New Results on Heilbronn Problem in Three-Dimensional Space

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Abstract

In this thesis, the following problem is considered.

Let $S$ be a point set in a three-dimensional Euclidean space, and it consists of $n$ (greater than 1) points.

We define that

$$D(S) = \max_{A,B \in S, A \neq B} |AB|$$

$$d(S) = \min_{A,B \in S, A \neq B} |AB|$$

$$\lambda_{n,3} = \inf \frac{D(S)}{d(S)}$$

And we prove that

$$3\sqrt[3]{\frac{\sqrt{18}}{\pi}} \sqrt[n]{n} - 1 \leq \lambda_{n,3} < 3\sqrt[3]{\frac{\sqrt{18}}{\pi}} \sqrt[n]{n} + 4$$

$$\lim_{n \to \infty} \frac{\lambda_{n,3}}{\sqrt[n]{n}} = 3\sqrt[3]{\frac{\sqrt{18}}{\pi}}$$

We also design a program to get approximate solutions for certain cases of small “$n$”s.
Chapter 1

Introduction

The following problem is called the “Heilbronn Problem”:

Consider a point set $S$, which consists of $n$ (great than 1) distinct points in a plane. Connect each two of them and we get $\binom{n}{2}$ line segments.

Let $D(S)$ be the length of the longest one and $d(S)$ the shortest.

The problem is to find

$$\lambda_{n,2} = \inf \frac{D(S)}{d(S)}$$

Fejes Toth in 1940 proved that

$$\lim_{n \to \infty} \frac{\lambda_{n,2}}{\sqrt{n}} = \sqrt{\frac{12}{\pi}}$$

Tian Zhengping in [3] and [4] proved that

$$\sqrt{\frac{12}{\pi}} \sqrt{n} - 1 \leq \lambda_{n,2} \leq \sqrt{\frac{12}{\pi}} \sqrt{n}$$

Our thesis focuses on a problem of the same type, but it comes to a three-dimensional Euclidean space. (See Abstract for more details of the problem)

In Chapter 2 we give $\lambda_{n,3}$ (defined in Abstract) a lower bound

$$\lambda_{n,3} \geq \sqrt[3]{\frac{18}{\pi}} \sqrt[3]{n} - 1$$
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which is more optimal than the lower bound given in [8]

\[ \lambda_{n,3} \geq \gamma_3 \left( \sqrt[3]{n} - 1 \right) \]

where \( \gamma_3 = \left[ \frac{\sqrt{2}}{12 \arctan \left( \frac{1}{\sqrt{2}} \right) - 2} \right]^{1/3} \approx 1.0865. \)

In Chapter 3 we get our inspiration from the face-centered cubic packing and use a polyhedron to fill the space, which gives \( \lambda_{n,3} \) an upper bound for \( n > 1024 \), say

\[ \lambda_{n,3} < \sqrt[3]{\frac{18}{\pi} \sqrt{n}} + 4 \]

Then we use a program with the same structural method to verify the upper bound for \( 2 \leq n \leq 1024 \), and we are glad to find out that the upper bound holds for \( 2 \leq n \leq 1024 \). Thus we prove that \( \forall n \geq 2, \lambda_{n,3} \leq \sqrt[3]{\frac{18}{\pi} \sqrt{n} + 4} \).

Still, it’s more optimal than the following upper bound given in [8] when it comes to a three-dimensional space,

\[ \lambda_{n,k} \leq \delta_k \sqrt[n]{n - 1} + \sqrt{\frac{k(k+1)}{2}} \]

where \( \delta_k = \sqrt{\frac{2}{\pi} \left[ k \sqrt{k + 1} \Gamma \left( \frac{k}{2} \right) \right]}^{1/k} \).

In Chapter 4 we use the Squeeze Rule, the lower bound and the upper bound of \( \lambda_{n,3} \) to get the limit of \( \frac{\lambda_{n,3}}{\sqrt[n]{n}} \) when \( n \to \infty \), which is

\[ \lim_{n \to \infty} \frac{\lambda_{n,3}}{\sqrt[n]{n}} = \sqrt[3]{\frac{18}{\pi}} \]

And this proves the conjecture Zhu Yuyang posed in 1995.

In Chapter 5 we use the Steepest Descent Approach to design a program to get some approximate solutions for cases where \( 5 \leq n \leq 13 \)
Chapter 2

A New Lower Bound

Hong Yi, Wang Guoqiang and Tao Zhisui in [8] give $\lambda_{n,3}$ a lower bound, which is

$$\lambda_{n,3} \geq \gamma_3 \left( \sqrt[3]{n} - 1 \right)$$

where

$$\gamma_3 = \left[ \frac{\sqrt{2}}{12 \arctan \left( \frac{1}{\sqrt{2}} \right) - 2\pi} \right]^{1/3} \approx 1.0865.$$  

Here in this chapter, we give $\lambda_{n,3}$ a more optimal lower bound,

$$\lambda_{n,3} \geq 3 \sqrt[3]{\frac{18}{\pi}} \sqrt[3]{\sqrt{n} - 1}$$

Theorem 2.1. Let $S \in \mathbb{R}^3$ and

$$\lambda_{n,3} = \inf \frac{\max_{A,B \in S, A \neq B} |AB|}{\min_{A,B \in S, A \neq B} |AB|}$$

\forall n \geq 2, we have

$$\lambda_{n,3} \geq 3 \sqrt[3]{\frac{18}{\pi}} \sqrt[3]{\sqrt{n} - 1}$$

Proof. To prove this theorem, we need to know the following two lemmas first.

