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Packing up to 50 Equal Circles in a Square

K. J. Nurmela and P. R. J. Östergård*

Department of Computer Science, Helsinki University of Technology,
FIN-02150 Espoo, Finland
Kari.Nurmela@hut.fi
Patric.Ostergard@hut.fi

Abstract. The problem of maximizing the radius of n equal circles that can be packed into a given square is a well-known geometrical problem. An equivalent problem is to find the largest distance d, such that n points can be placed into the square with all mutual distances at least d. Recently, all optimal packings of at most 20 circles in a square were exactly determined. In this paper, computational methods to find good packings of more than 20 circles are discussed. The best packings found with up to 50 circles are displayed. A new packing of 49 circles settles the proof that when n is a square number, the best packing is the square lattice exactly when $n \leq 36$.

1. Introduction

The problem to be discussed in this paper is one that many of us have encountered in everyday life: How many bottles of a given size can be packed into a square box of a given size and how should this be done? The problem can be geometrically expressed as follows: determine r_n, the maximum radius of n nonoverlapping circles in a unit square. By solving the latter problem, the former problem is also solved. Namely, the radius of the bottles is divided by the side of the box and this quotient is compared with the values in the nonincreasing series r_n. The largest n for which r_n is greater than the quotient is the demanded solution.

There is another equivalent formulation of the problem, which we adopt in this paper: maximize the minimum distance between n points in a unit square. We denote this value

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by d_n, and have the following relation between r_n and d_n:

$$r_n = \frac{d_n}{2(d_n + 1)}.$$

A packing corresponding to d_n (or r_n) is called an *optimal packing*. For some small values of n and some n where the optimal packing has a nice structure, exact values of d_n have been proved by hand. Recently exact values of d_n were determined for n up to 20 [4] (as explicit values or as the smallest root of a polynomial equation). The proofs involve extensive use of computers; as of today this is about as far as we can come with that approach. However, even if we are not able to find the exact values of d_n for larger values of n, we can try to find as good packings as possible, thereby lower-bounding d_n. In this research we try to find such good packings by computer search.

The paper is outlined as follows. Old results on the problem are surveyed in Section 2. In Section 3 we consider how computers can be used in the search for packings. We first discuss methods that have been mentioned in the literature; thereafter our approach is treated in detail. The best packings found are displayed and discussed in Section 4.

2. Old Results

The problem of packing circles into different geometrical shapes has received much attention since the seminal work of Fejes Tóth [7]. A recent survey of results and problems still open can be found in [3]. One of the most natural and most studied of these problems is that of packing circles in a square.

This problem was solved for up to nine circles in the 1960s by Graham, Meir and Schaer; the proofs of these cases have been reported in [12], [18], [20], and [22]. The proofs for $n \le 5$ are easy, whereas the cases $6 \le n \le 9$ require more elaborate mathematical tools. For example, for $n = 5$ we can divide the square into four subsquares as indicated in Fig. 1. Now at least one square must contain two points due to the pigeonhole principle, so the length of the diagonals in the subsquares ($\sqrt{2}/2$) upper-bounds d_5. This is also a lower bound, since in the solution in Fig. 1 (which is the only possible optimal solution), this is the smallest distance between two points. Thereby $d_5 = \sqrt{2}/2$.

For $n \ge 10$, only the optimal packings of 14 [26], 16 [24], 25 [25], and 36 [10] circles have been proved by hand.

Recently, de Groot *et al*. [5] used computers to find good packings for $n \le 22$. They

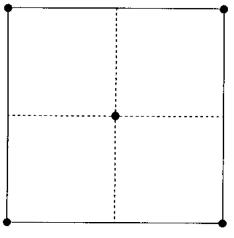

Fig. 1. Optimal packing of five points in a square.

were later even able to give a computer proof of the best packings with up to 20 circles [4], [15]. In particular, this ended a series of articles on packings of 10 circles (and conjectures about the optimality of the respective packings); see [8], [19], [21], [23], and some further references in [5]. Furthermore, for n up to 27 and for some sporadic values of n greater than 27, good packings were given by Goldberg in [8].

