The History of Packing Circles in a Square

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Introduction

There are many interesting optimization problems associated with the packing and covering of objects in a closed volume or bounded surface. Typical examples can be found in classical physics or chemistry where questions arise of the kind "What does the densest packing of atoms or molecules look like when a crystal or macro-molecule is formed with the lowest energy?" Also engineering and information science confront us with extremal problems associated with the packing and covering of objects. One of the most prominent examples arises from the study and design of spherical codes which have important applications in information processing. A spherical code is a set of real vectors on the unit sphere's surface in n-dimensional Euclidean space. In this case, one searches for an arrangement so that the minimum separating angle between the vectors becomes as large as possible.

However, it was another closely related problem, the optimal packing of n circles in a square, which has fascinated mathematicians over the last few years. The circle packing problem is equivalent to the problem of scattering n points in a unit square, such that the minimum distance m between any two of them becomes as large as possible. The relation between the maximum radius r of the circles and the scattering distance m between the points is then given by $r = \frac{m}{2(m+1)}$. It is very surprising that such a problem, which at first looks rather simple, has brought to us a series of interesting papers with a continuous improvement of the results.

In this article we give a review on the packing problem of up to $n = 20$ equal circles in a square. We report briefly how the optimal solutions were found by an elimination procedure and we sketch the proof of uniqueness. In addition we present the closed form solutions for all packings. The role Maple played in this work was to obtain these exact formulae for the optimal scattering diameter m. More precisely, we were able to compute the *minimal polynomial* corresponding to the optimal solution. We describe how these polynomials can be computed in Maple by explicitly showing the computation for $n = 10$.

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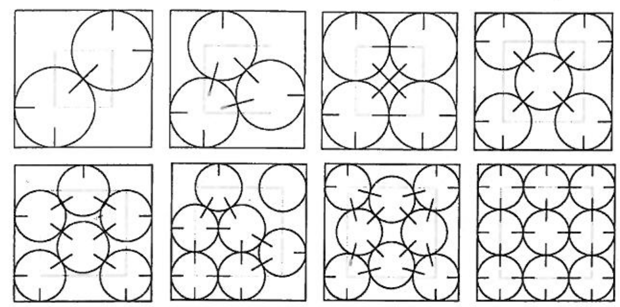

Figure 1: *Cases n=2–9*

History of the Packing Problem

Cases $n = 2 - 9$: The situation for packing of up to 9 circles in a square was already solved in 1964. Here, the cases $n = 2$, 3, 4, and 5 are solved easily. For $n = 6$ it was R.L. Graham, mentioned in [1], who found the optimal solution. The proofs for $n = 7$ and $n = 8$ were done by J. Schaer [1], and the one for $n = 9$ by J. Schaer and A. Meir [2]. Of interest in the optimal packing of 7 circles is the fact that one circle can be moved freely within a bounded region.

Case $n = 10$: This problem has a long history, beginning in 1970 when M. Goldberg [3] proposed a symmetric arrangement consisting of 4 rows of 3-2-3-2 circles which have a radius of $r \sim 0.14706$. In 1971, J. Schaer [4] increased the radius to $r \sim 0.14777$ (Fig. 2a), even though his packing contains two free circles in opposite corners of the square. Sixteen years later, R. Milano [5] proved that his packing with $r \sim 0.14792$ (Fig. 2b) is the best *symmetric* one. But in 1989, G. Valette [6] found a better *chaotic* solution without any symmetry in the arrangement of the circles in the square. The radius now increased to $r \sim 0.14818$ (Fig. 2c). His solution also did not survive very long. Later, in the *Zbl. Math.* [7], we find the note that "this packing has been improved, in 1989, by B. Grünbaum [8]" to $r \sim 0.148197$. However, this was not the end of the story.

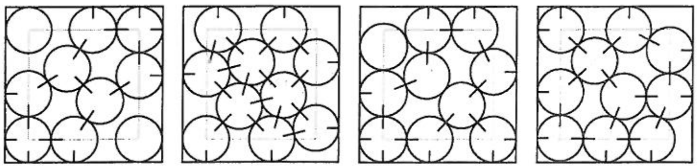

Figure 2: *Cases n=10–a, b, c, d*

We [9] [10] found an even better packing with a radius of $r \sim 0.148204$ (Fig. 2d) and showed that it was the *optimal* one. Furthermore, we are able to give the exact result for the optimal scattering distance m. It is the smallest positive zero of this irreducible polynomial of degree 18 with integer coefficients.

