos v) + f(-\cos(\frac{\pi}{3} - u)).$$

Let $u_1 = \frac{\pi}{3} - \theta_0$, $u_{i+1} = u_i + \epsilon$, $u_{N+1} = \frac{\pi}{2}$, where $\epsilon = \frac{6\theta_0 - \pi}{6N}$ and u_i is a point on $[\frac{\pi}{3} - \theta_0, \frac{\pi}{6}]$ for $i = 1, 2, \ldots, N+1$. If $\theta_1 \in [u_i, u_{i+1}]$, then $h_2 \le \Phi_2([u_i, u_{i+1}]) = f(1) + f(-\cos u_{i+1}) + f(-\cos(\frac{\pi}{3} - u_i))$. Thus $h_2 \le \lambda_2(N, \frac{\pi}{3}, \theta_0) := \max_{1 \le i \le N} \{\Phi_2([u_i, u_{i+1}])\}$. For $m = 3$. Suppose $m = 3$ and $\Delta_3 = y_1y_2y_3$ is a regular simplex. Assume $D := \{e_0 \in \Delta_3; \frac{\pi}{3} - \theta_0 \le \theta_1 \le \theta_2 \le \theta_3 \le \theta_0\}$. Let $K(4, \theta_0)$ be a 3-dimension cube with length θ_0, $K(4, \theta_0)$ contain Δ_3, $L(N)$ is a cube of side length ϵ, where $\epsilon = \frac{\theta_0}{N}$ and $K(4, \theta_0)$ consists of $L(N)$. There exists cube $L'(N)$ in $L(N)$ such that $L'(N) \bigcap D \ne \emptyset$. Let $\tilde{L}(N)$ be the subset of $L'(N)$ in $L(N)$, there exist a cube in $\tilde{L}(N)$ such that h_3 attains its maximum. Thus $h_3 \le \lambda_3(N, \frac{\pi}{3}, \theta_0) := \max_{L'(N,D) \in \tilde{L}(N)} \{\Phi_3(L'(N, D))\}$. The case $m = 4$ can be proven in the same way as the case $m = 3$.

For $m = 5$. Suppose $m = 5$ and Δ_5 is isometric to $p_5(\alpha)$ for some $\alpha \in [\frac{\pi}{3}, \frac{\pi}{2}]$. We fixed vertices y_1, y_2, y_3 of $p_5(\alpha)$. Then vertices y_4, y_5 are determined by α. The distance $\theta_4(\alpha) :=$ dist(e_0, y_4) increases and $\theta_5(\alpha)$ decreases in α. Let $u_1 = \frac{\pi}{3}$, $u_{i+1} = u_i + \epsilon$, $u_{N+1} = \frac{\pi}{2}$, where $\epsilon = \frac{\pi}{6N}$ and u_i is a point on $[\frac{\pi}{3}, \frac{\pi}{2}]$ for $i = 1, 2, \ldots, N+1$. Then

$\theta_4(\alpha_i) < \theta_4(\alpha_{i+1})$, $\theta_5(\alpha_i) > \theta_5(\alpha_{i+1})$, we have $f(-\cos\theta_4(\alpha_i)) > f(-\cos\theta_4(\alpha_{i+1}))$, $f(-\cos\theta_5(\alpha_i)) < f(-\cos\theta_5(\alpha_{i+1}))$. And using the proof of the case $m = 3$, we get $h_5 \leq \lambda_5(N, \frac{\pi}{3}, \theta_0) := f(1) + \max_{L'(N)\in\tilde{L}(N)}\{f_{1,2,3}(L'(N)) + \max_{1\leq i\leq N}\{f_{4,5}(\alpha_i)\}\}$. ■

Lemma 3.10.2. [11] Suppose $n = 4$, $f \in \Phi^*(\frac{1}{2})$, $\sqrt{\frac{1}{2}} > t_0 > \frac{1}{2}$, $\theta_0' \in [\frac{\pi}{4}, \theta_0]$. Then $h_6 \leq \max\{f(-\cos\theta_0') + \lambda_5(\frac{\pi}{3}, \theta_0), f(-\frac{1}{\sqrt{2}}) + \lambda_5(\frac{\pi}{3}, \theta_0')\}$.

