Optimal separation of points

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Abstract

How should n points be distributed in a given region $\mathcal{F}$ in $\mathbb{R}^d$ such that they are separated as much as possible? This general problem is studied in this paper, for some combinations of $\mathcal{F}$, d ,n, and the ways one can state this problem mathematically. Some numerical optimization methods are suggested and tested, both on the point separation problem and the closely related circle packing problem. The results are compared with some known analytical results. The main conclusion is that the suggested numerical methods are useful general tools to obtain optimal solutions to the considered problems.

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1 Introduction

1.1 Background

An early example of the problem of separating points as far as possible was raised by the botanist P. M. L. Tammes in 1930. He wanted to explain the observed distribution of the pores on a grain of pollen. He proposed that for the sake of maximum biological efficiency the pores on a grain of pollen should be placed as far away from each other as possible. This problem is related to an even earlier problem that was stated by J. J. Thompson 1904, which was to determine the minimum energy configuration of N electrons on the surface of a sphere that repel each other with a force given by Coulomb's law. The problem to separate points as far as possible is also related to packing problems, which involve the every day attempt to bring objects together as densely as possible. The general problem formulation, that is to separate points on a region as far as possible, is an important problem, not only in the industry but in nature as well.

1.2 Aim of the thesis

The aim of this thesis is to suggest and test algorithms for solving the general problem formulation stated in the abstract, that is how are n number of points going to be distributed in a given region $\mathcal{F}$ in $\mathbb{R}^d$ such that they are separated as much as possible? There are analytical results for certain combinations of $\mathcal{F}$ and d, but in general it is not possible to solve the problem analytically. Even numerically it should be difficult, at least of finding a global solution.

We will suggest different numerical methods which more or less uses the actual specialized structure of the problem, these methods and the results respectively will be compared later on and discussed. Numerical methods will also be suggested to the closely related circle packing problem.

1.3 Related work

This section review some of what is known in optimizing the distance between a given number of points within a region. But also the packing problem, that is how to pack objects together as densely as possible. In this paper we will focus on circular objects packed within a circle, a square and a cub.

In the paper of Bhaskar Bagchi [1] the so called Tammes' Problem is discussed. The essence of this problem is how to separate n points to its maximum on a spherical universe. He states that if you want to maximize the minimum distance for n points on the surface of a sphere, you must place the points at the the vertices of the Platonic solids, and that is the unique solution. But this cannot be used for all $n = 4, 6, 8, 12, 20$.

Some optimal solutions for $n \leq 12$ can be seen in the following table (1). Note that the convex hull of any n points on the sphere is a convex polyhedron whose vertices are precisely the n points that we began with. So it is often convenient to describe a solution to an instance of Tammes' problem as (the set of vertices of) a convex polyhedron. In the first column of Table (1) is the number n, and in the second is the geometry of the solutions and third if possible, the optimal length between the vertices of the Platonic solids inside a unit sphere [2].

Moreover, there are known optimal solutions for the maximal minimal distance (Tammes problem) and the minimal potential (Thomson problem) for $n = 4, 6, 9, 12, 16, 25$ for the region surface of the unit sphere listed in Table (2) [10] [24]. In the first column of Table (2) is the number n, the second column is the solutions for the Tammes problem and in the third column is the solutions of Thomson problem.

n	Vertices of:	Distance between vertices	Uniqueness
4	Tetrahedron	$\sqrt{8/3} = 1.6329932$	Unique
5	Octahedron minus a vertex	$\sqrt{2} = 1,4142136$	Not unique
6	Octahedron	$\sqrt{2} = 1,4142136$	Unique
8	Square anti-prism	$2\sqrt{4 - \sqrt{2}/7} = 1.2155625$	Unique
11	Icosahedron minus a vertex	$2p/\sqrt{1+p^2} = 1,0514622$	Not unique
12	Icosahedron	$2p/\sqrt{1+p^2} = 1,0514622$, where $p = \frac{\sqrt{5}-1}{2}$.	Unique

Table 1: Proven optimal solutions for certain n on a surface of a unit sphere

n	Min dist for Tammes	Min pot for Thomson
4	1.632993	3.674235
6	1.414214	9.985281
9	1.154701	25.759987
12	1.051462	49.165253
16	0.8805742	92.911655
25	0.7107762	243.812760

Table 2: Proven optimal solutions for certain n on a surface of a unit sphere

For the closely related packing problem there are some proven results for $n \leq 25$, for the regions unit circle and the unit square [22] [14] [23] [18]. Below is a table for each region, Table 3 that is for the container unit circle and the unit square respectively. The values that are shown in table 3 are maximal radius for identical circles packed inside a unit circle and identical circles packed inside a unit square as densely as possible. Note that for $n \leq 13$ and for $n = 19$ for the circular container, the values are proven to be globally optimal. And for the square container all $n \leq 25$ are proven to be globally optimal.

n	Circular container	Square container
	Optimal radius	Optimal radius
2	0.5000	0.2929
3	0.4641	0.2543
4	0.4142	0.2500
5	0.3702	0.2071
6	0.3333	0.1877
7	0.3333	0.1745
8	0.3026	0.1705
9	0.2769	0.1666
10	0.2623	0.1482
11	0.2549	0.1424
12	0.2482	0.1400
13	0.2361	0.1400
14	0.2310	0.1303
15	0.2212	0.1272
16	0.2167	0.1250
17	0.2087	0.1172
18	0.2056	0.1155
19	0.2056	0.1123
20	0.1952	0.1114
21	0.1904	0.1068
22	0.1838	0.1057
23	0.1803	0.1029
24	0.1769	0.1014
25	0.1738	0.1000

Table 3: The maximal radius when packing equal circles within a unit circle and a unit square. For $n \leq 13, n = 19$ the values are proven optimal for the circular container. For the square container all $n \leq 25$ are proven to be optimal

2 Mathematical formulations

In this chapter, the mathematical formulations of the considered problems are stated and discussed.

2.1 Max-min optimization problem

The general problem formulation can be stated as to maximize the distance between the points in the region. One approach is to use the theory of optimization and state this problem as an optimization problem. One way of doing that is to calculate all the distances possible and choose the one that which is the least, then maximize that distance and thus the "Max-min" optimization problem is risen. What does it really mean mathematically? Since this problem is an optimization problem, we need to determine what the objective function is and what the constraints are. One can state this optimization problem by to maximize the least distance between points. First of all we must determine what we mean by distance. From now on the distance is dermined by the Euclidean norm since we assume that the space is an Euclidean space.

By constructing a variable w and say that this variable is the minimal distance between all the points, i.e $w \leq \|\mathbf{p}_i - \mathbf{p}_j\|$, where $\mathbf{p}_i$ is the coordinate vector for point i in $\mathbb{R}^d$. To maximize w, which is equivalent to minimize $-w$. Thus we have our first optimization problem

$$\begin{array}{ll} \text{minimize} & -w \\ \text{subject to} & w \leq \|\, \mathbf{p}_i - \mathbf{p}_j \|, \quad (i,j) \in \mathcal{J}, \\ & \mathbf{p}_i \in \mathcal{F}, \quad i = 1, \dots, n. \end{array} \tag{1}$$

where $\mathcal{J} = \{\, (i,j) \mid 1 \leq i < j \leq n \,\}$, $\mathbf{p} = (\mathbf{p}_1^T, \dots, \mathbf{p}_n^T)$ and $\mathbf{p}_i = (x_i, y_i, z_i)^T$ or $\mathbf{p}_i = (x_i, y_i)^T$. With this mathematical problem we can theoretically solve the problem of separating points within a region, by maximizing the smallest distance.

2.2 Minimum potential problem

The real nature of the problem is that the points wants to be as far from each other as possible. So the question is if we can formulate that problem in a more natural way and less as a mathematical. It is a very interesting point of view since the effect where points want to stay away from each other as far as possible actually occurs in nature, namely for identically charged particles. This gives us the ability to write the general problem in a more physical manner, but still as an optimization problem.

We begin by formulating the mathematical description of the problem. In a system with identically charged particles there will be an electrostatic interaction between each and every one of them, that is the electrical potential. The potential describes how much energy the system of charged particles has. Say for simplicity there are only two particles in a physical system. The electrical potential in that system of two identically charged particles will be lesser if the the two particles are more far way from each other, that statement is followed by Columb's law [3]. If the particles are contained within a region and minimize the potential of the particle system, the particles will be stationed far away of each other as possible, within the region. The potential of two identically charged particles is $\frac{k_e q^2}{\| \mathbf{p}_i - \mathbf{p}_j \|}$, where k_e is the Coulombs constant and q is the charge of each particle. For more than two particles, the potential function for a system of n identical particles is given by

$$f(\mathbf{p}) = \sum_{(i,j)\in\mathcal{J}} \frac{k_e q^2}{\| \mathbf{p}_i - \mathbf{p}_j \|} \qquad (2)$$
$$\mathbf{p}_i \in \mathcal{F}, \quad i = 1, \ldots, n.$$

where $\mathcal{J} = \{ (i,j) \mid 1 \leq i < j \leq n \}$, $\mathbf{p} = (\mathbf{p}_1^T, \ldots, \mathbf{p}_n^T)$ and $\mathbf{p}_i = (x_i, y_i, z_i)^T$ or $\mathbf{p}_i = (x_i, y_i)^T$. For simplicity $q = k_e = 1$. This is valid mathematically since that does not affect the optimization. The solution of the problem is the interesting part, that is the distribution of the particles in the region after minimizing the potential. The following optimization problem follows, that is to minimize the potential of the particles within the region $\mathcal{F}$

$$\text{minimize} \quad f(\mathbf{p}) = \sum_{(i,j)\in\mathcal{J}} \frac{1}{\| \mathbf{p}_i - \mathbf{p}_j \|} \qquad (3)$$
$$\text{subject to} \quad \mathbf{p}_i \in \mathcal{F}, \quad i = 1, \ldots, n.$$

where $\mathcal{J} = \{ (i,j) \mid 1 \leq i < j \leq n \}$. In optimization methods gradients are important since the negative gradient describes in what direction the directional derivative is most negative. The gradient of the potential function (3) is given by

$$\nabla f(\mathbf{p}) = (\nabla_{\mathbf{p}_1} f(\mathbf{p})^T, \ldots, \nabla_{\mathbf{p}_n} f(\mathbf{p})^T)^T \qquad (4)$$

where

$$\nabla_{\mathbf{p}_i} f(\mathbf{p}) = \sum_{j\neq i} -\frac{\mathbf{p}_i - \mathbf{p}_j}{\|\mathbf{p}_i - \mathbf{p}_j\|^3} \qquad (5)$$

