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Japan Advanced Institute of Science and Technology

Optimal Packings of 8, 9, and 10 Equal Circles in an Isosceles Right Triangle

By Tomohiro Harayama

A thesis submitted to School of Information Science, Japan Advanced Institute of Science and Technology, in partial fulfillment of the requirements for the degree of Master of Information Science Graduate Program in Information Science

> Written under the direction of Professor Tetsuo Asano

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Preface

"Computer science is no more about computer than astronomy is about telescope." Dijkstra.

Is computer science a science of man and computer, for man and computer, and by man and computer? If so, what kind of exploration is possible in this science? As is usually said, computer provides us with a chance to think over the large-scaled, huge-finite, or complicated problems. And it also can help us to investigate many mathematical problems which seem strange, unknown, or hardly conquered. For the latter cases, there are a lot of subjects in mathematics or computer science which sometimes can't be handled by the simple (abstract?) and comprehensive theories. But what shall we do in such a case? Can we really use computers as telescopes?

The subject of this thesis, computation of finite circle packings, is one of the open problems in combinatorial geometry [1], and has been intensively studied during the last three decades. Several interesting results were obtained by R. L. Graham and B. D. Lubachevsky [3, 4, 5], K. Schlüter [20], M. Goldberg [2], G. Wengerodt [22, 23, 24], M. Mollard et al. [11], C. de Groot et al. [6], R. Peikert [6], H. Melissen [10]. As is often said, the progresses of these problems are being made in alternations of good conjectures and their proofs; after guessing the configuration of circles and the lower bound of packing radius we try to prove or frequently disprove their optimality. In spite of these efforts, however, it still remains very difficult to find out something like structural properties, as we often expect, or packing radius r(n) over arbitrary n. For example, when we look at the case of the densest 19 circle packing in a square, there is surely no theory which can explain why it is slightly non-symmetric. Besides, as increases the number of circles, it becomes almost impossible to conjecture such good packings and prove their optimality by hand. Recently, an interesting computing scheme has been developed by C. de Groot et al., K. J. Nurmela and P. R. J. Ostegård etc., which is called *computer-aided proof method*. Though this idea in packing problems originates from the manual proof technique of 9 circles in a square by J. Schaer [18], we can see the similar principles in numerical analysis, too. The important feature of these principles is that after computing the approximate solutions, we try to guarantee their quality with respect to the optimal ones. In this thesis, I have further applied this computer-aided proof method to the case of isosceles right triangle and depicted the optimal packings up to n = 10.

During the study at JAIST, my thanks go to Prof. T. Asano, Dr. K. Obokata, and all members of our laboratory for several comments and advices on network, LEDA, etc. My special thanks go to Dr. Subhas C. Nandy who had stayed at our department as a visiting researcher for the last year. Actually I started these problems during our discussion over his wife, Hindu's curry and somen-spaghetti. I thank Dr. H. Melissen for sending us his fantastic Ph.D. thesis, and also thank Dr. K. J. Nurmela for giving us several comments and their paper on computer-aided proof method. Outside computer science, my deep thanks always go to my parents, Tatsuo and Mieko, who have been supporting me physically and mentally with their consistent love for years. My hope is always to make a telescope which enable us together to view the coming new era.

Abstract

The densest packings of equal circles in a square have been determined earlier for $n \leq 27$, 36 and several results have been proved with the aid of computer. In a case of isosceles right triangle, the range of the densest packings is known for $n \leq 7$ and has been conjectured for up to n = 16. As the fact that isosceles right triangle is a half of square usually doesn't help us in the computing schemes, we should think of them separately. In this thesis, the computer-aided proof method is further applied to the case of isosceles right triangle and the range of optimal packings is extended to n = 10.

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Chapter 1

Introduction

Densest Circles Packings

Densest circle packing problem is one of the interesting open questions in combinatorial geometry as well as other possible variations of packing. We try to place n equal circles inside a given convex region in \mathbb{R}^2 like square, triangle, circle etc., such that the radius is maximized without overlapping.

The packing problem is usually regarded as distributing n points uniformly in the region P in such a way that the minimum distance d_n among the points is maximized, which we call maximum point separation problem. Suppose we define the separation distance as

$$d_n \stackrel{def}{=} \max_{S \subset P, \ |S|=n} \min_{p,q \in S, \ p \neq q} \ d(p,q) \tag{1.1}$$

(d(,)) is Euclidean distance), then the densest packing problem corresponds to that of optimizing the separation distance.

For example, let P be a triangle whose inscribed circle has radius r_{in} and r_n be the packing radius of n circles in P. Because the inward parallel body $(1 - \frac{r_n}{r_{in}})P$ contains n center points of the packing, by easy calculation the configuration of centers has the maximum separation distance $d = 2r_n$ inside $(1 - \frac{r_n}{r_{in}})P$.

On the other hand, if we have the optimal configuration of n points S inside P with separation distance d_n , then S consists of the center points of a packing in the outward body $(1 + \frac{d_n}{2r_{in}})P$ whose radius is $r = \frac{d_n}{2}$. Therefore we obtain the relation between r_n and d_n in P s.t.

$$d_n = \frac{2r_{in}r_n}{r_{in} - r_n},\tag{1.2}$$

$$r_n = \frac{r_{in}d_n}{2r_{in} + d_n}.\tag{1.3}$$

A configuration of n points with the maximum separation distance is called an *optimal* point configuration.

