International Journal of Computational Geometry & Applications

COMPUTING ROUNDNESS IS EASY IF THE SET IS ALMOST ROUND*

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Received 7 June 2001
Revised 4 March 2002
Communicated by P. K. Agarwal

ABSTRACT

In this paper we address the problem of computing the thinnest annulus containing a set of points $S \subset R^d$. For $d = 2$, we show that the problem can be solved in $O(n)$ expected time for a fairly general family of *almost round* sets, by using a slight modification of Sharir and Welzl's algorithm for solving LP-type problems. We also show that, for points in convex position, the problem can be solved in $O(n)$ deterministic time using linear programming. For $d = 2$ and $d = 3$, we propose a *discrete local optimization* approach. Despite the extreme simplicity and worst case $O(n^{d+1})$ complexity of the algorithm, we give empirical evidence that the algorithm performs very well (close to linear time) if the input is *almost round*. We also present some theoretical results that give a partial explanation of this behavior: although the number of local minima may be quadratic (already for $d = 2$), almost round configurations of points having *more than one* local minimum are very unlikely to be encountered in practice.

Keywords: Geometric optimization, tolerancing metrology, linear programming, roundness

1. Introduction

The problem of computing the thinnest annulus containing a given set of points $S \subset R^2$, the so called *roundness* problem, has been extensively studied. The main motivation for this problem comes from tolerancing metrology: given an object that has to be tested for circularity, take a sample of points from the object and measure the circularity of this sample set; then accept the object if the circularity

*A preliminary version of this paper appeared as Ref. [16]. Part of this work has been done while the second author was visiting INRIA. Partially supported by the French-Spanish collaboration program Picasso and by grants DGES-MEC-PB98-0933, DGES-MEC-PB98-0713-C02-01 and Universidad de Alcalá E041/2000.

is good enough and reject it otherwise. The measure for circularity recommended by international standards is the width of the thinnest annulus containing the set (see pp. 40-42 of Ref. [10] or p. 14 of Ref. [12]). Despite this fact, alternative measures, such as least squares fit, are used in industry, mainly because the problem of computing the thinnest annulus is algorithmically challenging and the algorithms available are either too slow or too complicated.

In order to summarize the long history of this problem let us mention that the first non-trivial observation, namely, that the center of the optimal annulus is a vertex of the diagram obtained by merging the closest and furthest point Voronoi diagrams of the set or, equivalently, that there are four points on the boundary of the annulus, has been independently rediscovered in several papers.[9,17,18] Up to our knowledge, Rivlin[17] is the first author who gives a stronger formulation of this result: he shows that the center is always the intersection of an edge of each Voronoi diagram or, equivalently, that there are two points on the inner circle and two points on the outer circle of the annulus and, furthermore, points on the inner circle interlace angle-wise with points on the outer circle as seen from the center of the annulus.

The best asymptotic bound for the complexity of the problem is due to Agarwal and Sharir,[2] who reduce the problem to a width-type problem in R^3 by lifting the points to the unit paraboloid and give an $O(n^{3/2+\varepsilon})$ randomized algorithm using parametric search and decomposition of arrangements of algebraic surfaces in R^4. Because the problem can have $\Omega(n^2)$ local minima (even for sets of points in convex position, see Ref. [11]), there is little hope that the complexity can be significantly improved for *non-restricted* data.

A promising approach to get algorithms that are useful in practice is try to make some assumptions on the input. As it has been pointed out by de Berg et al.,[6] one of the reasons why many algorithms developed in computational geometry are complicated or slow is because they have to be designed to handle very complicated, hypothetical inputs. A possible way to overcome this situation is try to take advantage of additional properties of the input data that are presented in some specific family of problems. As we shall see, the roundness problem, with some assumptions suggested by the metrology-type input is a good example of how successful this strategy can be.

A first step has been given by Mehlhorn et al. in Ref. [15], where the authors derive some results using what they call the *minimum quality assumption*. Following a similar idea, García et al.[11] show that, if the angular order of the points around the center of the solution is given as part of the input, there is at most one local minimum of the problem consistent with the given order and, furthermore, it can be computed in $O(n \log n)$ time using a simple algorithm. In the same paper, the authors show that, if points are in convex position, the problem can be solved in $O(n)$ time.

