2

Problem Definitions and Formulations

In this chapter we will specify the densest packing of equal circles in a square problem, and discuss some equivalent problem settings. Since, besides the geometric investigations, we also consider the problem from a global optimization point of view, some possible mathematical programming models will be included here.

2.1 Geometrical models

Informally speaking, the packing circles in a square and its related problems can be described in the following ways:

Problem 2.1. Place $n \geq 2$ equal and non-overlapping circles in a square, such that the common radius of the circles is maximal.

Problem 2.2. Place $n \geq 2$ points in a square, such that the minimum of the pairwise distances is maximal.

Problem 2.3. Place $n \geq 2$ equal and non-overlapping circles with the common radius in the smallest possible square.

Problem 2.4. Place $n \geq 2$ points with pairwise distances of at least a given positive value in the smallest possible square.

Of course, in order to investigate these problems and their relations in detail, we need their formal definitions and a consistent system of notation.

Formal description of Problem 2.1:

Definition 2.5. $P(r_n, S) \in P_{r_n}$ *is a* circle packing *with the common radius* r_n *in the square* $[0, S]^2$, *where* $P_{r_n} = \{((x_1, y_1), \dots, (x_n, y_n)) \in [0, S]^{2n} \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq 4r_n^2; x_i, y_i \in [r_n, S - r_n]\ (1 \leq i < j \leq n)\}$. $P(r_n, S) \in P_{\overline{r}_n}$ *is an* optimal circle packing, *if* $\overline{r}_n = \max\limits_{P_{r_n} \neq \emptyset} r_n$.

Problem $\mathcal{P}_1^n$. Determine the optimal circle packings for a given $n \geq 2$ integer.

Formal description of Problem 2.2:

Definition 2.6. $A(m_n, \Sigma) \in A_{m_n}$ *is a* point arrangement *with the minimal pairwise distance* m_n *in the square* $[0, \Sigma]^2$, *where* $A_{m_n} = \{((x_1, y_1), \ldots, (x_n, y_n)) \in [0, \Sigma]^{2n} \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq m_n^2; (1 \leq i < j \leq n)\}$. $A(m_n, \Sigma) \in A_{\overline{m}_n}$ *is an* optimal point arrangement, *if* $\overline{m}_n = \max\limits_{A_{m_n} \neq \emptyset} m_n$.

Problem $\mathcal{P}_2^n$. Determine the optimal point arrangements for a given $n \geq 2$ integer.

Formal description of Problem 2.3:

Definition 2.7. $P'(R, s_n) \in P'_{s_n}$ *is an* associated circle packing *with the common radius* R *in the square* $[0, s_n]^2$, *where* $P'_{s_n} = \{((x_1, y_1), \ldots, (x_n, y_n)) \in [0, s_n]^{2n} \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq 4R^2; x_i, y_i \in [R, s_n - R]\ (1 \leq i < j \leq n)\}$. $P'(R, s_n) \in P'_{\overline{s}_n}$ *is an* optimal associated circle packing, *if* $\overline{s}_n = \min\limits_{P'_{s_n} \neq \emptyset} s_n$.

Problem $\mathcal{P}_3^n$. Determine the optimal associated circle packings for a given $n \geq 2$ integer.

Formal description of Problem 2.4:

Definition 2.8. $A'(M, \sigma_n) \in A'_{\sigma_n}$ *is an* associated point arrangement *with the minimal pairwise distance* M *in the square* $[0, \sigma_n]^2$, *where* $A'_{\sigma_n} = \{((x_1, y_1), \ldots, (x_n, y_n)) \in [0, \sigma_n]^2 \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq M^2\ (1 \leq i < j \leq n)\}$. $A'(M, \sigma_n) \in A'_{\overline{\sigma}_n}$ *is an* optimal associated point arrangement, *if* $\overline{\sigma}_n = \min\limits_{A'_{\sigma_n} \neq \emptyset} \sigma_n$.