As one of the features of this finite circle packing it is often said "progress in proving lags that of conjecturings" [4]. That is, we need good packings in advance to compute the optimal packings.

Currently, the optimal packings in a unit square are known for $n \leq 9$ in [2, 13], n = 14, 16, 25, 36 in [7, 22, 23, 24]. The optimal packings for $10 \leq n \leq 20$ had been

obtained by C. de Groot et al. in [6] by using the computer searching and recently $21 \le n \le 27$ were presented by K. J. Nurmela et al. in [13, 15]. Other best packings in a square are known for up to 50 in [14], and $n \le 50$, n = 51, 52, 54, 56, 60, 61 including partial improvements of the conjectures in [14].

On the other hand, in a case of isosceles right triangle, the optimal packings were previously determined for $n \leq 7$ in [25] and the best packings are up to 16 in [10].

Method

Though this problem is very difficult in spite of the intensive efforts during decades, the current development of computer could facilitate to raise up the number of circles optimally packed in a region like a unit square, triangle or circle, and the progress is still going on.

As the examples of intensive use of computer to conjecture the good packings, there have been published about the densest packings of up to 50 circles in a square by nonlinear optimization technique about the separation distance in [14] or about a particular pattern of the number of circles in a square along certain values of n by computer simulations called *billiards* algorithm [4].

Usually after the best packings are conjectured by optimization of separation distance or simulations by billiards algorithms, we have to do two things. One is to show the existence of such packings. Just conjecturing the packings doesn't mean that such packings really exist. And the other thing is to prove their optimality.

With respect to these roles of computer use in packings, the method called *computer-aided proof* is one of the powerful candidates to make an exciting progress in this problem. In a series of papers in a case of square like $10 \le n \le 20$ in [6] by C. de Groot et al. and $21 \le n \le 27$ in [13, 15] by K. J. Nurmela et al., computer-aided proof could play an important role in order to verify whether the best known packings really exist and are optimal or not.

One of the common techniques in computing the optimal packings is that we try to restrict the possible area in the bounding region only in which each of n points can reside without violating the conjectures. That is, when we are maximizing the separation distance, the conjectured distance is regarded as the lower bound of the optimal distance. So we can eliminate such areas in the region as will violate the lower bound if the points of optimal configuration are placed in. Computer-aided proof can simulate this reducing procedure to narrow the possible areas in the region, and can prove both the existence and optimality of the conjectured packings.

In Chapter 2, we give the general steps of computer-aided proof method one by one and then in Chapter 3, we will show the results from our computer experiments by these methods for an isosceles right triangle and depict up to 10 optimal packings. The packing for n = 8, 9, and 10 were newly proved their optimality.

Chapter 2

Computer-Aided Proof Method

In chapter 2 we consider the maximum point separation problem for $n \ge 2$ points in an isosceles right triangle. The computing schemes described later use a good *lower* bound d_{low} of the separation distance d_n s.t.

$$d_n = \max_{S \subset P, |S|=n} \min_{p,q \in S, p \neq q} d(p,q)$$

obtained numerically in the best known packings [14]. Computer runs in our experiment showed that the sharper d_{low} could eliminate after the initial step the more combinations which never had the optimal configurations. So it is very preferable to get a sharp lower bound when we conjecture it as far as the appropriate error estimate of floating point representation of real number is taken into consideration.

In the following sections, we describe each general step of computer-aided proof method in detail. Though we have restricted the domain P to the isosceles right triangle, these schemes are possibly applicable to other simple geometrical domains like circle, equilateral triangle, etc. The experimental results for actual n by computer runs are in chapter 3.

2.1 Initial Combinations

Even if we know a quite good packing and its separation distance, we don't have any geometrical information like neighboring relationships among circles in the optimal solutions, or any numerical guarantee of its quality as an approximate solution. Computer-aided proof method begins with searching exhaustively for all the possible distributions of points in the domain.

2.1.1 Tilings

For $t, n \in \mathbb{N}$, $2 \leq n \leq t$, let P be an isosceles right triangle whose isosceles edges have unit length. Then we make a *tiling* $\mathcal{T} = \{T_0, T_1, \ldots, T_{t-1}\}$ of P with axis-parallel congruent squares and isosceles right triangles, which covers a whole of P (see Figure 2.1).

In order that each tile T_i $(0 \le i \le t-1)$ should contain at most one point of the optimal configurations for given n, P is tiled in such a way that an inequality

$$diameter(T_i) < d_{low} \tag{2.1}$$

is satisfied. Table 2.1 shows the diameter of T_i in each case. We have applied the same number of rows as that of columns in tiling which facilitated the implementation of computer programs.



Figure 2.1: Tilings of isosceles right triangle.

Tiling	Diameter	Number of tiles	Possible number of circles
(3,3)	$\sqrt{2}/3 \approx 0.471404521$	6	$2\sim 6$
(4,4)	$\sqrt{2}/4 \approx 0.353553391$	10	~ 8
(5,5)	$\sqrt{2}/5 \approx 0.282842712\ldots$	15	~ 12

Table 2.1: Diameter of tiles.

2.1.2 Choice of n Tiles

As each tile of \mathcal{T} has at most one point of the optimal point configurations by (2.1), we next choose all the possible *n*-tiles $\mathcal{P} = \{P_1, P_2, \ldots, P_n\}$ from \mathcal{T} . There are $\binom{t}{n}$ ways to select *n* tiles, but we can reduce such combinations by taking symmetries into account.