Lemma 2.2. (the Bieberbach inequality) For any set $A \in \mathbb{R}^n$, we have the inequality

$$V(\text{conv } A) \leq \frac{v_n}{2^n} (\text{diam } A)^n$$

(2.1)
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where conv $A$ is a convex hull of $A$, and diam $A$ is the diameter of $A$, while $v_n$ is the volume of the unit ball in $\mathbb{R}^n$. Here the equality sign in (2.1) holds if and only if $A$ is a ball (in $\mathbb{R}^n$) from which a zero-dimensional set may have been removed. (see [9])

Lemma 2.3. (the Kepler Conjecture) No packing of congruent balls in Euclidean three space has density greater than that of the face-centered cubic packing. This density is $\frac{\pi}{\sqrt{18}}$. (see [7])

For a point set $S$, without losing generality, we assume that $d(S) = 1$.

With these $n$ points being the centers, we draw $n$ spheres whose radii equal to $\frac{1}{2}$. Since $d(S) = 1$, it is obvious that no two spheres may intersect.

Let $G$ be the convex hull of the $n$ spheres, and $d = \text{diam } G$.

Because a convex set and its convex hull has the same diameter, there must be two points, $P$ and $Q$, while $P$ is on $\odot A$, and $Q$ is on $\odot B$, and $PQ$ is a diameter of $G$. Here $A$ and $B$ are two points in $S$ and $\odot A$ and $\odot B$ are two spheres we draw.

Thus we have

$$|PQ| \leq |PA| + |AB| + |BQ|$$

(2.2)

Here $|PQ| = d$, and $|PA| = |BQ| = \frac{1}{2}$.

Obviously we have $|AB| \leq D(S)$, hence

$$d \leq D(S) + 1$$

(2.3)

According to Lemma 2.2, we have the inequality

$$V(G) \leq \frac{4}{3} \pi \cdot d^3 = \frac{1}{6} \pi d^3$$

(2.4)

where $V(G)$ is the volume of $G$.

We all know that $\frac{1}{6} \pi d^3$ is the volume of a sphere of diameter $d$, so (2.4) implies that of all convex hulls of diameter $d$, the sphere bounds the greatest volume.
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According to Lemma 2.3, we have

\[ \frac{nV_0}{V(G)} \leq \frac{\pi}{\sqrt{18}} \quad (2.5) \]

where \( V_0 = \frac{\pi}{6} \), denoting the volume of each sphere we draw.

Use (2.4) to eliminate \( V(G) \) in (2.5), and we have

\[ \frac{n \cdot \frac{\pi}{6}}{\frac{1}{6} \pi d^3} \leq \frac{\pi}{\sqrt{18}} \]

which can be transformed to be

\[ d \geq \sqrt[3]{\frac{\sqrt{18}}{\pi} \sqrt[3]{n}} \quad (2.6) \]

Use Inequality (2.3) to eliminate \( d \) in (2.6), and it gives

\[ \frac{D(S)}{d(S)} = D(S) \geq d - 1 \geq \sqrt[3]{\frac{\sqrt{18}}{\pi} \sqrt[3]{n}} - 1 \quad (2.7) \]

Therefore, we can draw the conclusion that

\[ \lambda_{n,3} \geq \sqrt[3]{\frac{\sqrt{18}}{\pi} \sqrt[3]{n}} - 1 \]

And that completes the proof of Theorem 2.1
Chapter 3

A New Upper Bound

Hong Yi, Wang Guoqiang and Tao Zhisui in \cite{8} give $\lambda_{n,k}$ an upper bound, which is

$$\lambda_{n,k} \leq \delta_k \sqrt[3]{n-1} + \sqrt{\frac{k(k+1)}{2}}$$

where $\delta_k = \sqrt{\frac{2}{\pi}} \left[ k \sqrt{k+1} \Gamma\left(\frac{k}{2}\right) \right]^{1/k}$.

When in a three-dimensional space, it comes to be

$$\lambda_{n,3} \leq \delta_3 \sqrt[3]{n-1} + \sqrt{6}$$

where $\delta_3 \approx 1.685$.

Here in this chapter, we give $\lambda_{n,3}$ a more optimal upper bound

$$\lambda_{n,3} < 3 \sqrt[3]{\frac{18}{\pi}} \sqrt[3]{n} + 4$$

3.1 An Upper Bound for \( n \) greater than 1024

Here we give an upper bound of $\lambda_{n,3} \forall n > 1024$.