More recently, Duncan et al.[8] have shown that if the mean radius of the annulus is fixed, the problem is easier and can be solved in $O(n \log n)$ time while de Berg et al.[5] independently, have shown that the same bound holds if the inner, mean or outer radius of the annulus is fixed. Bose and Morin[3] extend the results of Mehlhorn et al.[15] to the case where the set is not convex by making some assumptions on the input which are essentially equivalent to the restricted roundness hypothesis that we use below. Devillers and Preparata[7] have shown that the annulus of minimum area (which can be computed using linear programming) is a very good approximation of the minimum width a nnulus for almost round sets.

Finally, Agarwal et al.[1] and Chan[4] give a variety of approximation algorithms for arbitrary dimension and Chan points out that the exact solution to the roundness problem in R^d can be obtained in $O(n^{\lfloor d/2 \rfloor + 1})$ time by optimizing inside a convex polytope in R^{d+2}.

1.1. Our Results

In this paper, instead of looking for simple algorithms that give an approximate solution to the problem, we propose simple algorithms that give the *exact* solution for families of input sets which are specially relevant in tolerancing metrology applications.

We will deal with *almost round* sets of points. Roughly speaking, we say that a set is almost round if it is contained inside a thin annulus centered at a given point, called the *nominal center*, and we call *nominal radius* the distance from each point to the nominal center.

- For $d = 2$, if we further assume a bound on the local variation of the nominal radius (but allowing sets which are not in convex position), we are able to show that the problem can be solved in $O(n)$ expected time with a slight modification of Sharir and Welzl's algorithm for solving LP-type problems.
- If S is a set of points in convex position in R^2, the problem can be solved in $O(n)$ (deterministic) time using linear programming.
- For $d = 2$ and $d = 3$, we propose a *discrete local optimization* method that performs very well (close to linear time) in the experiments. This is, to the best of our knowledge, the first practical algorithm to get the exact solution to the problem for $d = 3$. We also present some theoretical results that give a partial explanation of this behavior, showing that almost round configurations of points having *more than one* local minimum are quite degenerate and thus very unlikely to be encountered in practice.

2. Preliminaries

Let $S = \{p_1, \ldots, p_n\}$ be a set of points in R^d and let $\operatorname{conv} S$ denote its convex hull. The unit hypersphere is denoted by $\mathcal{S}^{d-1}$ and $d(p,q)$ is the Euclidean distance between points p and q. $\mathcal{V}_c(S)$ and $\mathcal{V}_f(S)$ denote, respectively, the closest and furthest-point Voronoi diagrams of S. We define the *roundness diagram* of S, denoted by $\mathcal{RD}(S)$, as the subdivision of the plane obtained by merging the closest and furthest-point Voronoi diagrams of S.

The closed ball centered at c with radius r is denoted by $\mathcal{B}(c, r)$ and the locus of points between two concentric spheres of radius r and R is called d-annulus and denoted $\mathcal{A}(c, r, R)$, that is,

$$\mathcal{A}(c, r, R) = \{\, x \in R^d \,|\, r \leq d(x, c) \leq R \,\}.$$

Finally, $w = R - r$ and $r_m = (R + r)/2$ are, respectively, the *width* and the *mean radius* of the annulus.

Given a point $x \in R^d$, we denote by $N(x)$ and $F(x)$ the set of nearest and furthest neighbors of x in S. Then, the *roundness function* can be defined in the following way:

$$\mathcal{R}(x) = d(x, F(x)) - d(x, N(x)).$$

The *roundness problem* can be formulated now as computing the annulus of smallest width containing S or, equivalently, finding

$$\mathcal{R}(S) = \inf_{x \in R^d} \mathcal{R}(x).$$

The following theorem gives a complete characterization of the local minima of $\mathcal{R}(x)$ in R^d which will be useful later:

Theorem 1 ([11]) *$x_0 \in R^d$ is a local minimum of $\mathcal{R}(x)$ if, and only if, when projected onto a common hypersphere centered at x_0, nearest and furthest neighbors of x_0 cannot be separated by a hyperplane.*