Why are we considering two different optimization problems (1) and (3) which seems to solve the same general problem? The reason is that the Max-min optimization problem is different from the Minimum potential problem, despite that both problems are striving for separation of points. The reason is how each problem solves the general problem of optimally separate points within a region. The following trivial case will explain why they are different in calculating the final distribution of the separated points by solving it for a simple trivial region and for a small number of points. Then a comparison of the solutions from the both optimization problems can be done.

Let the region for the points to be contained in be the interval $[-1, 1] \in \mathbb{R}$ with only 4 points to optimize, i.e $n = 4$. Firstly, the Max-min optimization problem will solve the problem through maximizing the minimal distance. It can be seen that two of the 4 points will be found in each boundary of the interval and two of the other points will remain somewhere between the origin and its closest boundary. By symmetry,

$$x_1 = -1, \quad x_2 = -t, \quad x_3 = t, \quad x_4 = 1, \quad t \in [0, 1] \qquad (6)$$

Since the Max-min optimization searches for the minimal distance and then maximize that distance, the equilibrium of the system is trivial and finds it self distributed evenly through the interval $[-1, 1]$, i.e $t = \frac{1}{3}$. The Minimum potential problem solves this problem in a different manner. As spoken of earlier the Minimum potential problem uses that the system can be modeled in a more physical manner, and represent the 4 points to identically charged particles. Since they are charged particles of the same charge there will be an electrical force that distributes the particles through the interval, since the force is the negative gradient of the potential, i.e $\mathbf{F}_i = -\nabla_{\mathbf{p}_i} f(\mathbf{p})$ where as $\mathbf{p} = (\mathbf{p}_i^T, \ldots, \mathbf{p}_n^T)$ Two of the particles will be forced to be stationed at each end of the interval, as before. But the remaining two particles will be positioned somewhere between the origin and its closest boundary as before, i.e $x_1 = -1, \quad x_2 = -t, \quad x_3 = t, \quad x_4 = 1, \quad t \in [0, 1]$. The force on each particle within the system must be investigated since it is the force that distributes the particles. The force from charged particles are $F = \frac{1}{d_{ij}^2}$, where d_{ij} is the distance between particle i and j. The force equilibrium equation on particle x_3 becomes

$$\frac{1}{(1-t)^2} = \frac{1}{(2t)^2} + \frac{1}{(1+t)^2} \tag{7}$$

This equation becomes a fourth grade polynom equation with the solution $t \approx 0.36148 > \frac{1}{3}$. Thus the final distribution for the Minimum potential solution is

$$x_1 = -1, \quad x_2 \approx -0.36, \quad x_3 \approx 0.36, \quad x_4 = 1 \tag{8}$$

Conclusively using the Max-min optimization problem we found that $t = \frac{1}{3}$, but with the Minimum potential problem we got $t \approx 0.36148 > \frac{1}{3}$. The Max-min optimization problem wants to maximize the minimum distance, but the Minimum potential problem wants to minimize the potential of the system. This is the major differens between the two optimization problems, and why we study both of them.

2.3 Packing problem formulation

Packing means that one tries to bring non-overlapping objects together (e.g. inside a container) as densely as possible. Since packing problems very much depends on the geometry of the objects and the region the objects are attempted to be contained within, the problem cannot be solved generally. Instead by using certain constraints the packing problem can be solved. The objects are in this work assumed identical and has the geometry of unit circles. We are looking at two containers, they are both in $\mathbb{R}^2$. The containers are the unit circle and the unit square with corners in $(\pm 0.5, \pm 0.5)$.

It is trivial to say that the method to packing is optimization, that is to maximize the number of circles within a unit circle. The model of the problem is an optimization formulation since instead of the circles there are points that represents the center of each circle. For every optimization problem, one need to declare the variables. Let the variables be the coordinates of each center of the circles, $\mathbf{p}_i \in \mathbb{R}^2$, i.e $\mathbf{p}_i = (x_i, y_i)^T$ for each point i. Let the radius of a circle be a variable since they are identical, thus add r to the collection of variables. To maximize the number n of small circles within the unit circles can be solved by instead for $n = 1, 2, 3, \ldots$ solve maximizing the radius of the small circles.

Since the circles can not overlap an important constraint is risen, that is that the distance between the centers can not exceed the diameter of the circle (since the diameter is twice the radius). And thus the constraint becomes $2r \leq \|\mathbf{p}_i - \mathbf{p}_j\|$. The centers of the circles cannot reach the boundary of the larger unit circle. Meaning that the points, i.e the centers of the circles are bounded to the circle with a radius $1 - r$, where 1 is the radius of the unit circle. That is the next constraint.

What is to be maximized? I.e what is the objective function? As discussed before the objective is to maximize the distance between the centers of the identical circles. Since the circles are identical, the objective function is to maximize the radius r. Instead of maximizing one can transform it to minimizing due to the convention of optimizing. Thus the objective function becomes, minimize $-r$. The packing problem becomes an optimization problem

$$\begin{aligned} \text{minimize} \quad & -r \\ \text{subject to} \quad & 2r \leq \| \mathbf{p}_i - \mathbf{p}_j \|, \quad (i,j) \in \mathcal{J}, \\ & \|\mathbf{p}_i\| \leq 1 - r, \quad i = 1, \dots, n. \end{aligned} \tag{9}$$

where $\mathcal{J} = \{\, (i,j) \mid 1 \leq i < j \leq n \,\}$, $\mathbf{p}_i = (x_i, y_i)^T$. Note that n circles with given radius r_0 can be placed in the unit circle if and only if $r_0 \leq \hat{r}(n)$ where $\hat{r}(n)$ is the optimal r in (9).

Next is the case with the container being the unit square with corners in $(\pm 0.5, \pm 0.5)$. The same logical argument is true in this case except for the regional constraint, that is the walls of constraint where the center of the circles can not cross over. Thus the optimization formulation for packing identical circles within a unit square

$$\begin{aligned} \text{minimize} \quad & -r \\ \text{subject to} \quad & 2r \leq \| \mathbf{p}_i - \mathbf{p}_j \|, \quad (i,j) \in \mathcal{J}, \\ & r - 0.5 \leq x_i \leq 0.5 - r, \quad i = 1, \dots, n. \\ & r - 0.5 \leq y_i \leq 0.5 - r, \quad i = 1, \dots, n. \end{aligned} \tag{10}$$

where $\mathcal{J} = \{\, (i,j) \mid 1 \leq i < j \leq n \,\}$, $\mathbf{p}_i = (x_i, y_i)^T$. As one can see, that the mathematical formulation of packing problems is naturally derived to becoming an optimization problem. To be more exact it becomes more like a Max-min optimization problem, as discussed earlier.

2.4 Convexity

The discussion of convexity is highly important since the mathematical problems stated are optimization problems. There is a theorem that states that if the optimization problem is convex then every local minimizer is a global minimizer [6]. Thus if the optimization problems formulated earlier are convex then only global solutions can be found. Let us first talk about convexity.

A set S is convex if, for any element $\mathbf{p}$ and $\mathbf{q}$ of S

$$\alpha \mathbf{p} + (1 - \alpha)\mathbf{q} \in S \tag{11}$$

for all $0 \leq \alpha \leq 1$. In other words, if $\mathbf{p}$ and $\mathbf{q}$ are in S, then the line segment connecting the $\mathbf{p}$ and $\mathbf{q}$ is also in S. Moreover a function f is convex function on a convex set S if it satisfies

$$f(\alpha\mathbf{p} + (1-\alpha)\mathbf{q}) \leq \alpha f(\mathbf{p}) + (1-\alpha) f(\mathbf{q}) \tag{12}$$

for all $0 \leq \alpha \leq 1$ and for all $\mathbf{p}, \mathbf{q} \in S$. This definition says that the line segment connecting the points $(\mathbf{p}, f(\mathbf{p}))$ and $(\mathbf{q}, f(\mathbf{q}))$ lies on or above the graph of the function. Let us return to the local and global solutions. We define a convex optimization problem to be an optimization problem where the region is convex and the function to be minimized is convex on the convex region.