Problem $\mathcal{P}_4^n$. Determine the optimal associated point arrangements for a given $n \geq 2$ integer.

Theorem 2.9. *The Problems* $\mathcal{P}_1^n$, $\mathcal{P}_2^n$, $\mathcal{P}_3^n$, *and* $\mathcal{P}_4^n$ *are equivalent in the sense that, if someone is able to solve one of the problem types for a fixed* $n \geq 2$ *integer, then this solution yields the solutions of all the other problem types. That is, for each* n *the optimal solutions of the particular problems can be derived from each other.*

The theorem will be proved through four lemmas, each of them giving the equivalence of two different problems. First, we prove that the circle centres of a $P(r_n, S)$ optimal circle packing result in an $A(m_n, \Sigma)$ optimal point arrangement. Then we show that the circles drawn around the points of an $A(m_n, \Sigma)$ optimal point arrangement with a proper radius result in a $P'(R, s_n)$ optimal associated circle packing. In the next step, we prove that circle centres of a $P'(R, s_n)$ optimal associated circle packing result in an $A'(M, \sigma_n)$ optimal associated point arrangement. Then we show that the circles drawn around the points of an $A'(M, \sigma_n)$ optimal associated point arrangement with a proper radius result in a $P(r_n, S)$ optimal circle packing.

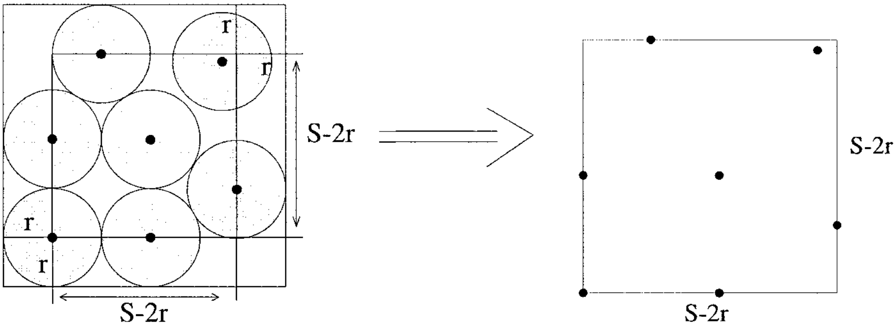

Fig. 2.1. Each circle packing corresponds to a point arrangement.

Lemma 2.10. *Let $P(r_n, S)$ be an optimal circle packing. Then the centres of the circles correspond to an $A(m_n, \Sigma)$ optimal point arrangement with $\Sigma = S - 2r_n$, $m_n = 2r_n$.*

PROOF. Assume the opposite of the statement of the lemma, i.e. that $A(2r_n, S - 2r_n)$ is not optimal. Then there exists an $A(m'_n, S - 2r_n)$ point arrangement with $m'_n > 2r_n$. Create a circle packing from $A(m'_n, S - 2r_n)$ by drawing a circle of radius $m'_n/2$ from each point of the packing (see Figure 2.1). Clearly, each such circle is located in a square of side $S - 2r_n + m'_n$. Reduce this square to a square of side S, using the midpoint of the square as the centre of the transformation. The transformation changes the common radius of the circles to

$$\frac{m'_n S}{2(S - 2r_n + m'_n)}.$$

$P(r_n, S)$ is an optimal circle packing, thus

$$r_n \geq \frac{m'_n S}{2(S - 2r_n + m'_n)}$$

holds, from which we get $(2r_n - m')(S - 2r_n) \geq 0$. Since it is easy to see that $S - 2r_n > 0$ holds for all $n \geq 2$, we obtain $2r_n - m' \geq 0$, but this contradicts the original assumption that $m' > 2r_n$. This contradiction completes the proof. □

Lemma 2.11. *Let $A(m_n, \Sigma)$ be an optimal point arrangement. Then the circles drawn around the points with a common radius of $R = m_n/2$ form a $P'(R, s_n)$ optimal associated circle packing with $s_n = \Sigma + m_n$.*