3. Computer Search for Packings

Computers have certainly played a central role in many searches for packings. Unfortunately, this is very seldom mentioned and even if it is, only brief details are given. It is very natural (for a given n) to define the problem as an optimization problem. A solution of this optimization problem can then be a set of either n scattered points or n centers of circles in a unit square. We now first take a look at what can be found in the literature and thereafter discuss our approach.

3.1. *Earlier Approaches*

In [5] the problem is considered as a maximizing problem. A solution is a set of centers of circles in the unit square. The maximum possible radius for circles with these centers that do not overlap and are within the boundaries of the square is easily calculated by considering the distances between the points and between the points and the boundaries. This is then the value that is maximized by moving the centers of the circles.

The optimization methods used in [5] are the simplex (polytope) algorithm and the quasi-Newton BFGS algorithm. Further details on the implementation of these methods are omitted in the paper. For $n \leq 20$, they fail to find optimal packings for $n = 14, 15, 17$. In the papers where the optimality of packings with $n \leq 20$ is proved [4], [15], the authors report a better performance of a (stochastic) Langevin equation formalism than of the two aforementioned methods; see also [6].

Mollard and Payan [13] found good packings of 11, 13, and 14 circles that improved on the results in [8] by using their own Cabri-Géomètre geometry software. They were further able to improve the packing of 13 circles by hand.

Graham and Lubachevsky [9] used an event-driven simulation algorithm to pack circles in an equilateral triangle. The algorithm simulates the idealized movement of billiard balls inside a triangular box; the size of the balls is increased slowly until the movement is blocked.

Clare and Kepert [2] and Kottwitz [11] found good packings of circles on a sphere by computer. They did not consider the minimum pairwise distance between points, but minimized the total potential energy of repulsion. The optimization methods used were variants of the Fletcher–Powell–Davidon quasi-Newton method [17] and a simple gradient method combined with Newton's method, respectively. The approximate solutions then found were refined by identifying the points at minimum pairwise distance and solving iteratively a system of equations using Newton–Raphson methods. This method was recently generalized for searching for higher-dimensional spherical codes in [14], where some packings of [11] were also improved by using simple packing heuristics combined with simulated annealing.

3.2. *Our Approach*

Our approach is closely related to that of [2] and [11]. It is based on the minimization of the energy function

$$E = \sum_{1 \le i < j \le n} \left(\frac{\lambda}{d_{ij}^2} \right)^m, \tag{1}$$

where d_{ij} is the distance between points i and j representing the centers of the circles, λ is a scaling factor to prevent numerical overflows, and m is a positive integer.

We transform the constrained optimization problem into an unconstrained one by using the simple coordinate transformation defined as follows:

Let (x_i, y_i) be the center of circle i. Define

$$\begin{aligned} x_i &= \sin(\tilde{x}_i), \\ y_i &= \sin(\tilde{y}_i), \end{aligned}$$

where $\tilde{x}_i$ and $\tilde{y}_i$ range over $\mathbb{R}$. We now have an unconstrained optimization problem in variables $\tilde{x}_i, \tilde{y}_i$ $(1 \le i \le n)$, where the coordinates of the centers of the circles fulfill $-1 \le x_i \le 1$, $-1 \le y_i \le 1$ as required (the square, of course, need not be a unit square).

The energy function (1) is twice continuously differentiable (except where two points coincide). In the optimization we use (for each value of m) a hybrid algorithm that consists of a simple steepest-descent algorithm with Goldstein–Armijo backtracking line search in the beginning and a modified Newton method in the end.

We start with a moderately small value of m (in the range $10 \le m \le 100$) and find a local optimum of the energy function. Then we double the value of m and repeat the optimization step. As m tends to infinity, only the smallest distances between the centers of the circles have an effect on the energy of the configuration. In some cases in this work we used as large final values for m as 10^{50}, although optimization can usually be ended when m reaches 10^6. For each n, at least 50 optimization runs were performed with random initial solutions.