The permutation group G (a subgroup of t-symmetry group S_t) which consists of all the *automorphisms* on \mathcal{T} , is generated by a mirror reflection for isosceles right triangle. (If P is a square and its tiling is made of axis-parallel congruent squares and rectangles, both 90° or 180° rotation and a mirror reflection become the generators of G [13].)

Suppose τ is the mirror reflection on \mathcal{T} , a simple backtracking algorithm with *Schreiner-Sims representation* $\overrightarrow{G} = [G_0, G_1, \ldots, G_{t-1}]$ of G generates each element uniquely from its set product $G_0 \times G_1 \times \cdots \times G_{t-1}$ [8].

For example in (4,4)-tiling of Figure 2.1, the cyclic representation of τ is

$$(0)(1,4)(2,7)(3,9)(5)(6,8), (2.2)$$

so τ generates G with the Shreiner-Sims representation $\overrightarrow{G} = [G_0, G_1, \dots, G_{t-1}]$, where

$$\begin{aligned}
G_0 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_1 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9), (0)(1, 4)(2, 7)(3, 9)(5)(6, 8))\}, \\
G_2 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_3 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_4 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_5 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_6 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_7 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_8 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}, \\
G_9 &= \{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9)\}.
\end{aligned}$$
(2.3)

Thus the permutation group acting on $\mathcal{T} = \{0, 1, \dots, 9\}$ is

$$\{(0)(1)(2)(3)(4)(5)(6)(7)(8)(9), (0)(1,4)(2,7)(3,9)(5)(6,8)\}.$$
(2.4)

In the family of all *n*-tiles from \mathcal{T} , the number of *orbits* by *G*'s action is determined by *Burnside's lemma*. Assume that N_n is the number of orbits, then *the initial combinations* in this step consist of all the *n*-tile *representatives* from these orbits under the action.

Proposition 1 (Burnside's Lemma) For $n, t \in \mathbb{Z}, t \geq 1, 0 \leq n \leq t$, and $\mathcal{T} = \{0, 1, \ldots, t-1\}$, let G be a permutation group acting on \mathcal{T} , and N_n be the number of orbits in the family of n-subsets in \mathcal{T} , then

$$N_n = \frac{1}{|G|} \sum_{g \in G} \mathcal{X}_n(g) \tag{2.5}$$

where $\mathcal{X}_n(g) = \# \{ \mathcal{P} \subset \mathcal{T} | g(\mathcal{P}) = \mathcal{P}, |\mathcal{P}| = n \}$ for $g \in G$.

In (4,4)-tiling, the number of 8-tiles N_8 in \mathcal{T} is 25, so the initial combinations are

 $\{1, 2, 3, 5, 6, 7, 8, 9\}, \{1, 2, 3, 4, 6, 7, 8, 9\}, \{1, 2, 3, 4, 5, 6, 8, 9\}, \{1, 2, 3, 4, 5, 6, 7, 9\}, \\ \{1, 2, 3, 4, 5, 6, 7, 8\}, \{0, 2, 3, 5, 6, 7, 8, 9\}, \{0, 1, 3, 5, 6, 7, 8, 9\}, \{0, 1, 3, 4, 5, 6, 8, 9\}, \\ \{0, 1, 2, 5, 6, 7, 8, 9\}, \{0, 1, 2, 4, 5, 6, 8, 9\}, \{0, 1, 2, 4, 5, 6, 7, 8\}, \{0, 1, 2, 3, 6, 7, 8, 9\}, \\ \{0, 1, 2, 3, 5, 7, 8, 9\}, \{0, 1, 2, 3, 5, 6, 8, 9\}, \{0, 1, 2, 3, 5, 6, 7, 9\}, \{0, 1, 2, 3, 5, 6, 7, 8\}, \\ \{0, 1, 2, 3, 4, 6, 8, 9\}, \{0, 1, 2, 3, 4, 6, 7, 9\}, \{0, 1, 2, 3, 4, 6, 7, 8\}, \{0, 1, 2, 3, 4, 5, 8, 9\}, \\ \{0, 1, 2, 3, 4, 5, 7, 9\}, \{0, 1, 2, 3, 4, 6, 7, 9\}, \{0, 1, 2, 3, 4, 5, 6, 9\}, \{0, 1, 2, 3, 4, 5, 6, 8\}, \\ \{0, 1, 2, 3, 4, 5, 7, 9\}, \{0, 1, 2, 3, 4, 5, 7, 8\}, \{0, 1, 2, 3, 4, 5, 6, 9\}, \{0, 1, 2, 3, 4, 5, 6, 8\}, \\ \{0, 1, 2, 3, 4, 5, 6, 7\}.$

The corresponding tilings are in Figure 2.2.

As is mentioned in [15], an easy unranking function constructs the corresponding combination (subset or binary string) immediately when a rank of it is given. We also stored them by rank, where the sample program C.A.G.E.S. [8] generated the minimum lexicographically ordered (i.e., minimum ranked) representatives from the orbits.



Figure 2.2: 25 initial combinations for 8-tile.

2.2 Polygon Reducing

This step decreases the number of initial combinations by the lower bound of the separation distance.

