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Packing equal circles in a square — bounds, repeated patterns and minimal polynomials

Results of the dissertation

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1. Introduction

The dissertation deals with the problem of the densest packing of equal circles in a square. This optimization problem, which arises from discrete geometry, has become a well-studied problem in the past decades [2, 3, 4, 5, 6, 7, 12]. Approximately 50 scientific publications have investigated it, from which will we give a short overview in the dissertation.

The dissertation studies the circle packing problem from three aspects:

a) How the numerical parameters of the optimal circle packings can be determined, such as bounds for the radius, and the density. We studied it in a theoretical way and also used computer-aided methods to find ways of improving them.

b) The kind of structuralproperties that is in the optimal and the best known circle packings have and how we might improve the theoretical lower bounds using them.

c) How we should calculate the minimal polynomials of the circle packings in a theoretical way and by a CAS (Computer Algebra System) and how they should be used for the classification of the circle packings.

The majority of the results in the dissertation are published in the articles [1, 8, 9, 10, 11] of the present bibliography.

2. The problem and its equivalent models

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

Problem $\mathfrak{P}_1^n$: Determine the optimal circle packings for $n \geq 2$.

Definition 2 $A(m_n, \Sigma) \in A_{m_n}$ is a *point arrangement* with minimal distance m_n in $[0, \Sigma]^2$, 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 $\mathfrak{P}_2^n$: Determine the optimal point arrangements for $n \geq 2$.

Definition 3 $P'(R, s_n) \in P'_{s_n}$ is an *associated circle packing* with radius R in $[0, s_n]$, where $P'_{s_n} = \{((x_1, y_1), \ldots, (x_n, y_n)) \in [0, s_n]^{2n} \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq 4R^2; x_i, y_i \in [R, s_n - R]\ (1 \leq i < j \leq n)\}$. $P'(R, s_n) \in P'_{\overline{s}_n}$ *optimal associated circle packing*, if $\overline{s}_n = \min\limits_{P'_{s_n} \neq \emptyset} s_n$.

Problem $\mathfrak{P}_3^n$: Determine the optimal associated circle packings for $n \geq 2$.

DEFINITION 4 $A'(M, \sigma_n) \in A'_{\sigma_n}$ is an *associated point arrangement* with the minimal distance M in $[0, \sigma_n]$, where $A'_{\sigma_n} = \{((x_1, y_1), \ldots, (x_n, y_n)) \in [0, \sigma_n]^2 \mid (x_i - x_j)^2 + (y_i - y_j)^2 \geq M^2 \ (1 \leq i < j \leq n)\}$. $A'(M, \sigma_n) \in A'_{\overline{\sigma}_n}$ *optimal associated point arrangement*, if $\overline{\sigma}_n = \min\limits_{A'_{\sigma_n} \neq \emptyset} \sigma_n$.

Problem $\mathfrak{P}_4^n$: Determine the optimal associated point arrangements for $n \geq 2$.

THEOREM 1 [9] *Problem $\mathfrak{P}_1^n$, $\mathfrak{P}_2^n$, $\mathfrak{P}_3^n$ and $\mathfrak{P}_4^n$ are equivalent in the sense that if $\mathfrak{P}_i^n$ can be solved for a fixed n and i, then the other $\mathfrak{P}_i^n$ can be solved for all $1 \leq i \leq 4$.*

In the dissertation the following corollary of THEOREM 1 is frequently used.

COROLLARY 1 [9] *The relations between the parameters $\overline{m}_n$, $\overline{r}_n$, $\overline{s}_n$ and $\overline{\sigma}_n$ take the following form:*

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

Since viewed the problem as an optimization problem, I decided to classify the mathematical models into problem classes suitable for mathematical programming.

This problem can be considered as

a) a continuous nonlinear constrained global optimization problem,
b) a max-min problem,
c) a DC programming problem, or as an
d) all-quadratic optimization problem [10].

3. Lower and upper bounds for the optimum values

THEOREM 2 *For every $n \geq 2$*

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

K. J. Nurmela and his coauthors [6] once published the following inequality

$$\sigma^2 + \frac{1-\sqrt{3}}{2}\sigma \leq \frac{\sqrt{3}}{2}n$$

which gives a lower bound for the number of an $A'(1,\sigma)$ associated point arrangement. Multiplying the previous inequality by $\frac{2}{\sqrt{3}}$ implies that

$$\frac{2}{\sqrt{3}}\sigma^2 + \frac{1-\sqrt{3}}{\sqrt{3}}\sigma \leq n.$$

In the proof of THEOREM 2 I proved an inequality which eliminated the linear term with the negative $\frac{1-\sqrt{3}}{\sqrt{3}}$ coefficient from this inequality, to give a better lower bound for $\overline{m}_n$.