Proof. Let Y be an optimal $\frac{\pi}{3}$-code on S^3. Assume $\theta_1 \leq \theta_2 \leq \ldots \leq \theta_6$. By the Corollary 3.7.4, we have $\theta_0 \geq \theta_6 \geq \theta_5 \geq \frac{\pi}{4}$. Then we consider two cases: (a) $\theta_0 \geq \theta_6 \geq \theta_0'$, (b) $\theta_0' \geq \theta_6 \geq \frac{\pi}{4}$. In the case(a), since $f(1) + f(-\cos\theta_1) + \ldots + f(-\cos\theta_5) \leq h_5 = \lambda_5(\frac{\pi}{3}, \theta_0)$ and $\theta_6 \geq \theta_0'$, $f(-\cos\theta_6) \leq f(-\cos\theta_0')$. Thus $h_6 \leq h_5 + f(-\cos\theta_6) \leq \lambda_5(\frac{\pi}{3}, \theta_0) + f(-\cos\theta_0')$. In the case(b), $\theta_0' \geq \theta_i$ for $i = 1, 2, \ldots, 6$. Since $f(1) + f(-\cos\theta_1) + \ldots + f(-\cos\theta_5) \leq h_5 = \lambda_5(\frac{\pi}{3}, \theta_0')$ and $\theta_6 \geq \frac{\pi}{4}$, $f(-\cos\theta_6) \leq f(-\frac{1}{\sqrt{2}})$. Then $h_6 \leq h_5 + f(-\cos\theta_6) \leq \lambda_5(\frac{\pi}{3}, \theta_0') + f(-\frac{1}{\sqrt{2}})$. ■

By the above lemmas, we have the following theorem.

Theorem 3.10.3. [11] Suppose $n = 4$, $f \in \Phi^*(\frac{1}{2})$, $\sqrt{\frac{1}{2}} > t_0 > \frac{1}{2} > 0$ and N is a positive integer. Then

(1) $h_0 = f(1)$, $h_1 = f(1) + f(-1)$.

(2) $h_m \leq \lambda_m(\frac{\pi}{3}, \theta_0) \leq \lambda_m(N, \frac{\pi}{3}, \theta_0)$ for $2 \leq m \leq 5$.

(3) $h_6 \leq max\{f(-\cos\theta_0') + \lambda_5(\frac{\pi}{3}, \theta_0), f(-\frac{1}{\sqrt{2}}) + \lambda_5(\frac{\pi}{3}, \theta_0')\}$, $\theta_0' \in [\frac{\pi}{4}, \theta_0]$.

Now we proof of Lemma 3.3.2.

Proof. The polynomial $f_4(t)$ is a monotone decreasing function on $[-1, -t_0]$, $t_0 \approx 0.60794$ and $f_4 \leq 0$ for $t \in [-t_0, \frac{1}{2}]$.(Figure 3.10.1) Thus $f_4 \in \Phi^*(\frac{1}{2})$. Since $t_0 > 0.6058$, then $m \leq 6$ by Corollary 3.7.4. We calculate h_m with $\theta_0 = \arccos t_0 \approx 52.5588°$. Then $h_0 = f(1) = 18.774$ and $h_1 = f(1) + f(-1) = 24.48$. The h_2 achieves its maximum at

$\theta_1 = 30°$, then $h_2 = f(1)+f(-\cos\theta_1)+f(-\cos\theta_2) = f(1)+2f(-\cos 30°) = 24.864$. For $m = 3$, $h_3 = \lambda_3(60°, \theta_0) \approx 24.8435$ at $\theta_3 = \theta_0$, $\theta_1 = \theta_2 \approx 30.0715°$. The case $m = 4$, we have $h_4 \approx 24.818$ at $\theta_1 = \theta_2 \approx 30.2310°$, $\theta_3 = \theta_4 \approx 51.6765°$. h_5 attains its maximum $h_5 \approx 24.6836$ at $\alpha = 60°$, $\theta_1 \approx 42.1569°$, $\theta_2 = \theta_4 \approx 32.3025°$, $\theta_3 = \theta_5 = \theta_0$. In the case $m = 6$, let $\theta_0' = 50°$, $f(-\cos 50°) \approx 0.0906$, $f(-\cos 45°) \approx 0.4533$. $\lambda_5(\frac{\pi}{3}, \theta_0) = h_5 \approx 24.6856$, $\lambda_5(\frac{\pi}{3}, 50°) \approx 23.9181$, then $h_6 \le max\{f(-\cos 50°) + h_5, f(-\cos 45°) + \lambda_5(\frac{\pi}{3}, 50°)\} \approx 24.7762$. Thus $h_{max} = h_2 < 25$ and by the (3.5.1), we have $S(X) < 25M$.

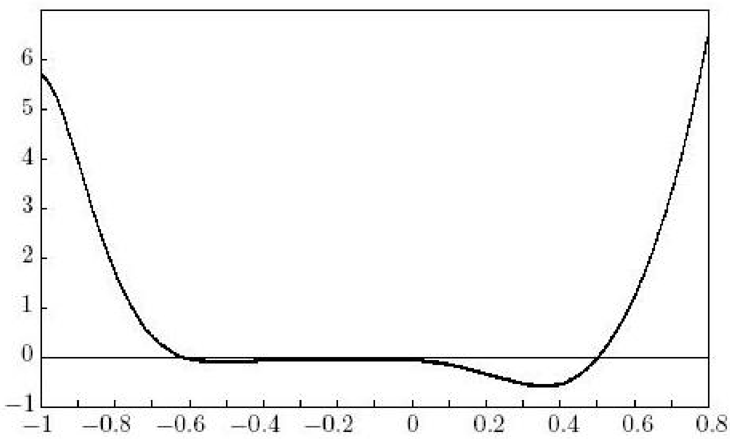

Figure 3.10.1: The graph of f_4

■

第 4 章　Applications

The kissing number problem in three dimension has applications in geometry, error correcting codes in telecommunications, string theory, sphere packing, chemistry and crystallography.