Let us fix a *n*-tile $\mathcal{P} = \{P_1, P_2, \ldots, P_n\}$ selected in the previous step. In the beginning a tile P_i $(1 \leq i \leq n)$ of \mathcal{P} is called a *full tile* (or *full region*), and after several rounds of the procedure, a reduced non-empty region from P_i , if exists, is called an *active region*. If the whole area in P_i disappears while reducing, such a combination of *n*-tile is found invalid for the optimal point configurations. Therefore the tiling is removed. The *polygon reducing* is repeatedly operated for each pair of tiles to narrow the active area in the region.

2.2.1 Reducing between Two Tiles

Let d be d_{low} , S denote the optimal point configuration for given n, and initially consider two tiles, A and B of \mathcal{P} . As we have tiled P with squares and isosceles right triangles in such a way that whose diameter is less than d, both A and B may possibly include one point of S. If a point in A is not far away from all points in B by the distance d, then this point is not a member of S. So the area A';

$$A' \stackrel{def}{=} \{a \in A \mid d(a,b) \le d, b \in B\}$$

$$(2.7)$$

$$= \bigcap_{b \in B} \mathbf{B}(b\,;d) \cap A,\tag{2.8}$$

where $\mathbf{B}(b; d)$ is a circular disc with center b and radius d, can be eliminated from A and it is possible to reduce A into the rest active area $A'' = A \setminus A'$.

Let ext(A), ext(B) be a set of (extreme) vertices of A and B respectively. Because of the convexity of A and B (initially square or isosceles right triangle), an easy calculation shows that a point in A at a distance less than d from all points in B is also at a distance less than d from all vertices of B. Thus the area to be eliminated is also regarded as

$$A' = \{ a \in A \mid d(a,b) \le d, \ b \in ext(B) \}$$
(2.9)

$$= \bigcap_{b \in ext(B)} \mathbf{B}(b;d) \cap A, \tag{2.10}$$

which means that it is only enough to round all the vertices of B to obtain it.

When repeating these reductions, as we always keep the convexity of both two active regions, a whole part of A' should not be eliminated from A (If so, A'' becomes non-convex). Consider a circle $\mathbf{C}(b;d) = \partial \mathbf{B}(b;d)$. Then we determine the rest area A_{rest} as a convex hull among all of the vertices of A which are outside $\mathbf{C}(b;d)$ for some vertex of B, and of the intersections between the edges of A and $\mathbf{C}(b;d)$ for the vertices of B, which is constructed by rounding them one by one, i.e., A_{rest} is defined as a convex hull of

$$\{ a \in ext(A) | a \notin \mathbf{B}(b ; d), \exists b \in ext(B) \}$$

$$\bigcup$$

$$\{ x \in edge(A) | x \in edge(A) \cap \mathbf{C}(b ; d), b \in ext(B) \}$$

$$(2.11)$$

where edge(A) is a set of edges of A. If the *eliminated area* A_{elim} is

$$A \setminus A_{rest},\tag{2.12}$$

then arbitrary point $a \in A_{elim}$ is apparently located in A' of (2.10).

One thing that should be remarked is that by taking a convex hull for the rest area about (2.11), we can avoid the particular cases like very *thin* active regions where the connectivity is occasionally broken. For example in Figure 2.3, because the vertices, $\mathbf{a_1}$, $\mathbf{a_2}$ and intersections, $\mathbf{x_1}$, $\mathbf{x_2}$, $\mathbf{x_3}$, $\mathbf{x_4}$ are added as the points of the rest area, the connectivity of $\mathbf{A_{rest}}$ is always kept as well as its convexity.

Figure 2.3: Thin active region.

2.2.2 Error Estimate

As is carefully discussed the rest and eliminated area in an active region, it is important to notice that we *never* eliminate points or area which should not be eliminated. In the implementation of these schemes, it is necessary to make an appropriate estimate on errors caused by real arithmetic system of computers like floating point representation. There are two kinds of operations of real numbers which are affected by the system.

- 1. Comparison between a distance d(a, b) and d_{low} .
- 2. Calculation of intersections between a circle $\mathbf{C}(b; d_{low})$ and an edge of A.

For case 1, IEEE double-precision floating point representation has the precision $\epsilon = 2^{-52} \approx 1.1 \times 10^{-16}$. Let *E* be 10^{-15} (larger than actual ϵ), and e_0 and e_1 be error upper bounds about d_n and d_{low} , then in our implementation we assumed an inequality

$$E < e_1 < d_n - d_{low} < e_0. (2.13)$$

Because the guessed value of d_n is from the best known packings and d_{low} should be a pretty good lower bound, if we set e_1 for 10^{-9} and such d_n for a given range of n have no consecutive decimal zeros in 8th and 9th digits below point, the middle inequality in (2.13) is attained by using a truncated value into exactly 7 digits below point for d_{low} . Therefore we can set e_0 for 10^{-7} .

