Chapter 1

GLOBAL OPTIMIZATION IN GEOMETRY — CIRCLE PACKING INTO THE SQUARE

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Abstract The present review paper summarizes the research work done mostly by the authors on packing equal circles in the unit square in the last years.

1. Introduction

The problem of finding the densest packing of n equal objects in a bounded space is a classical one which arises in many scientific and engineering fields. For the two-dimensional case, it is a well-known problem of discrete geometry. The Hungarian mathematician Farkas Bolyai (1775–1856) published in his principal work ('Tentamen', 1832–33 Bolyai (1904)) a dense regular packing of equal circles in an equilateral triangle (see Figure 1.1). He defined an infinite packing series and investigated the limit of *vacuitas* (the gap in the triangle outside the circles). It is interesting that these packings are not always optimal in spite of the fact

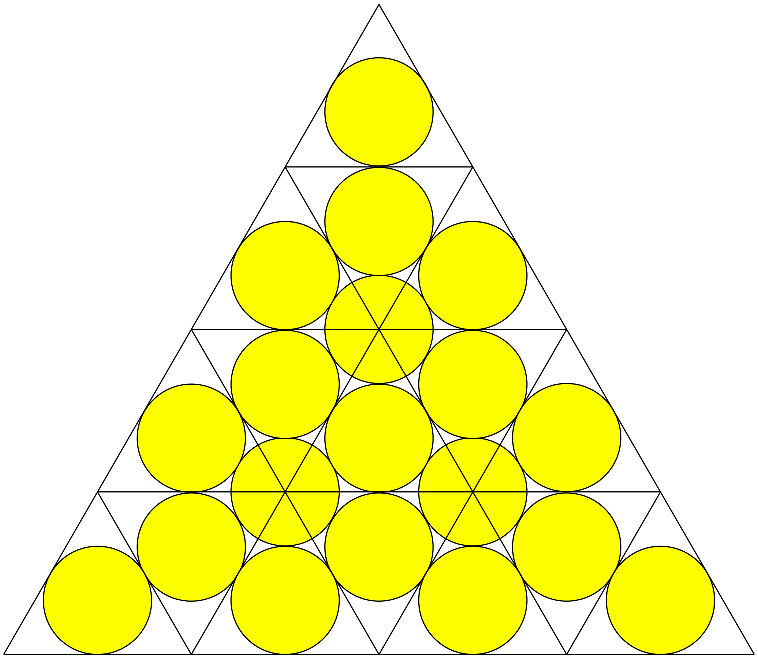

Figure 1.1. The example of Bolyai for packing 19 equal circles in an equilateral triangle.

that they are based on hexagonal grid packings (Szabó (2000)). Bolyai was probably the first author in the mathematical literature who studied the density of a series of packing circles in a bounded shape.

Of course, the work of Bolyai was not the very first in packing circles. There were other interesting early packings in fine arts, relics of religions and in nature (Tarnai (1997)), too. The old Japanese sangaku problems (Fukagawa and Pedoe (1989); Szabó (2001)) contain many nice results related to the packing of circles. Figure 1.2 shows an example of packing 6 equal circles in a rectangle.

The problem of finding the densest packing of n equal and non-overlapping circles has been studied for several shapes of the bounding region, e.g. in a rectangle (Ruda (1969)), in a triangle (Graham and Lubachevsky (1995)) and circle (Graham, Lubachevsky, Nurmela, and Östergård (1998)). Our work focuses only on the 'Packing of Equal Circles in a Square'-problem.

The Hungarian mathematicians Dezső Lázár and László Fejes Tóth have already investigated the problem before 1940 (Staar (1990); Szabó and Csendes (2001)). The problem first appeared in literature in 1960, when Leo Moser (1960) guessed the optimal arrangement of 8 circles.

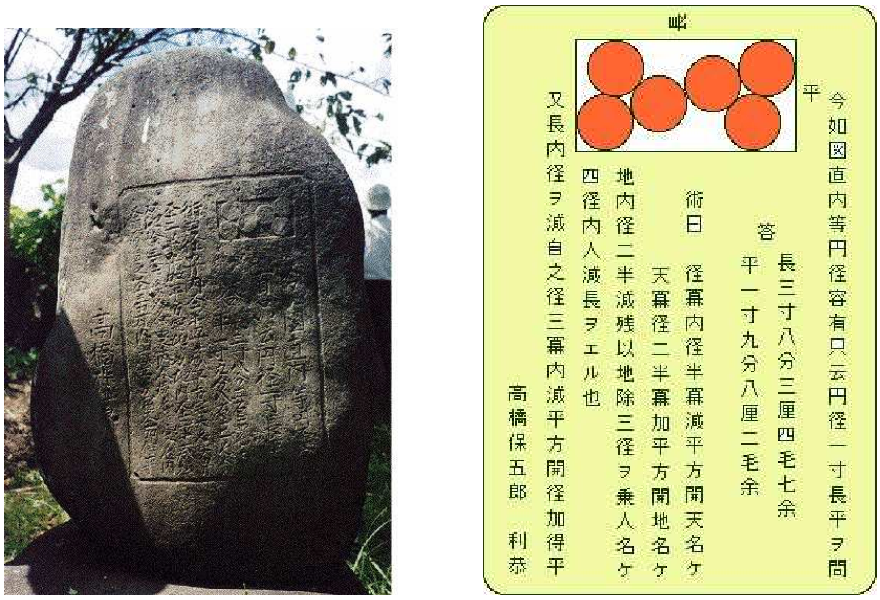

Figure 1.2. Packing of 6 equal circles in a rectangle on a rock from Japan.

Schaer and Meir (1965) proved this conjecture and Schaer (1965) solved the $n = 9$ case, too. Schaer has given also a proof for $n = 7$ in a letter to Leo Moser in 1964, but he never published it. There is a similar unpublished result from R. Graham in a private letter for $n = 6$. Later Schwartz (1970) and Melissen (1994) have given proof for this case (up to $n = 5$ circles the problem is trivial).

The next challenge was the $n = 10$ case. de Groot, Peikert, and Würtz (1990) solved this after many authors published new and improved packings: Goldberg (1970); Milano (1987); Mollard and Payan (1990); Schaer (1971); Schlüter (1979) and Valette (1989). Some unpublished results are known also in this case: Grünbaum (1990); Grannell (1990); Petris and Hungerbüler (1990). The proof based on a computer aided method, and nobody published a proof using only pure mathematical tools. There is an interesting mathematical approach of this case in Hujter (1999). Peikert, Würtz, Monagan, and de Groot (1992) found and proved optimal packings up to $n = 20$ using a computer aided method. Based on theoretical tools only, G. Wengerodt solved the problem for $n = 14, 16$ and 25 (Wengerodt (1983); Wengerodt (1987); Wengerodt (1987b)), and with K. Kirchner for $n = 36$ (Kirchner and Wengerodt (1987)).

In the last decades, several deterministic (Locatelli and Raber (2002); Markót (2003); Markót and Csendes (2004); Nurmela and Östergård (1999); Peikert, Würtz, Monagan, and de Groot (1992)) and stochastic (Boll, Donovan, Graham, and Lubachevsky (2000); Casado, García, Szabó, and Csendes (2001); Graham and Lubachevsky (1996)) methods were published. Proven *optimal* packings are known up to $n = 30$ (Nurmela and Östergård (1999); Peikert, Würtz, Monagan, and de Groot (1992); Markót (2003); Markót and Csendes (2004)) and for $n = 36$ (Kirchner and Wengerodt (1987)).

Approximate packings (packings determined by computer aided numerical computations without a rigorous proof) and *candidate* packings (best known arrangements with a proof of existence but without proof of optimality) were reported in the literature for up to $n = 200$: Boll, Donovan, Graham, and Lubachevsky (2000); Casado, García, Szabó, and Csendes (2001); Graham and Lubachevsky (1996); Nurmela and Östergård (1997); Szabó and E. Specht (2005). At the same time, some other results (e.g. repeated patterns, properties of the optimal solutions and bounds, minimal polynomials of packings) were published as well (Graham and Lubachevsky (1996); Locatelli and Raber (2002); Nurmela, Östergård, and aus dem Spring (1999); Tarnai and Gáspár (1995-96); Szabó (2000b); Szabó, Csendes, Casado, and García (2001); Szabó (2004)).