**Theorem 3.1.** Let $S \in \mathbb{R}^3$ and

$$\lambda_{n,3} = \inf \max_{A,B \in S, A \neq B} \frac{|AB|}{\min_{A,B \in S, A \neq B} |AB|}$$

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∀n > 1024, we have

\[ \lambda_{n,3} < \frac{\sqrt[3]{18}}{\pi} \sqrt[3]{n} + 4 \]

**Proof.** To prove this theorem, we need to structure a polyhedron.

![Figure 3.1: The center cube and the side cubes](image1)

![Figure 3.2: The structural method of the polyhedron](image2)

Firstly, we draw seven cubes (see Figure 3.1). The center one of them is called the *Center Cube* and the other six ones are called the *Side Cubes*, while each *Side Cube* has a common face with the *Center Cube*. Then, we connect the center of each *Side Cube* with the vertices of its corresponding common face with the *Center Cube*, and we get a red polyhedron (let’s call it a *Super Cube*) marked out in Figure 3.2.

Figure 3.3 shows how the Super Cube looks like when separated from the cubes. It is easy to know its central symmetry.

Now, for each integral point \( P(x, y, z) \) in the space, we use it as a center to draw a unit cube whose faces are parallel to the coordinate planes.

We say that an integral point \( Q(x, y, z) \) is an *Even Point* if \( x + y + z \equiv 0 \pmod{2} \). And for each *Even Point* we use its unit cube as a *Center Cube* to structure a *Super Cube*. Finally we get a space thoroughly filled with *Super Cubes.*
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Figure 3.3: Super Cube

Furthermore we draw a sphere, $T$, whose center is $O (0, 0, 0)$, of diameter $d$.

Let $A$ and $B$ be two Even Point sets. We say that an Even Point $P$ is in $A$ if it is inside or on $T$. We say that an Even Point $Q$ is in $B$ if it is out of $T$ and its Super Cube intersects with $T$. If we use $H (P)$ to denote the Super Cube of an Even Point $P$ and $V (X)$ to denote the volume of a solid figure $X$, we can easily get the following equation.

$$V (T) = V \left( \bigcup_{P \in A} H (P) \right) \cap T + V \left( \bigcup_{Q \in B} H (Q) \right) \cap T \quad (3.1)$$

Obviously $\forall P \in A$, $V (H (P) \cap T) \leq V (H (P))$. We know Super Cubes are central symmetrical, so $\forall Q \in B$, $V (H (Q) \cap T) < \frac{1}{2} V (H (Q))$, which is proved in Lemma 3.2 as follow.

**Lemma 3.2.** $\forall Q \in B$, $V (H (Q) \cap T) < \frac{1}{2} V (H (Q))$.

**Proof.** We say that a plane is an Equatorial Plane if it passes through $Q$ $(Q \in B)$.

Because Super Cubes are central symmetrical, if we divide $H (Q)$ into two parts with an Equatorial Plane, they bound the same volume.

Since $Q \in B$, the Equatorial Plane with $\overrightarrow{OQ}$ being its normal vector won’t intersect with $T$. And this Equatorial Plane divides $H (Q)$ into two isometric parts, one of which has $H (Q) \cap T$ inside. This implies that $V (H (Q) \cap T) < \frac{1}{2} V (H (Q))$.
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That completes the proof of Lemma 3.2.

Because we use unit cubes to structure the Center Cubes, it is easy to know that the volume of a Super Cube is 2. So we get the following inequality from (3.1) and Lemma 3.2

\[ V(T) < |A| \cdot 2 + |B| \cdot 1 \quad (3.2) \]

Here we consider \(|A|\) as \(n\), that is, we consider \(S = A\). Now we’re to prove that \(|B| < \pi (d + \sqrt{3} + \sqrt{6})^2\)

Draw an inscribed cube whose faces are parallel to the coordinate planes, of \(T\) (see Figure 3.4). Here \(\odot T'\) is the circumcircle of Square ABCD, and we get a spherical crown above Plane ABCD.

![Figure 3.4: Inscribed cube of T and circumcircle of Square ABCD](image)

Let \(C\) be a subset of \(B\). We say that a point is in \(C\) if it’s an Even Point above Plane \(ABCD\) and its Super Cube intersects with the spherical crown. To continue our proof, we need to prove a very important lemma.

**Lemma 3.3.** If two points, for example \(P(x_P, y_P, z_P)\) and \(Q(x_Q, y_Q, z_Q)\), are in \(C\), they can’t have the same objection on Plane \(xOy\).

**Proof.** We use proof by contradiction to prove this lemma.
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If this lemma is not true, there must be two points, \( P \) and \( Q \), in \( C \). Here \( Q \) is above \( P \), while they have the same objection on Plane \( xo\text{y} \).

Here comes the first part of the proof.