For case 2, let x_{low} be an intersection between $\mathbf{C}(b; d_{low})$ and an edge of A, and $x_{low}^{(1)}$ be the approximate point of x_{low} calculated here. If an error upper bound e_2 is estimated as 10^{-13} , i.e.,

$$d(x_{low}, x_{low}^{(1)}) < e_2,$$
 (2.14)

then

$$E < e_2 < e_1$$
 (2.15)

is achieved. From (2.13) to (2.15), we obtain

$$E < e_2 < e_1 < d_n - d_{low} < e_0. (2.16)$$

2.2.3 Adjustment of Intersections

For technical reasons by case 2, the following adjustment about x_{low} is required. Let $\mathbf{x_1}$ be an intersection between edge $\mathbf{a_1a_2}$ of \mathbf{A} and $\mathbf{C}(b; d_n)$ for some vertex b of B, and $\mathbf{x_{1,low}}$ be an intersection between $\mathbf{a_1a_2}$ and $\mathbf{C}(b; d_{low})$ (similarly for $\mathbf{x_k}$ and $\mathbf{x_{k,low}}$ in Figures 2.4, 2.5 and 2.6). If $\mathbf{x_{1,low}}$ happens to be calculated inside \mathbf{A} , like $\mathbf{x_{1,low}^{(1)}}$, the points in the neighborhood of $\mathbf{x_1}$ which must not be eliminated might be left outside the convex hull determined by $\{\ldots, \mathbf{a_1}, \mathbf{x_{1,low}^{(1)}}, \mathbf{x_{k,low}^{(1)}}, \mathbf{a_k}, \ldots\}$.

Figure 2.4: Error of intersection.

So with the adjustment length e_{ad} , we recalculate the adjusted point $\mathbf{x}_{1,low}^{(2)}$ for $\mathbf{x}_{1,low}^{(1)}$ s.t.

$$\mathbf{x}_{1,\mathbf{low}}^{(2)} = e_{ad} \,\overrightarrow{\mathbf{n}} + \mathbf{x}_{1,\mathbf{low}}^{(1)},\tag{2.17}$$

where $\overrightarrow{\mathbf{n}}$ is the outer normal vector of $\mathbf{a_1}\mathbf{a_2}$, in order to make the convex hull of $\{\ldots, \mathbf{a_1}, \mathbf{x_{1,low}^{(2)}}, \mathbf{x_{k,low}^{(2)}}, \ldots\}$ include all the near points around $\mathbf{x_1}$. By setting e_{ad} for 10^{-10} in our programs, such a case as the adjusted point crosses over

By setting e_{ad} for 10^{-10} in our programs, such a case as the adjusted point crosses over the half line $\mathbf{x_1}\mathbf{X}$, which again causes the same situation about the neighborhood of $\mathbf{x_1}$ is avoided by the easy observation. Let us call the area $\angle \mathbf{X}\mathbf{x_1}\mathbf{a_2}$ a *permissible area* in Figure 2.6, then we get the following fact.

Proposition 2 If $e_{ad} = 10^{-10}$, then the adjusted point $x_{1,low}^{(2)}$ (2.17) for $x_{1,low}^{(1)}$ is always inside the permissible area.

Proof. By (2.16), we get

$$d(x_{1,low}^{(2)}, b) \leq d(x_{1,low}^{(2)}, x_{1,low}) + d(x_{1,low}, b)$$

$$\leq e_2 + e_{ad} + d_{low}$$

$$= 10^{-13} + 10^{-10} + d_{low}$$

$$< 10^{-9} + d_{low}$$

$$= e_1 + d_{low}$$

$$< d_n.$$

Figure 2.5: Adjustment of intersection.

Figure 2.6: Adjusted point may cross over half line $\mathbf{x_1}\mathbf{X}$.

Figure 2.7 shows the sequential pictures in reducing for 8-tile. After these processes, we call the sets of n active regions *rest combinations*. In general it doesn't always occur that only such combinations as include (an) optimal configuration(s), say *optimal combinations*, survive after these polygon reducings.

Figure 2.7: Polygon reducing of 8-tile.

2.3 **Proof of Optimality and Uniqueness**

About circle packing problems, the terminology "computer-aided proof method" derives from this final step. We have already n active regions after the previous step only in which (an) optimal configuration(s) of n points can be placed. As we will see in Chapter 3 these active regions are usually small, but some *loose* points can move freely in relatively larger areas.

2.3.1 Guessing the Adjacency among *n* Points

After n active regions remain by polygon reducing, it is certain that if it is an optimal combination, each region has exactly one point of the optimal configuration(s). But we have to guess which pairs of points are really achieving the separation distance, which leads to simultaneous equations.

There are several criteria for guessing the adjacency among points. In [14], after the nonlinear optimization as a max-min problem of separation distance, all the distances between two points are stored in an increasing order. Then we try to locate the first sudden increase bigger than a given threshold value in the sequence. Similarly the relationships between points and the boundary are found by giving another threshold value. In any way of guessing, we should confirm two facts. One is whether the true *n*-point solved from the simultaneous equations is surely located in the *n*-active region because the guessed relation must be from its original initial combination. And the other is whether or not the packing with guessed relationship (i.e., simultaneous equations) really exists. Actually second question is never trivial, but interestingly the following discussion verifies whether such a guessing is correct or not, even if these simultaneous equations cannot be solved algebraically in practice (if solved, we know the packing surely exists).

2.3.2 Local Optimality and Uniqueness

Let P be the isosceles right triangle, S_{eq} be one of the guessed relationships and assume that the coordinates of n points $\{p_1, p_2, \ldots, p_n\}$ from S_{eq} are surely included in the rest active regions $\mathcal{P} = \{P_1, P_2, \ldots, P_n\}$. We also assume a point set $\{p'_1, p'_2, \ldots, p'_n\}$ is an approximation of the true solution s.t. for a certain error upper bound e_{eq} ,

$$d(p_i, p'_i) \le e_{eq} \quad (1 \le i \le n).$$
 (2.18)

(i.e., S_{eq} is solved at least numerically with satisfying this bound.)