2. The packing circles in a square problem

The packing circles in a square problem can be described by the following equivalent problem settings:

PROBLEM 1 *Find the value of the maximum circle radius, r_n, such that n equal non-overlapping circles can be placed in a unit square.*

PROBLEM 2 *Locate n points in a unit square, such that the minimum distance m_n between any two points is maximal.*

PROBLEM 3 *Give the smallest square of side ρ_n, which contains n equal and non-overlapping circles where the radius of circles is 1.*

PROBLEM 4 *Determine the smallest square of side σ_n that contains n points with mutual distance of at least 1.*

2.1 Optimization models

The problem is at one hand a geometrical problem and on the other hand a continuous global optimization problem. Problem 2 can be written shortly as a $2n+1$ dimensional continuous nonlinear constrained (or max-min) global optimization problem in the following form:

$$\max_{s_k \in [0,1]^2,\ 1 \le k \le n} \ \min_{1 \le i < j \le n} \|s_i - s_j\| \,.$$

This problem can be considered in the following ways:

a) *as a DC programming problem* Horst and Thoai (1999):

A DC (difference of convex functions) programming problem is a mathematical programming problem, where the objective function can be described by a difference of two convex functions. The objective function of the problem can be stated as the difference of the following two convex functions g and h:

$$g(z) = 2\sum_{j=1}^{2n} z_j^2,$$

$$h(z) = \max\left\{\left(2\sum_{j\in J\setminus J_{ik}} z_j^2 + (z_i + z_k)^2 + (z_{n+i} + z_{n+k})^2\right) : 1 \le i < k \le n\right\},$$

where

$$J = \{1, \dots, 2n\},$$
$$z = (x_1, \dots, x_n, y_1, \dots, y_n),$$
$$J_{ik} = \{i, k, n+i, n+k\}.$$

b) *or as an all-quadratic optimization problem.*

The general form of an all-quadratic optimization problem (Raber (1999)) is

$$\min \quad \left[x^{\mathrm{T}} Q^0 x + (d^0)^{\mathrm{T}} x\right]$$
subject to
$$x^{\mathrm{T}} Q^l x + (d^l)^{\mathrm{T}} x + c^l \le 0 \qquad l = 1, \dots, p$$
$$x \in P,$$

where Q^l $(l = 0, \dots, p)$ are real $(n+1)\times(n+1)$ matrices, d^l $(l = 0, \dots, p)$ are real $(n+1)$-dimensional vectors, c^l $(l = 1, \dots, p)$ are real numbers, p is the number of constraints and P is a polyhedron. Solving the general case of an all-quadratic optimization problem is NP-hard.

The problem with the following values is a special all-quadratic optimization problem with a linear objective function (Szabó and E. Specht (2005)):

$$Q^0 = \mathbf{0}, \quad x^{\mathrm{T}} = (x_0, x_1, \ldots, x_{2n}), \quad (d^0)^{\mathrm{T}} = (-1, 0, \ldots, 0),$$

$$(d^l)^{\mathrm{T}} = \underline{\mathbf{0}}, \;\; c^l = 0, \;\; p = \frac{n(n-1)}{2}, \;\; P = [0, \sqrt{2}] \times [0,1]^{2n},$$

$$[Q^l]_{ij} = Q_{ij}^{l'l''} = \begin{cases} -1, & \text{if } i = j = \begin{cases} 2l', \\ 2l'', \\ 2l'+1, \\ 2l''+1, \end{cases} \\ 1, & \text{if } i = j = 1, \\ & \quad i = 2l''+1 \text{ and } j = 2l'+1, \\ & \quad i = 2l'' \quad\;\; \text{and } j = 2l', \\ & \quad i = 2l'+1 \;\text{ and } j = 2l''+1, \\ & \quad i = 2l' \quad\;\;\; \text{and } j = 2l'', \\ 0, & \qquad \text{otherwise}, \end{cases}$$

$$1 \le i, j \le 2n+1,$$
$$1 \le l' < l'' \le n.$$

In this model, x_0 is the minimal distance between the points. The coordinates of the i^{th} point ($1 \le i \le n$) are (x_{2i-1}, x_{2i}).

These models can be of interest, to be used for mathematical programming solvers as hard optimization problems. The investigations show that those approaches are effective that utilize the geometrical properties of the problem.

3. Properties of optimal packings and bounds

Recently, Locatelli and Raber (2002) proved two engaging properties that must be satisfied by at least one optimal solution of Problem 2. These theorems state the intuitive fact that as many points as possible should be located along the boundary of the square.

THEOREM 1.1 *(Locatelli and Raber (2002)) There exists always an optimal solution of Problem 2 such that at each vertex of the square one and only one of the following conditions hold:*

- *at least one point of the optimal solution coincides with that vertex of the square,*
- *two points of the optimal solution belong to the edge determined by the vertices and have a distance of $\overline{m}_n$, where $\overline{m}_n$ denotes the minimal distance between the points in the optimal solution.*

THEOREM 1.2 *(Locatelli and Raber (2002)) There exists always an optimal solution of Problem 2 such that along each edge of the square there is no portion of the edge of width greater than or equal to twice the optimal distance* $\overline{m}_n$ *which does not contain any point of the optimal solution.*

Using two another generalized theorems we can give lower and upper bounds for $\overline{m}_n$.

THEOREM 1.3 *(Hadwiger (1944)) Let us denote by* X *a subset on the plane by bordering a Jordan curve. If* M_n *denotes the maximum of minimal distance between* n *points in* X*, then*

$$\sqrt{\frac{2A(X)}{\sqrt{3}n}} \leq M_n,$$

where $A(X)$ *is the area of* X*.*

THEOREM 1.4 *(Folkman and Graham (1969)) Let us denote by* X *a compact convex subset on the plane. The number of points with mutual distance of at least 1 can be at most*

$$\frac{2}{\sqrt{3}}A(X) + \frac{1}{2}P(X) + 1,$$

where $A(X)$ *is the area and* $P(X)$ *is the perimeter of* X*.*

After a short calculation it can easily be shown that these inequalities are equivalent with the following lower and upper bounds for $\overline{m}_n$, where X is a unit square:

$$\sqrt{\frac{2}{\sqrt{3}n}} \leq \overline{m}_n \leq \frac{1}{n-1} + \sqrt{\frac{1}{(n-1)^2} + \frac{2}{\sqrt{3}(n-1)}}. \tag{1.1}$$

Using these inequalities one may find that, if n tends to infinity,

$$\lim_{n\to\infty} \sqrt{n}\,\overline{m}_n = \sqrt{\frac{2}{\sqrt{3}}}, \quad \text{thus}$$

$$\overline{m}_n \approx \sqrt{\frac{2}{\sqrt{3}n}}.$$

Szabó, Csendes, Casado, and García (2001) have provided another lower bound using regular patterns and in Szabó, Csendes, Casado, and García (2001); Tarnai and Gáspár (1995-96) heuristic upper bounds were studied based on the computation of the areas of circles and minimum gaps among the circles.

3.1 Computer aided approaches

In this subsection we give an overview of the most important earlier methods to find approximate packings. Several strategies were used, e.g. nonlinear programming solver (MINOS, Maranas, Floudas, and Pardalos (1995)) and Cabri-Geométry software (Mollard and Payan (1990)).

Unfortunately, these approaches were good only for small numbers of circles. Here we summarize some useful earlier approaches to find approximate packings for higher n.