An investigate of the optimization problems is needed to conclude that either the optimization problems are either convex or not. The Min-max optimization problem has a convex function because every linear function is a convex function. But the region or the set is not convex, due to the constraint $w \leq \|\mathbf{p}_i - \mathbf{p}_j\|$. The following example disproves that the set $w \leq \|\mathbf{p}_i - \mathbf{p}_j\|$ is convex, since there exist a convex combination that does not appear in the set, i.e there exist an $\alpha \in [0,1]$ such that (11) is not fulfilled. Let us use the notation $\mathbf{p} = (\mathbf{p}_1^T, \ldots, \mathbf{p}_n^T)$, $\mathbf{p}_i = (x_i, y_i)^T$. Assume $n = 2$ and define the 2 points $\mathbf{p}^{(1)}$ and $\mathbf{p}^{(2)}$ with the corresponding w value

$$\begin{gathered} \mathbf{p}_1^{(1)} = (0,0)^T, \quad \mathbf{p}_2^{(1)} = (1,0)^T, \quad w^{(1)} = 1 \\ \mathbf{p}_1^{(2)} = (0,0)^T, \quad \mathbf{p}_2^{(2)} = (-0.8,0)^T, \quad w^{(2)} = 0.8 \end{gathered} \tag{13}$$

Note that the points $\mathbf{p}^{(1)}$ and $\mathbf{p}^{(2)}$ are feasible. A convex combination of the points $\mathbf{p}^{(1)}$, $\mathbf{p}^{(2)}$ with $\alpha = 0.5$ gives

$$\mathbf{p}^{(3)} = \frac{1}{2}\mathbf{p}^{(1)} + \frac{1}{2}\mathbf{p}^{(2)}, \quad w^{(3)} = \frac{1}{2}w^{(1)} + \frac{1}{2}w^{(1)} \tag{14}$$

Thus the third point calculated is

$$\mathbf{p}_1^{(3)} = (0,0)^T, \quad \mathbf{p}_2^{(3)} = (0.1,0)^T, \quad w^{(3)} = 0.9 \tag{15}$$

But $\mathbf{p}^{(3)}$ is not feasible since the values of $\mathbf{p}^{(3)}$ and $w^{(3)}$ does not fulfill the constraint $w \leq \|\mathbf{p}_i - \mathbf{p}_j\|$. Thus we conclude that the Max-min optimization problem is not a convex optimization problem.

How about the second optimization formulation, i.e the potential optimization problem? One can see that the objective function, that is the potential function of the system is not a convex function because it does not fulfill equation (12). To prove that the Potential function is not a convex function the same can be done with same mathematical example as before. Remember the potential function

$$f(\mathbf{p}) = \sum_{(i,j)\in\mathcal{J}} \frac{1}{\|\,\mathbf{p}_i - \mathbf{p}_j\|} \tag{16}$$

where $\mathcal{J} = \{\,(i,j) \mid 1 \leq i < j \leq n\,\}$. Define the following points with the corresponding potential function value

$$\begin{gathered} \mathbf{p}^{(1)} = (\mathbf{p}_1^{(1)}, \mathbf{p}_2^{(1)}) = (0,0,1,0)^T, \quad f(\mathbf{p}^{(1)}) = 1 \\ \mathbf{p}^{(2)} = (\mathbf{p}_1^{(2)}, \mathbf{p}_2^{(2)}) = (0,0,-0.8,0)^T, \quad f(\mathbf{p}^{(2)}) = \frac{1}{0.8} \end{gathered} \tag{17}$$

A convex combination is done of the points $\mathbf{p}^{(1)}$, $\mathbf{p}^{(2)}$ with $\alpha = 0.5$, and thus the third convex combinated point with the corresponding potential value becomes

$$\mathbf{p}^{(3)} = \frac{1}{2}\mathbf{p}^{(1)} + \frac{1}{2}\mathbf{p}^{(2)} = (0, 0, 0.1, 0)^T, \quad f(\mathbf{p}^{(3)}) = \frac{1}{0.1} \tag{18}$$

The potential function values of the points $\mathbf{p}^{(1)}$, $\mathbf{p}^{(2)}$ and $\mathbf{p}^{(3)}$ does not satisfy equation (12) and thus the potential function is not a convex function.

Since the packing problem formulation is originally a Max-min optimization formulation it cannot be a convex optimization problem. None of the optimization problem (1), (3), (9) nor (10) are convex optimization problems. We can not conclude that every local minimizer found is a global minimizer, and thus we cannot be sure that every calculated solution is a global solution to the problem.

3 Methods

To solve the general problem there are a couple of mathematical problems, but to actually solve them a method is needed. In this section we present the methods used to implement the mathematical problems stated earlier. The methods used are the Fmincon in the Matlab software, but also a method based on differential equations.

3.1 Fmincon algorithm

Fmincon is one of the algorithm used in the mathematical software Matlab. Matlab is a programming environment for algorithm development, data analysis, vizualization and numerical computation. Matlab is used here for algorithm development. Fmincon is an optimization problem solver that attempts to find a constrained minimum of a scalar function of several variables starting at an initial estmate. The algoritm we are using in Fmincon is the Active-set method.

The definition of what it means to have an active-constraint or an active-set needs to be clarified. Given a point $\mathbf{p}$ in the feasible region, a constraint $g_i(\mathbf{p}) \geq 0$ is called active at $\mathbf{p}$ if $g_i(\mathbf{p}) = 0$. The active set at $\mathbf{p}$ is made up of those constraints $g_i(\mathbf{p})$ that are active at the current point [7]. Problems that have inequality constraints are significantly more difficult to solve than problems in which all constraints are equations. The reason is that it is not known in advance which inequality constraints are active at the solution. Active-set methods attempt to overcome this difficulty by moving sequentially from one choice of active constraint to another choice that is guaranteed to produce at least as good a solution.

The Fmincon algorithm needs an initial estimate (starting points) as well as the stopping criteria. The initial estimate are the points of a spiral, see Figure (1) The spiral initial estimate is good choice since the points are distributed evenly and in way that no points coincide with another, it provides the Active-set with a nice initial estimate. The Fmincon stops when the stopping criteria are fulfilled. There are two stopping criteria for the algorithm Fmincon, the first-order optimality measure and the maximum constraint violation. The definition of the first order optimality measure is based on the Karush-Kuhn-Tucker (KKT) conditions [6]. The KKT conditions are analogous to the condition that the gradient must be zero at a minimum, modified to take constraints into account. The criteria for the first-order optimality measure is that it must not be greater than 10^{-6}. The second stopping criteria is when the maximum constraint violation do not exceed the limit of 10^{-6}.

The method of Fmincon is used for both the Max-min optimization problem and the Minimum potential problem.

3.2 Differental equation algorithm

In this section, we suggest a method for the Minimum potential problem (3) based on a system of differential equations obtained from Newton's and Coulumbs laws. Instead of using optimization we simply use a system of differential equations, and solve the problem in a more physical manner. What is about to be done is to discretize in time and apply Newtons law in every particle in each time instant. The mathematical description of the problem must be formulated at first. The following notations are used though out, $\mathbf{p} = (\mathbf{p}_1^T, \dots, \mathbf{p}_n^T)$, $\mathbf{p}_i = (x_i, y_i, z_i)^T$ or $\mathbf{p}_i = (x_i, y_i)^T$. We assume that all particles are identical in mass and in charge. Since there are electrical charges, the forces between them must be studied. For simplicity let there be two particles, and calculate the force from particle j to i. The notation of this force is $\mathbf{F}_{i,j}$ since it's applied to the parcticle i affected from particle j. The magnitude of the force is

$$\|\mathbf{F}_{i,j}\| = \frac{k_e q^2}{\|\mathbf{p}_i - \mathbf{p}_j\|^2} \tag{19}$$

Where q is the charge of each particle and k_e is the Coulomb's physical constant. As earlier mentioned we let the constants $q = k_e = 1$ since it does not affect the solution. The force must be in the direction $\mathbf{p}_i - \mathbf{p}_j$, and thus

$$\mathbf{F}_{i,j} = \frac{\mathbf{p}_i - \mathbf{p}_j}{\|\mathbf{p}_i - \mathbf{p}_j\|^3} \tag{20}$$

Since there are n particles in the system, the force $\mathbf{F}_i$ on particle i from all other particles is

$$\mathbf{F}_i(\mathbf{p}) = \sum_{j \neq i} \frac{\mathbf{p}_i - \mathbf{p}_j}{\|\mathbf{p}_i - \mathbf{p}_j\|^3} \tag{21}$$

Note that the force (21) is actually the negative gradient of the potential function (3) with respect to $\mathbf{p}_i$, i.e $\mathbf{F}_i(p) = -\nabla_{\mathbf{p}_i} f(\mathbf{p})$. Moving on to the differential equation system. We assume the particles are in a medium which slows the particles in proportion to the velocity, $\mathbf{F}_i^{med} = -c\mathbf{v}_i$ where c is the attenuation constant. With the notation $\mathbf{v}_i = \dot{\mathbf{p}}_i = (\frac{dx_i}{dt}, \frac{dy_i}{dt}, \frac{dz_i}{dt})^T$ the follwoing differential system is derived using Newton's law.

$$\begin{aligned} m\dot{\mathbf{v}}_i &= \mathbf{F}_i(\mathbf{p}) - c\mathbf{v}_i \\ \dot{\mathbf{p}}_i &= \mathbf{v}_i \end{aligned} \tag{22}$$

To simplify this system, assume that $\frac{m}{c} \to 0$, since the masses of the particles are so small this approximation can be done. The differential equation system becomes

$$\dot{\mathbf{p}}_i = \frac{\mathbf{F}_i(\mathbf{p})}{c}, \quad i = 1, \dots, n \tag{23}$$

This is the system of equation that should be solved numerically. That can be done through the Euler forward method. Then the following system is obtained:

$$\mathbf{p}_i(t_{k+1}) = \mathbf{p}_i(t_k) + \alpha_k \mathbf{F}_i(\mathbf{p}(t_k)), \quad i = 1, \dots, n \tag{24}$$

where $\alpha_k = (t_{k+1} - t_k)/c$.

