On the circle closest to a set of points

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Abstract

The objective of this paper is to find a circle whose circumference is as close as possible to a given set of points. Three objectives are considered: minimizing the sum of squares of distances, minimizing the maximum distance, and minimizing the sum of distances. We prove that these problems are equivalent to minimizing the variance, minimizing the range, and minimizing the mean absolute deviation, respectively. These problems are formulated and heuristically solved as mathematical programs. Special efficient heuristic algorithms are designed for two cases: the sum of squares, and the minimax. Computational experience is reported. © 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

We wish to find a circle such that its circumference is as close as possible to a given set of points in the plane. Three criteria for closeness are considered: minimizing the sum of squares of distances from the circumference of the circle, minimizing the maximum of these distances, and minimizing the sum of these distances. The problem is of considerable interest in quality control for production processes and has generated a considerable literature; for example see Shunmugam [1], Van Ban and Lee [2], Ventura and Yeralan [3], Yeralan and Ventura [4]. This problem is often required to monitor the closeness of the actual features of a manufactured product to the specified features. Such features could include straightness, roundness, flatness, cylindricity, etc.; circular features are...
very common. Monitoring is often done with coordinate measuring machines (CMMs), which are becoming very widespread [5]. These machines measure a number of points on the surface of a product with high precision. These points are then used to “fit” the features of the product being manufactured so that they can be compared to the specifications. Use of such machines allows problems to be quickly detected and corrected. Methods of fit include least-squares, minimax, and minisum criteria.

Other possible applications are in irrigation and forestry. Suppose one needs to use a circular irrigation system to water some plants. The sprinkler covers an area between two circles and we would like to find a location for it such that the plants will be covered with the narrowest band, which provides for the least waste of water. A common problem in forestry is to cut a trunk of a tree into a telephone or electrical pole. If one needs a perfect cylinder, then the problem is to find the largest circle enclosed within a set of points describing the periphery of the trunk. One needs to project the periphery of the trunk at various levels and use the intersection of all the peripheries. Note that if the direction of the cylinder is not given, finding that direction adds complexity to the problem. If one can allow for an imperfect cylindrical pole, then the correct objective is to fit the circle as close as possible to the periphery of the tree. If minimizing the maximum depth of missing wood is desired (for structural soundness), then a minimax criterion is appropriate.

As these applications indicate, the objective function measuring the closeness to a circle may have several formulations:

1. One may wish to find the circle that minimizes the sum of squares of distances from its circumference. This objective is widely used in similar contexts, and a prime example is least-squares regression where the sum of squares of the distances (parallel to the y-axis) to a line is minimized. This objective is termed the least-squares objective.
2. One may wish to minimize the maximum distance to the circumference of the circle. This is a common objective when the maximal “error” in the approximation is minimized. This objective is equivalent to finding the narrowest ring that covers all points. This objective is termed the minimax objective.
3. Another common objective in location models is minimizing the sum of distances [6–9]. This objective is termed the minisum objective.

Some papers treat the mathematical aspects of the problem [10,11], and Coope [10] proposed a different objective. The difference between the square of the distance to the circumference of the circle and the square of the radius is calculated for each point. This objective replaces the difference between the distance and the radius in calculating the least squares of the differences. This objective can be transformed to a convex optimization problem which can be explicitly solved.

In this paper we show that these objectives are equivalent to equity objectives used in facility location [12–17]. The least-squares objective is equivalent to minimizing the variance of the distances from the center of the circle (minimizing the variance in facility location is discussed in Carrizosa [18], Eisel and Laporte [13], Maimon [19], Plastria [17] and also mentioned in Plastria [20]); the minimax objective is equivalent to minimizing the range of the distances [12,13] and the minisum objective is equivalent to minimizing the mean absolute deviation (MAD) of the distances [13]. Some heuristic solution approaches have been developed.
2. Formulation