Draw a circumscribed sphere, \( E \), of \( H(Q) \). And \( X \) is a point inside \( E \). Connect \( X \) and \( P \). We assume \( \overrightarrow{PX} = (x, y, z) \) and we’re to prove that \( z^2 > 2(x^2 + y^2) \). (see Figure 3.5)

![Figure 3.5: P’s and Q’s Super Cubes](image)

Without losing generality, we assume that \( P(0, 0, 0) \) in this part of the proof, which can simplify it. According to the description of structuring a Super Cube, we know that the radius of \( E \) equals to 1. So we have \( Q(0, 0, t) \) where \( t \geq 2 \), and that \( X(x, y, z) \) must satisfy \( x^2 + y^2 + (z - t)^2 \leq 1 \) because \( X \) is inside \( E \). To prove \( z^2 > 2(x^2 + y^2) \), we only need to prove

\[
1 < \frac{z^2}{2} + (z - t)^2 \tag{3.3}
\]

since we know \( x^2 + y^2 + (z - t)^2 \leq 1 \).
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Because $t \geq 2$, it’s easy to know that $1 < z^2 + (z - t)^2$ holds for $\forall z \in \mathbb{R}$, which implies that for each point $X$ inside $E$, we have $z^2 > 2(x^2 + y^2)$, and then for each point $X$ inside $H(Q)$, we also have

$$z^2 > 2(x^2 + y^2) \quad (3.4)$$

The following is the second part of the proof.

Let $K(x_K, y_K, z_K)$ be any point of intersection of $H(Q)$, and the spherical crown. Let $P'$ be the objection of $P$ on Plane $xOy$. If line $PP'$ intersects with the spherical crown, let $W(x_W, y_W, z_W)$ be the point of intersection. Otherwise, let $W$ be the objection of $P$ on Plane $ABCD$.

We assume that $PK = (x, y, z)$ and $KW = (x, y, z)$. Since $Q$ is above $P$, we know $K$ is above $P$. And obviously $P$ is either above $W$ or the same point as $W$, hence

$$z_0 \leq z \quad (3.5)$$

Here we are to prove that $z^2 \leq 2(x^2 + y^2)$. Since the value of $z^2$ and $x^2 + y^2$ won’t change no matter how we rotate Plane $xOy$, circling round the $Z$-axis, there is no harm in assuming that $y_W = 0, x_W > 0$.

Hence, we have

$$z^2 - 2(x^2 + y^2) = (z_W - z_K)^2 - 2[(x_W - x_K)^2 + (0 - y_K)^2]$$
$$\leq (z_W - z_K)^2 - 2 \left[ (x_W - \sqrt{x_K^2 + y_K^2})^2 + (0 - 0)^2 \right] \quad (3.6)$$

Here we define that $K'(x_{K'}, y_{K'}, z_{K'})$ which is also on the spherical crown, while $(x_{K'}, y_{K'}, z_{K'}) = \left( \sqrt{x_K^2 + y_K^2}, 0, z_K \right)$. And (3.6) implies that for $WK' = (x_1, y_1, z_1), (y_1 = 0)$

$$z_1^2 - 2(x_1^2 + y_1^2) \geq z^2 - 2(x^2 + y^2) \quad (3.7)$$

Let’s consider the situation where $W$ is a point on the spherical crown first.

Specially, when $W$ is the same point as $K'$ which implies the fact that $WK' = (x_1, y_1, z_1) = (0, 0, 0)$, we have $z_1^2 \leq 2(x_1^2 + y_1^2)$. 55
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Figure 3.6: Sectional plane passing through $K'$, $W$ and $O$

Otherwise, $K'$ and $W$ are two distinct points. Let’s see Figure 3.6 for instance. Figure 3.6 shows the sectional plane passing through $K'$, $W$ and $O$.

Here, according to the properties in geometry

$$|OU| : |OV| : |UV| = \sqrt{3} : \sqrt{3} : 2\sqrt{2}$$  \hspace{1cm} (3.8)

Let $M(x_M, y_M, z_M)$, $(y_M = 0)$ be the midpoint of $WK'$. So $\overrightarrow{WK'} \perp \overrightarrow{OM}$, and then

$$\frac{z_{K'} - z_W}{x_{K'} - x_W} : \frac{z_M - 0}{x_M - 0} = -1$$  \hspace{1cm} (3.9)

It is the case where $x_M \neq 0$.

According to (3.8), we have

$$\frac{z_M - 0}{x_M - 0} \in \left( -\infty, -\frac{1}{\sqrt{2}} \right] \cup \left[ \frac{1}{\sqrt{2}}, \infty \right).$$

Then according to (3.9) we have

$$\frac{z_{K'} - z_W}{x_{K'} - x_W} \in [-\sqrt{2}, \sqrt{2}],$$

that is, $\frac{z_1}{x_1} \in [-\sqrt{2}, \sqrt{2}]$. And this still holds when $x_M = 0$, because in that case $z_{K'} = z_W$, which means $z_1 = 0$.

Hence, we have $z_1^2 \leq 2x_1^2 = 2(x_1^2 + y_1^2)$. According to (3.5) and (3.7), we have

$$0 \geq z_1^2 - 2(x_1^2 + y_1^2) \geq z^2 - 2(x^2 + y^2) \geq z_0^2 - 2(x^2 + y^2)$$  \hspace{1cm} (3.10)

As for the situation where $W$ is a point on Plane $ABCD$, let’s see Figure 3.7 for instance, which is similar to Figure 3.6. It shows the sectional plane which contains $K'$, $W$ and $O$. 