The scaling factor λ needs to be recalculated from time to time during the optimization run, because otherwise the cost becomes impractically small, especially with large m. We adjust λ after each optimization step by setting it equal to the square of the length of the shortest distance between two points of the packing.

The packing resulting from the optimization run can be further improved by constructing a system of nonlinear equations corresponding to the contacts between the circles and between the circles and the boundary and by solving that system numerically. We first sort all the distances between the points into increasing order and find the location where the distance shows a sudden increase. The distances up to this location are assumed to be equal, and points very close to the boundary are assumed to be on the boundary. We then form a system of equations from these assumptions. This procedure can be done automatically by giving two threshold values, one for the largest admitted difference between a candidate distance and the shortest distance of the configuration, and the other for the largest admitted distance between a point and the boundary.

In most cases the system of equations has a solution, which can be found numerically using, for example, a modified Newton–Raphson method [1]. However, in a few cases the

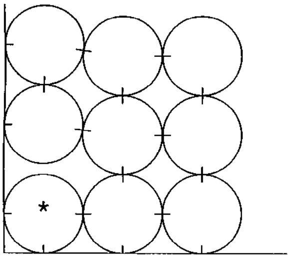

Fig. 2. Poor local optimum.

gaps between the circles or between the circles and the boundary are so narrow that this method results in a system of equations for which no solution exists, indicating that one or more equations should be removed from the system. On the other hand, if some contacts between circles are not included in the system, the solution of the system may have circles overlapping. In such cases we can try to make the set of shortest distances more clearly visible by continuing the optimization to locate the optimum more accurately. If this strategy fails, we finally remove and add equations through trial and error until a solvable system representing a nonoverlapping packing is found.

Sometimes the packing resulting from an optimization run has a circle that is in contact with the boundary and that can be moved toward the center of the square without causing overlap with any other circles. In Fig. 2 this situation occurs with the circle marked with a star. The arrangement, which is a local optimum of the energy function (1), can be further improved by moving the circle away from the boundary slightly and then continuing the optimization with a relatively large m.

Starting with a random initial solution, our implementation of the optimization algorithm performs an optimization run for 50 circles in about 20 minutes of CPU-time on a current workstation. After the structure of the packing has been detected, the numerical solution to the corresponding system of equations can be found in a few seconds with a mathematical software supporting arbitrary-precision numbers.

4. Best Packings Found

The best packings found for $21 \leq n \leq 50$ are displayed in Fig. 3. The nine packings for $n = 22, 23, 24(a), 25, 27, 30, 36, 39$, and 42 are old [5], [8], [10]—all other packings are new. The packing for $n = 21$ improves on the results in [5], and several packings improve on the results in [8]; see also [3]. There are three different best known packings of 24 circles and three packings of 35 circles. (A similar situation occurs with 17 circles—there are two different optimal such packings [15].) Only the packings of 25 and 36 circles have been proved optimal [10], [25].

In Table 1 we tabulate some properties of the packings. In addition to the diameter d of the circles, we show the density of the packing (that is, the area of the circles divided by the area of the square), the number of loose circles in the structure, the total number of contacts between the circles and between the circles and the boundary, and the order of the symmetry group [16].