Let 

\( n \) be the number of points,

\((x_i, y_i)\) be the location of point \( i \) for \( i = 1, \ldots, n \),

\((x, y)\) be the center of the best circle,

\( R \) be the radius of this circle,

\( d_i(x, y) \) be the distance between point \( i \) and the center of the circle:

\[
d_i(x, y) = \sqrt{(x - x_i)^2 + (y - y_i)^2}.
\]

In order to eliminate discontinuity in the derivatives of the distance when \( d_i(x, y) = 0 \) one may use the \( \varepsilon \)-approximation to the distance, i.e., adding \( \varepsilon^2 \) under the square root sign. Note that the possibility for \( d_i(x, y) = 0 \) is unlikely because a solution tends to be far from demand points.

The three objectives are:

\[
\text{Least squares: } \min_{x, y, R} \left\{ \sum_{i=1}^{n} [d_i(x, y) - R]^2 \right\}, \tag{1}
\]

\[
\text{Minimax: } \min_{x, y, R} \left\{ \max_i \{ |d_i(x, y) - R| \} \right\}, \tag{2}
\]

\[
\text{Minisum: } \min_{x, y, R} \left\{ \sum_{i=1}^{n} |d_i(x, y) - R| \right\}. \tag{3}
\]

These problems are not convex. Therefore, a global optimization procedure is required. For example, if all the points are colinear, then the optimal solution is at infinity (in the direction perpendicular to that line). At infinity, in that direction, the radius of the circle is infinite and its circumference is a line passing through all points yielding a zero objective which must be optimal. However, if it can be assumed that the points are “quite close” to the circle, then the search for the center of the circle can be restricted to quite a small area, and some global optimization procedure can be adopted. The “Big Square Small Square” [20,21] approach can perform an exhaustive search in the area close to the perceived center of the circle and result in an optimal solution. The properties proved in the next section are true for any point configuration. The procedures proposed in the rest of the paper are useful only for the case that the points are “quite close” to a circle and the location of the center of the circle can be estimated to be in a small area. This assumption is used by other papers in the literature which investigate this problem.

3. Properties of the various objectives

In this section we prove some properties of the solutions to the three objectives.
3.1. Properties of the least-squares problem

The properties of the least-squares problem are stated in Coope [10]. We give them here for completeness.

**Lemma 1.** For the least-squares distances (1), the optimal $R$ is the average of all distances.

**Proof.** By differentiating Eq. (1) with respect to $R$ we get the condition

$$\sum_{i=1}^{n} [d_i(x, y) - R] = 0,$$

which leads to

$$R = \frac{1}{n} \sum_{i=1}^{n} d_i(x, y)$$

which proves the lemma. □

**Theorem 1.** The center of the optimal circle solving problem (1) is the point at which the variance of the distances to the points is minimized.

**Proof.** The Theorem follows Lemma 1. The objective function (1) when substituting the optimal $R$ by Lemma 1, is the variance of the distances to the center of the circle. □

It follows that objective function (1) is equivalent to

$$\min_{x,y} \left\{ \sum_{i=1}^{n} d_i^2(x, y) - \frac{1}{n} \left[ \sum_{i=1}^{n} d_i(x, y) \right]^2 \right\}.$$  \hspace{1cm} (4)

3.2. Properties of the minimax problem

The following theorem characterizes the local optima to the minimax problem.

**Theorem 2.** A local optimum to the minimax problem consists of at least two points with an equal maximum distance and at least two points with an equal minimum distance to the center point.

**Proof.** The minimax problem is

$$\min_{x,y} \left\{ \max_i \{d_i(x, y)\} - \min_i \{d_i(x, y)\} \right\}.$$  \hspace{1cm} (5)