3.1.1 Energy function minimization. By virtue of

$$\min_{1\le i<j\le n} \|s_i - s_j\| = \lim_{m\to -\infty} \left(\sum_{1\le i<j\le n} \|s_i - s_j\|^m \right)^{\frac{1}{m}}$$

the problem is relaxed as

$$\min_{s_i\in[0,1]^2,\ 1\le i\le n} \sum_{1\le i<j\le n} \frac{1}{\|s_i - s_j\|^m}.$$

This objective function can be interpreted as a potential or energy function. A physical analogon of this approach is to regard the points as electrical charges (all positive or all negative) which are repulsing each other. If the minimal distance between the charged particles increases, the corresponding value of the potential function decreases. Nurmela and Östergård (1997) used a similar energy function with large positive integer m values, where λ is scaling factor to prevent numerical overflows:

$$\sum_{1\le i<j\le n} \left(\frac{\lambda}{||s_i - s_j||^2} \right)^m.$$

Introducing $x_i = \sin(x_i^{'})$ and $y_i = \sin(y_i^{'})$, it transforms into an unconstrained optimization problem in variables $x_i^{'}, y_i^{'}$, where the coordinates of the centers of the circles fulfill the constraints $-1 \le x_i \le 1$, $-1 \le y_i \le 1$.

They published candidate packings up to 50 circles using a combination of Goldstein-Armijo backtracking linear search and the Newton method for the optimization.

3.1.2 Billiard simulation. The billiard simulation method is physically motivated too. Let us consider a random arrangement of the points. Draw equal circles around the points without overlapping. Each circle can be considered as a ball with an initial radius, moving direction and speed. Start the balls and increase slowly the common radius of them. The swing of each ball during the process will be less and less. The algorithm stops when the packing or a substructure of the packing becomes rigid. Using billiard simulation Graham and Lubachevsky (1996) reported several candidate packings for up to 50 circles and for some values beyond.

3.1.3 A perturbation method. Boll, Donovan, Graham, and Lubachevsky (2000) used a stochastic algorithm which gave improved packings for $n = 32, 37, 48$, and 50. A brief outline of their method is

1. *Step:* Consider n random points in the unit square,
2. *Step:* define $s = 0.25$ as an initial value,
3. *Step:* for each point
   - *a)* perturb the place of the center by s in the directions of North, South, East, or West,
   - *b)* if during the movement the distance between the point and its nearest neighbour becomes greater, update the new location of the point,
4. *Step* repeat *Step 3* while movable points exist,
5. *Step* $s := s/1.5$, and if $s > 10^{-10}$ then continue with *Step 3*.

Using the previous simple algorithm good candidate packings can be found after some millions of iterations. They have found unpublished approximate packings up to $n = 200$. Douglas Hanson, an 8^{th} grade student from Texas, has recently improved some of them using Donovan's program (see `http://www.packomania.com`).

3.1.4 TAMSASS-PECS. The TAMSASS-PECS (Threshold Accepting Modified Single Agent Stochastic Search for Packing Equal Circles in a Square) method is based on the Threshold Accepting global optimization technique and a modified SASS local optimization algorithm Solis and Wets (1981). The algorithm starts with a pseudorandom initial packing, a standard deviation and with a threshold level. The algorithm improve the current solution by an iterative procedure. At every step it tries to find a better position of the actual point using a local search. The stopping criterion is based on the value of the standard deviation, which is decreased at every iteration. The framework of the method is the Threshold Accepting approach. It is a close alternative of the Simulated Annealing algorithms. It accepts every move that leads to a new approximate solution not much worse than the current one and rejects other moves. Using TAMSASS-PECS Casado, García, Szabó, and Csendes (2001) reported approximate packings up to $n = 100$ and improved some earlier packings.

3.1.5 A deterministic approach based on LP-relaxation.

The circle packing problem can be regarded as an all-quadratic optimization problem, i.e. an optimization problem with not necessarily convex quadratic constraints. The hardness is due to the large number of constraints. This approach provides a rectangular subdivision branch-and-bound algorithm. To give an upper bound at each node of the branch-and-bound tree, M. Locatelli and U. Raber used the special structure of the constraints and gave an LP-relaxation Locatelli and Raber (2002). They have found candidate packings for up to 39 circles proving the optimality theoretically within a given accuracy.

3.1.6 The MBS algorithm. The basic idea of the approach MBS (Modified Billiard Simulation) is as follows (Szabó and E. Specht (2005)): Distribute randomly n points inside the unit square and blow them up in a uniform manner. This can be done by incrementing the radii gradually from an initial value of $r_0 = \sqrt{\frac{10}{23n\pi}}$ (which is a safe lower bound). In early stages of the process, when the distance between the small circles is much greater than their size and no collisions occur, there is no need to change their positions. As the circles grow, we have to deal with collisions (also among the circles and the boundaries). During the process when the decrease is too small or the number of iterations is larger than a given number, the calculation stops.

The efficiency of the MBS algorithm comes from a significant reduction of computational costs. The basic idea is as follows: It is not necessary to calculate and store the mutual distance between two circles if they are too far from each other and will never meet. For the numerical calculation the program uses two matrices CCD and CED. Matrix CCD stores the adjacency between the objects themselves, and matrix CED holds these between the objects and the sides of the square. At start, all matrix elements are set to NEAR which means that only such pairs of circles will be checked during the calculation. When (after thousands of collisions) a mutual distance of a pair is great enough, then the value is set to FAR which means that this contact will never occur in later iterations. As long as the program runs, the cost of the subroutine which determines the contacts will become less and less.

n	exact r_n	exact m_n	approximate m_n	d_n
2	$\frac{1}{2}(2-\sqrt{2})$	$\sqrt{2}$	1, 4142135624	0, 5390120845
3	$\frac{1}{2}(8-5\sqrt{2}+4\sqrt{3}-3\sqrt{6})$	$\sqrt{6}-\sqrt{2}$	1, 0352761804	0, 6096448087
4	$\frac{1}{4}$	1	1, 0000000000	0, 7853981634
5	$\frac{1}{2}(-1+\sqrt{2})$	$\frac{1}{2}m_2$	0, 7071067812	0, 6737651056
6	$\frac{1}{46}(-13+6\sqrt{13})$	$\frac{1}{6}\sqrt{13}$	0, 6009252126	0, 6639569095
7	$\frac{1}{13}(4-\sqrt{3})$	$4-2\sqrt{3}$	0, 5358983849	0, 6693108268
8	$\frac{1}{4}(1+\sqrt{2}-\sqrt{3})$	$\frac{1}{2}m_3$	0, 5176380902	0, 7309638253
9	$\frac{1}{6}$	$\frac{1}{2}$	0, 5000000000	0, 7853981634
10	–	–	0, 4212795440	0, 6900357853
11	(see separately)	(see separately)	0, 3982073102	0, 7007415778
12	$\frac{1}{382}(-34+15\sqrt{34})$	$\frac{1}{15}\sqrt{34}$	0, 3887301263	0, 7384682239
13	–	–	0, 3660960077	0, 7332646949
14	$\frac{1}{33}(6-\sqrt{3})$	$\frac{2}{13}(4-\sqrt{3})$	0, 3489152604	0, 7356792555
15	$\frac{1}{2}r_3$	$2\,r_8$	0, 3410813774	0, 7620560109
16	$\frac{1}{8}$	$\frac{1}{3}$	0, 3333333333	0, 7853981634
17	–	–	0, 3061539853	0, 7335502633
18	$\frac{1}{262}(-13+12\sqrt{13})$	$\frac{1}{2}m_6$	0, 3004626063	0, 7546533579
19	–	–	0, 2895419920	0, 7523078967
20	$\frac{1}{482}(65-8\sqrt{2})$	$\frac{1}{16}(6-\sqrt{2})$	0, 2866116524	0, 7794936869
21	–	–	0, 2718122554	0, 7533577029
22	–	–	0, 2679584016	0, 7716801121
23	$\frac{1}{2}(-7-5\sqrt{2}+4\sqrt{3}+3\sqrt{6})$	$\frac{1}{4}m_3$	0, 2588190451	0, 7636310321
24	$\frac{1}{92}(21-5\sqrt{2}+3\sqrt{3}-4\sqrt{6})$	r_3	0, 2543330950	0, 7749632598
25	$\frac{1}{10}$	$\frac{1}{4}$	0, 2500000000	0, 7853981634
26	–	–	0, 2387347572	0, 7584690905
27	$\frac{1}{3022}(-89+40\sqrt{89})$	$\frac{1}{40}\sqrt{89}$	0, 2358495283	0, 7723114565
28	–	–	0, 2305354936	0, 7718541114
29	–	–	0, 2268829007	0, 7789062418
30	$\frac{1}{1202}(126-5\sqrt{10})$	$\frac{1}{75}(20-\sqrt{10})$	0, 2245029645	0, 7920190265

Table 1.1. The numerical results for n=2 – 30.