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

Later, we also made public the work of K. Schlüter [11] from 1979, in which this solution could be found. The paper of K. Schlüter was written in German, and this may be the reason that it was not known in the scientific community. Schlüter's solution was also found by M. Grannell [12], by J. Petris and N. Hungerbühler [13], and by M. Mollard and C. Payan [14]. None of them proved optimality, but Schlüter already conjectured that his solution may be the optimal one. Now we know from our investigations [10] that his conjecture was true.

Cases $n = 11 - 13$: We [15] have also presented the optimal solutions for 11, 12, and 13 circles. For 11 circles the optimal solution with a scattering diameter $m \sim 0.421280$ was only about 0.05% larger compared to the previously known result of Goldberg [3]. The case $n = 12$ shows a diamond structure leading to an m value of 0.388730. And indeed it is this highly symmetric structure which is the optimal one. When considering one more circle, the situation becomes much more complicated. How to arrange an additional circle in the highly compact configuration of 12? There must be a complete rearrangement leading to a highly chaotic structure with an optimal scattering diameter $m \sim 0.366096$.

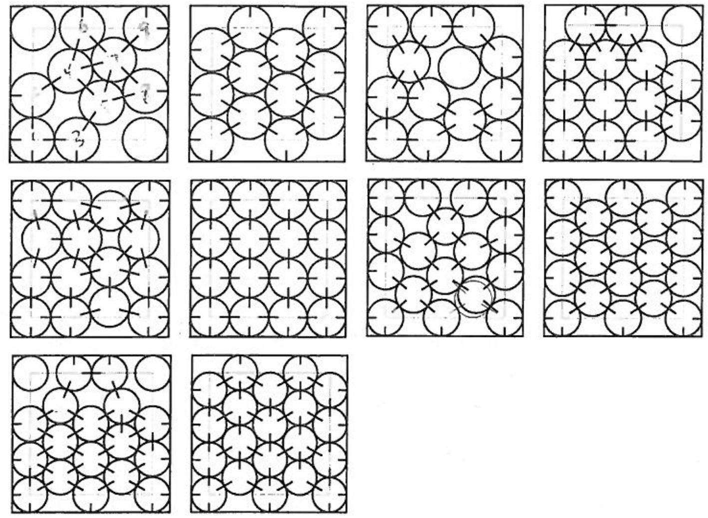

Figure 3: *Cases n=11–20*

The solution is difficult to find, since there exist two narrow gaps between two circles of the order 10^{-4} times the scattering distance. The optimal solution of Peikert *et al.* [15] is more than 3.5% better than the regular 3-2-3-2-3 structure proposed by M. Goldberg [3] with $m \sim 0.35355$. Independently of Peikert *et al.*, M. Mollard and C. Payan [14] found the optimal packings for $n = 11, 13$ (and also for 14) without proving optimality. In all three cases we [15] obtained the exact result as the smallest positive zero of a polynomial. The most difficult case was $n = 13$, resulting in a polynomial of degree 40.

Cases: $n = 14 - 20$: Furthermore, we [15] have also investigated *numerically* the problem for $n = 14$ to $n = 22$. However, with an increasing number of circles, it becomes more and more difficult to converge to the global optimum. For even larger n, we become more likely to get trapped in local optima containing hexagonal clusters. Nevertheless, all solutions found by Peikert *et al.* [15] were better or at least as good as those already known from the work of M. Goldberg [3]. One of the cases where we did not find the global optimum by optimization methods alone was for $n = 14$. J. Petris and N. Hungerbühler [16] showed that their packing could be improved by performing a few rearrangements. After this, Peikert *et al.* [15] improved their method which could now be applied for the range $n = 14..20$. In the case of $n = 17$, they found two degenerated optimal packings, one of which is axially symmetric. The packing for $n = 19$ is not symmetric. However, the lower 13 circles are invariant under a 180 degree rotation.