Assume that the minimum distance is measured to one point only (and the distances to all other points are greater than this value), and we reach a contradiction. Moving away from this minimum distance point a small distance $\varepsilon$, in exactly the opposite direction, increases the shortest distance by exactly $\varepsilon$. The maximum distance cannot increase by more than $\varepsilon$ by the triangle inequality. The only possibility that the difference stays the same is when the solution point $(x, y)$, the closest point $(x_j, y_j)$,
and one of farthest points \((x_i, y_i)\) are colinear in that order (i.e., the closest point is between the solution and the farthest point). Let us rotate the system of coordinates so that the solution is at \((0, 0)\), the minimum distance is to the point \((a, 0)\), and the maximum distance is to the point \((b, 0)\) for \(b > a \geq 0\). Now, moving in the direction of the \(y\)-axis to a point \((0, \varepsilon)\) for a small \(\varepsilon\) (positive or negative) gives the following change in the difference between the distances to points \((a, 0)\) and \((b, 0)\):

\[
\sqrt{b^2 + \varepsilon^2} - b - \{\sqrt{a^2 + \varepsilon^2} - a\} = \begin{cases} 
\varepsilon^2 \left( \frac{1}{2|\varepsilon|} - \frac{1}{2a} \right) + O(\varepsilon^3) & \text{for } a > 0 \\
- \varepsilon + O(\varepsilon^2) & \text{for } a = 0 
\end{cases} < 0
\]

in contradiction to this configuration being a local minimum. Note that when the solution is located at a point (i.e., \(a = 0\)), then Eq. (6) holds as well.

Now assume that the maximum distance is measured to one point only and the distances to all other points are smaller than this value. We show that this leads to a contradiction as well. Moving exactly towards this maximum distance point a small distance \(\varepsilon\) decreases the maximum distance by exactly \(\varepsilon\). The minimum distance cannot decrease by more than \(\varepsilon\) by the triangle inequality. The only possibility that the difference stays the same is when the solution point \((x, y)\), one of the closest points \((x_i, y_i)\), and the farthest point \((x_i, y_i)\) are colinear in that order. This is the same configuration as above which leads to a contradiction. In conclusion, the minimal distance is equal to at least two points, and the maximum distance is equal to at least two points.

**Theorem 3.** The center of the optimal circle solving problem (2) is the point at which the range of the distances to the points is minimized.

**Proof.** Follows directly from Eq. (5).  

### 3.3. Properties of the minisum problem

**Lemma 2.** For the minisum of distances (3), the optimal \(R\) is the median of all distances.

**Proof.** The lemma follows by direct definition of a median and can also be proven by the proof utilized in the rectilinear minisum problem [9].

**Theorem 4.** The center of the optimal circle solving problem (3) is the point at which the mean absolute deviation of the distances to the points is minimized.

**Proof.** The Theorem follows Lemma 2. The objective function (3) when substituting the optimal \(R\) by Lemma 2, is the mean absolute deviation of the distances to the center of the circle.

### 4. Computational experiments with AMPL

We coded the three objectives in AMPL [22] AMPL is a general mathematical programming solver which uses MINOS 5.4 as its optimizer. The programs for our problems are very simple. The
program for the least-squares objective is given below, and the other two programs are very similar to this one. The vectors \( xx \) and \( yy \) are the data points. \((x, y)\) and \( R \) are the center of the circle and its radius, respectively. These variables are given the starting guess of a random uniform variable in \([0, 1]\).

### 4.1. AMPL code for the least-squares problem

```AMPL
param n;
set I := 1..n;
param xx{i in I};
param yy{i in I};
var x := Uniform(0,1);
var y := Uniform(0,1);
var R := Uniform(0,1);
var L = sum {i in I} (sqrt((x-xx[i])^2 + (y-yy[i])^2 + 1.e-16) - R)^2;
minimize objective: L;
```

To illustrate the procedure we constructed a problem with nine points. The points and the various local optima are depicted in Fig. 1. The data file prepared for AMPL is given below, and the coordinates of the points can be extracted from this file.