It is worth noting that, as a consequence, if x_0 is a local minimum of $\mathcal{R}(x)$, then $|N(x_0)|$ and $|F(x_0)|$, the number of closest and furthest neighbors of x_0, satisfy the equation $|N(x_0)| + |F(x_0)| \geq d + 2$, with $|N(x_0)| \geq 2$ and $|F(x_0)| \geq 2$. From this, it follows that local minima are vertices of the roundness diagram of S which are not vertices of the closest or the furthest point Voronoi diagram of S. Furthermore, the result generalizes in a natural way to "points at infinity", if we interpret a hyperplane as a hypersphere centered at infinity, characterizing thus the situations when the optimal annulus degenerates to a slab.

Although the roundness function can have as many as $\Omega(n^2)$ local minima even for sets of points in convex position, García et al.[11] have shown that the situation changes drastically if we assume that the angular order of the points around the center of the solution is known in advance.

More formally, let $S = \{p_1, \ldots, p_n\}$ be a *labeled* set of points in the plane such that the polygon $\mathcal{P}$ with vertices $p_1, \ldots, p_n$ is *simple* and define the *kernel* of S, denoted $\ker S$, as the locus of points from which the points of S are seen in the given angular order. We point out that, if $\ker S \neq \emptyset$, then $\mathcal{P}$ is a star-shaped polygon and $\ker \mathcal{P} = \ker S \cap \operatorname{conv} S$.

Theorem 2 ([11]) *Inside* $\ker S$ *there is at most one local minimum of* $\mathcal{R}(x)$.

In the next section we exploit this result and show that the *restricted roundness problem*, defined below, can be solved in linear expected time because it is "almost LP-type".

3. The Restricted Roundness Problem

Throughout this section, S is a set of points in the plane. Furthermore, motivated by properties of the data coming from tolerancing metrology applications, we assume that points of S are sampled around a point which is called *nominal center*, the set is contained inside a *nominal annulus* centered at the nominal center and with a given *nominal width*, the sample of points is well distributed around the circle and, finally, there is a bound on the local variation of the distance from the points to the nominal center.

More formally, we put the origin of the coordinate system O at the nominal center and denote by (ρ_i, θ_i) the polar coordinates of the point p_i. We assume that $\theta_1 < \theta_2 < \ldots < \theta_n$ and indices are understood modulo n (obviously, the expression $\theta_1 - \theta_n$ should be understood as $2\pi + \theta_1 - \theta_n$). Finally, we scale the problem in such a way that the mean radius of the nominal annulus is 1. We say that S satisfies the Restricted Roundness Hypothesis if[a]:

$$|\rho_i - 1| \leq \delta = 0.1 \tag{C1}$$

$$\theta_{i+1} - \theta_i \leq \frac{\pi}{2} \tag{C2}$$

$$|\rho_{i+1} - \rho_i| \leq \theta_{i+1} - \theta_i \tag{C3}$$

It is worth pointing out that condition (C1) is referred to as the *minimum quality assumption* in[3], while condition (C3) is looser than the convexity required in[15] and the star-shape assumption in[3] can be derived as a consequence of (C3).

In this section, we deal with this restricted version of the problem, that we shall refer to as the Restricted Roundness Problem. It is worth noting that this is actually the *real* problem in tolerancing metrology applications, either because we can make a minimum quality assumption on the manufacturing process or because shapes that do not satisfy these assumptions can be easily rejected.

The following result guarantees that the center of the optimal annulus is inside the kernel of S.

Lemma 1 *If S satisfies the Restricted Roundness Hypothesis, there exists a unique $x_0 \in R^2$ such that $\mathcal{R}(S) = \mathcal{R}(x_0)$ and, furthermore, $x_0 \in \mathcal{B}(O, 1/2) \subset \ker S$.*

Proof. First, we show that $\mathcal{B}(O, 1/2) \subset \ker S$. Let p and q be two consecutive points of S with coordinates $p = (r, 0)$ and $q = (r_q \cos\theta, r_q \sin\theta)$ (see Figure 1.a). Let ℓ be the line through p and q. For a fixed value of θ, $d(O, \ell)$ is minimum when r is minimum and r_q is maximum and, because of (C1) and (C3), we have $r \geq 0.9$ and $r_q \leq r + \theta$. Therefore,

$$d(O, \ell) = \frac{r r_q \sin\theta}{\sqrt{r_q^2 + r^2 - 2 r r_q \cos\theta}} \geq \frac{0.9(0.9+\theta)\sin\theta}{\theta\sqrt{1.81 + 0.9\theta}}$$

[a] The choice of the constants has been made in order to simplify the exposition and is not restrictive at all in applications. Moreover, it can be further relaxed with some careful analysis of the sequel.