Next, we define the congruent error squares $\mathcal{R} = \{R_1, R_2, \dots, R_n\}$ with side r > 0 s.t.

$$R_i \supset P_i, \ R_i \text{ is fit into } P \text{ with center } p_i \ (1 \le i \le n),$$
 (2.19)

and similarly we draw the approximate error squares $\mathcal{R} = \{R'_1, R'_2, \dots, R'_n\}$ with side r > 0 s.t.

$$R'_i \supset P_i, \ R'_i \text{ is fit into } P \text{ with center } p'_i \ (1 \le i \le n).$$
 (2.20)

It should be noted that we may construct only the approximate error squares \mathcal{R}' but always confirm the conditions (2.18) and (2.19). (It is important to *confirm* (2.19). This

can be done by drawing the approximate error squares with side $r + 2e_{eq}$.)

Remember that we have inequality (2.16). If we define a value d_{low2} in such a way that

$$d_{low2} \stackrel{def}{=} d_{low} + 2e_{eq} + e_2 < d_n, \qquad (2.21)$$

and can show the existence of decreasing sequences of error square from $\mathcal{R} = \{R_1, R_2, \ldots, R_n\}$ where each R_i converges into its center p_i by a constant factor, then this means that such a guessed S_{eq} has the optimal solution $\{p_1, p_2, \ldots, p_n\}$ uniquely with respect to the error squares.

Theorem 1 Fix the rest active regions $\mathcal{P} = \{P_1, P_2, \ldots, P_n\}$ after polygon reducing procedure, and assume that error squares $\mathcal{R} = \{R_1, R_2, \ldots, R_n\}$ and its approximate error squares $\mathcal{R}' = \{R'_1, R'_2, \ldots, R'_n\}$ with constant length of side r > 0 under the conditions (2.18) and (2.19). Let d_{low2} be another reducing distance in (2.21). If there exists a polygon reducing about \mathcal{R}' with d_{low} and a constant q s.t. 0 < q < 1 where each $R'_i \in$ \mathcal{R}' $(1 \leq i \leq n)$ is reduced into an active approximate error region which is inside the smaller approximate error square qR'_i by q, then the guessed packing is optimally and uniquely determined about the error squares.

Proof. We try to verify that there are *n* decreasing sequences of error square $R_i \to qR_i \to q^2R_i \cdots$.

Let D' be a polygon reducing procedure about $\mathcal{R}' = \{R'_1, R'_2, \ldots, R'_n\}$ in the assumption which proceeds a finite number of rounds between approximate error squares, and D_k be a polygon reducing from $q^{k-1}\mathcal{R} = \{q^{k-1}R_1, q^{k-1}R_2, \ldots, q^{k-1}R_n\}$ to $q^k\mathcal{R} = \{q^kR_1, q^kR_2, \ldots, q^kR_n\}$ s.t. $q^kR_i = D_k(q^{k-1}R_i)$ $(1 \le i \le n)$.

Existence of D_1 : If a point x'_i in R'_i is far from at a distance less d_{low} for arbitrary point x'_i in R'_i , i.e.,

$$d(x'_i, x'_j) \leq d_{low}$$
 for all $x'_j \in R'_j$ $(1 \leq i \leq n)$.

If the homothetic point of x'_i (resp. x'_j) in R_i is denoted as x_i (resp. x_j), then from (2.18) and (2.21)

$$d(x_i, x_j) \leq d(x_i, x_i') + d(x_i', x_j') + d(x_j', x_j)$$

$$\leq 2e_{eq} + d_{low}$$

$$< 2e_{eq} + d_{low} + e_2$$

$$= d_{low2}$$

$$< d_n$$

is obtained (see Figure 2.8 (left)). The corresponding point x_j of x'_j runs arbitrarily in R_j , so the point x_i is far from all points in R_j at a distance less than d_{low2} (so, less than d_n). This means that there exists a polygon reducing D_1 about \mathcal{R} by the same number of rounds as D' s.t.

$$D_1(\mathcal{R}) = \{ D_1(R_1), D_1(R_2), \dots, D_1(R_n) \}$$

= $\{ qR_1, qR_2, \dots, qR_n \}$
= $q\mathcal{R}.$

Existence of general D_k : Consider $q^{k-1}R_i$ and $q^{k-1}R_j$ after k-1 th step. We assume that there exists a polygon reducing D_k in k th step s.t.

$$q^k R_i = D_k(q^{k-1}R_i),$$

$$q^k R_j = D_k(q^{k-1}R_j),$$

and also that a point $y_i \in q^{k-1}R_i$ is far away from $y_j \in q^{k-1}R_j$ at a distance less than d_n . Let z_i be $p_i + q(y_i - p_i)$ and z_j be $p_j + q(y_j - p_j)$ then

$$d(z_i, z_j) < d_n \tag{2.22}$$

is obtained because of the convexity of the quadrilateral $p_i p_j y_j y_i$ and the fact $d(p_i, p_j) = d_n$. y_j is an arbitrary point in $q^{k-1}R_j$, so z_j runs arbitrarily in $q^k R_j$. Let w_i be $p_i + q(z_i - p_i)$ and w_j be $p_j + q(z_j - p_j)$. Then

$$d(w_i, w_j) < d_n$$

is again obtained because of the convexity of the quadrilateral $p_i p_j z_j z_i$, (2.22) and $d(p_i, p_j) = d_n$. This means that $w_i \in q^k R_i$ is far away from arbitrary points in $q^k R_j$ at a distance less than d_n . So a polygon reducing occurs between w_i and w_j , too, which means the existence of D_{k+1} (see Figure 2.8 (right)).