### 4.2. The data file

```text
param n 9;
param: xx yy :=
1  -9.  2.
2  -11. -1.
3   2.  10.
4   -1. -10.
5   4.  9.
6   9.  -5.
7   7.  7.
8   7.  -7.
9  10.  1.
;
```

Obtaining a local optimum for the example problem by AMPL took less than a second of computer time. However, we encountered difficulties in the solution of the minisum problem because AMPL is not reliable for nondifferentiable functions. When the solution was started from various randomly generated values, we obtained many different solution points, many of them clearly not local minima. We therefore modified the AMPL code for the minisum objective to an equivalent formulation, obtaining a stable program that always converged to the same point without any error messages. The modified formulation removes the discontinuity in the derivative of the objective function and is based on additional \( 2n \) variables \( u_i \geq 0 \) and \( v_i \geq 0 \) used to define
Table 1
Results for the example problem using AMPL.

<table>
<thead>
<tr>
<th>Method</th>
<th>x</th>
<th>y</th>
<th>R</th>
<th>Objective</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least squares</td>
<td>-0.0522</td>
<td>-0.1064</td>
<td>10.0747</td>
<td>1.7895</td>
</tr>
<tr>
<td>Minimax</td>
<td>-0.0820</td>
<td>-0.7213</td>
<td>10.1228</td>
<td>0.7988</td>
</tr>
<tr>
<td>Minisum</td>
<td>0.1429</td>
<td>-0.1429</td>
<td>9.9232</td>
<td>2.5991</td>
</tr>
</tbody>
</table>

$\mathbf{d}_i(x, y) - R$ and its absolute value. We add $n$ constraints to the problem: $\mathbf{d}_i(x, y) - R = \mathbf{u}_i - \mathbf{v}_i$ and replace the absolute value in the objective function by $\mathbf{u}_i + \mathbf{v}_i$. The results for the example problem are given in Table 1.

5. Analysis of the least-squares problem

In practical applications it might be required to obtain extremely fast estimates for the best-fitting circle. Real-time application may require a solution within a pre-specified short period
of time. If obtaining the optimal solution takes too long, one might wish to obtain an approximate solution within the pre-specified length of time. An approximation to the least-squares version of the problem is given in Shunmugam [1]. In this section we propose another approximation for this problem.

The minimal variance version of problem (4) is solved. It is suggested to use the ε-approximation for the distance to avoid numerical problems when the distance is zero. The derivatives of \( F(x, y) \) (4) by \( x \) and \( y \) (ignoring a factor of “2”, and for simplicity of notation ignoring the \( (x, y) \) for the distances) are

\[
F_x = \sum_{i=1}^{n} (x - x_i) \left[ 1 - \frac{\sum_{j=1}^{n} d_j}{nd_i} \right], \quad F_y = \sum_{i=1}^{n} (y - y_i) \left[ 1 - \frac{\sum_{j=1}^{n} d_j}{nd_i} \right].
\]

(7)

The second derivative by \( x \) is

\[
F_{xx} = \sum_{i=1}^{n} \left[ 1 - \frac{\sum_{j=1}^{n} d_j}{nd_i} - (x - x_i) \frac{\sum_{j=1}^{n} (x - x_j)/d_j - (x - x_i)/d_i \sum_{j=1}^{n} d_j}{nd_i^2} \right]
\]

(8)

Algebraic manipulations (and similar ones for the other two derivatives) lead to

\[
F_{xx} = \frac{1}{n} \left\{ n^2 - \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{(y - y_i)^2}{d_i^3} - \left[ \sum_{i=1}^{n} \frac{x - x_i}{d_i} \right]^2 \right\},
\]

(9)

\[
F_{yy} = \frac{1}{n} \left\{ n^2 - \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{(x - x_i)^2}{d_i^3} - \left[ \sum_{i=1}^{n} \frac{y - y_i}{d_i} \right]^2 \right\},
\]

(10)

\[
F_{xy} = \frac{1}{n} \left\{ \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{(x - x_i)(y - y_i)}{d_i^3} - \sum_{i=1}^{n} \frac{x - x_i}{d_i} \sum_{i=1}^{n} \frac{y - y_i}{d_i} \right\}
\]

(11)