It is useful to consider not only random arrangements for the initial packing but hexagonal or regular lattice packings too. Sometimes the relationship between the number of the circles and the structure of packing can provide a good initial configuration. The code and the found packings (up to $n = 300$) can be downloaded from the Packomania web-site: `http://www.packomania.com/`.

In Table 1.1 we have summarized the numerical results of the known optimal packings.

$r_{11} = \frac{1}{568}\ \ 176 - 9\sqrt{2} - 14\sqrt{3} - 13\sqrt{6} - 2\sqrt{-16523 + 12545\sqrt{2} - 9919\sqrt{3} + 6587\sqrt{6}}\ $, and

$m_{11} = \frac{1}{4}\ \ -4 - 3\sqrt{2} + 2\sqrt{3} + 3\sqrt{6} +\ \ 4 + \sqrt{2} - 2\sqrt{3} - \sqrt{6}\ \ \sqrt{1 + 2\sqrt{2}}\ \ .$

4. Repeated patterns in packings

Sometimes, there is a connection between the structures of the packings and the number of circles. When the structure of a packing follows a kind of regularity (e.g. a lattice arrangement), then the coordinates of the centers of the circles can easily be calculated and these structures are called *patterns*.

It is easy to see the pattern when the number of the circles is a square number ($n = k^2,\ 1 \leq k \leq 6$). In this case, the circles are in a $k \times k$ lattice arrangement (**PAT1**) and $m_n = \frac{1}{k-1}$. This pattern gives the optimal solutions considering the mentioned cases, however, if $n = 49$, then there exist denser packings (cf. Nurmela and Östergård (1997)). The patterns proposed by Nurmela and Östergård (1997) and Graham and Lubachevsky (1996) are summarized in Table 1.2. The fourth column of Table 1.2 gives those cases which can ensure optimal packings for the patterns, while in the fifth column, we can find the ones with the best known packings. We will show examples of them in Figure 1.3. Here $d = nr^2\pi$ denotes the density of the packing, c is the number of connections and f stands for the number of free circles.

Pattern	n	m_n	Optimal (k)	The best (k)
PAT1	k^2	$\frac{1}{k-1}$	2,3,4,5,6	—
PAT2	k^2-1	$\frac{1}{k-3+\sqrt{2+\sqrt{3}}}$	3,4,5(3)	6
PAT3a	k^2-2	$\frac{1}{k-2+\frac{1}{2}\sqrt{3}}$	3,4	—
PAT3b	k^2-2	$\frac{1}{k-5+2\sqrt{2+\sqrt{3}}}$	5	6(4)
PAT4	$k(k+1)$	$\frac{k^2-k-\sqrt{2k}}{k^3-2k^2}$	4	5,6,7
PAT5	$k^2+\lfloor k/2 \rfloor$	$\sqrt{\frac{1}{k^2}+\frac{1}{(2k-2)^2}}$	2, 4, 5	6, 7

Table 1.2. Patterns for the optimal and for the currently best known arrangements.

If $n = k^2-1$ then (**PAT2**) pattern can be recognized, or for $n = k^2-2$ (**PAT3a, PAT3b**). These patterns are similar to **PAT1**, but in this case we remove 1 or 2 circles and press the remaining ones into their columns and rows. There exist 3 different optimal solutions for $n = 24$ (**PAT2**) and 4 different good packings for $n = 34$ (**PAT3b**), in both cases with the same radius values. **PAT4** and **PAT5** are patterns, which represent the points (or centers of the circles) in a lattice arrangement. A generalized pattern of **PAT5** is discussed by Szabó, Csendes, Casado, and García (2001).

After studying these patterns, we can recognize that always exists a threshold number k_0 such that the patterns give the optimal or the

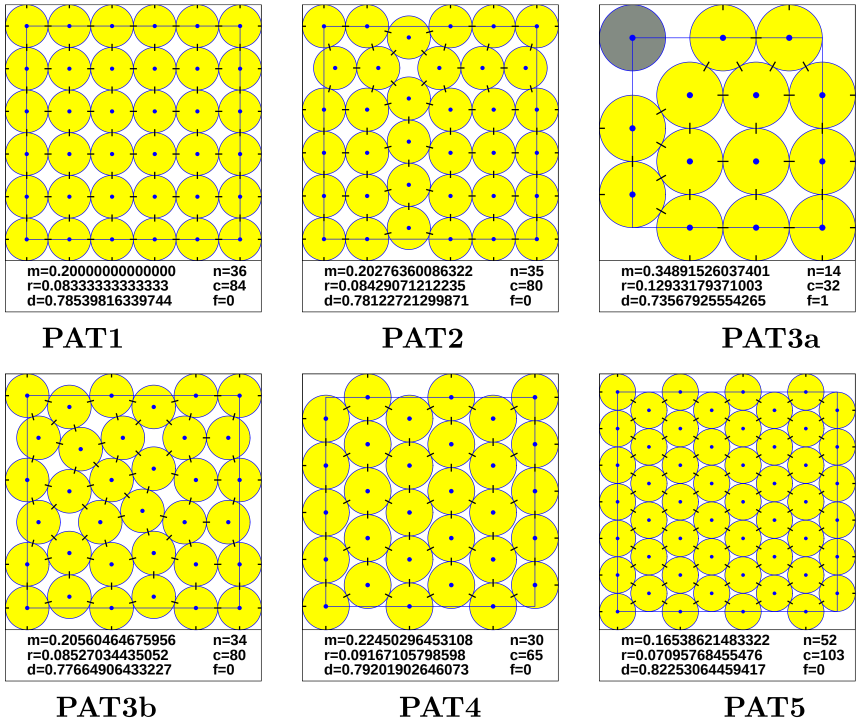

Figure 1.3. Examples for the repeated patterns.

currently best known packings up to this dimension, but later on these packings will provide only lower bounds for the optimal values.

It is an interesting question whether there is a universal pattern with an infinite packing series in which all packings are optimal. This is a natural question, originating from an analogous problem: find the densest packing for n equal circles in an equilateral triangle and $n = \frac{k(k+1)}{2}$, $k \geq 1$. In this case there exists an infinite series of optimal packings, see Lubachevsky, Graham, and Stillinger(1997). Here the circles are in the hexagonal arrangement (the centers of the circles are in a hexagonal grid) which is the densest packing of equal circles in the plane.

A similar conjecture exists for equal circles packing in a square problem (Nurmela, Östergård, and aus dem Spring (1999); Szabó (2000b)). Consider the following recursive sequences ($k \geq 3$):

$$\begin{aligned} a_1 &= 1, \quad a_2 = 3, & \qquad b_1 &= 1, \quad b_2 = 5, \\ a_k &= 4a_{k-1} - a_{k-2}, & \qquad b_k &= 4b_{k-1} - b_{k-2}. \end{aligned} \tag{1.2}$$

Dividing the side of the square into a_k and b_k equal parts, we obtain $a_k \times b_k$ rectangulars. Put the first point into a corner of the square, then place the points in each second corners of the rectangulars as on Figure 1.4. It is open for which values of a_k and b_k these packings are optimal.

