Interval Methods for Verifying Structural Optimality of Circle Packing Configurations in the Unit Square

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Abstract

The paper is dealing with the problem of finding the densest packings of equal circles in the unit square. Recently, a global optimization method based exclusively on interval arithmetic calculations has been designed for this problem. With this method it became possible to solve the previously open problems of packing 28, 29, and 30 circles in the numerical sense: tight guaranteed enclosures were given for all the optimal solutions and for the optimum value. The present paper completes the optimality proofs for these cases by determining all the optimal solutions in the geometric sense. Namely, it is proved that the currently best-known packing structures result in optimal packings, and moreover, apart from symmetric configurations and the movement of well-identified free circles, these are the only optimal packings. The required statements are verified with mathematical rigor using interval arithmetic tools.

Key words: interval analysis, circle packing, computer-assisted proof
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1 Introduction

The class of problems considered is classically described as that of 'placing a given number n of equal circles in the unit square without overlapping, in such a way that the common radius of the circles is maximal'. However, in numerical calculations it is more convenient to investigate an equivalent ([17]) 'point packing problem': 'Place n points in the unit square in such a way that the minimal distance between the pairs of points is maximal'. A point

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packing configuration is derived from the locations of the centres of the corresponding circle packing configuration and from the smallest square enclosing these centres. The point packing approach leads to a bound-constrained global optimization problem in the form of *maximizing*

$$\min_{1\le i\ne j\le n} \|(x_i, y_i), (x_j, y_j)\|_2^2 = f_n(x, y), \qquad \text{s.t.} \quad x_i, y_i \in [0, 1] \ \forall i, \tag{1}$$

where $\|\cdot,\cdot\|_2$ is the Euclidean distance, and the ith point is placed at (x_i, y_i). We are interested in all the optimal solutions *and* the optimal value of (1).

In our studies the necessary numerical computations are performed using interval arithmetic, which enables us to compute reliable bounds on the results of floating point calculations, and thus to prove mathematical statements on computers. Below, some basic concepts of interval arithmetic will be introduced together with the notation used in the paper. For more details on interval analysis the reader can refer e.g. to [5,11,16].

Throughout the paper, the set of compact *interval*s is denoted by $\mathbb{I}$. The real numbers and vectors are denoted by lower-case letters, while capital letters denote the intervals and interval vectors (boxes). The *lower and upper bounds of an interval* X are denoted by $\mathrm{lb}(X)$ and $\mathrm{ub}(X)$, respectively, i.e. $X = [\mathrm{lb}(X), \mathrm{ub}(X)]$. The *real arithmetic operators* and *standard mathematical functions* (such as $\sqrt{\ }, \log, \sin$) can easily be extended to interval arguments by using the interval bounds and monotonicity properties. A real *multivariate function* $f(x)$ can be extended to interval arguments by using e.g. the *natural interval extension* $F(X)$ for $x \in X$: replace all the occurrences of the variable x_i with X_i and apply the corresponding interval extensions for the arithmetic operators and standard functions occurring in f. (In the present paper, all interval functions will be constructed by natural interval extension.) The above interval functions have the *inclusion property* $f(x) \in F(X), \forall x \in X$. Moreover, the natural interval extension is *inclusion isotone*, i.e. $F(X) \subseteq F(Y)$ whenever $X \subseteq Y$.

Prior to the studies of the author's group, the circle packing problems for $n = 2, \ldots, 27$ and 36 were solved, most of them by computer-assisted techniques [2,3,13–15]. In the last few years, we introduced numerically reliable methods, fully based on interval calculations, to tackle the next few open problems $n > 27$. In [8] the first reliable solutions for $n = 28$ were published. [9] contains a multi-stage optimization algorithm based on an interval Branch and Bound (B&B) procedure and various problem-specific interval tools, and reports the tight enclosures of all solutions and the optimal values for $n = 28, 29, 30$, while [10] describes the applied interval algorithms in detail and presents proofs of correctness. (The main interval B&B method follows the scheme of a classical rectangular B&B algorithm for global optimization – see e.g. [6] – and utilizes the fact that interval arithmetic provides convenient tools to compute bounds of functions over boxes.) The objective of the present paper is to complete the above optimality proofs and extend the numerical results by geometric results concerning the *structures* of the optimal packings.