How to Find the Optimal Solutions

In the following, we briefly describe the method of Peikert *et al.* [15]. First let us start with same notations and definitions. Let us denote the closed unit square $[0, 1] \times [0, 1]$ by S. Then by $\mathcal{A}_{nm}$ we denote the *set of arrangements* of n points in S with minimal distance m, i.e.,

$$\mathcal{A}_{nm} = \{ (\langle x_1, y_1 \rangle, \cdots, \langle x_n, y_n \rangle) \in S^n \mid \\ (x_i - x_j)^2 + (y_i - y_j)^2 \geq m^2 \text{ for all } 1 \leq i < j \leq n \}$$

$\mathcal{A}_{nm}$ consists of one or more *connected components* which we call *packings of* n *circles of diameter* m. Hence, a packing P is a sequence $\langle P_1, \cdots, P_n \rangle$, where P_i is the set of possible center points of the i-th circle. Two packings P and P' are considered identical if P' is obtained from P by a symmetry transformation and/or an index permutation. The i-th circle is called a *fixed circle* if P_i consists of a single point. It is called a *free circle* if P_i includes an open neighborhood.

For a given number n, let m_n denote the maximal diameter $\max\{m \mid \mathcal{A}_{nm} \neq 0\}$. As *optimal packings* we can then define the packings $P \subseteq \mathcal{A}_{nm_n}$. Given the number n, our problem consists now in finding m_n and a member of each optimal packing. For a fixed n, the following procedure has been used by Peikert *et al.* [15] to find m_n and to prove its maximality: 1) Find a good lower bound m for m_n by standard and Monte-Carlo optimization methods. 2) For each optimal packing, find a small $2n$-dimensional interval bounding the center points. Prove that every packing with a diameter $\geq m$ is contained in one of the intervals. 3) Knowing the centers of the fixed circles up to a small tolerance, *guess* the optimal packing. That means: guess the connectivity graph and derive the diameter m_n from it.

Step 1) Finding sharp lower bounds: The search for the best radius was inspired by considering the problem as a typical numerical optimization task. Applying a standard BFGS quasi-Newton algorithm [17] and starting from a random initial position for the centers of the circles a local minimum of the objective function was found. Within about a dozen trials we found for $n = 10$ in typically 30% of the solutions the optimal one. However, for larger numbers of circles the solutions got stuck in local, hexagonal substructures. Using a (stochastic) Langevin equation formalism, as described in [18] we were able to find near optimal or even optimal solutions.

Step 2) The elimination procedure: Assume that we have a lower bound m. This rational number m is used to decompose S into a set of rectangular *tiles* in such a way that the *diameter* of any tile is $\leq m$. If we denote by t the number of "empty" tiles and by n the "full" tiles which do contain a center point C_i, there are $\binom{t}{n}$ combinations for distributing

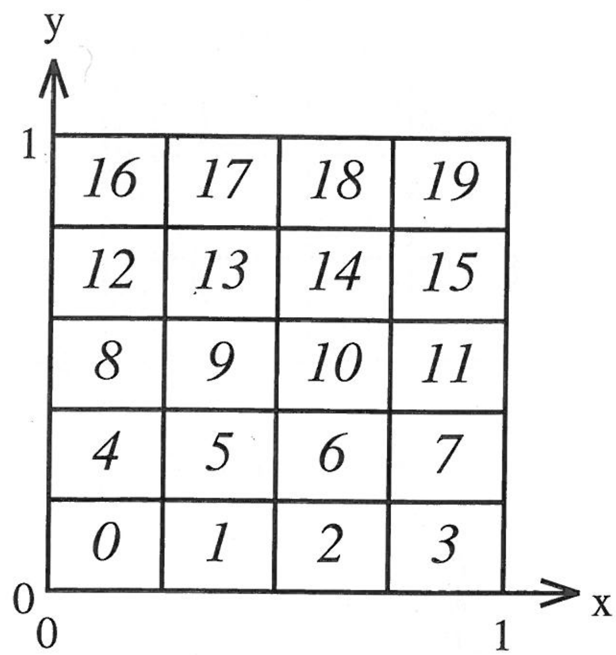

Figure 4: *Rectangular Tiling*

$C_0, \cdots, C_{n-1}$ among t tiles. *Tiles* are numbered as shown in Fig. 4. *Combinations* are first assigned a binary number, whose i^{th} bit is set iff the i^{th} tile is full. Then, combinations are ordered with increasing binary numbers, skipping those combinations which have a symmetric image. For each combination, we will now try to show individually that it *cannot be assumed* by a packing $P \subseteq \mathcal{A}_{nm}$. We start with partitioning S into a grid of quadratic *cells*. It is advantageous to have cells contained in single tiles. We will call *active cells* those cells which are still candidates for containing a center point. Since we assumed a fixed combination, we can immediately reduce the set of active cells to those not completely covered by one or more empty tiles.