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Figure 3.7: The sectional plane of another situation

Here $V$ is a point on $\odot T'$ (defined above) and it is the closest point to $W$. We assume that $\overrightarrow{VK'} = (x_2, y_2, z_2)$. Obviously we have

\[ z_2 = z_1 \]  \hspace{1cm} (3.11)

\[ x_2^2 + y_2^2 < x_1^2 + y_1^2 \]  \hspace{1cm} (3.12)

where $\overrightarrow{WK'} = (x_1, y_1, z_1)$ which is mentioned above.

If we use the method which is similar to the previous one, we can prove that

\[ z_2^2 \leq 2 \left( x_2^2 + y_2^2 \right) \]  \hspace{1cm} (3.13)

According to (3.5), (3.7), (3.11), (3.12) and (3.13), we have

\[ 0 \geq z_2^2 - 2 \left( x_2^2 + y_2^2 \right) > z_1^2 - 2 \left( x_1^2 + y_1^2 \right) \geq z_0^2 - 2 \left( x^2 + y^2 \right) \]  \hspace{1cm} (3.14)

We see (3.10) and (3.14) are contradictory to (3.4).

And thus we prove Lemma 3.3. \hfill \square

Now let’s prove $|C| < \frac{1}{6} \pi \left( d + \sqrt{3} + \sqrt{6} \right)^2$

Lemma 3.4. $|C| < \frac{1}{6} \pi \left( d + \sqrt{3} + \sqrt{6} \right)^2$

Proof. Look at Figure 3.8. It shows Plane $ABCD$ while $T'$ is the center of $Square \ AB CD$.  

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Figure 3.8: A view of Plane $ABCD$

It is easy to know that $T'A = T'B = T'C = T'D = \frac{d}{\sqrt{6}}$. If we draw a larger circle $\odot T'$ with radius of $\frac{d}{\sqrt{6}} + \frac{1}{\sqrt{2}} + 1$, we can cover all the unit squares which are objected from the unit cubes of points in $C$. Hence, according to Lemma 3.3, we have the inequality

$$|C| \cdot S_0 < S(\odot T') \quad (3.15)$$

where $S_0 = 1$, denoting the area of a unit square. And $S(\odot T') = \pi\left(\frac{d}{\sqrt{6}} + \frac{1}{\sqrt{2}} + 1\right)^2$, denoting the area of $\odot T'$.

Hence we have $|C| < \frac{1}{6} \pi \left(d + \sqrt{3} + \sqrt{6}\right)^2$, which proves Lemma 3.4.

To prove $|B| < \pi \left(d + \sqrt{3} + \sqrt{6}\right)^2$, we only need to prove $|B| \leq 6 |C|$

Lemma 3.5. $|B| \leq 6 |C|$

Proof. Let's again consider the inscribed cube of $T$, see Figure 3.4. Here the six faces of the cube are in six distinct planes. For each plane, it divides the space into two regions, one of which doesn't have $O$, the center of $T$, in it.

We say a point is beyond a plane if this point is on the plane or in the region this plane makes that doesn’t have $O$ in it. For each plane, we use a
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point set to describe all the points in point set \( B \) that are beyond it, and we get six point sets, say \( C_1, C_2, \cdots, C_6 \).

According to the symmetry of the sphere, the cube and the Super Cube, we know that all the six sets have exactly the same number of points, and that one of the six sets is \( C \), we have

\[
|C_1| = |C_2| = \cdots = |C_6| = |C| \quad (3.16)
\]

Obviously, every point in \( B \) is in at least one of the six sets. (If not, there must be a point in \( B \) being in the inscribed cube of \( T \), and that is contradictory to the definition of \( B \)) So we have

\[
B \subseteq \bigcup_{i=1}^{6} C_i \quad (3.17)
\]

and that gives

\[
|B| \leq \left| \bigcup_{i=1}^{6} C_i \right| \leq \sum_{i=1}^{6} |C_i| = 6 |C| \quad (3.18)
\]

which completes the proof of Lemma 3.5.

Now according to Lemma 3.4 and Lemma 3.5, we have

\[
|B| < \pi \left( d + \sqrt{3} + \sqrt{6} \right)^2 \quad (3.19)
\]

Use (3.19) to eliminate \( |B| \) in (3.2), we have

\[
\frac{1}{6} \pi d^3 < 2n + \pi \left( d + \sqrt{3} + \sqrt{6} \right)^2 \quad (3.20)
\]

Expend and rearrange it, we have

\[
\frac{12}{\pi} n + 18 \left( 3 + 2\sqrt{2} \right) > d^3 - 6d^2 - 12 \left( \sqrt{3} + \sqrt{6} \right) d \quad (3.21)
\]

To make it simpler, we assume that

\[
d^3 - 6d^2 - 12 \left( \sqrt{3} + \sqrt{6} \right) d \geq d^3 + 3ad^2 + 3a^2 d \quad (3.22)
\]