2 Packing structures and previous numerical results

The structure of a point packing configuration (or an equivalent circle packing one) describes that

(a) which points are located on the sides of the square (which circles are touching the side of the square),
(b) which pairs of points have the minimal distance (which circles are touching each other), and
(c) which are the free points [1] (free circles) of the packing.

Obviously, the question of whether the distance between two points (given by two binary floating point numbers) is exactly the minimal pairwise distance cannot be answered on computers by simply calculating distances or interval enclosures of distances. This fact causes the main difficulty in proving structural properties.

From the numerical results of [9] we have the following numerical information in hand for $n = 28, 29, 30$:

- An interval enclosure of all global optimizers (apart from symmetric cases): $(X, Y)^*_n = (X_1, \ldots X_n, Y_1, \ldots Y_n) \subset [0, 1]^{2n}$. Each component of $(X, Y)^*_n$ has a width of $\approx 10^{-13} - 10^{-15}$, with the exception of components enclosing a possibly free point for $n = 28, 29$.
- An enclosure of the global optimum value: $F^*_n \in \mathbb{I}$. The width of this interval is about 10^{-14}.
- For $n = 28$ and 29, an enclosure $(X_{free}, Y_{free})_n \subset (X_k, Y_k)^*_n$ of a point (x_{free}, y_{free}), such that

$$\mathrm{lb}(\|(X_{free}, Y_{free})_n, (X'_j, Y'_j)_n\|_2^2) > \mathrm{ub}(F^*) \geq f^* \quad (2)$$

  for $(X_j, Y_j)^*_n \subseteq (X'_j, Y'_j)_n$ and for all $j = 1, \ldots, n$, $j \neq k$. $(X_{free}, Y_{free})_n$ is used to temporarily reduce those components of the search boxes which probably enclose free points, and thus to prevent the B&B algorithm from performing unnecessary subdivisions on these components.

[1] A free point of a packing configuration can be slightly moved without affecting the minimal pairwise distance, i.e. the objective function value. See [9] for the precise definition used in our studies.

- A real-type high-precision approximate solution computed from a configuration what is thought to be an optimal packing: $(x_{appr}, y_{appr})_n \in [0,1]^{2n}$.

To simplify notation, in the rest of the paper we neglect the lower n indices unless they are explicitly required.

The above mentioned best available packing structures were discovered in [1] for $n = 28$ and in [12] for $n = 29, 30$, respectively. The graphical representations of these structures are (as we will soon prove) identical to those shown in Figure 1.

In the rest of the paper the term *rigid points* will be used for those points of a packing configuration that are not free (or in the case of interval enclosures, those which are conjectured to be fixed). The component vectors corresponding to (conjectured) rigid points are denoted by an upper r index.

The verification procedures were implemented using the PROFIL/BIAS v.2.0 interval package [7]. The source codes and the numerical results are available at `http://www.inf.u-szeged.hu/~markot/packcirc.htm`.

In the following section three assertions and their computer-assisted verifications will be given to prove the optimality and uniqueness of the guessed packing structures.

3 Optimality and uniqueness properties

ASSERTION 1 *For $n = 28, 29$, and 30, the system of equations describing the rigid part of the best-known packing structure has exactly one $(\bar{x}, \bar{y})^r$ solution in the particular components $(X, Y)^{*,r}$ of $(X, Y)^*$.*

To verify this assertion, at first the rigid structures of the best-known packings were determined in terms of the properties (a) and (b) of Section 2. These properties can be expressed by a quadratic system of equations using the coordinates of the points and the minimal pairwise distance. For $n = 28$ and 29, the exact solutions of these systems are not known. Thus, after performing some simplifications – variable substitutions – these systems were solved numerically by the interval Newton–Gauss–Seidel iteration method of the toolbox [4]. To demonstrate the existence and uniqueness of a solution on a large box, the search region was determined by blowing up $(X, Y)^{*,r}$ and $\sqrt{F_n^*}$ to the width of 0.01. Still, the interval Newton method was able to prove the existence and uniqueness of a solution and to give its proper tight $(\bar{X}, \bar{Y})^r$ enclosure. Finally, the verification of the inclusion property $(\bar{X}, \bar{Y})^r \subseteq (X, Y)^{*,r}$ implying Assertion 1 was also successful.