As an example, Fig. 5 shows the active cells (unshaded) at this stage for $n = 10$, $m = .4212795$, a 4 by 4 tiling, a 32 by 32 grid, and for the 500^{th} combination. Figs. 6 and 7 show what the elimination process does. One of the cells of tile 0 (shown at the left in Fig. 6) contains a C_i (drawn in black). Then the shaded area of tile 1 cannot contain a C_i. When repeating this for all active cells of tile 0, some cells of tile 1 lie in the shaded area each time. That means, these cells cannot contain a C_i and can therefore be made inactive, as shown in Fig. 7. The procedure is easily generalized and iterated

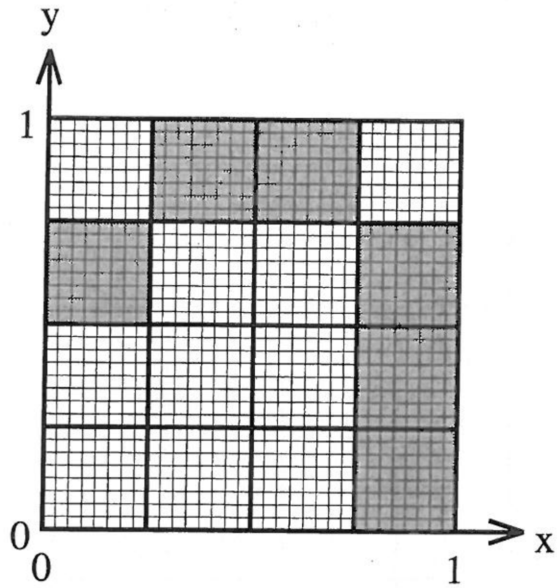

Figure 5: *Active Cells*

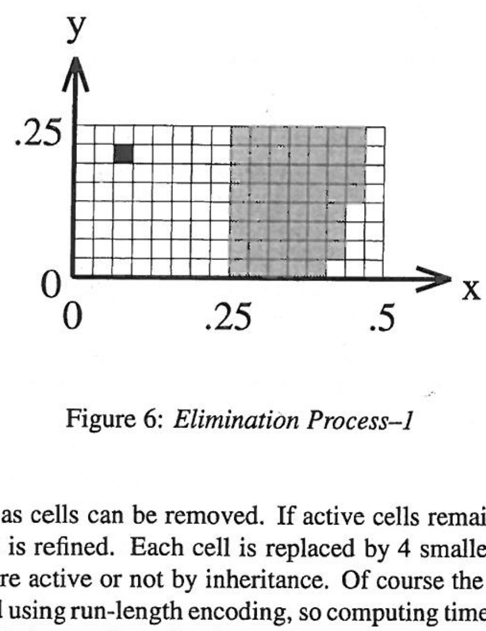

Figure 6: *Elimination Process–1*

as long as cells can be removed. If active cells remain, then the grid is refined. Each cell is replaced by 4 smaller cells, which are active or not by inheritance. Of course the matrix is stored using run-length encoding, so computing time grows only with the number of active cells, not with the total number of cells. For a few combinations however, the number of active cells grows fast enough to make further computation infeasible.

To overcome this difficulty, two heuristics can be introduced. *(i)* Because free circles lead to large areas of active cells, remove them after a certain number of grid refinements. This is legitimate because to remove constraints for one of the centers means to generalize the problem. *(ii)* Split a problem (for a particular combination) into two sub-problems by selecting a coordinate variable x_i or y_i ($1 \leq i \leq n$) and a threshold value k. Then the two cases $x_i \leq k$ and $x_i \geq k$

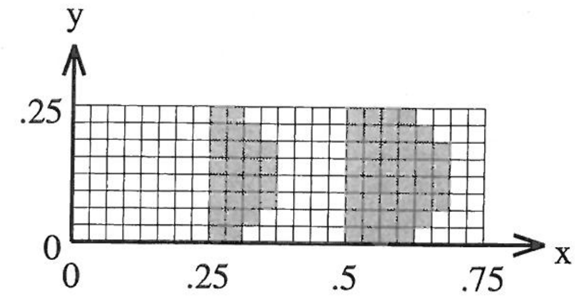

Figure 7: *Elimination Process–2*

($y_i \leq k$ and $y_i \geq k$, respectively) are treated separately. If k is well chosen, the number of active cells can be better reduced in the two sub-problems.