Here, \( a \) is a parameter. Transform (3.22) into another equivalent inequality, and we have

\[
-(3a + 6) d \geq 3a^2 + 12 \left( \sqrt{3} + \sqrt{6} \right) \quad (3.23)
\]
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This inequality won’t hold for all cases. But since $3a^2 + 12(\sqrt{3} + \sqrt{6}) > 0$, $d > 0$, so for $d$ and $a$ satisfying the following conditions, inequality (3.22) holds.

\begin{align*}
  a &< -2 \quad (3.24) \\
  d &\geq \frac{3a^2 + 12(\sqrt{3} + \sqrt{6})}{3a + 6} \quad (3.25)
\end{align*}

According to (3.21) and (3.22), we have

\[ \frac{12}{\pi} n + 18 \left(3 + 2\sqrt{2}\right) + a^3 > (d + a)^3 \quad (3.26) \]

Hence

\[ d < \sqrt{\frac{12}{\pi} n + 18 \left(3 + 2\sqrt{2}\right) + a^3 - a} \quad (3.27) \]

For a simpler inequality, we let $a = -3\sqrt{\frac{3}{18} \left(3 + 2\sqrt{2}\right)} < -2$, and we have

\[ d < \sqrt{\frac{12}{\pi} \sqrt{n} + \sqrt{18 \left(3 + 2\sqrt{2}\right)}} \quad (3.28) \]

We know that the shortest distance between two Even Points is $\sqrt{2}$, so according to Theorem 2.1, we have

\[ \frac{d}{\sqrt{2}} \geq \frac{D(S)}{d(S)} \geq \lambda_{n,3} \geq \sqrt{\frac{18}{\pi}} \sqrt{n} - 1 \quad (3.29) \]

Therefore, for each $n$ satisfying

\[ \sqrt{\frac{18}{\pi}} \sqrt{n} - 1 \geq \frac{1}{\sqrt{2}} \frac{3a^2 + 12(\sqrt{3} + \sqrt{6})}{3a + 6} \quad (3.30) \]

\[ a = -\sqrt{\frac{18}{3 + 2\sqrt{2}}} \quad (3.31) \]

the inequality (3.28) holds. That is, $\forall n > 1024$, we have

\[ \lambda_{n,3} \leq \frac{D(S)}{d(S)} \leq \frac{d}{\sqrt{2}} < \sqrt{\frac{12}{\pi} + \sqrt{\frac{18 \left(3 + 2\sqrt{2}\right)}{\sqrt{2}}}} < \sqrt{\frac{18}{\pi}} \sqrt{n} + 4 \quad (3.32) \]

Thus we prove Theorem 3.1.
3.2 An Upper Bound for $n$ not greater than 1024

**Theorem 3.6.** Let $S \in \mathbb{R}^3$ and

$$\lambda_{n,3} = \inf \max_{A,B \in S, A \neq B} |AB| \min_{A,B \in S, A \neq B} |AB|$$

$\forall 2 \leq n \leq 1024$, we have

$$\lambda_{n,3} < \sqrt[3]{\frac{3\sqrt{18}}{\pi}} \sqrt[3]{n} + 4$$

**Proof.** For these cases, we design a program to simulate the structural method (see Section 3.1) to get the solutions for cases where $2 \leq n \leq 1024$ to see if the upper bound holds.

The algorithm goes like this:

1. Let the initial value of $R$ be zero. Here $R$ is the radius of the sphere.

2. Consider the point set $S$ as an empty set, and consider all the Even Points as unmarked.

3. Add the unmarked Even Points in the sphere into $S$ one by one. Each time renew $f_{|S|,3}$ ($f_{|S|,3} = \frac{\max_{A,B \in S, A \neq B} |AB|}{\min_{A,B \in S, A \neq B} |AB|}$) and mark the point.

4. If $|S| > 1024$, exit.

5. Use $R + r$ to renew $R$. Here $r$ is a small positive number.

6. Go to 3.

The figure on the right shows the flowchart of the simulating program.

![Flowchart of the simulating program](image)
CHAPTER 3. A NEW UPPER BOUND

Use this program we get some solutions and we find that for each \(2 \leq n \leq 1024\), \(\lambda_{n,3} < 3\sqrt{\frac{18}{\pi}} \sqrt[3]{n} + 4\) (see Appendix A).

Thus we prove \textbf{Theorem 3.6}.

\[\square\]

3.3 A New Result on Upper Bound

\textbf{Theorem 3.7}. Let \(S \in \mathbb{R}^3\) and

\[
\lambda_{n,3} = \inf \max_{A,B \in S, A \neq B} \frac{|AB|}{\min_{A,B \in S, A \neq B} |AB|}
\]

\(\forall n \geq 2\), we have

\[
\lambda_{n,3} < 3\sqrt{\frac{18}{\pi}} \sqrt[3]{n} + 4
\]

\textbf{Proof}. According to \textbf{Theorem 3.1}, we have \(\forall n > 1024\), \(\lambda_{n,3} < 3\sqrt{\frac{18}{\pi}} \sqrt[3]{n} + 4\).

According to \textbf{Theorem 3.6}, we have that for each \(n\) between 2 and 1024, \(\lambda_{n,3} < 3\sqrt{\frac{18}{\pi}} \sqrt[3]{n} + 4\).