To make sure that the potential decreases it is necessary to take small time steps, since for enough small α_k the potential will decrease. That the function do decrease can be proven in this way. Assume that the vector $\mathbf{d}$ satisfies the following inequality in a point $\mathbf{p}$

$$\mathbf{d}^T \nabla f(\mathbf{p}) < 0 \tag{25}$$

We do a lineseach in the direction of $\mathbf{d}$ using the step length α. Taylors theorem gives that

$$f(\mathbf{p} + \alpha\mathbf{d}) = f(\mathbf{p}) + \alpha\mathbf{d}^T\nabla f(\mathbf{p}) + \mathcal{O}(\alpha^2). \tag{26}$$

But since $\mathbf{d}^T\nabla f(\mathbf{p}) < 0$, the objective function value is guaranteed to decrease if α is sufficiently small. In our case, through physics it is known that the force is equal to the negative gradient of the potential, where the potential is our objective function. We choose our direction as the negative gradient of the potential, and that direction is in fact a descent direction since $\mathbf{d}^T\nabla f(\mathbf{p}) = -\|\nabla f(\mathbf{p})\|^2 < 0$. With that fact proven, we can make sure that the potential remains to decrease by adjusting the time step (step length). That is done by in every iteration controlling that the new potential is less than the previous potential, if not decrease the time step by a half.

If a point $\mathbf{p}_i$ is at the boundary of $\mathcal{F}$ and the force $\mathbf{F}_i(\mathbf{p})$ points out of $\mathcal{F}$ then the force is projected on the tangent plane of $\mathcal{F}$ at $\mathbf{p}_i$. The projected force (if not the zero vector) is still a descent direction of the potential function. The projection of the force depends on the region of calculation, and thus the mathematical explanation of how to project the forces comes in the next section with the description of the regions. Also, if the new point $\mathbf{p}_i + \alpha\mathbf{d}_i$ is outside $\mathcal{F}$, it is projected on $\mathcal{F}$.

One iteration of the suggested algorithm can be described as follows:
$\mathbf{d}_i = \mathbf{F}_i(\mathbf{p}(t_k))$ or $\text{proj}(\mathbf{F}_i(\mathbf{p}(t_k))), \quad i = 1, \ldots, n,$
$\bar{\alpha} = \min\{0.01,\, 0.1/\max_i \|\mathbf{d}_i\|\},$
$\mathbf{p}_i(t_{k+1}) = \mathbf{p}_i(t_k) + \alpha_k\mathbf{d}_i$ or $\text{proj}(\mathbf{p}_i(t_k) + \alpha_k\mathbf{d}_i), \quad i = 1, \ldots, n,$
where α_k is the largest of $\bar{\alpha}, \bar{\alpha}/2, \bar{\alpha}/4, \ldots$ such that $f(\mathbf{p}(t_{k+1})) < f(\mathbf{p}(t_k))$.

Since this is an algorithm, it needs an initial estimate, i.e starting point. It is natural to have the same initial estimate as the Fmincon, because a comparison can be done. The initial estimate is also the points of a spiral. So how about the stopping criteria? A possible stopping criteria for this method is when the points stop moving, and that is the one that is used. Numerically the stopping criteria is $\|\mathbf{p}_i(t_{k+1}) - \mathbf{p}_i(t_k)\| \leq 10^{-8}$ for all i. So if the points are not moving more than 10^{-8}, the points has stopped moving and thus the calculate solution is the final solution.

4 Test regions

The mathematical problems and the methods derived, have been tested on different regions $\mathcal{F}$ which are described in this chapter. For comparison reasons, the regions $\mathcal{F}$ have been chosen such that there are some known analytical results.

4.1 Inside a unit circle

The first region is the unit cricle, so the points that are about to be separated are bounded inside the unit circle in $\mathbb{R}^2$. Mathematically the region is described

$$\mathcal{F} = \{\mathbf{p}_i \in \mathbb{R}^2 \mid \|\mathbf{p}_i\| \leq 1\} \tag{27}$$

With the region mathematically written, a solution of the Max-min optimization problem and the Minimal potential problem by using the method Active-set in the algorithm Fmincon can be calculated. But with the differential equation problem the Fmincon cannot be used, since the algorithm Fmincon is only used for optimization systems. Since the method of differential equations is not a optimization problem, the points that are numerically calculated needs to stay within the region, in this case the unit circle.

The difficulty is how to state that the points can not move past the circular region when using the differential equation problem (24). To solve this problem the concept of projection must be used. Assume that point i was calculated to be outside the region, to bring it back to a corresponding point on the boundary a projection down must be made, i.e $\|\mathbf{p}_i\| = 1$. The following calculation make it happen $\mathbf{p}_i^{proj} = \frac{\mathbf{p}_i}{\|\mathbf{p}_i\|}$.

What happens with the forces at the boundary of the region? If the particles position $\mathbf{p}_i$ is at the boundary of the region and the force points out of $\mathcal{F}$, the same argument is used, i.e to bring it down to the tangent plane of the boundary a projection must be made. Lets say that a particle is stationed at the boundary of the region, and its force is directed out from the region. If that is the case, project that force down on the tangent plane. Let the projected force be denoted $\mathbf{F}_i^{proj}$. Then the following relation holds

$$\mathbf{F}_i^{proj} + t\mathbf{p}_i = \mathbf{F}_i \tag{28}$$

Where t is a parameter that is to be calculated. It is trivial that $\mathbf{p}_i^T \mathbf{F}_i^{proj} = 0$. From this relationship t can be calculate, multiply the equation (28) with $\mathbf{p}_i^T$ and thus $t = \mathbf{F}_i^T \mathbf{p}_i$. And now

$$\mathbf{F}_i^{proj} = \mathbf{F}_i - (\mathbf{F}_i^T \mathbf{p}_i)\mathbf{p}_i \tag{29}$$

4.2 Surface of a unit sphere

Next is the region of a surface of a unit sphere, that is that the points are bounded on that region, which gives us the mathematical description of $\mathcal{F}$

$$\mathcal{F} = \{\mathbf{p}_i \in \mathbb{R}^3 \mid \|\mathbf{p}_i\| = 1\} \tag{30}$$

The same argument is used to this region, that is Fmincon cannot be used here on the formulation of differential equations (24), so the exakt same projection is made, i,e projection of the forces to force the points to project down to the corresponding point as did in the previous region. The equation (28) is used and the following calculations to do so.

4.3 Inside a unit sphere

The upcoming region is now the whole unit sphere, interior and exterior. With n representing the number of points, the region $\mathcal{F}$ becomes

$$\mathcal{F} = \{\mathbf{p}_i \in \mathbb{R}^3 \;\mid\; \|\mathbf{p}_i\| \leq 1\} \tag{31}$$

As explained before, the samething is made here. That is to use projection to maintain that the points cannot escape $\mathcal{F}$. The use of equation (28) becomes again useful in this region and the calculation that follows.

4.4 Inside a square

The next region is different, namely the square with side length of 2. This means that the region $\mathcal{F}$ is written as, if for clarification since $\mathcal{F} \in \mathbb{R}^2$, the notation $\mathbf{p}_i = (x_I, y_i)^T$ is used

$$\mathcal{F} = \{\mathbf{p}_i \in \mathbb{R}^3 \;\mid\; |x_i| \leq 1, |y_i| \leq 1\} \tag{32}$$

As before the Fmincon only solves the first two mathematical problems, that is the Max-min optimization problem and the Minimum potential problem. Meaning that numerically force the points to be inside the region of $\mathcal{F}$ when using the differential equation formulation. The points calculated need to stay in the region, in this case the square. For simplicity, study the case where we have a wall at $x_i = 1$. To make sure that the point cant go through that wall, the value of the x-coordinate is substituted with the minimum between the value of the x-coordinate and 1. I.e $x_i^{proj} = min(x_i, 1)$. The same thought is applied to all other walls in the square.

How about the forces in this region? The same thing can be deduced as with the positions of the particles moving. If a particle is at a wall of a square, that force can't be directed in the same direction as the normal of that wall, since the particle can move past the wall. As before for simplicity, study the case where there is a wall at $x_i = 1$. If a particle is at the wall or beyond we substitute it with the minimum of its current value or the value 0. Or mathematically, $F_x^{proj} = min(F_x, 0)$.

4.5 Inside a cube

The last region to test the methods and mathematical problems is the cube with the side length of size 2. This means that the region $\mathcal{F}$ can be expressed in this way, if with the same analogous notation $\mathbf{p}_i = (x_i, y_i, z_i)^T$ since $\mathcal{F} \in \mathbb{R}^3$

$$\mathcal{F} = \{\mathbf{p}_i \in \mathbb{R}^3 \;\mid\; |x_i| \leq 1, |y_i| \leq 1, |z_i| \leq 1\} \tag{33}$$

The same logical calculations is done as with the square, both with the forces and how the positioning of the points cannot pass the walls of the cube.

5 Results

The mathematical problems are solved using the methods discribed earlier. With the different regions declared, solutions and test can be compared to each other. The mathematical problems, Max-Min optimization problems, Minimum potential problems and the problem of differential equations are labeled together with their methods as "Fmincon (max-min)", Fmincon (potential) and "Diff.eqn". With each method and mathematical formulation we have calculated the total potential of the system and the minimum distance, which is labeled as "Pot" and "Min dist" respectively below each of the mathematical problems in the tables. Note that the values that are highlighted are the best values for each row, the rows that does not have any highlighted values means that all values are the same. What does the tables show? All of the tables (4), (5), (6), (7) and (8) show that the maximum minimal distance is best obtained by using the Fmincon (max-min) method. The reason of why the Fmincon(max-min) gives the best optimal value of the maximum minimal distance is because it does not prioritize the potential value of the system. And thus it is the best at finding the optimal maximum minimal distance but at the cost of the potential value. Note that from table (4) for $n = 9$ and table (6) for $n = 12$ the maximal minimal distance value is not the best one for the Fmincon(max-min). The explanation is since none of the optimization problems are convex, each local minimum is not a global one. This rises the fact that the local minimum found using the Fmincon for the optimization problems can be a very bad local minimum. These values of table (4) for $n = 9$ and table (6) for $n = 12$ are such values.