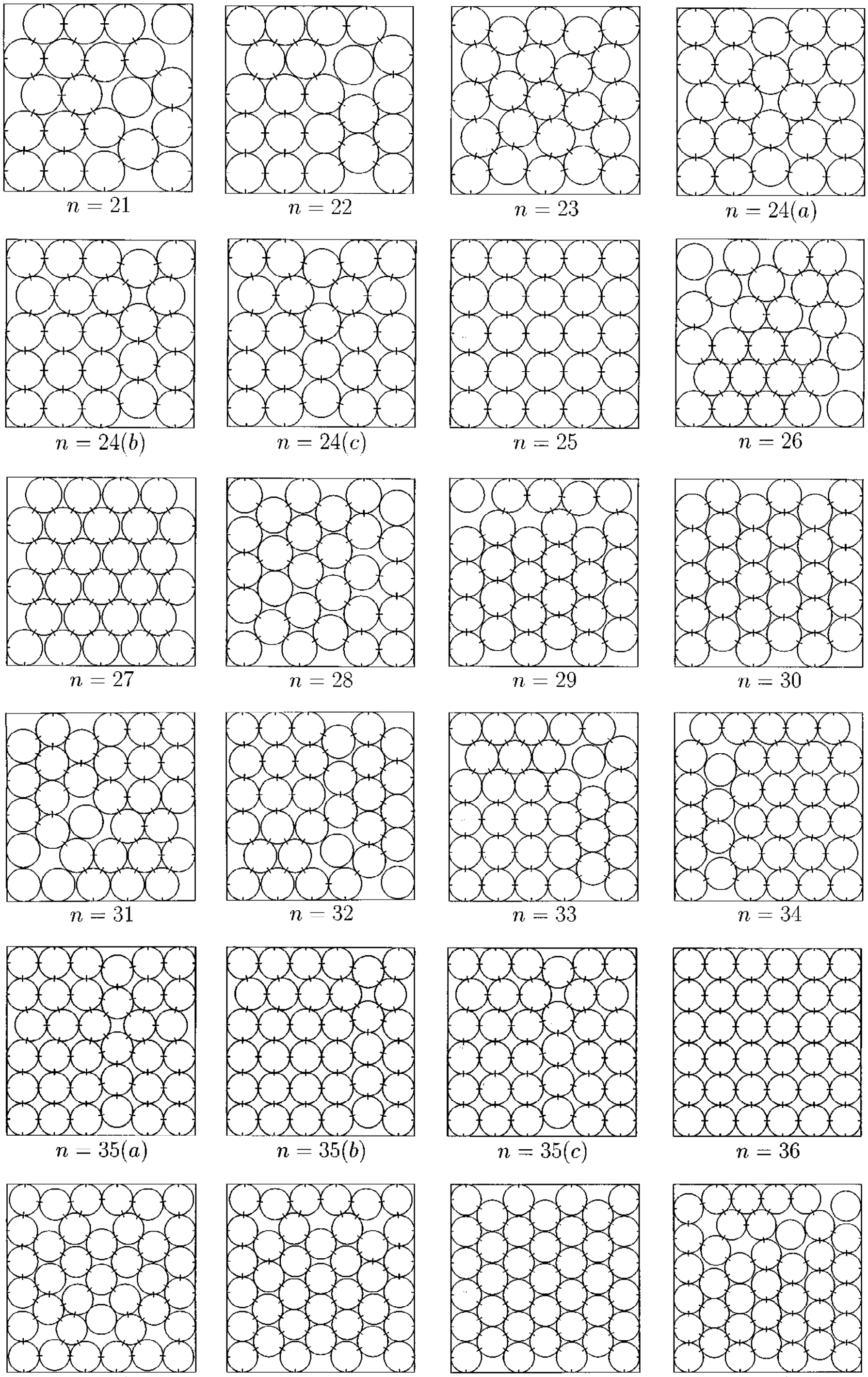

Fig. 3. Best known packings for $21 \leq n \leq 50$.