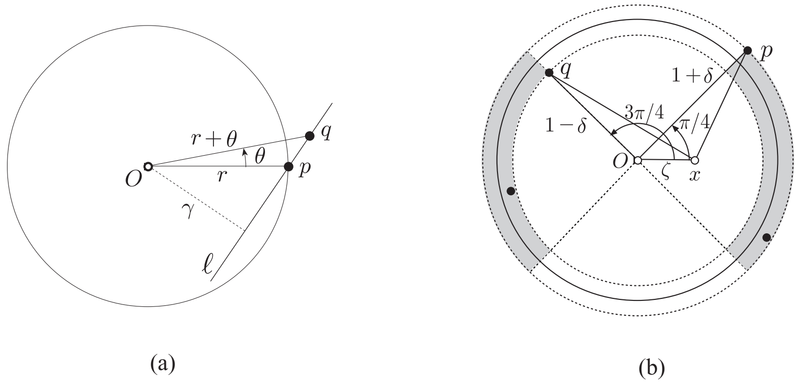

Fig. 1. Illustration for the proof of Lemma 1.

where in the last inequality we have used that $1 - \cos\theta \le \frac{\theta^2}{2}$. From this, it can be easily seen that $d(O,\ell) \ge 1/2$ if $\theta < \pi/2$.

Consider now a point x at distance ζ from O and choose a coordinate system in such a way that x has coordinates $(\zeta, 0)$ (see Figure 1.b). Let p and q be points with coordinates $(1+\delta)(\cos\pi/4, \sin\pi/4)$ and $(1-\delta)(\cos 3\pi/4, \sin 3\pi/4)$, respectively. Because of condition (C2), there must be at least one point inside the annulus within each of the angular intervals $(-\pi/4, \pi/4)$ and $(3\pi/4, 5\pi/4)$ and, therefore, $d(x, F(x)) \ge d(x,q)$ and $d(x, N(x)) \le d(x,p)$. Then, we have

$$\begin{aligned}\mathcal{R}(x) &= d(x,F(x)) - d(x,N(x)) \ge d(x,q) - d(x,p) \\ &\ge \left(\zeta^2 + (1-\delta)^2 + (1-\delta)\sqrt{2}\,\zeta\right)^{1/2} - \left(\zeta^2 + (1+\delta)^2 - (1+\delta)\sqrt{2}\,\zeta\right)^{1/2}.\end{aligned}$$

If $\zeta = d(O,x) \ge 0.5$ we have, $\mathcal{R}(x) > 0.2 \ge \mathcal{R}(O)$ and, therefore, x is not the global minimum of $\mathcal{R}(x)$. Therefore, the result follows from the continuity of $\mathcal{R}(x)$ and Theorem 2. $\square$

In order to show that the Restricted Roundness Problem can be solved in $O(n)$ expected time, we recall from[14] the definition of *LP*-type problems, which in the case of optimizing a function over a set of points can be rephrased as follows. Let $S \in R^d$ be a set of n points and $\omega : 2^S \to R$. We say that (S, ω) is an *LP-type problem* if it satisfies the following two conditions:

$$S_1 \subseteq S_2 \subseteq S \Rightarrow \omega(S_1) \le \omega(S_2) \tag{1}$$

$$\left.\begin{array}{c} S_1 \subseteq S_2 \subseteq S \\ \omega(S_1) = \omega(S_2) \\ p \in S \end{array}\right\} \Rightarrow \left\{\begin{array}{c} \omega(S_1 \cup \{p\}) > \omega(S_1) \\ \Leftrightarrow \\ \omega(S_2 \cup \{p\}) > \omega(S_2) \end{array}\right. \tag{2}$$

Conditions (1) and (2) are usually called *monotonicity* and *locality*, respectively. A set $B \subseteq S$ is called a base if $\omega(T) < \omega(B)$ for all $T \subsetneq B$ and B is a base of S if it is a base and, furthermore, $\omega(B) = \omega(S)$.