The results show that the Fmincon(max-min) does not obtain the best potential value. It is obvious that either Fmincon(potential) or the differential equation problem gives us the best potential value of the system of points (particles). Both Fmincon(potential) and the differential equation problem calculates very good values for the potential value of the system. The potential value from the methods Fmincon(potenial) and Diff.eqn show for the region surface of the a unit sphere, that they are optimal when compared with the known optimal solutions from Table (2). And thus both of them are good methods that provides good optimal results. Which of the methods provides best the best potential optimal value? Results show that it is inconclusive. It can not be determined which of the methods Fmincon(potential) or Diff.eqn gives the best optimal value of the potential. Note that the method Diff.eqn have both good potential value and good minimal distance value.

We have also solved the problem of packing circles in containers of a larger circle and a square. The maximum radius of each of the identical circles are shown below in table (9) for each value of n

n	Fmincon (max-min)		Fmincon (potential)		Diff.eqn	
	Pot	Min dist	Pot	Min dist	Pot	Min dist
4	3.8284	1.4142	3.8284	1.4142	3.8284	1.4142
6	12.1502	**1.0000**	**10.9641**	0.9999	**10.9641**	**1.0000**
9	32.1981	0.7547	**30.4389**	0.7650	**30.4389**	**0.7654**
12	62.5258	**0.6602**	**59.5757**	0.5634	**59.5757**	0.5635
16	128.3843	**0.5370**	117.3701	0.4669	**116.5320**	0.4367
25	345.6416	**0.4142**	320.6982	0.3223	**320.6035**	0.3614

Table 4: The potential and the minimum distance. **Within a CIRCLE**

n	Fmincon (max-min)		Fmincon (potential)		Diff.eqn	
	Pot	Min dist	Pot	Min dist	Pot	Min dist
4	3.6742	1.6330	3.6742	1.6330	3.6742	1.6330
6	9.9853	1.4142	9.9853	1.4142	9.9853	1.4142
9	25.8013	**1.1547**	**25.7600**	1.1355	**25.7600**	1.1355
12	49.1653	1.0515	49.1653	1.0515	49.1653	1.0515
16	93.0827	**0.8745**	**92.9117**	0.8281	92.9204	0.8472
25	244.2360	**0.7093**	**243.8128**	0.6727	**243.8128**	0.6734

Table 5: The potential and the minimum distance. **Surface of a SPHERE**

n	Fmincon (max-min)		Fmincon (potential)		Diff.eqn	
	Pot	Min dist	Pot	Min dist	Pot	Min dist
4	3.6742	1.6330	3.6742	1.6328	3.6742	1.6330
6	9.9853	1.4142	9.9853	1.4142	9.9853	1.4142
9	25.8013	**1.1547**	**25.7600**	1.1355	**25.7600**	1.1355
12	51.9231	1.0000	**49.1653**	1.0509	**49.1653**	**1.0515**
16	95.8606	**0.9026**	**92.9117**	0.8284	**92.9117**	0.8284
25	255.4664	**0.7340**	**243.8134**	0.6721	243.8135	0.6757

Table 6: The potential and the minimum distance. **Within a SPHERE**

n	Fmincon (max-min)		Fmincon (potential)		Diff.eqn	
	Pot	Min dist	Pot	Min dist	Pot	Min dist
4	2.7071	2	2.7071	2	2.7071	2
6	11.1984	**1.0718**	**8.9960**	0.9998	**8.9960**	1.0000
9	24.9417	**1.0000**	**24.8794**	0.6379	25.0172	0.7873
12	55.4296	**0.7775**	**49.4458**	0.6550	49.9682	0.5881
16	110.5579	**0.5999**	**98.3714**	0.4587	**98.3714**	0.4588
25	394.2342	**0.4844**	**271.5181**	0.3598	**271.5181**	0.3599

Table 7: The potential and the minimum distance. **Within a SQUARE**

n	Fmincon (max-min)		Fmincon (potential)		Diff.eqn	
	Pot	Min dist	Pot	Min dist	Pot	Min dist
4	2.1213	2.8284	2.1213	2.8284	2.1213	2.8284
6	6.5749	**2.0730**	6.1987	2.0000	**5.9873**	2.0000
9	18.4350	**1.5403**	**15.9883**	1.0271	15.8529	1.0000
12	35.8932	**1.3110**	32.0669	0.9184	**32.0352**	0.9182
16	70.0929	**1.1280**	61.5048	0.8651	**61.4565**	0.8966
25	173.8034	**1.0000**	**165.8150**	0.6009	167.1198	0.5642

Table 8: The potential and the minimum distance. **Within a CUBE**

n	Radius for packing in a circle	Radius for packing in a square
3	0.4641	0.2500
4	0.4142	0.2500
5	0.3702	0.1964
6	0.3333	0.1877
7	0.3333	0.1735
8	0.3026	0.1667
9	0.2740	0.1667
10	0.2601	0.1407
11	0.2549	0.1362
12	0.2294	0.1400
13	0.2240	0.1320
14	0.2188	0.1248
15	0.2080	0.1229

Table 9: The values calculated for the packing problem

6 Plots

The final distribution of plots provided from our mathematical problems and methods respectively are shown for different n and regions. The first Figure (1) shows graphically the initial estimate used for all the methods, that is the "spiral" intial condition. Figures for the 3D regions, surface of the unit sphere, the unit sphere and the cube are not stated since it is difficult to even see how the points actually are distributed, for that reason we omit these figures.

The solution figures show how different the mathematical problems solve the general problem of separating points within a region. Note the difference in distribution between the Max-min optimization problem and the Minimum potential problem, the plots show how the Max-min problem are distributed in a way that the maximum minimal distance is prioritized to be as great as possible. That is shown for example for the solution for the Max-min optimization problem in Figure (2) and Figure (3), and for the solution for the Minimum potential problem in Figure (6) and (7). The plots also shows that the Potential optimization problems provides solution that are different from the Max-min optimization problem graphically. The Minimal potential problems searches for solution where as the points optimized are stationed at the boundary, as long as it is a local minimum and an optimal solution. That is perfectly shown in Figures (8) and Figure (9) compared with Table (4) and Table (4). The Diff.eqn problem provides solution where as both the Max-min and the Pot values are good, the potential values are optimal sometimes but it is rare. The same sort of solutions are provided by the Diff.eqn problem as with the Potential optimization problems, that is that it strives for solutions which are stationed at the boundary. But not at the degree as the Minimal distance problem sense the Diff.Eqn problem provides good Min dist values.

The final distribution for the packing problem are provided for the circular container in Figure (14)-(20), and for the square container in Figure (21)-(27). Figure (28) and Figure (29) shows how the initial estimate influence the solution. In Figure (28)(a) and (29)(a) shows the final global optimal distribution and solution for the Max-min optimization problem and Minimum potential problem, where as Figures (28)(b) and (29)(b) show an another solution for a different initial estimate The initial estimate in those tables are chosen randomly. Below each figure are the calculated values Max-min and the potential value. And thus the initial estimate does influence the solution of the problem since the optimization problems are not convex and the method used for each optimization problem is the method of the Active-set which is dependent on the initial estimate.

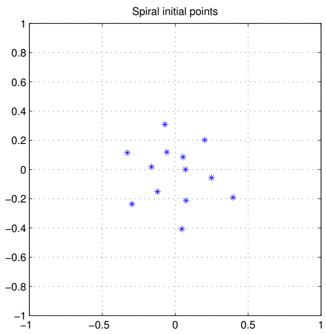
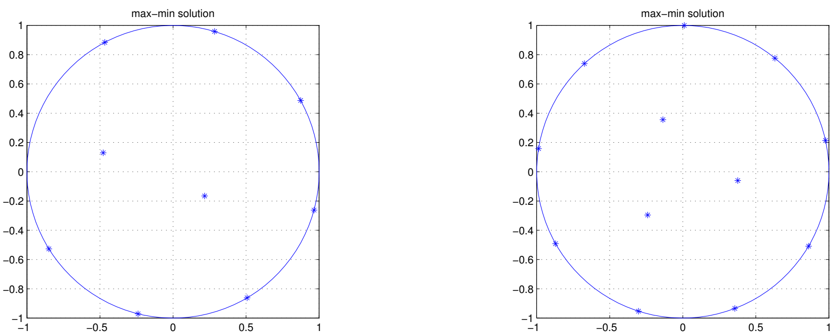


Figure 1: The "spiral" initial estimate shown for $n = 13$. This "spiral" initial condition is used in all methods.