PROOF. Assume that the $P'(m_n/2, \Sigma + m_n)$ associated circle packing is not optimal. Then there exists a $P'(m_n/2, s'_n)$ associated circle packing with $s'_n < \Sigma + m_n$. The centres of this latter packing are located in a square of side $s'_n - m_n$. Enlarge this square to a square of side Σ, using the midpoint of the square as the centre of the transformation. The enlargement changes the minimal pairwise distance between the circle centres to

$$\frac{m_n \Sigma}{s'_n - m_n}.$$

Since $A(m_n, \Sigma)$ is an optimal point arrangement,

$$m_n \geq \frac{m_n \Sigma}{s'_n - m_n}$$

holds. Using the obvious $m_n > 0$ condition, we can divide both sides by m_n, and after rearrangement we obtain $s'_n - m_n \geq \Sigma$. But this contradicts the assumption $s'_n < \Sigma + m_n$. □

Lemma 2.12. *Let $P'(R, s_n)$ be an optimal associated circle packing. Then the centres of the circles correspond to an $A'(M, \sigma_n)$ optimal associated point arrangement with $M = 2R, \sigma_n = s_n - 2R$.*

PROOF. Assume that $A'(2R, s_n - 2R)$ is not optimal. Then there exists an $A'(2R, \sigma'_n)$ associated point arrangement for which $\sigma'_n < s_n - 2R$. Create a circle packing from this latter arrangement by drawing a circle of radius R around each point. These circles are located in a square of side $\sigma'_n + 2R$. Since $P'(R, s_n)$ is an optimal associated circle packing, $s_n \leq \sigma'_n + 2R$, which contradicts our original assumption $\sigma'_n < s_n - 2R$. □

Lemma 2.13. *Let $A'(M, \sigma_n)$ be an optimal associated point arrangement. Then the circles drawn around the points with a common radius of $r_n = M/2$ form a $P(r_n, S)$ optimal circle packing with $S = \sigma_n + M$.*

PROOF. Assume that the $P(M/2, \sigma_n + M)$ circle packing is not optimal, that is, there exists a $P(r'_n, \sigma_n + M)$ circle packing with $r'_n > M/2$. The centres of this latter packing are located in a square of side $\sigma_n + M - 2r'_n$. Reduce this square (using the midpoint of the square as the centre of the transformation) in such a way that the minimal pairwise distance between the centres becomes M. Then the side of the reduced square is

$$\frac{M(\sigma_n + M - 2r'_n)}{2r'_n}.$$

Since $A'(M, \sigma_n)$ is an optimal associated point arrangement, we obtain

$$\sigma_n \leq \frac{M(\sigma_n + M - 2r'_n)}{2r'_n},$$

from which, after rearrangement, we get $0 \leq (\sigma_n + M)(M - 2r'_n)$. The first term on the right-hand side is positive, which yields $M - 2r'_n \geq 0$, but this contradicts the assumption $r'_n > M/2$. □

Table 2.1. Relations between the parameters of the problems.

	$P(r_n, S)$	$A(m_n, \Sigma)$
$P(r_n, S)$	1	$r_n = \frac{Sm_n}{2(m_n+\Sigma)}$
$A(m_n, \Sigma)$	$m_n = \frac{2\Sigma r_n}{S-2r_n}$	1
$P'(R, s_n)$	$s_n = \frac{RS}{r_n}$	$s_n = \frac{2R(m_n+\Sigma)}{m_n}$
$A'(M, \sigma_n)$	$\sigma_n = \frac{M(S-2r_n)}{2r_n}$	$\sigma_n = \frac{M\Sigma}{m_n}$

Table 2.2. Relations between the parameters of the problems.