The kissing number problem is the foundation of sphere packing problem, sphere packing problem are a class of optimization problems. It is a obviously real and the important issue. In mathematics, sphere packing problems concern arrangements of nonoverlapping identical spheres which fill a space.

In chemistry and crystallography, the coordination number of a central atom in a molecule or crystal is the number of its nearest neighbors. This number is determined somewhat differently for molecules and for crystals. The highest bulk coordination number is 12, two most common arrangements are called cubic close packing (or face center cubic) and hexagonal close packing. This value of 12 corresponds to the theoretical limit of the kissing number problem when all spheres are identical. For example, the two most common allotropes of carbon have different coordination numbers. In diamond each carbon atom is at the center of a tetrahedron formed by four other carbon atoms, so the coordination number is four as for methane. Graphite is made of two-dimensional layers in which each carbon is covalently bonded to three other carbons. Atoms in other layers are much further away and are not nearest neighbors, so the coordination number of a carbon atom in graphite is 3 as in ethylene. And in recent year, the carbon 60 (C60) study shows the geometry in chemistry.

第 5 章　Conclusion

The kissing number has a rich history. In 1694, Isaac Newton and David Gregory has a famous discussion about the kissing number in three dimension. Newton believed the answer was 12, while Gregory thought that 13 might possible. The problem was solved until 1953.

We use Fejes T**ó**th's lemma to estimate the area of spherical triangles and prove $k(3) = 12$. Kissing number problem in three dimension has applications in chemistry, crystallography and sphere packing problem. In chemistry and crystallography, the coordination number of a central atom in a molecule or crystal is the number of its nearest neighbors. This number is determined somewhat differently for molecules and for crystals. In recent year, the carbon 60 study shows the geometry in chemistry. The kissing number problem is a foundation of sphere packing problem concern arrangements of nonoverlapping identical spheres which fill a space. If tangent to the ball whose radius are not different. This is complexification. The sphere packing problem is one of the problems in geometry.

In four dimension, Delsarte developed a method to determine the upper bounds for the kissing number based on linear programming. Delsarte showed the bound is 25, in fact, kissing number in four dimension is 24. Musin proved it in 2003 and extension the method to high dimension.

Appendix. An algorithm for polynomials $f(t)$.[11]

In this paper, the polynomial $f(t)$ is a monotone decreasing function on the interval $[-1,-t_0]$ and $f(t) \leq 0$ for $t \in [-t_0, \frac{1}{2}]$, $t_0 > \frac{1}{2} > 0$. $f(t)$ satisfy the following conditions: $c_k \geq 0$, $1 \leq k \leq d$(c1), $f(a) > f(b)$ for $-1 \leq a < b \leq -t_0$(c2), $f(t) \leq 0$ for $-t_0 \leq t \leq \frac{1}{2}$(c3). 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 are at the distance of ρ_m from y_c, where

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

When $m = 2n-2$,Δ_m presumably is a regular $(n-1)$-dimensional crosspolytope. In this case $\cos\rho_m = \sqrt{z}$. Let $I_n = \{1,2,\ldots,n\} \cup \{2n-2\}$, $m \in I_n$, $b_m = -\cos\rho_m$, 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 $f(b_m) \leq \frac{F_0}{m}$, $m \in I_n$. And $f(t)$ 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 inequality at the points $a_j = -1 + \epsilon j$, $0 \leq j \leq N$, $\epsilon = \frac{1+z}{N}$:

Second use linear programming to find $F_0, c_1, \ldots, c_d$ so as to minimize $E - 1 = F_0 + \sum_{k=1}^{d} c_k$ subject to the constraints $c_k \geq 0$ for $1 \leq k \leq d$, and $\sum_{k=1}^{d} c_k G_k^{(n)}(a_j) \geq \sum_{k=1}^{d} c_k G_k^{(n)}(a_{j+1})$, $a_j \in [-1,-t_0]$; $1+\sum_{k=1}^{d} c_k G_k^{(n)}(a_j) \leq 0$, $a_j \in [-t_0, z]$; $1+\sum_{k=1}^{d} c_k G_k^{(n)}(b_m) \leq \frac{F_0}{m}$, $m \in I_n$. Let us note that $E \leq h_{max}$, and $E = h_{max}$ only if $h_{max} = H_{m0}(y_c)$ for some $m_0 \in I_n$.

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