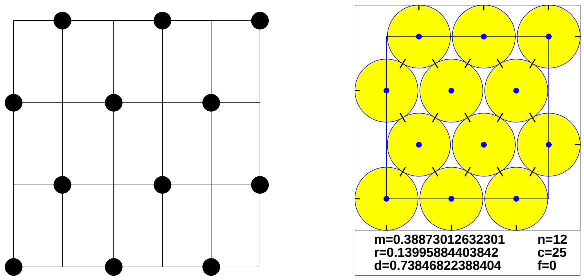

Figure 1.4. An example for a generalized pattern of **PAT5** with 12 points.

An interesting number theoretical statement is that when a_k and b_k are defined by the previous recursive series, then

a) $\lim\limits_{k\to\infty} \frac{a_k}{b_k} = \frac{\sqrt{3}}{3}$, and

b) $\left\{\frac{a_k}{b_k}\right\}_{k=1}^{\infty}$ is a subseries of the approximate fractions of the

$$\frac{\sqrt{3}}{3} = [0; 1, \overline{1, 2}] = 0 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{2 + \cfrac{1}{1 + \cfrac{1}{2 + \cfrac{1}{1 + \cfrac{1}{2 + \dots}}}}}}}$$

continued fraction. Looking at the previous packing sequence, the number of the circles is equal to

$$n = \frac{(a_k + 1)(b_k + 1)}{2}.$$

An explicit formula for n is the following:

$$n = \frac{\sqrt{3}}{6}(A_k - B_k)(A_k + B_k + 1) - \frac{1}{4}(A_k^2 + B_k^2) + \frac{1}{2},$$

where $A_k = (2+\sqrt{3})^k$ and $B_k = (2-\sqrt{3})^k$. The maximum m_n of the minimal distance is $m_n = \sqrt{\frac{1}{a_k^2} + \frac{1}{b_k^2}}$.

Here, the circles also approximate the hexagonal structure, but this alone, of course, does not prove the optimality. An interesting packing sequence can be found for the densest packing of equal circles in a *circle* problem in which $n = 3k(k+1)+1$. On the one hand, the hexagonal structure might be solved in this pattern as well and it presents the most spread packings when $n = 7, 19, 37$ and 61. On the other hand when $n = 91, 127, 169$ better ways of packing can be used (Lubachevsky and Graham (1997)).

5. Minimal polynomials of packings

Sometimes it is useful to have an algebraic description of a packing. The minimal polynomial is a polynomial with minimal degree and the first positive root of the polynomial is m_n. Sometimes it is easy to determine the minimal polynomial of a packing (e.g. the packing symmetric or contains optimal substructures Szabó (2004)). But if the structure of an optimal packing is not symmetric and it does not contain an optimal substructure then it is not trivial to calculate the minimal polynomial. In this case a possible way to determine the minimal polynomial is the following: Let us define a quadratic system of equations to the packing where an equation reflects the fact that the distance of two points is m_n. To determine the minimal polynomial we have to eliminate all variables with the exception of m_n. Using Buchberger's algorithm (based on Gröbner basis) or another technique utilizing the resultant and a symbolic algebra system (e.g. Maple, Mathematica, CoCoA, Macaulay2, Singular, etc.) this can be done, but sometimes this is also hard.

As an example, let us determine the minimal polynomial $p_{10}(m)$ for $n = 10$ (de Groot, Peikert, and Würtz (1990)). The corresponding quadratic system of equations is the following:

$$\begin{array}{rr}
(x_1-x_2)^2+(y_1-y_2)^2=m^2 & (x_1-x_4)^2+(y_1-y_4)^2=m^2 \\
(x_2-x_3)^2+(y_2-y_3)^2=m^2 & (x_2-x_5)^2+(y_2-y_5)^2=m^2 \\
(x_5-x_6)^2+(y_5-y_6)^2=m^2 & (x_3-x_6)^2+(y_3-y_6)^2=m^2 \\
(x_4-x_7)^2+(y_4-y_7)^2=m^2 & (x_5-x_7)^2+(y_5-y_7)^2=m^2 \\
(x_7-x_9)^2+(y_7-y_9)^2=m^2 & (x_7-x_{10})^2+(y_7-y_{10})^2=m^2 \\
(x_8-x_{10})^2+(y_8-y_{10})^2=m^2 & (x_6-x_8)^2+(y_6-y_8)^2=m^2
\end{array}$$

The points $P_1, P_2, P_3, P_4, P_6, P_8, P_9$, and P_{10} are on the side of the square thus $x_1 = x_4 = x_9 = y_2 = y_3 = 0$ and $x_6 = x_8 = y_9 = y_{10} = 1$. It is easy to see that $y_4 = y_1 + m$, $x_3 = x_2 + m$ and $y_8 = y_6 + m$. $P_2P_3P_5P_6$ is a rhombus thus $x_5 = 1 - m$ and $y_5 = y_6$. In the $P_4P_7P_9$ and $P_9P_7P_{10}$

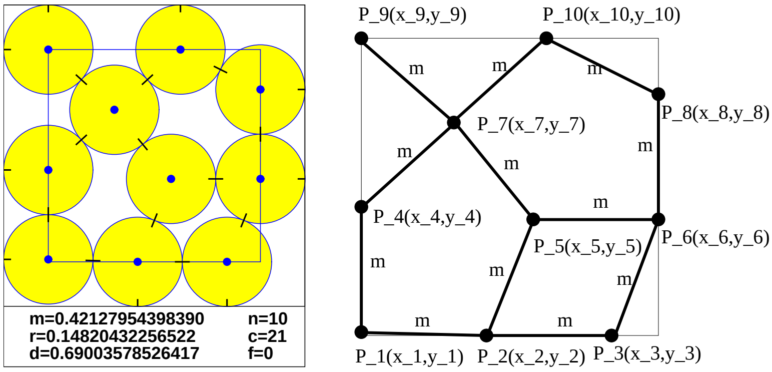

Figure 1.5. The optimal packing of 10 circles/points in the unit square.

isosceles triangulars these equalities holds: $y_7 = (1 + y_1 + m)/2$ and $x_7 = x_{10}/2$.

Using the previous observations, all variables are eliminated with the exception of x_2, x_{10}, y_1, y_5 and m. The system of equations is then reduced to the form ($y_1 \neq 0$):

$$\begin{aligned} x_2^2 + y_1^2 &= m^2, \\ x_{10}^2 + (1 - y_1 - m)^2 &= (2m)^2, \\ (1 - x_{10})^2 + (1 - y_5 - m)^2 &= m^2, \\ (1 - x_2 - m)^2 + y_5^2 &= m^2, \\ (2 - 2m - x_{10})^2 + (2y_5 - 1 - y_1 - m)^2 &= (2m)^2. \end{aligned}$$

Let us now determine the minimal polynomial with Maple 8 based on the Groebner package:

`>with(Groebner):univpoly(m,[polynomials],`$\{x_2, y_1, x_{10}, y_5, m\}$`);`.

The obtained minimal polynomial $p_{10}(m)$ is given in the following list.