	$P'(R, s_n)$	$A'(M, \sigma_n)$
$P(r_n, S)$	$r_n = \frac{RS}{s_n}$	$r_n = \frac{MS}{2(M+\sigma_n)}$
$A(m_n, \Sigma)$	$m_n = \frac{2R\Sigma}{s_n-2R}$	$m_n = \frac{M\Sigma}{\sigma_n}$
$P'(R, s_n)$	1	$s_n = \frac{2R(M+\sigma_n)}{M}$
$A'(M, \sigma_n)$	$\sigma_n = \frac{M(s_n-2R)}{2R}$	1

Moreover, of course, the transformed circle packings and point arrangements used in the previous proofs are in shifted squares, where the left lower corner of a square is in the (0,0) point.

Definition 2.14. *The density of a circle packing $P(r_n, S)$ is given by the formula*

$$d_n(r_n, S) = \frac{nr_n^2\pi}{S^2}.$$

Since the density of a circle packing is a quadratic function of the radius r_n, the following problem formulation is equivalent (in the sense of Theorem 2.9) to the Problems $\mathcal{P}_i^n$, $1 \le i \le 4$:

Problem $\mathcal{P}_5^n$. Determine the *densest* $P(r_n, S)$ circle packings for a given $n \ge 2$ integer.

Corollary 2.15. *The relations between the parameters of the circle packings, point arrangements, associated circle packings, and associated point arrangements* derived from each other *are the ones listed in Tables 2.1 and 2.2.*

PROOF. Each entry of Tables 2.1 and 2.2 is a straightforward consequence of the transformations used in the proofs of Lemmas 2.10 to 2.13. □

In the sequel, the Problems $\mathcal{P}_1^n$, $\mathcal{P}_2^n$, and $\mathcal{P}_5^n$ will be investigated *in the unit square*. (Obviously, one can fix the square this way without the loss of generality, since the different domain squares can be transformed to each other without affecting the structures of the packings.)

In the following, we consider two packings to be *identical*, if they can be transformed to each other by applying symmetry transformations or index permutations. Note that this consideration is obvious from a *geometrical point of view*. However, as we shall see later, one of the main difficulties the numerical methods have to cope with is finding one configuration and avoiding the other identical configurations.

Definition 2.16. *Let us suppose that there is a given solution of Problem (2.1) (or the equivalent ones (2.2)–(2.4)). We say that* a circle is free (or a rattler) *if its centre can be moved towards a positive distance point without causing the others overlap.*

Definition 2.17. *We say, that*

- *a circle is* fixed *if it isn't a free circle,*
- *a packing is* rigid *if all of its circles are fixed.*

We should point out here that when a packing contains one or more free circles, then the solution is obviously not unique. Moreover, the possible locations of the centre of any free circles form a non-empty interior and connected set. In the present volume the number of contacts will be denoted by c_n, and the number of free circles by f_n. In each figure a contact will be represented by a short line section and free circles will be indicated by dark shading.

2.2 Mathematical programming models

As we have already mentioned, the circle packing problem was originally a geometrical problem; on the other hand, it can also be viewed as a continuous global optimization problem.

In this book, we will usually refer to the following *bound-constrained, max-min optimization model* of the point arrangement problem in the unit square (that is, Problem 2.2 or Problem $\mathcal{P}_2^n$):

$$\begin{aligned} &\max_{x_i,y_i} \quad \min_{1\le i<j\le n} \sqrt{(x_i-x_j)^2+(y_i-y_j)^2} \\ &\text{subject to} \quad 0\le x_i,y_i\le 1 \qquad (1\le i\le n), \end{aligned} \tag{2.1}$$

where x_i, y_i are the coordinates of the i-th point. The goals are to find the global optimum of the problem (the maximum of the minimal pairwise distance of the points), *and also*, to find the global optimizer(s), that is, the respective locations of the points.