THEOREM 3 For every $n \geq 2$

$$\overline{r}_n \leq \min\left(\frac{1}{\sqrt{2\sqrt{3}n + (4\lfloor\sqrt{n}\rfloor - 2)(2-\sqrt{3})}}, \frac{1+\sqrt{1+\frac{2}{\sqrt{3}}(n-1)}}{2n + 2\sqrt{1+\frac{2}{\sqrt{3}}(n-1)}}\right).$$

Based on THEOREM 2 and the upper bound of THEOREM 3, I found an absolute error bound for the asymptotic approximation of $\overline{m}_n$ in the PROPOSITION 1

PROPOSITION 1 *An absolute error bound for the asymptotic approximation of* $\overline{m}_n \approx \sqrt{\frac{2}{\sqrt{3}n}}$ *is*

$$\frac{2}{n-1}.$$

4. Computer-aided methods for improving lower bounds

In [1] we improved the theoretical lower bounds using a stochastic global optimization algorithm and we obtained better results for some previously known circle packings. The TAMSASS-PECS algorithm is based on the TA (Threshold Accepting) method and a modified SASS (Single Agent Stochastic Search) local search technique that is especially suited for the circle packing problem.

The TAMSASS-PECS method

Selects an initial solution s
Selects an initial value for T_h
Selects an initial standard deviation σ
while $\sigma > \sigma_{final}$ **do**
    while *All centers are not visited* **do**
        $s = MSASS(s, \sigma, T_h, NextCenter(s))$
    Decrease T_h
    Decrease standard deviation σ
return *the best found solution*

The TAMSASS-PECS algorithm starts with a pseudorandom feasible solution, which is generated in the following way: Let us divide the square for $\lceil\sqrt{n}\rceil \times \lceil\sqrt{n}\rceil$ non-overlapping tiles. The first point is located randomly at the center of the first or second tile. The following points are located at the center of a tile that is separated from the previous one by one free tile in a row order. The remaining points are randomly allocated to the free tiles (putting one point in each tile). The initial value for the T_h threshold was 0.02 and the standard deviation σ was equal to the common diameter of the tiles.

The TAMSASS-PECS algorithm tries to improve an initial point arrangement in an iterative way. At every iteration step it starts the MSASS subroutine, for each point with the same σ deviation and T_h threshold. After finishing the MSASS subroutine for each point, the σ deviation and the T_h threshold were decreased by 1%. The TAMSASS-PECS algorithm works until the σ deviation becomes smaller than a given σ_{final} value.

The MSASS subroutine

```
 1  proc MSASS(s, σ0, Th, i)
 2     var scnt := 0; fcnt := 0; Fcnt := 3; ct := 0.5; σ := σ0;
 3        while fcnt < 4 · Fcnt and scnt = 0 do
 4              σ := { ct · σ   if fcnt > Fcnt
                     { σ        otherwise
 5              Generate a random ξ with N(0, σ) distribution;
 6              s'(i) := s(i) + ξ;
 7              if f(s) − f(s') ≤ f(s)Th
 8                 then
 9                    s(i) := s'(i);
10                    scnt := scnt + 1;
11                 else
12                    s'(i) := s(i) − ξ;
13                    if f(s) − f(s') ≤ f(s)Th
14                       then
15                          s(i) := s'(i);
16                          scnt := scnt + 1;
17                       else
18                          fcnt := fcnt + 1;
19        od
20  end
```

The input parameters of the MSASS procedure are: an initial feasible solution denoted by s (which is a vector that describes the points of the arrangement), an initial σ_0 deviation value, an initial T_h threshold level and an index i of a point in the arrangement, whose location will be changed the method. Note that in line 7 and in line 13 above there is not just the $f(s) < f(s')$ condition, but also the $f(s) \leq f(s') + f(s)T_h$ condition. In the MSASS subroutine the loop will be executed until there is an improved position for the ith point or the number of the unsucessful trials is greater than 11.

Computational results

The numerical results are reliable because the PROFIL/BIAS C++ program library routine uses interval arithmetic based procedures, and hence the determined numerical values will be proven lower bounds of the optimum value.

In [1h we published circle packings up to $n = 100$ using the TAMSASS-PECS algorithm. In our results of using 5 cases our results were an improvement on the best previously known packings (for $n = 32, 37, 47, 62$ and 72).

5. Repeated patterns in circle packings

When comparing the structures of the optimal and the best known packings, we noticed some common patterns. Sometimes there exists a connection between the given structure and the number of circles. Based on this, we can classify some packings into pattern classes [8,11].