We need to solve for the equations \( F_x = F_y = 0 \). Using first terms in the Taylor expansion of \( F_x \) and \( F_y \) we get for a small \( \Delta x \) and \( \Delta y \):

\[
F_x + F_{xx} \Delta x + F_{xy} \Delta y = 0, \quad F_y + F_{xy} \Delta x + F_{yy} \Delta y = 0.
\]

(12)

which leads to

\[
\Delta x = \frac{F_y F_{xy} - F_x F_{yy}}{F_{xx} F_{yy} - F_{xy}^2}, \quad \Delta y = \frac{F_x F_{xy} - F_y F_{xx}}{F_{xx} F_{yy} - F_{xy}^2}.
\]

(13)

5.1. Computational experience with a Newton–Raphson approach

In a manner similar to the Weiszfeld procedure [9,23] one can implicitly solve \( F_x = 0 \) and \( F_y = 0 \) for \( x \) and \( y \) and use the implicit expression as an iterative procedure. However, since the factors multiplying \((x - x_i)\) and \((y - y_i)\) in (7) are both positive and negative and add up to be close to zero, such an iterative scheme does not converge. Therefore, we construct a Newton–Raphson procedure that includes the second derivatives of \( F(x, y) \). This means using Eq. (13) in an iterative procedure.

We coded a Microsoft FORTRAN program on a PC486 33 MHz compatible computer. We found a local minimum of the example problem (plotted in Fig. 1) repeating the solution procedure.
Table 2
Computational experience with the Newton–Raphson method

<table>
<thead>
<tr>
<th>Square side</th>
<th>Iterations</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min</td>
<td>Max</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>5</td>
</tr>
</tbody>
</table>

*Initial guess was randomly generated in a square centered at the origin with side length of “square side”.

1000 times from randomly generated points in a square centered at the origin. A starting point farther away from the origin will conceivably result in a different local minimum. Therefore, we tested the procedure using different size squares for generating starting solutions. We stopped the iterations when the distance between two successive iterations is less than $10^{-5}$. In Table 2, we summarize the computational results for various sides of the square. The same local optimum was obtained in all experiments. The number of iterations and, consequently, the run times increase with the increase of the side of the square. This means that when a starting solution is located farther away from the optimum, more iterations are required until convergence is detected. The Newton–Raphson approach was empirically found to be very efficient.

5.2. Approximations to the least-squares local minimum

Let us show that the sum of $F_{xx}$ and $F_{yy}$ is approximately equal to $n$:

$$F_{xx} + F_{yy} = 2n - \frac{1}{n} \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{1}{d_i} \left\{ \left[ \sum_{i=1}^{n} \frac{x_i - x}{d_i} \right]^2 \left[ \sum_{i=1}^{n} \frac{y_i - y}{d_i} \right] \right\},$$  \hspace{1cm} (14)

If all $d_i$’s are approximately equal to a value $d$ then

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{1}{d_i} \approx nd \times \frac{n}{d} = n^2$$

and therefore by Eq. (14):

$$F_{xx} + F_{yy} \approx n - \frac{1}{n} \left\{ \left[ \sum_{i=1}^{n} \frac{x_i - x}{d_i} \right]^2 \left[ \sum_{i=1}^{n} \frac{y_i - y}{d_i} \right] \right\},$$

The last term is small compared to $n$ because each sum contains both positive and negative numbers that tend to cancel one another. In fact, for the minimum Weber solution point each of the two sums is equal to zero. Due to symmetry we can assume that each of them is about $n/2$. Also, the
absolute value of $F_{xy}$ is usually small compared to the other two second derivatives because the expected value of each term is zero and the final result is divided by $n$. Note that if these assumptions are true, the resulting solution is a local minimum and not a local maximum because $F_{xx}$ and $F_{xy}$ are positive, and the determinant of the second derivatives is positive. Making all these simplifying assumptions yields by Eq. (13):

$$\Delta x \approx -\frac{2}{n} F_x, \quad \Delta y \approx -\frac{2}{n} F_y.$$ (15)

We applied approximation (15) in an iterative procedure. Initial $x, y$ were generated and the next iterate was calculated as $(x + \Delta x, y + \Delta y)$. Experiments with this approximation were quite successful. Convergence was obtained in 6–8 iterations, each much simpler than using (13). When these iterations converge the first derivatives must vanish at the limit. Therefore, if the iterations converge, the limit must be a local optimum.