Besides (2.1), the mathematical programming models of Problem $\mathcal{P}_2^n$ can be represented in various different ways, for instance:

a) *as a continuous, nonlinear, inequality-constrained global optimization problem* [66]:

$$\max_{x_i, y_i} \ t,$$

subject to

$$\sqrt{(x_i - x_j)^2 - (y_i - y_j)^2} \geq t \qquad (1 \leq i < j \leq n),$$

$$0 \leq x_i, y_i \leq 1 \qquad (1 \leq i \leq n).$$

b) *as a DC programming problem* [48]:

A DC (difference of convex functions) programming problem is a mathematical programming problem, where the objective function is given by the difference between two convex functions. In [48], the *minimal pairwise squared distance* is treated as the objective function, and a DC decomposition of this function is given. That is, the point arrangement problem is formulated as

$$\max_{\substack{z_j \in [0,1]^2, \\ 1 \leq j \leq 2n}} \ \min_{1 \leq i < k \leq n} \left\{ (z_i - z_k)^2 + (z_{n+i} - z_{n+k})^2 \right\},$$

with

$$z = (x_1, \ldots, x_n, y_1, \ldots, y_n),$$

which is obviously equivalent to the original Problem $\mathcal{P}_2^n$. Using the additional notation

$$J = \{1, \ldots, 2n\},$$

$$J_{ik} = \{i, k, n+i, n+k\},$$

the objective function can be written as

$$\min_{1 \leq i < k \leq n} \left\{ (z_i - z_k)^2 + (z_{n+i} - z_{n+k})^2 \right\}$$

$$= \min_{1 \leq i < k \leq n} \left\{ (z_i - z_k)^2 + (z_{n+i} - z_{n+k})^2 - 2\sum_{j=1}^{2n} z_j^2 + 2\sum_{j=1}^{2n} z_j^2 \right\}$$

$$= 2\sum_{j=1}^{2n} z_j^2 + \min_{1 \leq i < k \leq n} \left\{ -2 \sum_{j \in J \setminus J_{ik}} z_j^2 - (z_i + z_k)^2 - (z_{n+i} + z_{n+k})^2 \right\}$$

$$= 2\sum_{j=1}^{2n} z_j^2 - \max_{1 \leq i < k \leq n} \left\{ 2 \sum_{j \in J \setminus J_{ik}} z_j^2 + (z_i + z_k)^2 + (z_{n+i} + z_{n+k})^2 \right\}.$$

Thus, the objective function can be specified as the difference of two *convex* functions $g : \mathbb{R}^{2n} \to \mathbb{R}^+$ and $h : \mathbb{R}^{2n} \to \mathbb{R}^+$:

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

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

c) *as an all-quadratic optimization problem (or QCQP – Quadratically Constrained Quadratic Problem)*:

The general form of an all-quadratic optimization problem [97] is

$$\min\ \left[x^T Q^0 x + (d^0)^T x\right],$$

subject to

$$x^T Q^l x + (d^l)^T x + c^l \le 0 \qquad l = 1, \ldots, p$$

$$x \in P,$$

where Q^l $(l = 0, \ldots, p)$ are real $(n+1) \times (n+1)$-dimensional matrices, d^l $(l = 0, \ldots, p)$ are real $(n+1)$-dimensional vectors, c^l $(l = 1, \ldots, p)$ are real numbers, p is the number of constraints, and P is a polyhedron.

Problem $\mathcal{P}_2^n$ can be written as a special case of the all-quadratic optimization problem with a linear objective function in the following way:

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

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

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

$$1 \le i, j \le 2n+1,$$

$$1 \le l' < l'' \le n.$$

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}).

The above models may be of interest for mathematical programming solvers as very hard optimization problems. To demonstrate the expected difficulty of the problem, we might mention the example of the sophisticated, interval arithmetic-based global optimization solver GlobSol [51], which was unable to return sufficient results even for the case of packing five circles/points with reasonable parameter settings [125]. However, as the previous and current numerical studies show, approaches that use not only optimization models, but also the geometrical aspects of the problem are often more effective (cf. the methods of Chapters 7 and 8). Hence in the next chapter some of these useful geometrical characteristics will be investigated in detail.