Finite pattern classes

We used the $\mathbf{PAT}(f(k))$ notation for the pattern classes and its patterns, where f: N→N is a function and $f(k)$ is the number of circles ($n = f(k)$).

In the dissertation, the following pattern classes are elaborated on [8,11]:

a) a $\mathbf{PAT}(k^2 - l)$ $(l = 0, 1, 2)$ pattern classes,
b) a $\mathbf{PAT}(k(k + 1))$ pattern class,
c) a $\mathbf{PAT}(k^2 + \lfloor k/2 \rfloor)$ pattern class.

Approximating the structure of the number of $k^2 - l$ $(l = 3, 4, 5)$ circle packings, I introduced and studied the

d) $\mathbf{STR}(k^2 - l)$ $(l = 3, 4, 5)$ structure classes [8] as well.

The most intense study has been on grid packings, since this pattern class probably contains some optimal circle packing sequences that are infinite.

A conjectured inifinite pattern class

K. J. Nurmela and his coauthors [6] published the following conjecture in 1999: Let us consider the simple continued fraction representation of $\frac{\sqrt{3}}{3}$, and let us consider that subsequence of the approximation sequences that consists of every second fraction of the previous sequence. Now let us associate the $\frac{p}{q}$ elements of this subseries with a point arrangement in the following way: Let us divide the two perpendicular sides of the square for p and q into equal parts and let us draw lines parallel to the sides of the dividing points. Then we will have $p \times q$ rectangles. Place one point in the left corner of the square (in the point (0,0)) and place a new point in every second rectangular gridpoint. It is not too hard to see that in this way we can find room for

$$\left\lceil \frac{(p+1)(q+1)}{2} \right\rceil$$

points. The conjecture is that every point arrangement which arises from the previous subseqence will be optimal. For obvious reasons I will call these packings grid packings.

Grid packings

Suppose that p and q are positive integers, where $\frac{p}{q} \in \left(\frac{\sqrt{3}}{3}, \sqrt{3}\right)$. Let $[[p,q]]$ represent a grid packing, and let $\frac{p}{q}$ is in the $\left(\frac{\sqrt{3}}{3}, \sqrt{3}\right)$ interval. Now let GP be a set of $[[p,q]]$ pairs (GP= 'Grid Packing').

Proposition 9 [9] *In GP the following operations are well definied*

$$[[p_1, q_1]] + [[p_2, q_2]] := [[p_1 + p_2, q_1 + q_2]],$$
$$\lambda[[p, q]] := [[\lambda p, \lambda q]],$$

where λ positive integer number, and if $p_2 < p_1$ and $q_2 < q_1$ then

$$[[p_1, q_1]] - [[p_2, q_2]] := [[p_1 - p_2, q_1 - q_2]],$$

and if $\frac{p}{\lambda}$ and $\frac{q}{\lambda}$ is an integer, then

$$\frac{1}{\lambda}[[p, q]] := [[\frac{p}{\lambda}, \frac{q}{\lambda}]].$$

Conjectured optimal grid packing series

The above grid packing sequence may have a recursion relation as well:

Proposition 10 [8] *Let us consider the subseries of the approximating series of the periodical simple continued fraction representation of $\frac{\sqrt{3}}{3}$ which consists of every second fraction of the sequence. These grid packings can be generated by using the following recursion relations:*

$$S_1 = [[1,1]], \quad S_2 = [[3,5]],$$
$$S_n = 4S_{n-1} - S_{n-2} \quad (n \geq 3).$$

The density of the packings of the elements of this series is very high and asymptotically tends to $\frac{\pi}{\sqrt{12}}$ (which is the density of the densest packing of equal circles in the plane). Based on the proved optimal packings and the best known packings I obtained four other circle packing sequences, which I hypothesize will contain only optimal elements.

PROPOSTION 12 *Let us consider the* $\{A_i\}, \{B_i\}, \{C_i\}, \{D_i\}$ *grid packing sequences, where* $(i \in \mathbb{Z}^+) : A_i := 2S_i, B_i := S_i + S_{i+1}, C_i := B_i/2, D_i := C_i + [3,5]$ *In this case* $\lim_{i\to\infty} d_{Xi} = \frac{\pi}{\sqrt{12}}$, *where* $X \in \{S, A, B, C, D\}$ *and* d_{Xi} *denotes the density of the circle packings.*

An improved lower bound using pattern classes

The pattern classes are useful for improving the theoretical lower bounds.