A list of the known minimal polynomials $p_n(m)$ $(2 \leq n \leq 100)$:

$n = 2$	$m^2 - 2$
$n = 3$	$m^4 - 16m^2 + 16$
$n = 4$	$m - 1$
$n = 5$	$2m^2 - 1$

$n=6 \quad 36m^2-13$

$n=7 \quad m^2-8m+4$

$n=8 \quad m^4-4m^2+1$

$n=9 \quad 2m-1$

$$n=10 \quad \begin{aligned} &1180129m^{18}-11436428m^{17}+98015844m^{16}-462103584m^{15}\\ &+1145811528m^{14}-1398966480m^{13}+227573920m^{12}+1526909568m^{11}\\ &-1038261808m^{10}-2960321792m^{9}+7803109440m^{8}-9722063488m^{7}\\ &+7918461504m^{6}-4564076288m^{5}+1899131648m^{4}-563649536m^{3}\\ &+114038784m^{2}-14172160m+819200 \end{aligned}$$

$n=11 \quad m^8+8m^7-22m^6+20m^5+18m^4-24m^3-24m^2+32m-8$

$n=12 \quad 225m^2-34$

$$n=13 \quad \begin{aligned} &5322808420171924937409m^{40}+58677395933804988617323 2m^{39}\\ &+13024448845332271203266928m^{38}-129884095670569099901704 32m^{37}\\ &-6697217539589294973937 2512m^{36}-271451157211281654252175360m^{35}\\ &+1438322342979585076139742976m^{34}-3354298954676639164979968 00m^{33}\\ &-6543699259726848821592216832m^{32}+944137136101134536216646860 8m^{31}\\ &+10182180602633501397232254976m^{30}-42246019864541071922661621760m^{29}\\ &+37620100408876038921186476032m^{28}+28699095956807539331396009984m^{27}\\ &-102587608293645346411004952576m^{26}+103509313296807875445571190784m^{25}\\ &-23909360523055293307841740800m^{24}-62735581440162634955836358656m^{23}\\ &+88454871551963142041952583680m^{22}-53012494559549527012040245248m^{21}\\ &+2135173605242212884072628224m^{20}+26378985900767549703436894208m^{19}\\ &-26497225761631816480192462848m^{18}+12731474183761933022491836416m^{17}\\ &-3984323399280382686621859 84m^{16}-4422001291286852186186711040m^{15}\\ &+3658751900977247115934695424m^{14}-1429726216634427968279543808m^{13}\\ &+577707736218287188266188 80m^{12}+275582370688699861317976064m^{11}\\ &-171632310725283375512289280m^{10}+46974915155899860050247680m^{9}\\ &+17600674325965992414412 80m^{8}-7491112055212411797372928m^{7}\\ &+3652998504696614282592256m^{6}-1072642406499215430647808m^{5}\\ &+217086289997205686190080m^{4}-30811405631471617048576m^{3}\\ &+2960075719794736758784m^{2}-174103532094609162240m\\ &+4756927106410086400 \end{aligned}$$

$n=14 \quad 13m^2-16m+4$

$n=15 \quad 2m^4-4m^3-2m^2+4m-1$

$n=16 \quad 3m-1$

$n=17 \quad m^8-4m^7+6m^6-14m^5+22m^4-20m^3+36m^2-26m+5$

$n=18 \quad 144m^2-13$

$$n=19 \quad \begin{aligned} &242m^{10}-1430m^9-8109m^8+58704m^7-78452m^6\\ &-2918m^5+43315m^4+39812m^3-53516m^2+20592m\\ &-2704 \end{aligned}$$

$n=20 \quad 128m^2-96m+17$

$n=23 \quad 16m^4-16m^2+1$

$n=24 \quad m^4-16m^3+20m^2-8m+1$

$n=25 \quad 4m-1$

$n=27 \quad 1600m^2-89$

$n=30 \quad 1202m^2-252m+13$

$n=34 \quad m^4+28m^3-10m^2-4m+1$

$n=35 \quad 46m^4-84m^3+50m^2-12m+1$

$n = 36$	$5m - 1$
$n = 39$	$1732m^2 - 68m - 17$
$n = 42$	$864m^2 - 360m + 37$
$n = 52$	$7056m^2 - 193$
$n = 56$	$1715m^2 - 588m + 50$
$n = 99$	$28900m^2 - 389$

6. A reliable computer-assisted optimization method for circle packing

The papers Markót (2000), Markót (2003) and Markót and Csendes (2004) introduced a computer-aided technique for proving optimality of certain problem instances. In contrast to the earlier computer methods (see Section 1), the presented algorithm is based fully on *interval arithmetic*. Thus, our method is capable to overcome the rounding and conversion problems occurring in finite precision floating point computations and in I/O routines.

6.1 Problem definition

We study the point packing problem, Problem 2, but with the square of distances. Denote the set of points to be located by $((x_1, y_1), \ldots, (x_n, y_n))$, all in $[0, 1]^2$. In the sequel we denote this point set briefly by (x, y). Moreover, denote the square of the distance between the points (x_i, y_i) and (x_j, y_j) by d_{ij}. Then the objective function to be maximized is:

$$f_n(x, y) = \min_{1 \le i < j \le n} (x_i - x_j)^2 + (y_i - y_j)^2 = \min_{1 \le i < j \le n} d_{ij}. \tag{1.3}$$

Prior to our investigation the optimal solutions of the cases $n = 2, \ldots, 27$ and 36 were known. Although a part of the optimality proofs were based on computer-assisted methods, still those methods used floating point arithmetic (with the exception of an interval based local result verification method of Nurmela and Östergård (1999)).

6.2 Interval analysis

The description of the algorithm requires a brief survey on the basic interval definitions and properties (for more details see e.g. Alefeld and Herzberger (1983); Hansen (1992); Moore (1966)):

The set of compact *intervals* is denoted by $\mathbb{I}$, where for all $A \in \mathbb{I}$ intervals $A = [\underline{A}, \overline{A}] = \{a \in \mathbb{R} \mid \underline{A} \le a \le \overline{A}\}$. Here $\underline{A}, \overline{A} \in \mathbb{R}$ mean the *lower* and *upper bounds* of A, respectively. In the case of $\underline{A} = \overline{A}$ we call

A a *point interval*. For a given set of reals $D \subseteq \mathbb{R}$, $\mathbb{I}(D)$ denotes the set of all intervals in D. The *width* of an interval is defined by $w(A) := \overline{A} - \underline{A}$.

The real *arithmetic operations* can be extended for intervals by applying the general definition $A \circ B := \{a \circ b \mid a \in A,\ b \in B\}$, which can be calculated by the following formulas:

$$A + B = [\underline{A} + \underline{B}, \overline{A} + \overline{B}],$$

$$A - B = [\underline{A} - \overline{B}, \overline{A} - \underline{B}],$$

$$A \cdot B = [\min\{\underline{A}\,\underline{B}, \underline{A}\,\overline{B}, \overline{A}\,\underline{B}, \overline{A}\,\overline{B}\}, \max\{\underline{A}\,\underline{B}, \underline{A}\,\overline{B}, \overline{A}\,\underline{B}, \overline{A}\,\overline{B}\}],$$

$$A/B = A \cdot [1/\overline{B}, 1/\underline{B}], \text{ if } 0 \notin B.$$

Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be an elementary real function which is continuous in all $A \in \mathbb{I}(D)$ intervals. Then the *interval extension of the elementary function* φ is $\Phi : \mathbb{I}(D) \to \mathbb{I}$, $\Phi(A) := \{\varphi(a) \mid a \in A\}$. For a given function the corresponding interval extension can be calculated e.g. by invoking monotonicity properties.

A vector of n intervals is called an *n-dimensional interval* (or shortly, a *box*): $X = (X_1, X_2, \ldots, X_n)$, $X \in \mathbb{I}^n$, and $X_i \in \mathbb{I}$ for $i = 1, 2, \ldots, n$. For a given n-dimensional set $D \subseteq \mathbb{R}^n$ we denote the set of n-dimensional boxes in D by $\mathbb{I}(D)$. The extension of the basic arithmetic operations and elementary functions for multidimensional intervals is defined componentwise, similarly as for real vectors.

In order to define interval extensions for compound real functions, we introduce the concept of *interval inclusion functions*. We call $F : \mathbb{I}(D) \to \mathbb{I}$ an *inclusion function* of $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$, if $f(X) = \{f(x) \,|\, x \in X\} \subseteq F(X)$ holds for all $X \in \mathbb{I}(D)$, where $f(X)$ denotes the range of f over X.

Beyond the theoretical reliability of interval computations, the inclusion properties should be guaranteed also in the case when finite precision floating-point computer arithmetic is applied, i.e. the rounding errors should be controlled. This is usually done by the computational environment using exactly representable floating-point numbers (also called machine numbers) together with directed outward rounding procedures.