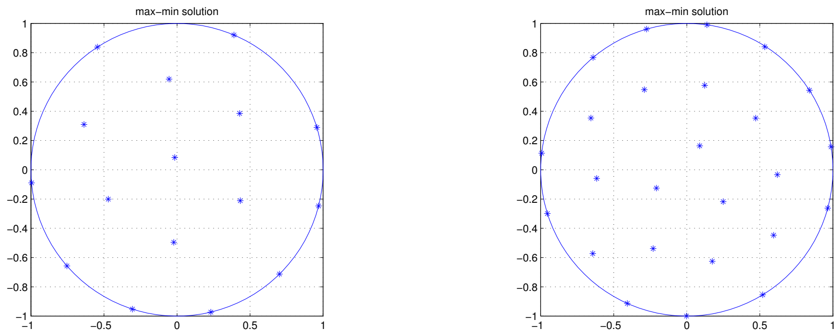
6.1 Max-min problem solutions



(a) The Max-min optimization problem solved for n=9 using a region of a circle

(b) The Max-min optimization problem solved for n=12 using a region of a circle

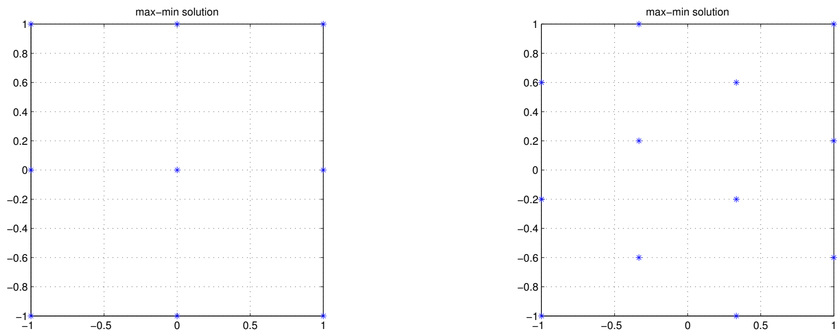
Figure 2



(a) The Max-min optimization problem solved for n=16 using a region of a circle

(b) The Max-min optimization problem solved for n=25 using a region of a circle

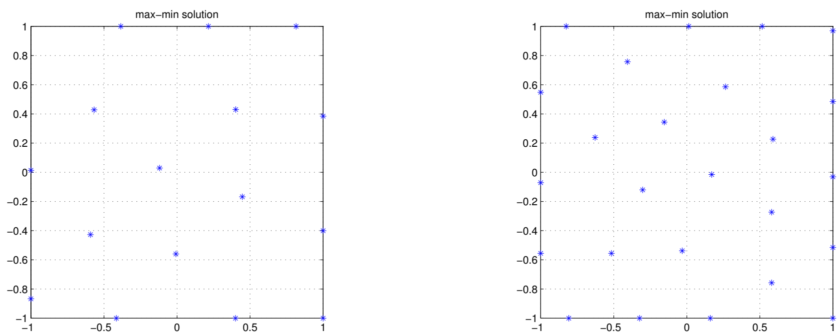
Figure 3



(a) The Max-min optimization problem solved for n=9 using a region of a square

(b) The Max-min optimization problem solved for n=12 using a region of a square

Figure 4

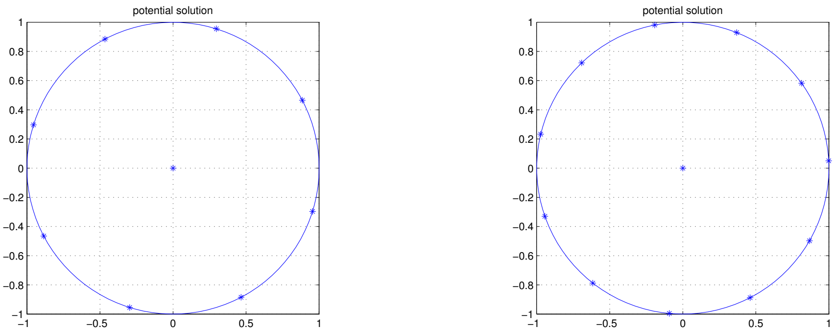


(a) The Max-min optimization problem solved for n=16 using a region of a square

(b) tThe Max-min optimization problem solved for n=25 using a region of a square

Figure 5

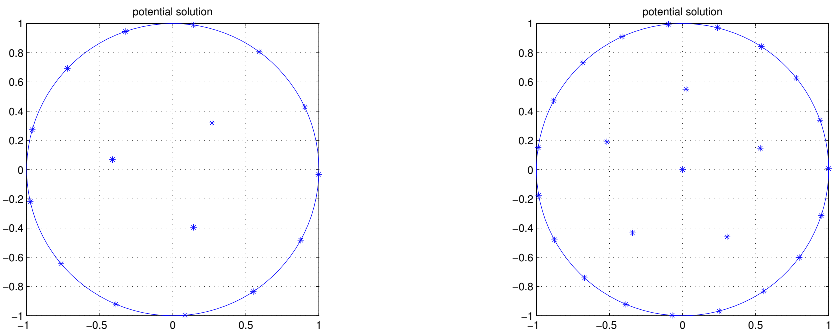
6.2 Potential problem solutions with Fmincon



(a) The Minimum potential problem solved for n=9 using a region of a circle

(b) The Minimum potential problem solved for n=12 using a region of a circle

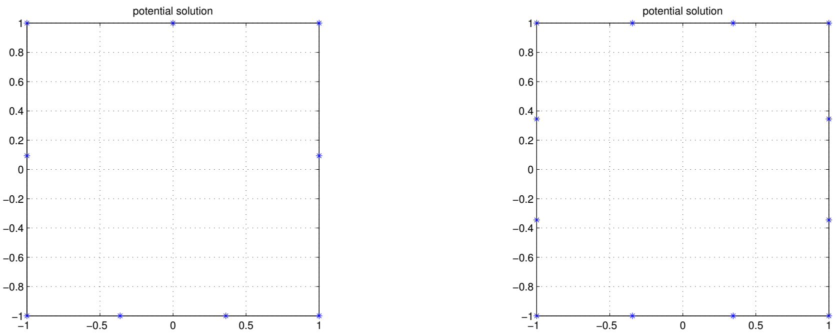
Figure 6



(a) The Minimum potential problem solved for n=16 using a region of a circle

(b) The Minimum potential problem solved for n=25 using a region of a circle

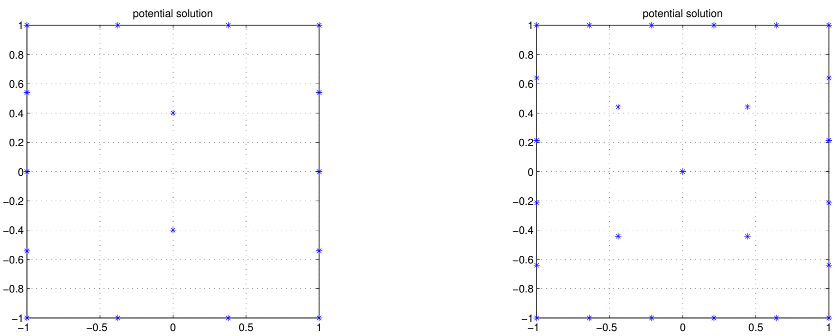
Figure 7



(a) The Minimum potential problem solved for n=9 using a region of a square

(b) The Minimum potential problem solved for n=12 using a region of a square

Figure 8

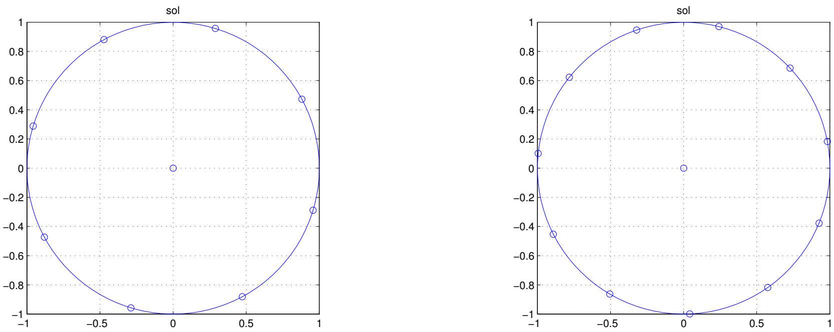


(a) The Minimum potential problem solved for n=16 using a region of a square

(b) The Minimum potential solved for n=25 using a region of a square

Figure 9

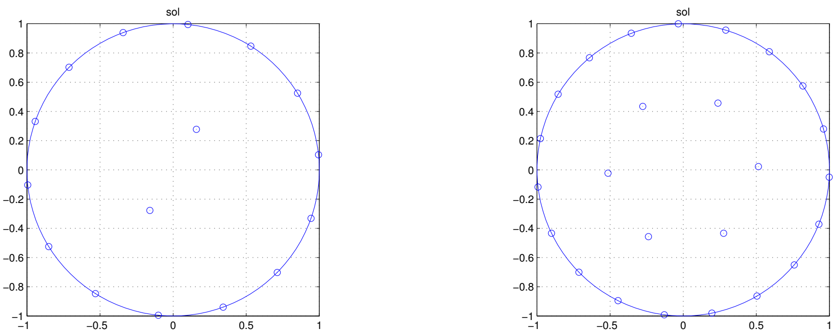
6.3 Potential problem solutions with Diff. eqn