On the contrary, for $n = 30$ the system variables are given in an exact analytic form (see e.g. [9]). Consequently, Assertion 1 could be proved in a straightforward way by evaluating the guaranteed enclosures $(\bar{X}, \bar{Y})^r$ of the exact coordinate values and then verifying $(\bar{X}, \bar{Y})^r \subseteq (X, Y)^{*,r}$ as before.

The importance of Assertion 1 is that it allows one to associate a unique point packing (i.e. a solution vector) located in the box $(X, Y)^{*,r}$ with the rigid part of the guessed optimal structure (with the geometric solution).

ASSERTION 2 *For* $n = 28, 29$, *the solution* $(\bar{x}, \bar{y})^r$ *of Assertion 1 can be extended by a free point located in that of the component* $(X_k, Y_k)^*$ *of* $(X, Y)^*$ *which is not considered in* $(X, Y)^{*,r}$.

Formally, Assertion 2 means that one has to prove the existence of a point $(x_k, y_k) \in (X_k, Y_k)^*$, for which

$$\|(x_k, y_k), (\bar{x}_j, \bar{y}_j)\|_2^2 > f^* \tag{3}$$

for each $j = 1, \ldots, n,\ j \neq k$. Although we do not know the exact values of either $(\bar{x}_j, \bar{y}_j)$ or f^*, we can test the existence of a small rectangle (X_k, Y_k) enclosing (x_k, y_k), such that $(X_k, Y_k) \subseteq (X_k, Y_k)^*$ and

$$\text{lb}\|(X_k, Y_k), (\bar{X}_j, \bar{Y}_j)\|_2^2 > \text{ub}(F^*) \tag{4}$$

for each $j = 1, \ldots, n,\ j \neq k$. Obviously, (4) implies (3). Comparing the latter equation with (2), (X_{free}, Y_{free}) turns out to be a suitable value for (X_k, Y_k). Theoretically, since $(\bar{X}_j, \bar{Y}_j) \subseteq (X_j, Y_j)^* \subseteq (X_j', Y_j')$, the inclusion isotone property of the natural interval extension would imply that (4) holds for $(X_k, Y_k) = (X_{free}, Y_{free})$. However, since the implementation does not necessarily guarantee the inclusion isotonicity with mathematical rigor, and additionally, since (3) was obtained in a slightly different coordinate range (see [9] and [10] for details), (4) had to be explicitly verified – successfully – using (X_{free}, Y_{free}) for (X_k, Y_k).

ASSERTION 3 *For* $n = 28, 29, 30$, $(\bar{x}, \bar{y})^r$ *is the only optimal point packing in* $(X, Y)^{*,r}$.

This assertion is proved by using the interval version of the theorem of Nurmela and Östergård, [13]:

THEOREM 1 *(based on [13]) Assume that we know an approximation* $(\hat{x}, \hat{y})^r$ *of* $(\bar{x}, \bar{y})^r$, *such that*

$$\|(\hat{x}_i, \hat{y}_i)^r, (\bar{x}_i, \bar{y}_i)^r)\|_2 < d' \quad \forall i \tag{5}$$

with a suitable $d' \in \mathbb{R}$*. Determine an error rectangle* $(\hat{X}_i, \hat{Y}_i)^r \subseteq [0,1]^2$ *for each* i*, such that*

$$(\hat{x}_i, \hat{y}_i)^r \in (\hat{X}_i, \hat{Y}_i)^r \quad \text{and} \quad (X_i, Y_i)^{*,r} \subseteq (\hat{X}_i, \hat{Y}_i)^r \quad \forall i, \tag{6}$$

and that the second statement of (6) holds also for an identical rectangle obtained by shifting the original rectangle with the vector $(\bar{x}_i - \hat{x}_i, \bar{y}_i - \hat{y}_i)$ *from* $(\bar{x}_i, \bar{y}_i)^r$*. Choose a proper real value (called as a cutoff value)* $\hat{f}$*, for which*

$$\hat{f} + 2d' < f^* \tag{7}$$

holds. Run an elimination algorithm on $(\hat{X}, \hat{Y})^r$ *which attempts to erase all* $(x, y)^r \in (\hat{X}, \hat{Y})^r$ *points, for which* $f(x, y) < \hat{f}$*. If we are able to reach the contraction of each* $(\hat{X}_i, \hat{Y}_i)^r$ *component, then it is guaranteed that* $(\bar{x}, \bar{y})^r$ *is the only optimal point packing within* $(\hat{X}, \hat{Y})^r$*, and thus, within* $(X, Y)^{*,r}$*.*