6.3 The optimization frame algorithm

We have applied an interval branch-and-bound optimization approach (see e.g. Csallner, Csendes, and Markót (2000); Csendes and Ratz (1997); Hammer, Hocks, Kulisch, and Ratz (1993); Hansen (1992); Kearfott (1996); Markót, Csendes, and Csallner (2000); Ratschek and Rokne

(1988)) designed for determining all the global maximizers of the general global optimization problem

$$\max_{z \in Z_0} f(z), \tag{1.4}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a continuous objective function and $Z_0 \in \mathbb{I}^n$ is the search space. The main building blocks of the algorithm are basically the same as the steps of the classical B&B methods. We utilize the fact that interval arithmetic provides a general tool to compute guaranteed enclosures $F(Z)$ of the range of the objective function $f(z)$ over a box Z. At each iteration cycle, we choose a box Z from the list of boxes (WorkList) waiting for further subdivision, and split it into *subboxes*, $U^1, \ldots, U^s$ (we used $s = 2$ in the present method).

Then for all U^i subintervals some shrinking tools, the so-called *accelerating devices* are applied, which delete some parts of U^i that cannot contain a global maximizer point. When the box $\hat{U}^i$ enclosing all the remaining parts of U^i fulfills a certain termination criterion, we put $\hat{U}^i$ into the list of the result boxes (ResultList), otherwise we store $\hat{U}^i$ for further processing in the WorkList. At each iteration we also try to update the best known lower bound $\tilde{f}$ of the global maximum value. $\tilde{f}$ is also called as *cutoff value*: we can delete all boxes U^i from the WorkList for which $\overline{F}(U^i) < \tilde{f}$ holds. The algorithm stops when the WorkList becomes empty: then the candidate boxes in the ResultList contain the enclosures of all the global maximizers, and moreover, the interval $[\tilde{f}\,, \max\{\overline{F}(Z) \,|\, Z \in \text{ResultList}\}]$ encloses the global maximum value.

In the following, we specify the algorithmic details by defining an inclusion function of (1.3) and introducing a special accelerating device. Note that already in the first phase of our study it turned out that the classical accelerating devices are not enough, we have to tune our algorithm by designing special interval-based tools utilizing the geometric properties of the problem class.

6.4 Introducing an interval inclusion function

Markót (2000) gives a non-trivial interval inclusion function of the objective function (1.3):

THEOREM 1.5 *(Markót (2000), slightly modified) Assume that* $(X, Y) \subseteq [0,1]^{2n}$*, and let*

$$D_{ij} = (X_i - X_j)^2 + (Y_i - Y_j)^2, \qquad \text{for all } 1 \le i \ne j \le n.$$

Define $a := \min_{1 \le i \ne j \le n} \underline{D_{ij}}$, $a \in \mathbb{R}$, *and* $b := \min_{1 \le i \ne j \le n} \overline{D_{ij}}$, $b \in \mathbb{R}$. *Then the interval* $F_n(X, Y) := [a, b]$ *encloses the range of* $f_n(x, y)$ *over the* (X, Y) *box.*

6.5 The method of active areas

This method played a key role in the earlier theoretical and computer-aided optimality proofs, e.g. in de Groot, Monagan, Peikert, and Würtz (1992); de Groot, Peikert, and Würtz (1990); Kirchner and Wengerodt (1987); Locatelli and Raber (2002); Nurmela and Östergård (1999); Nurmela and Östergård (1999b); Peikert, Würtz, Monagan, and de Groot (1992). The essence of the method is the following: assume that we have an $\tilde{f}_0$ lower bound for the maximum of the minimal pairwise distances. Let $C = (C_1, \ldots, C_n)$, $C_i \subseteq [0,1]^2, i = 1, \ldots, n$ be the currently investigated search set (with a suitable representation), where C_i contains the ith point of all packing configurations in C. Then, from each component C_i we can iteratively delete those points which have a distance smaller than $\tilde{f}_0$ to *all* points of the remained region of an other component.

Figure 1.6. Approximating the active regions by polygons (with exact arithmetic).

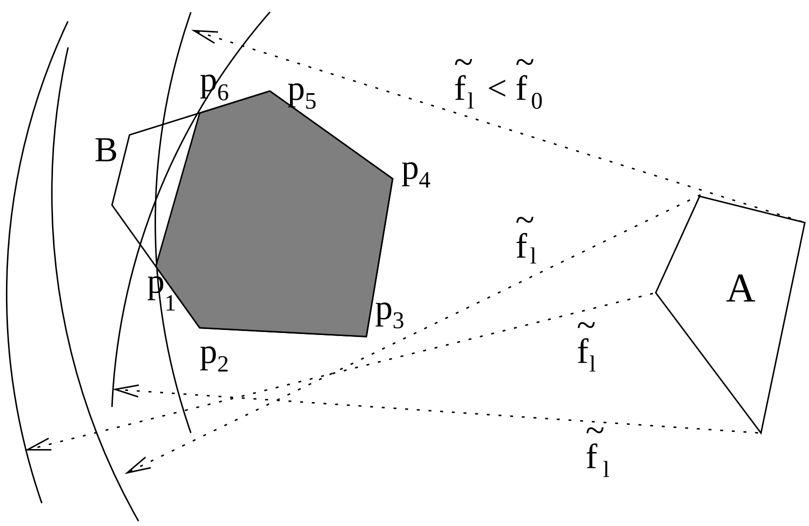

Figure 1.6 shows an example of eliminating a region (the shaded polygon) from polygon B using polygon A, when assuming exact computations.

In the first version of our interval approach (Markót (2000)) the remaining (active) region of each component was approximated by a rectangle (or unions of rectangles obtained after a horizontal and/or vertical quantization) during the basic elimination step. This matches the idea proposed by de Groot et al. and by Nurmela and Östergård. However, our algorithm variant using this device was only able to confirm the local optimality of the earlier found optimal packings.

Instead of representing the remaining regions simply by unions of cells, Nurmela and Östergård (1999) approximated the remaining sets by polygons. The proposed procedure raises several problems when using floating point computations. As a solution, in Markót and Csendes (2004) we developed a reliable version of this polygonal approach using interval arithmetic. This method proved to be the most efficient accelerating test of the present algorithm.

6.6 The method of handling free circles

The efficient way of handling free circles in the optimal solution (or equivalently, handling free points in the corresponding point packing problem) is crucial when circle packing problems are solved with interval algorithms, since free circles pose a positive measure, continuum set of equivalent global optimizers. The simple method below shows a suitable way to overcome this difficulty. The basic idea is that – under certain conditions – some remaining regions can temporarily be replaced by *machine points*, i.e. by pairs of two machine numbers without losing any global optimizers.

1. Let $(X, Y) \in \mathbb{I}^{2n}$ enclose all the remaining boxes (stored either in the WorkList or in the ResultList) after a certain number of iteration loops when executing the B&B algorithm. Let $\tilde{f}$ be the current cutoff value.

2. Assume that there exist *machine points* $p_{k_1}, \ldots, p_{k_t},\ p_{k_s} \in (X_{k_s}, Y_{k_s})$, $s \in \{1, \ldots, t\}$ within t different components of (X, Y) such that

$$\underline{D}(p_{k_s}, (X_j, Y_j)) > \overline{F}(X, Y) \geq \tilde{f}$$

holds for all $s \in \{1, \ldots, t\}$ and for all $j \neq k_s,\ j \in \{1, \ldots, n\}$. Let K denote the index set $\{k_1, \ldots, k_t\}$.

3. Replace the components (X_i, Y_i) with the point intervals p_i for each $i \in K$. Run the B&B algorithm on the resulting (X', Y') box ignoring the step of improving $\tilde{f}$ and stop it after a certain number of iterations.

4. Let $(X'', Y'') \in \mathbb{I}^{2n}$ include all the remaining boxes. The output box of the procedure is then given by (X_i, Y_i) for $i \in K$ and by (X''_j, Y''_j) for $j \notin K$.