THEOREM 4 [11] *The* $\overline{m}_n$ *value is not less than*

$$\max\left(L_1(n), L_2(n), L_{3a}(n), L_{3b}(n), L_4(n), L_5(n), L_6(n), L_7(n), L_8(n), L_9(n)\right),$$

where

$$\begin{aligned}
L_1(n) &= \frac{1}{\lceil\sqrt{n}\rceil - 1}, \\
L_2(n) &= \frac{1}{\lceil\sqrt{n+1}\rceil - 3 + \sqrt{2+\sqrt{3}}}, \\
L_{3a}(n) &= \frac{1}{\lceil\sqrt{n+2}\rceil - 2 + \frac{1}{2}\sqrt{3}}, \\
L_{3b}(n) &= \frac{1}{\lceil\sqrt{n+2}\rceil - 5 + 2\sqrt{2+\sqrt{3}}}, \\
L_4(n) &= \frac{1}{\lceil\sqrt{n+3}\rceil - 3 + \sqrt{3}}, \\
L_5(n) &= \frac{1}{\lceil\sqrt{n+4}\rceil - 3 + \sqrt{3}}, \\
L_6(n) &= \frac{1}{\lceil\sqrt{n+5}\rceil - 4 + 3\sqrt{3}/2}, \\
L_7(n) &= \frac{k^2 - k - \sqrt{2k}}{k^3 - 2k^2}, \text{ if } n = k(k+1), \text{ otherwise } 0, \\
L_8(n) &= \max_i \left\{\sqrt{\frac{1}{p_i^2} + \frac{1}{q_i^2}}\right\}, \text{ if } n = \left\lceil \frac{(p_i+1)(q_i+1)}{2} \right\rceil, p_i^2 \le 3q_i^2 \text{ and} \\
&\quad q_i^2 \le 3p_i^2, i \in \mathbb{N}, \text{ otherwise } 0, \\
L_9(n) &= \sqrt{\frac{2}{\sqrt{3}n}}.
\end{aligned}$$

I used the grid packing sequence in PROPOSITON 12 to prove the following theorem.

THEOREM 5 [9] *For every* $n \ge 2$

$$(3 - 2\sqrt{2})\pi \le d_n(\overline{r}_n, [0,1]^2) < \frac{\pi}{\sqrt{12}},$$

where $d_n(\overline{r}_n, [0,1]^2)$ *denotes the density of a circle packing, whose bounds are sharp.*

6. Minimal polynomials of circle packings

I have extended the concept of the minimal polynomial of a point arrangement (the minimal degree polynomial with the smallest positive root of m_n) to the other equivalent forms of the problem. Based on the general minimal polynomials of the optimal substructures, I found minimal polynomials of packings using the resultant of the general minimal polynomials of these substructures.

DEFINITION 15 [9] We call a circle packing/point arrangement an *optimal substructure* in the $X \subset [0,1]$ compact set, if the $d_{n'}(r_{n'}, [0,1]^2)$ density is maximal in X, where n' denotes the number of circles in X.

DEFINITION 16 [9] A $p_n^I(x)$ polynomial is a *generalized minimal polynomial*, if $x \in \{r, m, s, \sigma\}$ and $I \in \{S, \Sigma, R, M\}$ respectively, and $\overline{x}_n$ is the smallest positive root of the polynomial $p_n^I(x)$ and the degree of the polynom is minimal. For the sake of simplicity we use the notation $P_n(x) = p_n^1(x)$ notation.

PROPOSITION 13 [9] *The relation between the general minimal polynomials are described by the following:*

$$\begin{array}{rl|rl}
\mathbf{p_n^S}(r) = & p_n^{\Sigma:=S-2r}(m := 2r) & \mathbf{p_n^\Sigma}(m) = & p_n^{R:=\Sigma+m}(s := \frac{m}{2}) \\
& p_n^{R:=S}(s := r) & & p_n^{M:=\Sigma}(\sigma := m) \\
& p_n^{M:=S-2r}(\sigma := 2r) & & p_n^{S:=\Sigma+m}(r := \frac{m}{2}) \\
\hline
\mathbf{p_n^R}(s) = & p_n^{M:=R-2s}(\sigma := 2r) & \mathbf{p_n^M}(\sigma) = & p_n^{S:=M+\sigma}(r := \frac{\sigma}{2}) \\
& p_n^{S:=R}(r := s) & & p_n^{\Sigma:=M}(m := \sigma) \\
& p_n^{\Sigma:=R-2s}(m := 2s) & & p_n^{R:=M+m}(s := \frac{\sigma}{2})
\end{array}$$