In[14] it is shown that if, given a base B, the operations

– Is $\omega(B \cup \{p\}) > \omega(B)$?   violation test

– Compute a base of $B \cup \{p\}$ base computation

can be performed in constant time, then a call to the algorithm

Algorithm (Sharir, Welzl)

```
function procedure lptype(G,T)
    F := T; B := T;
    for all p ∈ G ∖ T in random order do
        F := F ∪ {p};
        if ω(B) < ω(B ∪ {p}) then
            B:=lptype(F,base(B ∪ {p}));
        end if;
    end do;
    return B;
```

---

of the form lptype$(S, \emptyset)$ computes the solution to the problem in $O(n)$ expected time (the constant hidden in the big-O notation depends exponentially on the *combinatorial dimension* of the problem, defined as the maximum cardinality of any base).

The Restricted Roundness Problem is not LP-type, because the locality condition can be violated in situations when the optimal annulus is not unique. Nevertheless, monotonicity is obviously satisfied and, for the locality condition, consider the following slight modification: choose $S_0 \subset S$ of constant size such that the nominal angle between two consecutive points of S_0 is at most $\pi/2$. Then, we have that

$$\left.\begin{array}{c} S_0 \subseteq S_1 \subseteq S_2 \subseteq S \\ \mathcal{R}(S_1) = \mathcal{R}(S_2) \\ p \in S \end{array}\right\} \Rightarrow \left\{\begin{array}{c} \mathcal{R}(S_1 \cup \{p\}) > \mathcal{R}(S_1) \\ \Leftrightarrow \\ \mathcal{R}(S_2 \cup \{p\}) > \mathcal{R}(S_2) \end{array}\right.$$

To see this, observe that S_1 and S_2 satisfy the Restricted Roundness Hypothesis: conditions (C1) and (C3) are obviously satisfied and we have chosen the set S_0 to guarantee condition (C2). Let $\mathcal{A}$ be the thinnest annulus containing S_2 and denote by c its center. We observe that from Lemma 1, $c \in \mathcal{B}(O, 1/2) \subset \ker S_2 \subset \ker S_1$ and since $\mathcal{R}(S_1) = \mathcal{R}(S_2)$, it follows from Theorem 2 that $\mathcal{A}$ is also the thinnest annulus containing S_1. Therefore,

$$\mathcal{R}(S_1 \cup \{p\}) > \mathcal{R}(S_1) \Leftrightarrow p \notin \mathcal{A} \Leftrightarrow \mathcal{R}(S_2 \cup \{p\}) > \mathcal{R}(S_2)$$

We can now slightly modify Sharir and Welzl's algorithm to solve our problem: instead of processing all points in random order, we first choose a set S_0 as before and compute the thinnest annulus containing it in $O(1)$ time. Furthermore, each time that a point fails to be inside the annulus and a recursive call to the algorithm

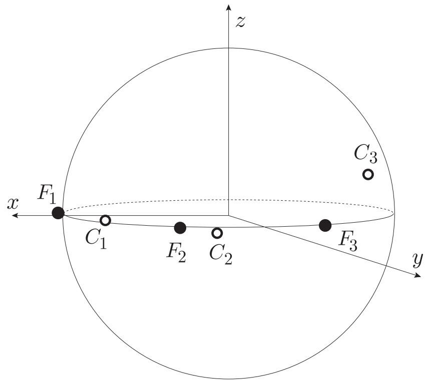

Fig. 2. A configuration of six points in convex position with two local minima.

for computing an optimal solution with some specific points on the boundary is made, we also add the points of S_0 to the set of points and compute the solution by brute force in constant time. The rest of the analysis of Ref. [14] is exactly the same and we have:

Theorem 3 *The Restricted Roundness Problem in R^2 can be solved in $O(n)$ randomized time.*