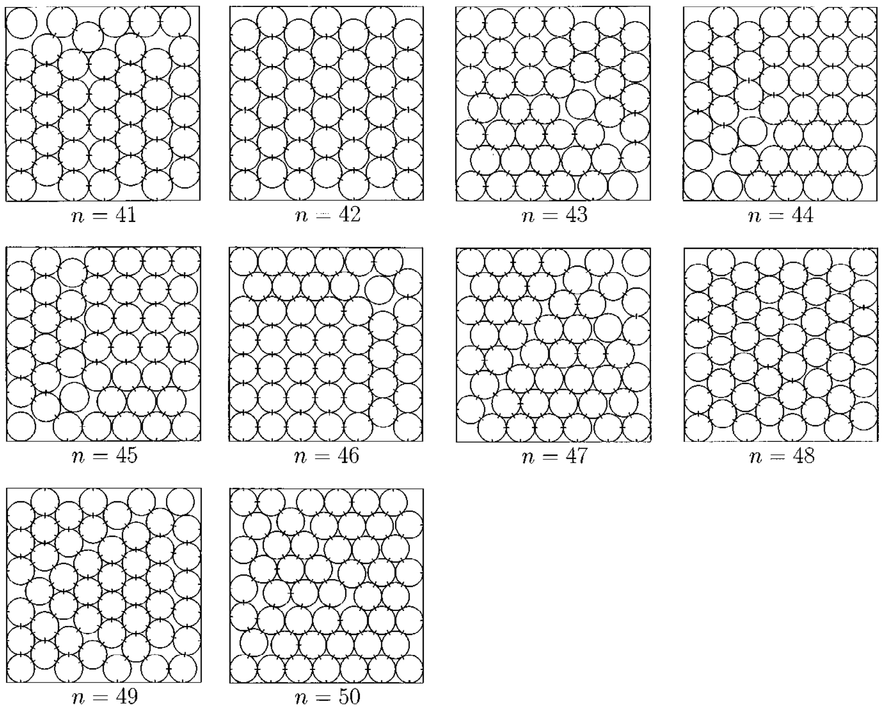

Fig. 3 (*continued*)

Some similarities can be found among the best known packings. For $n = k^2 - 1$, best known packings of 8, 15, 24, and 35 (but not 48) circles have similar structure. For $n = k^2 - 3$, that is also the case for packings of 22, 33, and 46 (but not 13) circles. Other examples are the cases $n = k^2 + k$, and $n = (2k^2 + k)/2$ for k even. For $n = k^2$, the optimal packing for $n \leq 36$ is the square lattice. The new packing for $n = 49$ found in this work concludes the proof that, for $n = k^2$, the square lattice packings are optimal exactly for $n \leq 36$. This disproves a conjecture of Wengerodt (who found denser packings for $n \geq 64$) that the square lattice packings are optimal for $n \leq 49$; see [3] and its references.

Some packings in Fig. 3 are almost symmetric (for example, the packings of 22, 33, and 46 circles); the packings are obtained by breaking the symmetry slightly. Two more examples where an almost symmetric packing is better than the nearby symmetric one can be found in the packings of 37 and 44 circles in this work. The packing of 37 circles is interesting for two reasons: it does not contain any corner circles, and 37 is the largest number of circles for which the best known packing has lower density than that of a square lattice packing. The packing of 44 circles very much resembles that of 31 circles and is possibly not optimal.

In some packings there are very narrow gaps between the circles or between the circles and the boundary. In the packing of 40 circles, the gap between one of the circles and the boundary is about $3 \cdot 10^{-15}$ times the diameter of the circles. The width of some of

Table 1. Properties of packings.

n	d	Density	Loose circles	Contacts	Order of symmetry group
21	0.271811687	0.753355227	2	40	1
22	0.267958402	0.771680112	1	43	1
23	0.258819045	0.763631032	0	56	4
24	0.254333095	0.774963260	0	56	8(a), 2(b), 2(c)
25	0.250000000	0.785398163	0	60	8
26	0.238734757	0.758469090	2	56	1
27	0.235849528	0.772311456	0	55	2
28	0.230534597	0.771849233	2	53	1
29	0.226882901	0.778906242	1	65	1
30	0.224502965	0.792019026	0	65	2
31	0.217547292	0.777297479	4	55	2
32	0.213082353	0.775450816	2	61	1
33	0.211328384	0.788852304	1	65	1
34	0.205021908	0.772999930	1	71	1
35	0.202763601	0.781227213	0	80	2(a), 2(b), 1(c)
36	0.200000000	0.785398163	0	84	8
37	0.196238101	0.782029274	1	73	1
38	0.195342304	0.797042557	0	77	2
39	0.194365063	0.811179027	0	80	4
40	0.188175077	0.787976383	2	79	1
41	0.186099512	0.792723899	1	100	1
42	0.184277072	0.798684279	0	90	2
43	0.180132785	0.786832179	2	83	1
44	0.178639224	0.793842645	4	82	1
45	0.175515450	0.787909640	2	87	1
46	0.174459361	0.797187132	1	91	1
47	0.171107017	0.788007250	2	95	1
48	0.169382110	0.790957782	0	101	1
49	0.167386077	0.791216990	1	120	1
50	0.166454626	0.799679429	0	104	1