(a) The differential equation problem solved for n=9 using a region of a circle

(b) The differential equation problem solved for n=12 using a region of a circle

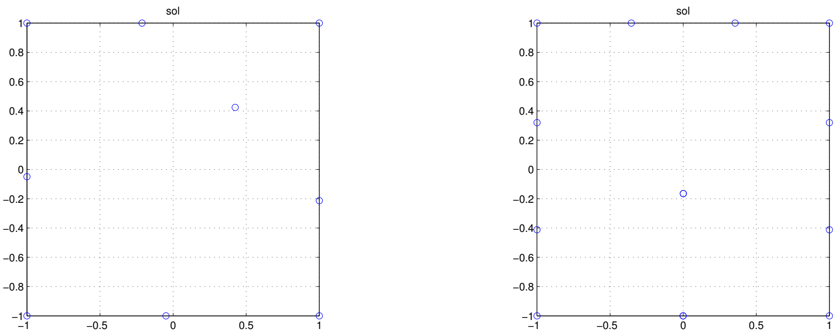
Figure 10



(a) The differential equation problem solved for n=16 using a region of a circle

(b) The differential equation problem solved for n=25 using a region of a circle

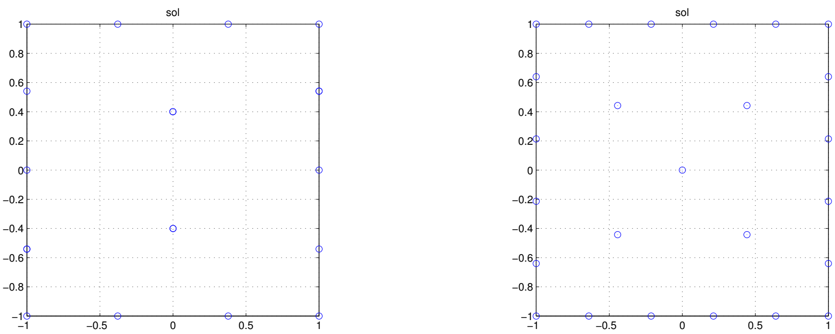
Figure 11



(a) The differential equation problem solved for n=9 using a region of a square

(b) The differential equation problem solved for n=12 using a region of a square

Figure 12

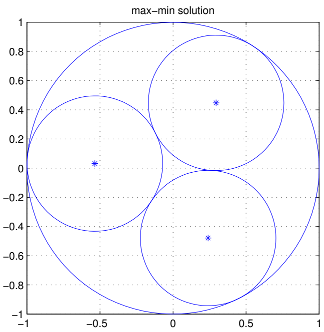


(a) The differential equation problem solved for n=16 using a region of a square

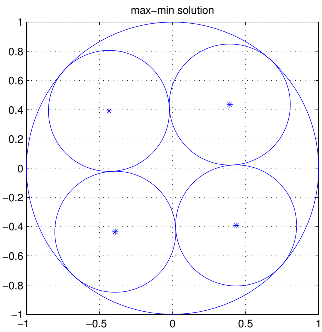
(b) The differential equation problem solved for n=25 using a region of a square

Figure 13

6.4 Packing problem solution

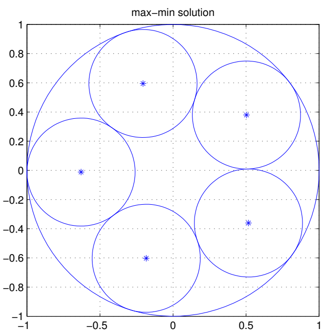


(a) Solving the problem of packing circles within a larger unit circle where as n=3. Global optimum

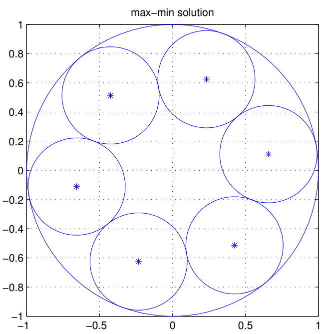


(b) tSolving the problem of packing circles within a larger unit circle where as n=4. Global optimum

Figure 14

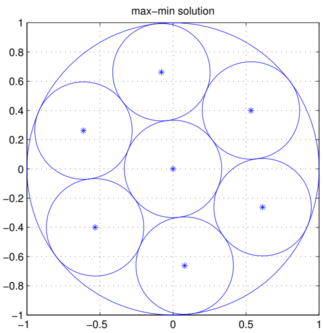


(a) Solving the problem of packing circles within a larger unit circle where as n=5. Global optimum

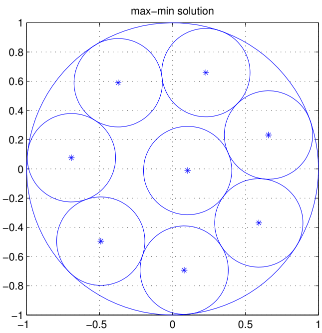


(b) Solving the problem of packing circles within a larger unit circle where as n=6. Global optimum

Figure 15

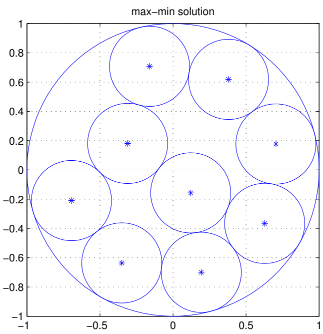


(a) Solving the problem of packing circles within a larger unit circle where as n=7. Global optimum

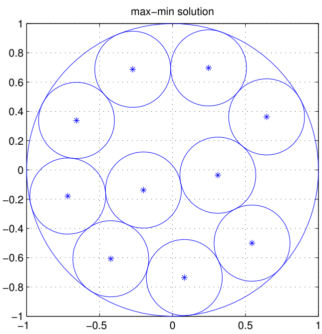


(b) Solving the problem of packing circles within a larger unit circle where as n=8. Global optimum

Figure 16

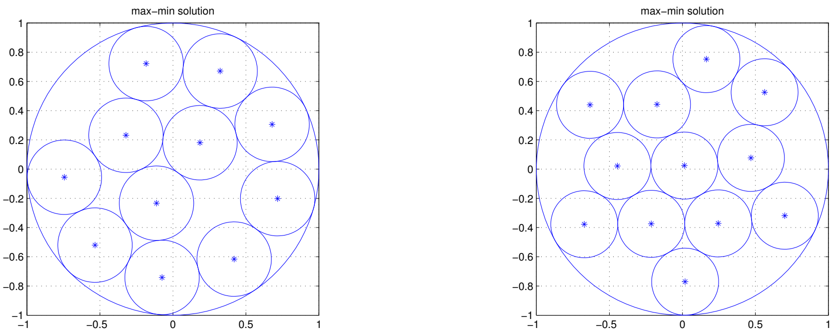


(a) Solving the problem of packing circles within a larger unit circle where as n=9



(b) Solving the problem of packing circles within a larger unit circle where as n=10

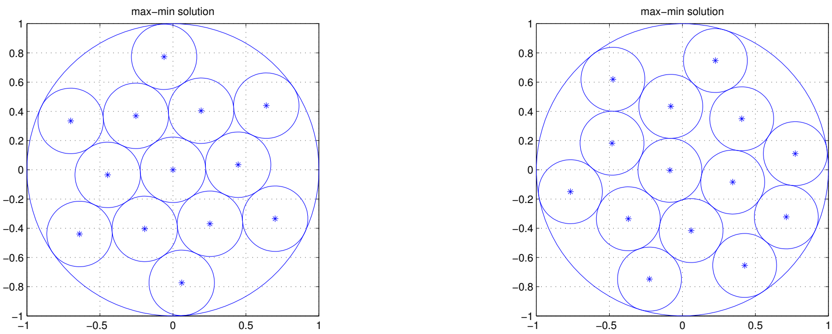
Figure 17



(a) Solving the problem of packing circles within a larger unit circle where as n=11. Global optimum

(b) Solving the problem of packing circles within a larger unit circle where as n=12

Figure 18



(a) Solving the problem of packing circles within a larger unit circle where as n=13

(b) Solving the problem of packing circles within a larger unit circle where as n=14

Figure 19

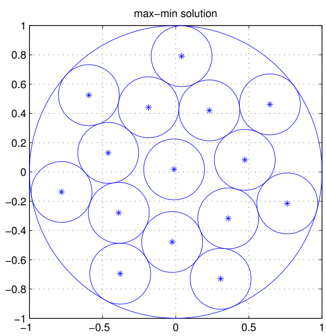
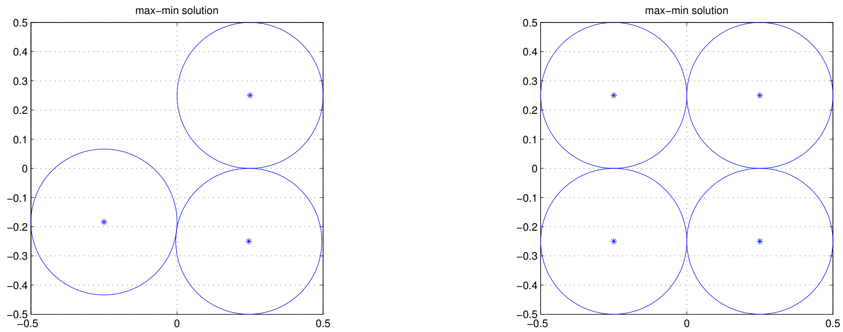


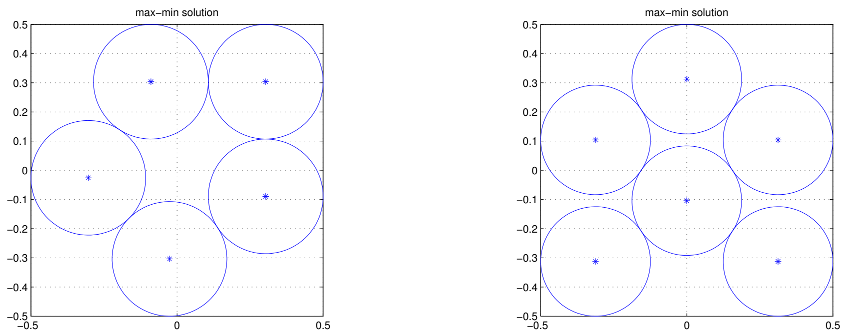
Figure 20: Solving the problem of packing circles within a larger unit circle where as n=15