Step 3) Guessing optimal packings: The previous steps gave us the packings in Fig. 1 – 3. Whenever two circles touch or one circle touches a square side this is indicated by a solid line. It must be verified that these arrangements represent a packing as defined. First of all, algebraic *solvability* has to be checked. But we must also check that distances $\overline{C_iC_j}$ not declared to be m are greater than m and that the positions of any free circle center form a non-empty and connected set. For our range of n, these verifications are immediate.

Proof of Uniqueness

The proof of uniqueness done by Peikert *et al.* [15] is similar to their elimination procedure. The main difference is that we don't work with sets of cells anymore but use instead convex regions bounded by lines and/or arcs. At the beginning, these regions R_i are error circles around the C_i of the guessed packing. The radii r_i are such that at least the $2n$-dimensional interval obtained in step 2 is contained. If C_i lies on a square side, R_i is a half circle only (or a quarter circle if C_i is a corner of the square). The cutting process shown in Figs. 6 and 7 is now used in a modified form. The basic idea is again that a region R_i is being used to exclude parts of a second region R_j. Instead of cutting off a set of cells, we remove everything lying outside a *straight line.* The endpoints of the line are found on the boundary of R_j by inspecting all "critical" points on the boundary of R_i. The goal is to reduce all regions belonging to fixed circles to *polygons* lying strictly inside the error circle.

If this can be achieved, we have managed to reduce the error radii by a (common) factor $0 < q < 1$. The trick is now that, scaled down by q, the same sequence of cuts can be performed again. That means we get sequences of concentric

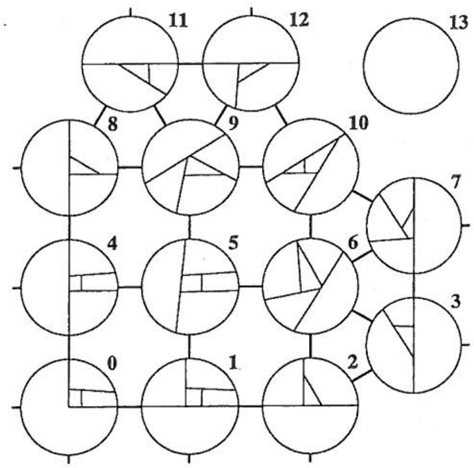

Figure 8: *Uniqueness Proof*

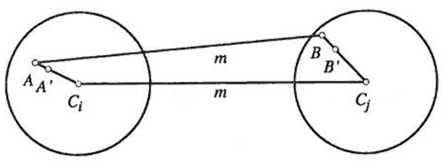

Figure 9: *Error Radii*

error circles which converge to the guessed optimal packing.

Fig. 9 shows why iteration is legitimate: Assume that the point B in the region R_j is determined by the point A in R_i. Then, the distances $\overline{C_iC_j}$ and $\overline{AB}$ are both equal to m. If A' and B' are chosen such that $\overline{C_iA'} = q\overline{C_iA}$ and $\overline{C_jB'} = q\overline{C_jB}$, then $\overline{A'B'} \leq m$. This is true even if the quadrilateral is concave or a "bowtie".

Again, this proof was carried out on a computer. A strategy was implemented to ensure that relatively wide segments are cut off at each step. In contrast to Fig. 8, for other values of n it may be necessary to use more than once each pair C_i and C_j of neighbors before a polygon is obtained. The highest number of cuts needed was 141, namely for $n = 13$.

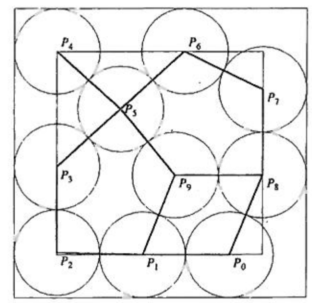

Figure 10: *Coordinates P for n=10*

Finding the Closed Form Solution for m

The packings in Fig. 1 – 3 tell us which circles touch which other circles and which circles touch the boundary of the square. From this information, we apply Pythagoras' Theorem for right angle triangles to write down equations relating centers of circles to other circles. Including boundary conditions, we obtain a system of quadratic equations to solve. Let us show how to do this for the case $n = 10$.