the gaps between the circles in the packing of 47 circles is less than $3 \cdot 10^{-11}$ times the diameter of the circles.

The system of equations corresponding to the structure of a packing can be reduced to a polynomial equation—of one variable—that has a zero at the diameter of the circles. In some cases the polynomials have been constructed [4], but large irregular packings have so complex polynomials that there is little hope of constructing them. The diameter of the circles of a large packing can be solved exactly only in special cases.

Finding a numerical solution to the system of equations corresponding to the proposed structure of the packing does not guarantee that the structure exists, because of the finite precision in calculations. The systems of equations in this work were solved numerically so that the overlaps of, or gaps between, contacting circles in the conjectured structure are less than 10^{-33}; it is thus highly improbable that any of these structures turns out to be nonexistent.

The densities of the best known packings of 1–50 circles are plotted in Fig. 4. The densities of hexagonal and square lattice packings are also shown by dotted lines. The

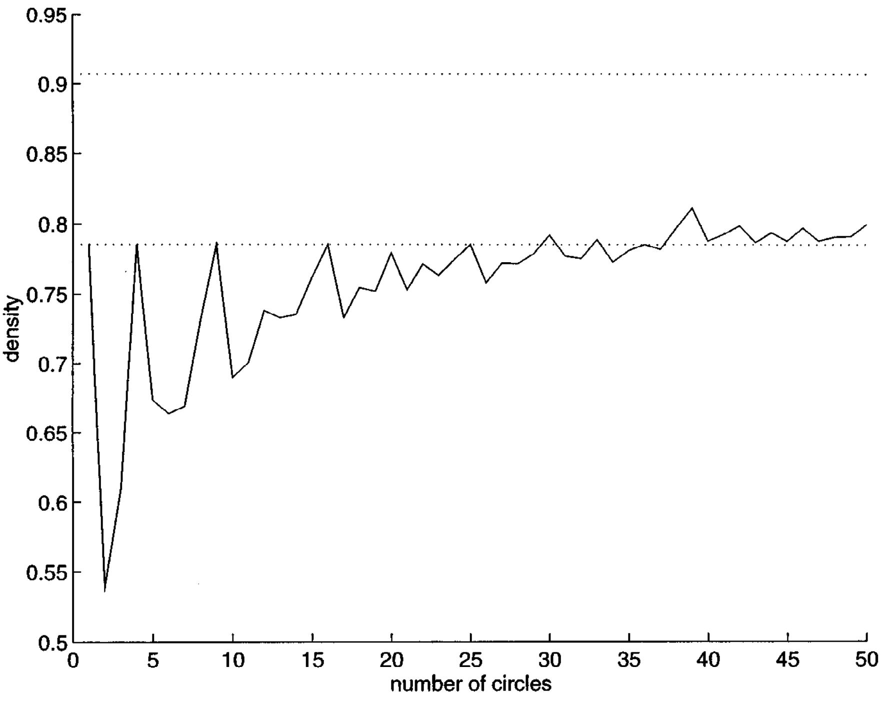

Fig. 4. Densities of best known packings.

density shows a clear tendency to increase as the number of circles increases, although the densities of all the packings in this work still remain clearly below the density of the hexagonal lattice packing—which the density approaches as n tends to infinity [7]. An open question stated in [3] is whether there are any values of n such that $d_n = d_{n+1}$. We conclude this paper by conjecturing that there are no such n.

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