Hence, we have \(\forall n \geq 2\), \(\lambda_{n,3} < 3\sqrt{\frac{18}{\pi}} \sqrt[3]{n} + 4\).

That completes the proof of \textbf{Theorem 3.7}.

\[\square\]
Chapter 4

The Limit of $\frac{\lambda_{n,3}}{3\sqrt[3]{n}}$

Zhu Yuyang in 1995 posed the following conjecture:

Use congruent $k$-dimensional balls to fill any convex figure in $\mathbb{R}^k$. And let $P_k$ be the supremum of the density. We have

$$\lim_{n \to \infty} \frac{\lambda_{n,k}}{\sqrt[3]{n}} = P_k^{-\frac{1}{k}}$$

When it comes to a three-dimensional space, the conjecture is

$$\lim_{n \to \infty} \frac{\lambda_{n,3}}{\sqrt[3]{n}} = \sqrt[3]{\frac{\sqrt{18}}{\pi}}$$

which is to be proved as follow.

**Theorem 4.1.** Let $S \in \mathbb{R}^3$ and

$$\lambda_{n,3} = \inf \frac{\max_{A,B \in S, A \neq B} |AB|}{\min_{A,B \in S, A \neq B} |AB|}$$

We have

$$\lim_{n \to \infty} \frac{\lambda_{n,3}}{\sqrt[3]{n}} = \sqrt[3]{\frac{\sqrt{18}}{\pi}}$$

**Proof.** According to **Theorem 2.1** and **Theorem 3.7**, we have

$$\sqrt[3]{\frac{\sqrt{18}}{\pi}} \sqrt[3]{n} - 1 \leq \lambda_{n,3} < \sqrt[3]{\frac{\sqrt{18}}{\pi}} \sqrt[3]{n} + 4 \quad (4.1)$$
CHAPTER 4. THE LIMIT OF $\frac{\lambda_{n,3}}{\sqrt[N]{N}}$

Divide (4.1) through by $\sqrt[3]{n}$. This gives

$$\sqrt[3]{\frac{\sqrt{18}}{\pi}} - \frac{1}{\sqrt[n]{n}} \leq \frac{\lambda_{n,3}}{\sqrt[n]{n}} < \sqrt[3]{\frac{\sqrt{18}}{\pi}} + \frac{4}{\sqrt[n]{n}}$$  (4.2)

Obviously

$$\lim_{n \to \infty} \sqrt[3]{\frac{\sqrt{18}}{\pi}} - \frac{1}{\sqrt[n]{n}} = \lim_{n \to \infty} \sqrt[3]{\frac{\sqrt{18}}{\pi}} + \frac{4}{\sqrt[n]{n}} = \sqrt[3]{\frac{\sqrt{18}}{\pi}}$$  (4.3)

According to the squeeze rule and (4.2), (4.3), we have

$$\lim_{n \to \infty} \frac{\lambda_{n,3}}{\sqrt[n]{n}} = \sqrt[3]{\frac{\sqrt{18}}{\pi}}$$

Thus we prove Theorem 4.1. \qed
Chapter 5

Near Optimal Solutions for some cases

For cases where $5 \leq n \leq 13$, we design a program using the Steepest Descent Approach to give some near optimal solutions.

Without losing generality, we assume that $d(S) = \min_{A,B \in S, A \neq B} |AB| = 1$. And we are to find the distribution of all points in $S$ which will minimize $D(S) = \max_{A,B \in S, A \neq B} |AB|$.

We define that $S = (A_1, A_2, \ldots, A_n)$ and $A_i = (x_i, y_i, z_i), (i = 1, 2, \ldots, n)$. Here $(x_i, y_i, z_i), (i = 1, 2, \ldots, n)$ are randomly valued. Let’s consider the vector

$$\vec{V} = (x_1, x_2, \cdots, x_n, y_1, y_2, \cdots, y_n, z_1, z_2, \cdots, z_n)$$

which describes how the points distribute in the space.

Each time we find another vector

$$\vec{u} = (\Delta x_1, \Delta x_2, \cdots, \Delta x_n, \Delta y_1, \Delta y_2, \cdots, \Delta y_n, \Delta z_1, \Delta z_2, \cdots, \Delta z_n)$$

which will make $\vec{V}' = \vec{V} + \vec{u}$ a more optimal vector. Here we say that a vector is more optimal if the distribution of points it describes has a smaller $D(S)$.

Because we assume that $d(S) = 1$, we have

$$|A_i A_j|^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \geq 1, (1 \leq i < j \leq n) \quad (5.1)$$
To emphasize this, we define a function

\[ F(S) = D(S) + \sum_{1 \leq i < j \leq n} M \cdot \max \left( 1 - \left| \overrightarrow{A_iA_j} \right|, 0 \right)^2 \]  

(5.2)

to see if the vector is optimal or not. Here \( M \) is a very large positive number. That means, if the distance of two points, for example \( A_i \) and \( A_j \), is smaller than 1, the value of \( F(S) \) can be very bad. So there’s no need to consider (5.1) any more.