The proof of the theorem matches that of the one in [13] and it is not repeated here. The essence of the proof is that if some regions can be eliminated from the $(\hat{X}_i, \hat{Y}_i)^r$ error rectangles around $(\hat{x}_i, \hat{y}_i)^r$ using the $\hat{f}$ cutoff value, then congruent regions can be eliminated from the (hypothetical) error rectangles around $(\bar{x}_i, \bar{y}_i)^r$ using the f^* cutoff value. That is, a contraction of the rectangles drawn around the approximate solution implies a contraction of the rectangles around the exact optimal solution.

To satisfy the conditions of Theorem 1, the following constructions were made: $(\hat{x}, \hat{y})^r$ was set to the existing approximate solution $(x_{appr}, y_{appr})^r$. Then the left-hand side of (5) was evaluated for each i using the interval enclosure of the arguments, resulting in a reliable d' bound. A mathematically correct $\hat{f}$ value was also evaluated in an interval way by using F^* and an enclosure of d' in (7). The error rectangles were determined as $\hat{X}_i = (X_i^* + \Delta) \cap [0, 1]$, $\hat{Y}_i = (Y_i^* + \Delta) \cap [0, 1]$ with $\Delta = [-10^{-5}, 10^{-5}]$. This implied (6), and it made possible to verify the required property for the shifted rectangles as well – after evaluating an interval enclosure of the shift vector. Note that the choice of the order of Δ has a demonstrative role: since d' has the order of 10^{-15}, the prerequisites would hold for much smaller error rectangles.

The required elimination algorithm of Theorem 1 was the core interval B&B optimization method of [9]. This algorithm provides the guarantee that only packings with $f(x, y) < \hat{f}$ are eliminated from $(\hat{X}, \hat{Y})^r$. The algorithm was able to verify the required contraction property in all components without particular difficulties (within 100 iteration steps), and consequently, to prove Assertion 3 for all three packing problems.

Corollary 1 *The packing structure guessed in [1] for* $n = 28$ *and in [12] for* $n = 29$ *and* 30 *results in the only optimal packing of* n *points in the unit*

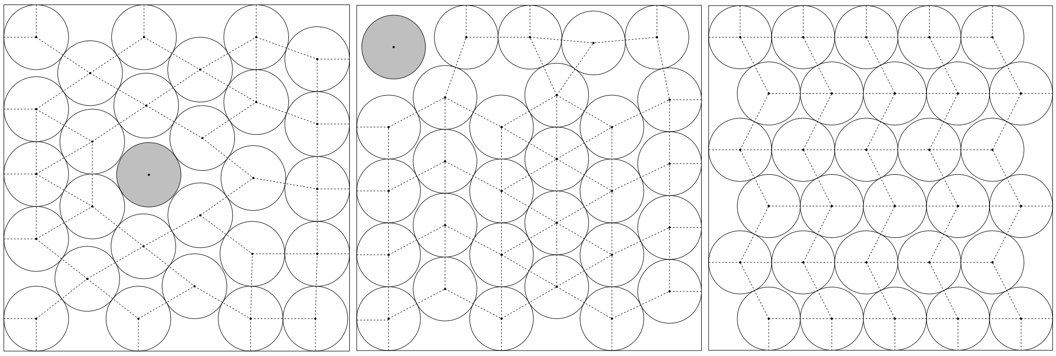

Fig. 1. The unique optimal packing structures of 28, 29, and 30 circles in the square.

square (disregarding symmetric cases and the movement of the free point for $n = 28, 29$*). Hence, the guessed optimal structure can be called as the unique optimal geometric solution of the particular packing problem.*

Proof. Let $f((\bar{x}, \bar{y})^r) = \bar{f}$, and let $(x', y') \subseteq (X, Y)^*$, $(x', y')^r \neq (\bar{x}, \bar{y})^r$ be an arbitrary point packing of n points. Then by Assertion 3, $f((x', y')^r) < \bar{f}$, that is, $f(x', y') < \bar{f}$. Since by Assertion 2 $(\bar{x}, \bar{y})^r$ can be extended to $(\bar{x}, \bar{y})$ such that $f(\bar{x}, \bar{y}) = \bar{f}$, we obtain that $\bar{f} = f^*$. Thus, $(\bar{x}, \bar{y})$ is optimal, unique (apart from symmetry and from a possible free circle), and by Assertion 1 it is determined by the guessed packing structure. □

Figure 1 shows the optimal packing structures of 28, 29, and 30 circles (points) in the square, also indicating the free and touching circles.