Let m be the diameter of the circles and let the circle with center P_i have co-ordinates (x_i, y_i). See Figure 10. Thus there are 21 unknowns: $x_0, y_0, \ldots, x_9, y_9$, and m. Applying Pythagoras' Theorem to the line connecting P_0 to P_8 we obtain the equation $(x_8 - x_0)^2 + (y_8 - y_0)^2 = m^2$. Let the inner square have unit co-ordinates. Hence $x_8 = 1$ and $y_0 = 0$ so the equation simplifies to $(1 - x_0)^2 + y_8^2 = m^2$. Applying Pythagoras' Theorem to all the heavy lines except the ones on the boundary, we obtain the following equations.

```
> pythagoras := {
>     (x[9]-x[8])^2+(y[9]-y[8])^2 = m^2,
>     (x[8]-x[0])^2+(y[8]-y[0])^2 = m^2,
>     (x[2]-x[1])^2+(y[2]-y[1])^2 = m^2,
>     (x[9]-x[1])^2+(y[9]-y[1])^2 = m^2,
>     (x[5]-x[3])^2+(y[5]-y[3])^2 = m^2,
>     (x[4]-x[5])^2+(y[4]-y[5])^2 = m^2,
>     (x[6]-x[5])^2+(y[6]-y[5])^2 = m^2,
>     (x[9]-x[5])^2+(y[9]-y[5])^2 = m^2,
>     (x[7]-x[6])^2+(y[7]-y[6])^2 = m^2   }:
```

By inspection, we have the following boundary conditions.

```
> boundary := { y[0]=0, x[0]=x[1]+m, y[1]=0,
>     x[2]=0, x[3]=0, y[3]=y[2]+m, x[4]=0,
>     y[4]=1, y[6]=1, x[7]=1, y[7]=y[8]+m,
>     x[8]=1 }:
```

Substituting the boundary conditions into the equations we obtain the following 9 equations in 9 unknowns.

```
> equations := subs(boundary,pythagoras)
>     minus {m^2 = m^2};
```

$$equations := \{(x_9 - x_5)^2 + (y_9 - y_5)^2 = m^2,\\ (1 - x_6)^2 + (y_8 + m - 1)^2 = m^2,\\ (x_6 - x_5)^2 + (1 - y_5)^2 = m^2, {x_5}^2 + (1 - y_5)^2 = m^2,\\ {x_5}^2 + (y_5 - y_2 - m)^2 = m^2, (x_9 - x_1)^2 + {y_9}^2 = m^2,\\ {x_1}^2 + {y_2}^2 = m^2, (1 - x_1 - m)^2 + {y_8}^2 = m^2,\\ (x_9 - 1)^2 + (y_9 - y_8)^2 = m^2\}$$

Now, in principle, we can solve for m by solving the equations. However, it is very difficult to solve this system of polynomial equations algebraically. We can help the solver if we can find any other equations which will simplify the computation. We note that from symmetry $x_5 = x_6/2$ and $y_5 = (1+y_3)/2 = (1+y_2+m)/2$. Also the points P_0, P_1, P_9, P_8 form a parallelogram; hence, we obtain the equations $y_9 = y_8$ and $x_9 = 1-m$. Substituting these conditions into our equations, we obtain the following system of 5 quadratic equations in $\{y_2, x_6, x_8, y_8, m\}$ to solve.

```
> symmetry := { x[5] = x[6]/2, y[5] =
>     (1+y[2]+m)/2, y[9]=y[8], x[9]=1-m }:
> equations := subs(symmetry, equations)
>     minus {m^2 = m^2};
```

$$equations := \left\{(1 - x_6)^2 + (y_8 + m - 1)^2 = m^2,\\ {x_1}^2 + {y_2}^2 = m^2, (1 - x_1 - m)^2 + {y_8}^2 = m^2,\\ \left(1 - m - \frac{1}{2}x_6\right)^2 + \left(y_8 - \frac{1}{2} - \frac{1}{2}y_2 - \frac{1}{2}m\right)^2 = m^2,\\ \frac{1}{4}{x_6}^2 + \left(\frac{1}{2} - \frac{1}{2}y_2 - \frac{1}{2}m\right)^2 = m^2\right\}$$