Remark

Theorem 1 deduces the local optimality and uniqueness of the guessed packing from the corresponding initial combination. Therefore global evaluation should be done by considering all the initial combinations. Furthermore, the rest active regions with relatively large area are treated separately because such regions in the guessed adjacency among points might not interact with others by the separation distance.

Figure 2.8: Reducing an approximate error square into a polygon (left). Induction process of an error square (right).

Chapter 3

Packings in an Isosceles Right Triangle

In this chapter, we describe the experimental results of packings by the computer-aided proof method. Most of our experiments were done by using LEDA (Library of Efficient Data types and Algorithms) implemented by a C++ class library. The optimal packings of up to 10 circles in an isosceles right triangle are depicted with their initial, rest and optimal combinations, reducing processes, and proofs by (approximate) error squares. The packings from 8 to 10 were newly proved their optimality.

3.1 n = 5, 6 and 7

From n = 1 to 4, the proofs of optimality are elementary. Figures 3.1, 3.2 and 3.3 show the sequential pictures in polygon reducings for n = 5, 6 and 7. There is one point which moves relatively freely in the rest error region around the acute corner for n = 5, and two points for n = 7. n = 5, 6 and 7 are obtained respectively from the optimal combinations

$$\{0, 1, 2, 4, 5\}, \{0, 1, 2, 3, 4, 5\}, \{0, 1, 3, 4, 6, 8, 9\}.$$
 (3.1)

Figure 3.1: Polygon reducing for 5-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figure 3.2: Polygon reducing for 6-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figure 3.3: Polygon reducing for 7-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figures 3.4, 3.5 and 3.6 show the proofs of local optimality and uniqueness from their corresponding rest combinations. The rest regions after polygon reducings in which loose

points can reside may not interact with other regions, but the simultaneous equations determined the unique separation distance in this proof. The loose points can be moved to the acute corners without decreasing the separation distance in n = 5 and 7. We used the side of approximate error square r = 0.05 in order to draw the figures, but careful treatments are definitely required about the size. The detail is referred in Conclusion.

Figure 3.4: Proof for n = 5 by (approximate) error squares.

Figure 3.5: Proof for n = 6 by (approximate) error squares.

Figure 3.6: Proof for n = 7 by (approximate) error squares.

Figure 3.7 shows the optimal point configurations with separation distances,

$$d_5 = 4 - 2\sqrt{3} \approx 0.535898384862246\dots, \qquad (3.2)$$

$$d_6 = 1/2 = 0.5, \tag{3.3}$$

$$d_7 = (\sqrt{44\sqrt{2} + 50} - 2 - 4\sqrt{2})/7 \approx 0.419542091095306\dots$$
 (3.4)

The edges drawn between points are attaining the separation distance.

Figure 3.7: Optimal configuration for n = 5, 6 and 7.

3.2 n = 8

There are two optimal packings, 8a and 8b (see Figure 3.12). Both are the same as the previously conjectured packings. For n = 8a there are two loose point around the acute corners in Figure 3.8. n = 8a is from the optimal combination

$$\{0, 2, 3, 5, 6, 7, 8, 9\}$$
(3.5)

and n = 8b in Figure 3.9 is from

$$\{0, 1, 3, 4, 5, 6, 8, 9\}.$$
(3.6)

Figure 3.8: Polygon reducing for 8a-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figure 3.9: Polygon reducing for 8b-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

In n = 8a the simultaneous equations were solved symbolically, so we have set e_{eq} for $E = 10^{-15}$. Two points on the isosceles edges were fixed by the neighboring points even if reducing between loose points and them hadn't occurred. The separation distance is obtained as

$$d_8 = 2\sqrt{2} - \sqrt{6} \approx 0.378937381963012\dots$$
(3.7)

Figure 3.10 and 3.11 show the proofs for n = 8a and 8b.

Figure 3.10: Proof for n = 8a by (approximate) error squares.

Figure 3.11: Proof for n = 8b by (approximate) error squares.

Figure 3.12: Optimal configuration for n = 8a (left) and 8b (right).

3.3 n = 9

There is one optimal packing the same as previously conjectured (see Figure 3.15) and the optimal combination in Figure 3.13 is

$$\{0, 2, 4, 6, 8, 9, 11, 13, 14\}.$$
(3.8)

The separation distance is

$$d_9 = \sqrt{2}/4 \approx 0.353553390593274\dots$$
(3.9)

Figure 3.14 shows the proof in this case.

Figure 3.13: Polygon reducing for 9-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figure 3.14: Proof for n = 9 by (approximate) error squares.

Figure 3.15: Optimal configuration for n = 9.

3.4 n = 10

There is one optimal packing the same as previously conjectured (see Figure 3.18) which is the half of n = 16 in a square, and the optimal combination in Figure 3.16 is

$$\{0, 1, 3, 4, 5, 6, 8, 12, 13, 14\}.$$
(3.10)

The separation distance is

$$d_{10} = 1/3 \approx 0.3333333333333333 \dots$$
(3.11)

Figure 3.17 shows the proof in this case.