4 Summary

The paper presented interval-based, computer-assisted verification methods for proving the structural properties of circle packing problems. It has been proved that for the cases of packing 28, 29, and 30 circles, the currently best-known packing structure results in an optimal and (apart from symmetry and the occurrence of a free circle) unique packing. That is, in all three cases the guessed optimal structure is the unique optimal geometric solution of the particular problem.

References

[1] R. L. Graham and B. D. Lubachevsky, *Repeated patterns of dense packings of equal disks in a square*, Electronic Journal of Combinatorics 3:R16 (1996).

[2] C. de Groot, M. Monagan, R. Peikert, and D. Würtz, *Packing circles in a square: review and new results*, in P. Kall (ed.): System Modeling and Optimization (Proc. 15th IFIP Conf. Zürich, 1991), pp. 45–54, Lecture Notes in Control and Information Services 180 (1992).

[3] C. de Groot, R. Peikert, and D. Würtz, *The optimal packing of ten equal circles in a square*, IPS Research Report 90-12, ETH, Zürich, 1990.

[4] R. Hammer, M. Hocks, U. Kulisch, and D. Ratz, *Numerical Toolbox for Verified Computing I.*, Springer-Verlag, Berlin, 1993.

[5] E. Hansen, *Global Optimization Using Interval Analysis*, Marcel Dekker, New York, 1992.

[6] R. Horst, P.M. Pardalos, and N.V. Thoai, *Introduction to Global Optimization*, Kluwer, Dordrecht, 1995.

[7] O. Knüppel, *PROFIL/BIAS V 2.0*, Bericht 99.1., Technische Universität Hamburg-Harburg, 1999.

[8] M. Cs. Markót, *Optimal Packing of 28 Equal Circles in a Unit Square — the First Reliable Solution.* Numerical Algorithms (37) 2004, pp. 253–261.

[9] M. Cs. Markót and T. Csendes, *A New Verified Optimization Technique for the "Packing Circles in a Unit Square" Problems*, to appear in SIAM J. Optimization. Available at `http://www.inf.u-szeged.hu/~markot/impcirc.ps.gz`.

[10] M. Cs. Markót and T. Csendes *A reliable area reduction technique for solving circle packing problems.* Submitted for publication. Available at `http://www.inf.u-szeged.hu/~markot/intpoly.ps.gz`.

[11] A. Neumaier, *Interval Methods for Systems of Equations*, Encyclopedia of Mathematics and its Applications 37, Cambridge Univ. Press, Cambridge, 1990.

[12] K. J. Nurmela and P. R. J. Östergård, *Packing up to 50 circles in a square*, Discrete and Computational Geometry 18 (1997), pp. 111–120.

[13] K. J. Nurmela and P. R. J. Östergård, *Optimal packings of equal circles in a square*, in Y. Alavi, D. R. Lick, and A. Schwenk (eds.): Combinatorics, Graph Theory, and Algorithms (Proc. 8th Quadrennial International Conference on Graph Theory, Combinatorics, Algorithms, and Applications), pp. 671–680 (1999).

[14] K. J. Nurmela and P. R. J. Östergård, *More Optimal Packings of Equal Circles in a Square*, Discrete and Computational Geometry 22 (1999), pp. 439–457.

[15] R. Peikert, *Dichteste Packungen von gleichen Kreisen in einem Quadrat*, Elemente der Mathematik 49 (1994), pp. 17–25.

[16] H. Ratschek and J. Rokne, *New Computer Methods for Global Optimization*, Ellis Horwood, Chichester, 1988.

[17] P. G. Szabó, *Some New Structures for the "Equal Circles Packing in a Square" Problem*, Central European Journal of Operations Research 8 (2000), pp. 79–91.