THEOREM 1.6 *Markót and Csendes (2004) The above procedure is correct in the sense that all the optimal solutions in* (X, Y) *are also contained in the output box.*

6.7 Investigating subsets of tile combinations

In order to avoid (a part of) the extra amount of work caused by geometrically equivalent packing configurations and to restrict the application of the method of active areas to a local investigation, most computer methods for circle packing include a preprocessing procedure called *tiling*:

Assume that a lower bound $\tilde{f}$ for the maximum value of the considered point packing problem instance is given. Split the unit square into regions (tiles) in such a way, that the square of distance between any two points within each tile is less than $\tilde{f}$ (or the distance between any two points within each tile is less than the $\tilde{f}_0$ value of Section 6.5). Then for a feasible solution having an objective function value greater than or equal to $\tilde{f}$, each tile can contain obviously at most one point of this solution. The optimal packings can be then found by running the search procedure on all possible tile combinations.

Prior to the results of the present studies, the main problem when solving circle packing problem instances for $n > 27$, $n \neq 36$ was the highly increasing number of initial tile combinations. For $n = 28$, a sequential process on those combinations would have required about 1000 times more processor time (about several decades) even with non-interval computations — compared to the case of $n = 27$.

The idea behind the newly proposed method is that we can utilize the local relations (patterns) between the tiles and eliminate groups of tile combinations together. Let us denote a generalized point packing problem instance by $P(n, X_1, \ldots, X_n, Y_1, \ldots, Y_n)$, where n is the number of points to be located, $(X_i, Y_i) \in \mathbb{I}^2$, $i = 1, \ldots n$ are the components of the starting box, and the objective function of the problem is given by (1.3). The theorem below shows how to apply a result achieved on a $2m$-dimensional packing problem to a $2n$-dimensional problem with $n \geq m \geq 2$.

THEOREM 1.7 *Markót and Csendes (2004) Assume that* $n \geq m \geq 2$ *are integers and let*

$$P_m = P(m, Z_1, \ldots, Z_m, W_1, \ldots, W_m) = P(m, (Z, W)), \text{ and}$$

$$P_n = P(n, X_1, \ldots, X_n, Y_1, \ldots, Y_n) = P(n, (X, Y))$$

be point packing problem instances $(X_i, Y_i, Z_i, W_i \in \mathbb{I}; X_i, Y_i, Z_i, W_i \subseteq [0, 1])$*. Run the B&B algorithm on* P_m *using an* $\tilde{f}$ *cutoff value in the ac-*

celerating devices but skipping the step of improving $\tilde{f}$. *Stop after an arbitrary preset number of iteration steps. Let* $(Z'_1, \ldots, Z'_m, W'_1, \ldots, W'_m) := (Z', W')$ *be the enclosure of all the elements placed on the WorkList and on the ResultList. Assume that there exists an invertable, distance-preserving geometric transformation* φ *with* $\varphi(Z_i) = X_i$ *and* $\varphi(W_i) = Y_i$, $\forall i = 1, \ldots, m$. *Then for each point packing* $(x, y) \in \mathbb{R}^{2n}$ *satisfying* $(x, y) \in (X, Y)$ *and* $f_n(x, y) \geq \tilde{f}$, *the statement*

$$(x, y) \in \begin{array}{l}(\varphi(Z'_1), \ldots, \varphi(Z'_m), X_{m+1}, \ldots, X_n, \\ \quad \varphi(W'_1), \ldots, \varphi(W'_m), Y_{m+1}, \ldots, Y_n) \end{array} := (X', Y')$$

also holds.

The meaning of Theorem 1.7 is the following: assume that we are able to reduce some search regions on a tile set S'. When processing a higher dimensional subproblem on a tile set S containing the image of the tile set of the smaller problem, it is enough to consider *the image of those of the remaining regions of* S' as the particular components of the latter problem.

Figure 1.7. The idea behind processing tile combinations.

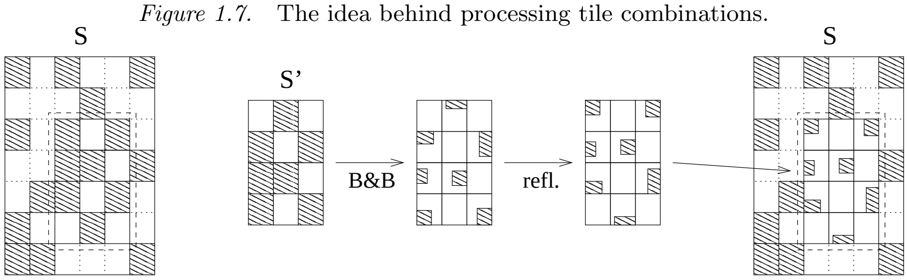

Figure 1.7 illustrates the application of the idea of handling sets of tile-combinations: the remaining regions of the tile combinations S and S' are given by the shaded areas. The transformation φ is a reflection to the horizontal centerline of the rectangular region enclosing S'.

COROLLARY 1.8 *Markót and Csendes (2004) Let* φ *be the identity transformation and assume that the B&B algorithm terminates with an empty WorkList and with an empty ResultList, i.e. the whole search region* $(Z, W) = (Z_1, \ldots, Z_m, W_1, \ldots, W_m) = (X_1, \ldots, X_m, Y_1, \ldots, Y_m)$ *is eliminated by the accelerating devices using (the same)* $\tilde{f}$. *Then* (X, Y) *does not contain any* $(x, y) \in \mathbb{R}^{2n}$ *vectors for which* $f_n(x, y) \geq \tilde{f}$ *holds.*

6.8 Tile algorithms used in the optimality proofs

The method of the optimality proofs is started by finding feasible tile patterns and their remaining areas on some small subsets of the whole set of tiles. Then bigger and bigger subsets are processed while using the results of the previous steps. Thus, the whole method consists of several phases. The two basic procedures are:

– `Grow()`: add tiles from a new column to each element of a set of tile combinations.

– `Join()`: join the elements of two sets of tile combinations pairwise.

The detailed description of `Join()` and `Grow()` and the strategy of increasing the dimensionality of the subproblems can be found in Markót and Csendes (2004).

6.9 Numerical results: optimal packings for $n = 28,\ 29, 30$

The results obtained with the multiphase interval arithmetic based optimality proofs are summarized below:

– Apart from symmetric cases, one initial tile combination (more precisely, the remaining areas of the particular combination) contains all the global optimal solutions of the packing problem of n points.

– The guaranteed enclosures of the global maximum values of PROBLEM 2 are

$$\begin{array}{ll} F_{28}^* = [\underline{0.23053549364266}73, \underline{0.23053549364267}43], & w(F_{28}^*) \approx 7 \cdot 10^{-15}, \\ F_{29}^* = [\underline{0.2268829007442}089, \underline{0.2268829007442}240], & w(F_{29}^*) \approx 2 \cdot 10^{-14}, \\ F_{30}^* = [\underline{0.22450296453108}81, \underline{0.22450296453109}03], & w(F_{30}^*) \approx 2 \cdot 10^{-15}. \end{array}$$

– The exact global maximum value differs from the currently best known function value by at most $w(F_n^*)$.

– Apart from symmetric cases, all the global optimizers of the problem of packing n points are located in an $(X, Y)_n^*$ box (see Markót and Csendes (2004)). The components of the result boxes have the widths of between approximately 10^{-12}–10^{-14} (with the exception of the components enclosing possibly free points).

– The differences between the volume of the whole search space and the result boxes are more than 711, 764, and 872 orders of magnitudes, respectively.

– The total computational time was approximately 53, 50, and 20 hours, respectively. The total time complexities are remarkably less than the forecasted execution times of the predecessor methods.

6.10 Optimality of the conjectured best structures

An optimal packing structure specifies which points are located on the sides of the square, which pairs have minimal distance, and which points of the packing can move while keeping optimality. The output of our methods serves only as a numerical approximation to the solution of the particular problems but it says nothing about the structure of the optimal packing(s). Extending the ideas given in Nurmela and Östergård (1999) to an interval-based context, in a forthcoming paper we intent to prove also some structural properties of the global optimizers (for details see Markót (2003b)).

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