Now, can Maple solve these equations? It turns out that there is an effective approach to solving polynomial equations based on the theory of Gröbner bases. Roughly speaking, given a set of polynomials, a Gröbner basis is an equivalent set of polynomials in a standard form which is more convenient for computational purposes. Equivalence here means that any zero of the input set of polynomials will be a zero of the Gröbner basis, and vice-versa. How does the Gröbner basis help use to solve for m? If the set of input polynomials has a finite number of solutions, the Gröbner basis will be a triangularized set of polynomials. It is then straight forward to solve using back substitution. We refer the reader to [19] and [20] for futher information about Gröbner bases. We compute a Gröbner basis in Maple using the `gbasis` command in the `grobner` package as follows. Note: the `gbasis` function expects its input to be polynomials, not equations. Hence

```
> polynomials := [seq(lhs(e)-rhs(e),
>     e=equations)]:
> GB := grobner[gbasis](polynomials,
>     [x[1],y[2],x[6],y[8],m], plex):
```

The Grobner basis obtained is too big to present here. It also took over 20 minutes on our computer to compute it. It contains 9 polynomials whose coefficients are larger than 60 digits in length. The option `plex` specifies a lexicographical ordering on the variables (i.e., $x_1 > y_2 > x_6 > y_8 > m$) is to be used. By specifying m to be the last variable in the ordering, we obain the polynomial in m that we want. We select it and factor it.

```
> a := select(type, GB, polynom(rational,m)):
> a := sort( factor( a[1] ) );
```

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

The optimal solution for m is therefore the smallest positive real root of this polynomial. The factor m corresponds to the uninteresting solution $m = 0$, a square with zero width. It turns out that the degree 18 polynomial cannot be solved exactly in terms of radicals. We can however solve for m numerically as follows.

```
> Digits := 20:
> fsolve(a,m,0..1);
```

$$.42127954398390343277, .58863320774543513596,\\ .85329426491606600846,\\ .85990342812346032974,\\ .95225192338964487310,\\ .97654789054414157453, 0$$

Thus the value of m is .4212795440 to 10 significant digits. The `grobner` package in Maple contains another function, `finduni`, that computes this polynomial in m directly for us. This function will often be somewhat faster in general. Thus the best approach in Maple is to do `finduni(m, polynomials);`.

The minimal polynomials for the circles problems for $n =$ 10..20 are given in the table below. The cases $n = 12, 14, 16$ are trivial. They are not included. The optimal solution for m is the smallest positive real root of these polynomials. An approximation is given. We note that we were not able to find the solution for $n = 13$ using the Gröbner basis method. Maple was not able to solve 7 quadratic equations. We found the solution using an elimination method based on computing polynomial resultants and greatest common divisors.

For $n = 10,\ m \approx 0.421279$ from

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

For $n = 11,\ m \approx 0.398297$ from

$$m^8 + 8\,m^7 - 22\,m^6 + 20\,m^5 + 18\,m^4 - 24\,m^3 - \\ 24\,m^2 + 32\,m - 8$$

For $n = 13,\ m \approx 0.366096$ from

$$5322808420171924937409\, m^{40} + \\ 5867739593380498886173232\, m^{39} +$$

...

$$2960075719794736758784\, m^{2} - \\ 1741035320946091622240\, m + \\ 47569271064100086400$$

For $n = 15,\ m \approx 0.341081$ from

$$2\,m^4 - 4\,m^3 - 2\,m^2 + 4\,m - 1$$

For $n = 17, m \approx 0.306154$ from

$$m^8 - 4\,m^7 + 6\,m^6 - 14\,m^5 + 22\,m^4 - \\ 20\,m^3 + 36\,m^2 - 26\,m + 5$$

For $n = 18,\ m \approx 0.300463$ from

$$13 - 144\,m^2$$

For $n = 19,\ m \approx 0.289542$ from

$$484\,m^{14} - 2376\,m^{13} - 19320\,m^{12} + 102620\,m^{11} \\ -31387\,m^{10} - 221444\,m^{9} + 159246\,m^{8} + 169172\,m^{7} - \\ 70723\,m^{6} - 105660\,m^{5} + 89292\,m^{4} - 26000\,m^{3} + \\ 2704\,m^{2}$$

For $n = 20,\ m =\approx 0.286612$ from

$$128\,m^2 - 96\,m + 17$$

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