THEOREM 6 [9] *Let us consider a point arrangement in the unit square. Let us further suppose that the point arrangement consists of $N \geq 2$ optimal substructures, on the sides of $\Sigma_1, \Sigma_2, \ldots, \Sigma_N$ squares. If f is such a polynomial with the respective indices $\Sigma_i = f(\Sigma_j)$, then the $p_n^\Sigma(m)$ minimal polynomial can be calculated by the ith and jth minimal polynomials of the optimal substructures using:*

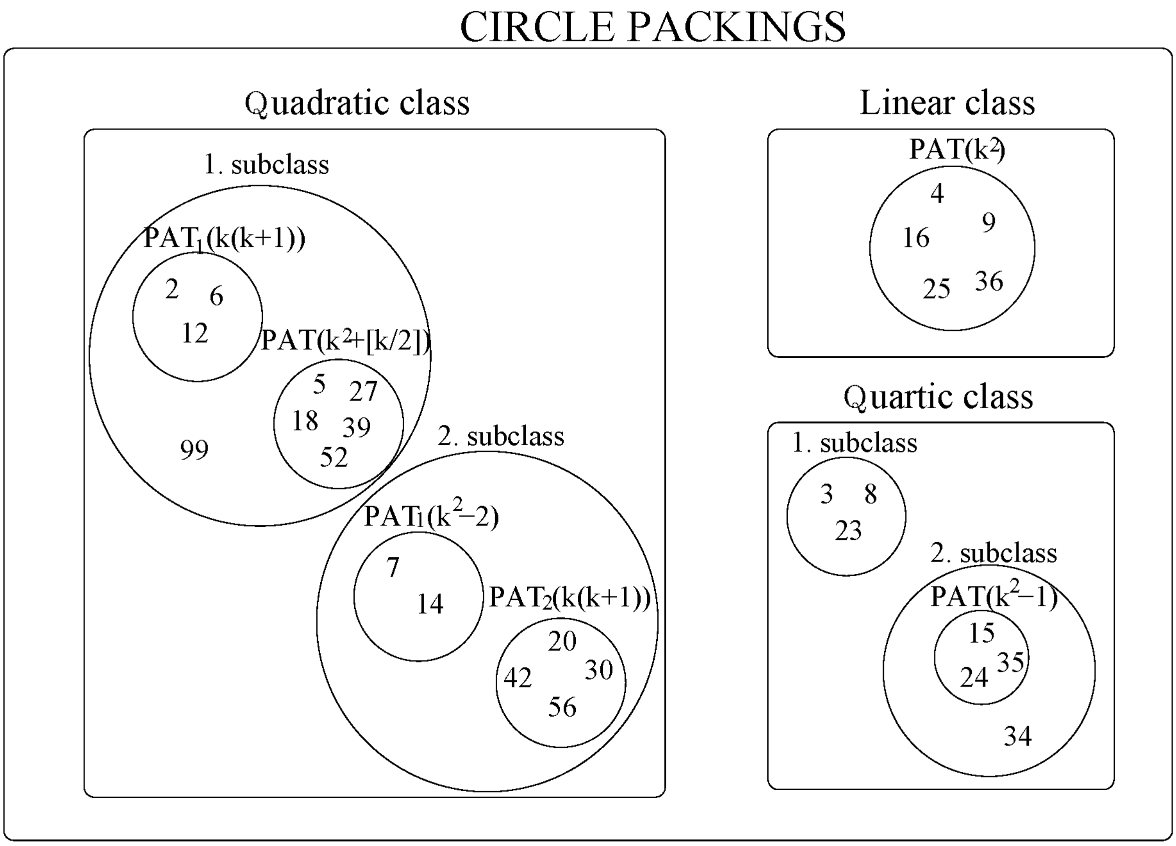
$$p_n^\Sigma(m) = \mathrm{Res}(p_{n1}^{\Sigma_j}(m), p_{n2}^{f(\Sigma_j)}(m), \Sigma_j) =$$
$$\det(\mathrm{Syl}(p_{n1}^{\Sigma_j}(m), p_{n2}^{f(\Sigma_j)}(m), \Sigma_j)).$$

I have published minimal polynomials for up to 100 circles, and using them, have also calculated the exact values of $\overline{m}_n$ and $\overline{r}_n$ in many cases. I studied separately the case $n = 11$, when the roots of the polynomial of degree 8 can be determined in an algebraic way. I also obtained the appropriate quadratic field where the roots can be found.

Classification based on minimal polynomials

The minimal polynomials of point arrangements are suitable for classifiying these packings. Based on the fact that a minimal polynomial is linear, quadratic or quartic

I found different kinds of packing classes and subclasses, where the connection between previous pattern classes can be seen in the following figure.



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