Figure 3.16: Polygon reducing for 10-tile. (The vertices randomly selected from each rest error region are emphasized in the rightmost figure.)

Figure 3.17: Proof for n = 10 by (approximate) error squares.

Figure 3.18: Optimal configuration for n = 10.

3.5 Results

In our implementations, we have applied $E = 10^{-15}$, $e_0 = 10^{-7}$, $e_1 = 10^{-9}$, $e_2 = 10^{-13}$, $e_{ad} = 10^{-10}$ and $e_{eq} = E = 10^{-15}$. As $e_0 = 10^{-7}$ we used the truncated value of separation distance for d_{low} . Table 3.1 shows the initial, rest and optimal combinations in polygon reducings. The initial combinations are described as the number of orbits, and rest and optimal combinations as *n*-tile which happened to coincide in this range of *n*. Table 3.2 is the maximum separation distance for $2 \le n \le 10$. Finally we see the optimal packings of up to 10 circles in Figure 3.19.

n	Tiling	d_{low}	N_n	Rest and optimal combinations
5	(3,3)	0.5358983	4	$\{0,1,2,4,5\}$
6	(3,3)	0.5	1	$\{0,1,2,3,4,5\}$
7	(4, 4)	0.4195420	64	$\{0,1,3,4,6,8,9\}$
8	(4, 4)	0.3789373	25	$\{0,2,3,5,6,7,8,9\}$ for 8a
				$\{0,1,3,4,5,6,8,9\}$ for 8b
9	(5,5)	0.3535533	2535	$\{0,2,4,6,8,9,11,13,14\}$
10	(5,5)	0.33333333	1527	$\{0, 1, 3, 4, 5, 6, 8, 12, 13, 14\}$

Table 3.1: Experimental results.

\overline{n}	d_n	
$\frac{n}{2}$	$\frac{\omega_n}{\sqrt{2}}$	$\approx 1.414213562373095\ldots$
3	1	= 1.0
4	$\sqrt{2}/2$	$\approx 0.707106781186547$
5	$4 - 2\sqrt{3}$	$\approx 0.535898384862246\dots$
6	1/2	= 0.5
7	$(\sqrt{44\sqrt{2}+50}-2-4\sqrt{2})/7$	$\approx 0.419542091095306$
8	$2\sqrt{2} - \sqrt{6}$	$\approx 0.378937381963012$
9	$\sqrt{2}/4$	$\approx 0.353553390593274\dots$
10	1/3	$\approx 0.333333333333333333$

Table 3.2: Maximum separation distance.

Figure 3.19: Optimal packings of up to 10 circles.

Chapter 4

Conclusion

In this thesis, we have applied the computer-aided proof method and newly proved the optimal packings for n = 8, 9 and 10.

Our computer programs mainly implemented by LEDA were found correct for these solutions. At first we implemented the schemes by using the known data for $6 \le n \le 27$ circles in a square developed by Nurmela and Östegård [15], and actually got all of the optimal packings in this range with the error estimate in Chapter 2 (Inequality 2.16). The polygon reducing program left all the rest and optimal combinations which shouldn't be excluded. The following is the general description of the computer-aided proof in this kind of problem.

- 1. Consider all the *n*-tile representatives from the tiling (initial combinations).
- 2. Apply polygon reducing to each *n*-tile, and obtain the corresponding rest regions (polygon reducing).
- 3. Guess the adjacency among n points which belong(s) to the rest combination.
- 4. Draw the approximate error squares. Check whether or not the approximate error squares are shrunk into a constant factor smaller squares after a finitely many number of rounds of reducings (proof of optimality and uniqueness).

One of the interesting parts of this method is that it is just enough in stage 4 to round finitely many times between approximate error squares (during several CPU-seconds in our case) so as to prove the *existence* of the error squares converging into the center points as an infinitely long sequence. Because we can verify whether or not the guessed adjacent relationship is really solvable, locally unique and locally optimal by the approximate solutions in stage 4, so we can prove both the geometrical or algebraical information of the guessed relationship like local uniqueness in the form of connectivity graph and simultaneous equations at the same time, and the numerical quality like local optimality of the separation distance. In our polygon reducings we could use the same procedure as was applied in eliminating the initial combinations, but generally, an exceptional treatment about adjustment of intersections is required when *outward* adjustment happens in shrinking.

It may occur in stage 3 that more than two solutions with same or similarly distances from a system of equations or even more than two systems of equations can be guessed as the candidates (especially when larger active regions remained after the reducings). In such cases a straightforward application of reducing procedure of stage 4 might not shrink the approximate error squares by a certain constant factor. About this situation, it is known that dividing the initial combinations into several *sub* initial combinations works well [15]. It is an open question whether the connectivity graph (i.e., simultaneous equations) determines the optimal packing uniquely or not. It should be remarked that Theorem 1 in Chapter 2 gives the locally optimal and unique packing with respect to not only the rest regions but also the *error squares*, so too large side of error square must be avoided. The final solutions with global optimality can be obtained by comparing all the rest combinations in stage 2.

We have seen in our experiment that the initial combinations rapidly increase as n grows up (for example in n = 16, our simple way of tiling with squares and isosceles right triangle generates $N_{16} = 15213963$ orbits), but it seems possible by modifying the way of tiling in stage 1 to apply this method up to the similar size of n (beyond 20?) as is currently reported in the case of square [15].

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