We found that using this approximation at the center of gravity point leads to a very good approximation to the location of the local minimum. The center of gravity is a convenient point because the sums of $x - x_i$ and $y - y_i$ vanish there. This means that at the center of gravity Eqs. (7) are simpler because the number “1” is no longer needed. First, calculate the center of gravity $(\bar{x}, \bar{y})$ as the average of the $n$ coordinates. Let $d_i$ be the distance between demand point $i$ and the center of gravity, then by using approximation (15) and Eqs. (7):

$$x \approx \bar{x} + \frac{2}{n^2} \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{\bar{x} - x_i}{d_i}, \quad y \approx \bar{y} + \frac{2}{n^2} \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \frac{\bar{y} - y_i}{d_i}.$$ (16)

For our example problem the center of gravity is quite far from the local minimum at $(2.0000, 0.6667)$ with an objective function of 23.1321! (which is 1193% over the best-known solution). The approximation (16) is at $(0.0138, -0.1159)$ with an objective of 1.8096 which is only 1.1% over the best-known objective. The best-known location is at $(-0.0522, -0.1064)$ with an objective of 1.7895.

In order to check the approximation we tested it on randomly generated problems. Since we wanted to have points located around the origin, the problems were generated in the following way. Points were generated in a ring whose lower radius is 9 and upper radius is 11. The ring is divided into $n$ equal sectors, each based on an angle of $2\pi/n$ centered at the origin. One point is randomly generated at each sector. For each value of $n$ 1000 such problems were generated and solved by using (13) yielding “the best-known solution” for each of these problems. In Table 3, we report the percentage of the objective function by the approximation formula (16) over the best-known value for these 1000 randomly generated problems, and the time required to find the best-known solution. The approximation is excellent, especially for larger $n$’s. We do not report results for $n > 25$ because the average percentage over the best-known objective is less than 0.001%.

6. On the solution of the minimax problem

The minimax solution is based on 4 points. Two are tied for the largest distance and two are tied for the shortest distance. Using Voronoi diagrams [24] the problem can be optimally solved in $o(n^2)$ time [2,25].
Table 3
The quality of the approximated formula

<table>
<thead>
<tr>
<th>n</th>
<th>Percentage over the best-known objective</th>
<th>Time for finding best known</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Minimum</td>
<td>Maximum</td>
</tr>
<tr>
<td>10</td>
<td>0.000</td>
<td>20.628</td>
</tr>
<tr>
<td>15</td>
<td>0.000</td>
<td>1.674</td>
</tr>
<tr>
<td>20</td>
<td>0.000</td>
<td>0.244</td>
</tr>
<tr>
<td>25</td>
<td>0.000</td>
<td>0.090</td>
</tr>
</tbody>
</table>

6.1. Finding a local minimum of the minimax problem

In this section we propose an efficient gradient search algorithm which exhibited in experiments a run time linear in \( n \).

The problem is

\[
\min_{x,y} \left\{ \max_i \{d_i(x, y)\} - \min_i \{d_i(x, y)\} \right\}. \tag{17}
\]

This problem is equivalent to

\[
\min_{x,y} \left\{ \max_{i,j} \{d_i(x, y) - d_j(x, y)\} \right\}. \tag{18}
\]

Problem (18) is in the traditional minimax formulation. It contains \( n(n - 1)/2 \) functions. For a given small \( \delta \), define

\[
I_\delta(x, y) = \left\{ i \mid d_i(x, y) \geq \max_j \{d_j(x, y)\} - \delta \right\}, \tag{19}
\]

\[
J_\delta(x, y) = \left\{ i \mid d_i(x, y) \leq \min_j \{d_j(x, y)\} + \delta \right\}. \tag{20!}
\]