(a) Solving the problem of packing circles within a larger square where as n=3

(b) Solving the problem of packing circles within a larger square where as n=4. Global optimum

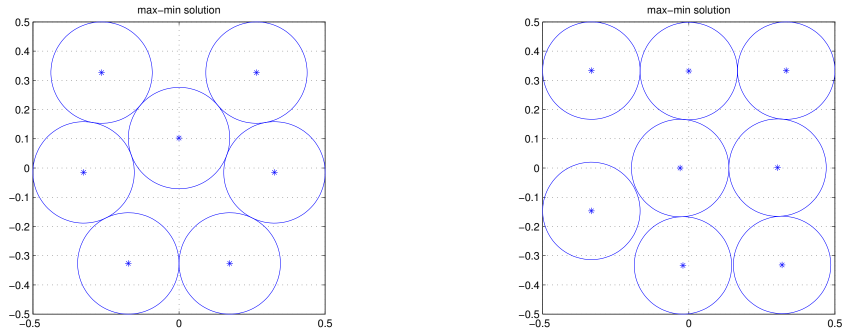
Figure 21



(a) tSolving the problem of packing circles within a larger square where as n=5

(b) Solving the problem of packing circles within a larger square where as n=6. Global optimum

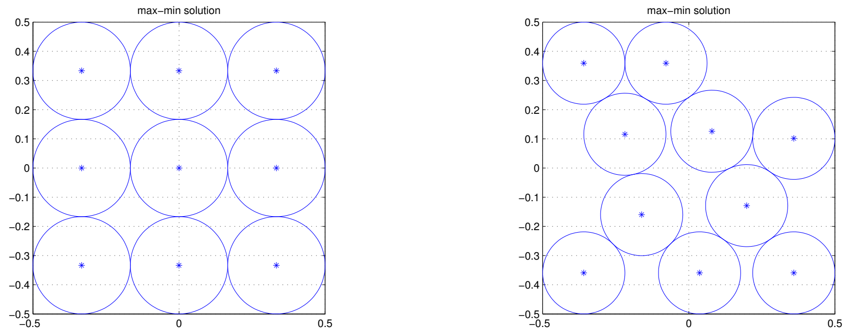
Figure 22



(a) Solving the problem of packing circles within a larger square where as n=7

(b) Solving the problem of packing circles within a larger square where as n=8

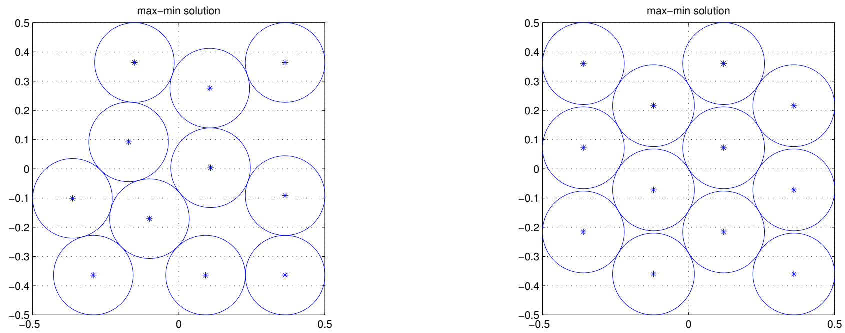
Figure 23



(a) Solving the problem of packing circles within a larger square where as n=9. Global optimum

(b) Solving the problem of packing circles within a larger square where as n=10

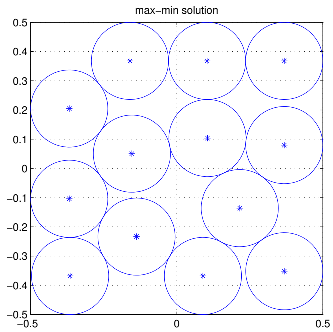
Figure 24



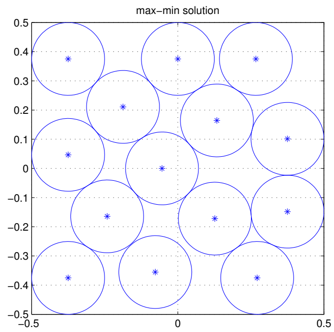
(a) Solving the problem of packing circles within a larger square where as n=11

(b) Solving the problem of packing circles within a larger square where as n=12. Global optimum

Figure 25



(a) Solving the problem of packing circles within a larger square where as n=13



(b) tSolving the problem of packing circles within a larger square where as n=14

Figure 26

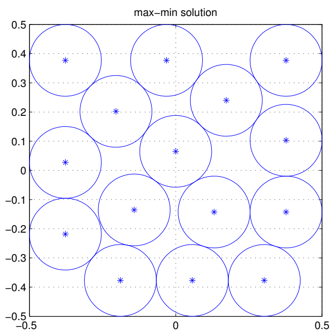
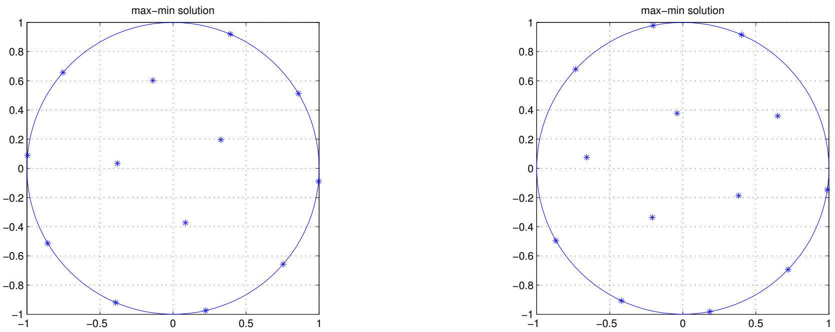


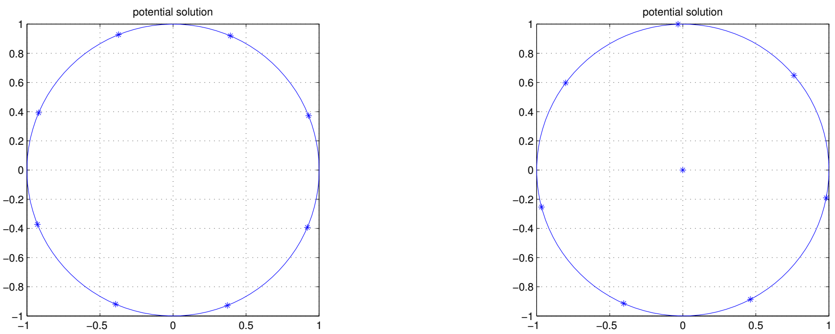
Figure 27: Solving the problem of packing circles within a larger square where as n=15



(a) Global optimal solution from solving the Max-min optimization problem for n=13 using a random initial estimate. The values of the maximum minimal distance and the potential are: $Min - dist = 0.6180, \quad Pot = 76.7786$

(b) Local optimal solution from solving the Max-min optimization problem for n=13 using a random initial estimate. The values of the maximum minimal distance and the potential are: $Min - dist = 0.6090, \quad Pot = 78.2893$

Figure 28



(a) Global Optimal solution from solving the Potential optimization problem for n=8 using a random initial estimate. The values of the maximum minimal distance and the potential are: $Min - dist = 0.7651, \quad Pot = 22.4389$

(b) Local optimal solution from solving the Potential optimization problem for n=8 using a random initial estimate. The values of the maximum minimal distance and the potential are: $Min - dist = 0.8676, \quad Pot = 23.1334$

Figure 29

7 Conclusions

The Max-min optimization problem using the Fmincon method provides in many cases globally optimal solutions. The Minimum potential problem prioritize the potential ahead of the maximum minimal distance and thus giving not as good maximal minimum distance compared with the Max-min optimization problem. The Differential equation problem gives both good values in the potential as with the maximal minimal distance, but still not as good as the Max-min optimization problem.

What methods provides global solutions? The value that are compared are the maximal minimal distance and the potential. Comparing the results from the test region of the surface of a unit sphere with Table (1), all of the methods gives global optimal maximal minimal distance value according to Table (5) for $n = 4, 6, 12$. For the region of a unit circle we have that for $n = 4, 6$ all methods gave globally optimal values on the maximal minimal distance. For $n = 12$ the Fmincon(max-min) obtains another global optimal solution, despite the other methods do not. Conclusively as expected the Fmincon (max-min) in general is better of finding maximal minimal value solutions than both the Fmincon(potential) and Diff.eqn. In some cases the Fmincon(potential) and Diff.eqn do find better maximal minimal values than the Fmincon(max-min). Note that the Fmincon(max-min) never finds the best potential value compared with the other methods. It cannot be concluded which of the methods Fmincon(potential) and the Diff.eqn are the best of finding the potential value. Note that the calculated optimal solution from the Max-min optimization problem has more points inside the region compared with the Minimum potential problem, where the calculated optimal solutions has more points at the boundary of the region.

The method for solving the packing problem obtains a couple of global optimum. The results from Table (9) show that for the circular container the radius for each of the smaller circles for $n = 3, 4, 5, 6, 7, 8, 11$ are all globally optimal solutions. The packing on these n are as dense as possible. For the square container there are a couple of globally optimal solutions. For $n = 4, 6, 9, 12$ the packing are globally optimal.

For comparison reasons, we have tested the methods on regions for which there are some known theoretical results, but the methods are general tools which can easily be adopted to other regions. It can be concluded that the studied numerical methods are useful tools for calculating optimal solutions to point separation problems and the packing problems

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