And now it’s the matter of finding \( \vec{u} \).

According to the Steepest Descent Approach, we can use the gradient vector, \( \vec{z} \), to get \( \vec{u} \). That is

\[ \vec{z} = \left( \frac{\partial F}{\partial x_1}, \frac{\partial F}{\partial x_2}, \ldots, \frac{\partial F}{\partial x_n}, \frac{\partial F}{\partial y_1}, \frac{\partial F}{\partial y_2}, \ldots, \frac{\partial F}{\partial y_n}, \frac{\partial F}{\partial z_1}, \frac{\partial F}{\partial z_2}, \ldots, \frac{\partial F}{\partial z_n} \right) \]  

(5.3)

\[ \vec{u} = \lambda \vec{z} \]  

(5.4)

Here \( \lambda \) is parameter which can lead us to a locally optimal solution. We use the Newton Iteration Method to find it.

After we find \( \vec{u} \), we use \( \vec{V}' = \vec{V} + \vec{u} \) to renew \( \vec{V} \), and then we repeat these steps until \( \vec{V}' = \vec{V} \).

Here goes the algorithm of our program:

1. Give each point in \( S \) a random coordinate. And we have \( \vec{V} \) for current distribution.

2. Find the gradient vector \( \vec{z} \), of \( F(S) \).

3. Use the Newton Iteration Method to find a \( \lambda \) and then we get \( \vec{u} \).

4. If \( \|\vec{u}\| < \epsilon \) (\( \epsilon \) is a very small positive number), exit.

5. Use \( \vec{V}' = \vec{V} + \vec{u} \) to renew \( \vec{V} \).

6. Go to 2
CHAPTER 5. NEAR OPTIMAL SOLUTIONS FOR SOME CASES

Figure 5.1 shows the flowchart of the algorithm of the program.

If we repeat this program many times, we can get solutions which are very close to the optimal solutions.

We use this program to get solutions for the problem of both the two-dimensional version and the three-dimensional version and we all get solutions better than what we currently know. Since the problem of two-dimensional space has little relevance to this thesis, we only provide with the solutions of the three-dimensional version.

The figures in the following pages are our solutions which show the distribution of the points.

Here the blue segments indicate the shortest segments and the yellow segments indicate the longest ones. Other segments are not shown in the figures below.

The coordinates of the points are given in Appendix B.
CHAPTER 5. NEAR OPTIMAL SOLUTIONS FOR SOME CASES

\[ \lambda_{4,3} = 1.000000000 \]

\[ \lambda_{5,3} \leq 1.3093073414 \]

\[ \lambda_{6,3} \leq 1.4142135624 \]

\[ \lambda_{7,3} \leq 1.5144098705 \]

\[ \lambda_{8,3} \leq 1.5537739740 \]

\[ \lambda_{9,3} \leq 1.5952200746 \]
CHAPTER 5. NEAR OPTIMAL SOLUTIONS FOR SOME CASES

\[ \lambda_{10,3} \leq 1.7611433799 \]

\[ \lambda_{11,3} \leq 1.8396119135 \]

\[ \lambda_{12,3} \leq 1.9021130326 \]

\[ \lambda_{13,3} \leq 1.9869300892 \]
This research project would not have been possible without the support of many people.

We wish to express our gratitude to our supervisor, Mr. Ling Xiaofeng, who abundantly offered invaluable assistance, support and guidance. We also want to thank Dr. Zhou Tianxiang, for his helping us in using Matlab 7.0.

Special thanks also to our friends, especially Chen Keqin and Pan Yuchao, who gave us inspiration and true help during the programming phase, and also Zhou Yuchen, who patiently taught us everything he knew about closest packing and crystal structure.

We would also give our love to our families, for their understanding, encouragement and endless care without which we would not have had the courage to overcome the difficult times during our studies.
Appendix A

Solutions of Theorem 3.6

See the file named “Solutions for Theorem 3.6.CHM”. This file shows the solutions of Theorem 3.6.

For each data, the first line contains a single number \(n\), which is the number of points.

The second line contains one real number, \(F(S)\), which is produced by our program; while the third line contains one real number evaluated by

\[
g(n) = \sqrt[3]{\frac{18}{\pi}} \sqrt{n} + 4
\]

By comparing to these two numbers, we can see that the inequality

\[
\lambda_{n,3} < \sqrt[3]{\frac{18}{\pi}} \sqrt{n} + 4
\]

holds for each \(n\) between 2 and 1024.

There are three numbers in each of the following \(n\) lines, which describe the coordinate of a point.

The Results is a list containing all the results:

Here each line contains three numbers. The first one is \(n\); the second one is \(F(S)\) and the third one is \(g(n)\).
Appendix B

Coordinates of the points of
Chapter 5

Here are the coordinates of the points of Chapter 5.
Each line contains three numbers, $x$, $y$ and $z$, describing the coordinate of a point.

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APPENDIX B. COORDINATES OF THE POINTS OF CHAPTER 5

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73
## Appendix B. Coordinates of the Points of Chapter 5

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Bibliography


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