If the cardinality of \( I_\delta(x, y) \) is \( r \) and the cardinality of \( J_\delta(x, y) \) is \( s \), then the cardinality of the set of functions whose value is equal to the maximum in (18) is \( rs \). The gradient, if it is a non-zero gradient, at \( (x, y) \) is calculated as given in Demjanov [26] and Drezner and Wesolowsky [27].

\[
\min \left\{ [\Delta x]^2 + [\Delta y]^2 \right\}
\]

subject to

\[
\begin{align*}
\frac{x - x_i}{d_i(x, y)} & - \frac{x - x_j}{d_j(x, y)} \Delta x + \left[ \frac{y - y_i}{d_i(x, y)} - \frac{y - y_j}{d_j(x, y)} \right] \Delta y \leq -1 \\
\text{for } i & \in I_\delta(x, y), \quad j \in J_\delta(x, y).
\end{align*}
\]
The exact gradient is defined for $\delta = 0$. If there is no feasible solution to (21), then the gradient is zero and $(x, y)$ is a local optimum.

Problem (21) is a quadratic programming problem [28] and can be easily solved directly. However, since the problem is defined by two variables, it can be solved much easier and faster as follows: the optimal solution can be either the unconstrained solution (which is $\Delta x = \Delta y = 0$, which does not fulfill the constraints), or with one or two tight constraints.

The problem contains $rs$ constraints. Rewriting problem (21) by defining the coefficients in the constraints yields:

$$\begin{align*}
\min & \quad \{ [\Delta x]^2 + [\Delta y]^2 \} \\
\text{subject to} & \quad a_k \Delta x + b_k \Delta y \leq -1 \quad \text{for } k = 1, \ldots, rs.
\end{align*}$$

(22)

Solving (22) is simple:

1. Assuming that constraint $k$ is tight yields the optimal solution

$$\Delta x = -\frac{a_k}{a_k^2 + b_k^2}, \quad \Delta y = -\frac{b_k}{a_k^2 + b_k^2}.$$ 

If the other constraints are not violated, this solution is feasible and should be considered for optimality.

2. Assuming that constraints $k$ and $m$ are tight leads to the solution (there is only one feasible point): 

$$\Delta x = \frac{b_k - b_m}{a_k b_m - a_m b_k}, \quad \Delta y = \frac{a_m - a_k}{a_k b_m - a_m b_k}.$$ 

If the other constraints are not violated, this solution is feasible and should be considered for optimality.

3. The best objective obtained in steps 1 and 2 is the solution to problem (22).

4. If no feasible solution is found in steps 1 and 2, then the gradient is zero at $(x, y)$.

The Demjanov gradient algorithm is very efficient. Experiments with problems up to 1000 points randomly generated in a unit square are reported in Table 4. The tolerance $\delta = 10^{-5}$ was used in the program. This algorithm exhibits a run time which is about linear in $n$.

7. Conclusions

The problem of finding a circle whose circumference is as close as possible to a given set of points is investigated. Three objectives are considered: minimizing the sum of squares of distances (least squares), minimizing the maximum distance (minimax), and minimizing the sum of distances (minisum). We proved that these problems are equivalent to minimizing the variance, minimizing the range, and minimizing the mean absolute deviation, respectively. These problems are formulated and solved as mathematical programs using standard mathematical programming software such as AMPL. Since the objective functions are not convex, many local optima may exist. However, when the configuration of the demand points is close to being circular, the
Table 4
Experiments with 1000 problems using the Demjanov gradient search

<table>
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<th>n</th>
<th>Time (s)</th>
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<th>Min.</th>
<th>Max.</th>
<th>Avg.</th>
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</table>

neighborhood of the optimal solution can be identified. Special efficient heuristic algorithms are
designed for two cases: the least squares and the minimax. These algorithms are very fast and easy
to implement.

Possible extensions to this problem may be formulated and analyzed. For example, one may
consider the weighted version of the problem. We may investigate such extensions in future papers
but at this point we could not find any applications for such extensions.

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