Unfortunately, this approach does not seem generalizable to higher dimensions because, as the next example shows, even for sets of points in convex position in R^3 we can have two local minima inside the convex hull (and arbitrarily close to each other). Consider the following points given in spherical coordinates:

$$
\begin{array}{ll}
F_1 = (1.05, \frac{\pi}{2}, 0) & C_1 = (0.95, \frac{\pi}{2} - \varepsilon, \frac{\pi}{8}) \\
F_2 = (1.05, \frac{\pi}{2}, \frac{\pi}{4}) & C_2 = (0.95, \frac{\pi}{2} + \varepsilon, \frac{5\pi}{8}) \\
F_3 = (1.05, \frac{\pi}{2}, \frac{3\pi}{4}) & C_3 = (r, \frac{19\pi}{40}, \frac{7\pi}{8})
\end{array}
$$

($\varepsilon = 0.001$ and r is a constant that will be fixed later) and let

$$S = \{F_1, F_2, F_3, C_1, C_2, C_3\}.$$

It is easy to see that the origin of the coordinate system is a local minimum of $\mathcal{R}(x)$ such that points C_1, C_2, F_1, F_2 and F_3 are on the boundary of the annulus. Now, if we move along the z-axis (i.e. along the edge of the roundness diagram defined by F_1, F_2 and F_3), we can see that the point $X_1 = (0, 0, 0.1)$ (rectangular coordinates) is also a local minimum of $\mathcal{R}(x)$ (the points on the boundary of the corresponding annulus are C_1, C_3, F_1, F_2 and F_3) for the value of r for which $d(X_1, C_1) = d(X_1, C_3)$ ($r \approx 0.955149$).

We observe that in the example there are four "almost coplanar" points in the five point set defining the local minimum configuration (points on the boundary of the annulus). We will see (Theorem 6) that, if this is not the case, the local minimum defined by the configuration of points can be shown to be the global minimum of the function. Because this configuration is quite degenerate, it is very unlikely to be encountered in practice. Our plan for Section 5 is to use a local optimization technique in order to locate a local minimum and then check whether or not there may be any other local minima in a neighborhood of it.

4. Roundness Using Linear Programming

A common approach in practice to compute the roundness of a set of points $S = \{p_1, \ldots, p_n\}$ is to use the width of the *minimum area* annulus containing the set S as an approximation of the width of the *minimum width* annulus prescribed by international standards. The main reason for this approach is that, as it is well known, the problem of computing the annulus of minimum area can be formulated as a linear programming problem. In order to do so, assume that p_i has coordinates (x_i, y_i) and let (α, β), r and R be the center, the inner and the outer radius of the optimal solution, respectively. Then, the problem of computing the annulus of minimum area containing S can be formulated as the optimization problem in the variables (r, R, α, β) of

$$\begin{cases} \text{Minimize} & R^2 - r^2 \\ \text{subject to} & r^2 \leq (x_i - \alpha)^2 + (y_i - \beta)^2 \leq R^2 \quad \text{for } i = 1, \ldots, n \end{cases}$$

If we introduce the variables

$$\begin{aligned} \hat{r} &= \alpha^2 + \beta^2 - r^2 \\ \hat{R} &= \alpha^2 + \beta^2 - R^2 \end{aligned}$$

the problem becomes

$$\begin{cases} \text{Minimize} & \hat{r} - \hat{R} \\ \text{subject to} & 2\alpha x_i + 2\beta y_i - \hat{r} \leq x_i^2 + y_i^2 \leq 2\alpha x_i + 2\beta y_i - \hat{R} \quad \text{for } i = 1, \ldots, n \end{cases} \tag{MA$_{LP}$}$$

which is a linear programming problem.

Let ω be the width of the minimum width annulus and ω_A be the width of the minimum area annulus. Devillers and Preparata[7] have shown that ω_A is a very good approximation of ω under the hypothesis that any sector of angle $\frac{\pi}{2}$ from the center of the minimum width annulus contain at least one point. Specifically, if R denotes the outer radius of the minimum width annulus, then

$$\omega_A \leq \omega + \frac{3\omega^2}{R}.$$

However, the situation in practice seems to be even better, in the sense that, as reported in[16], the solution to both problems appears to be exactly the same in most cases. In the remainder of this section we give an explanation of the frequent coincidence of the minimum width annulus and minimum area annulus for point sets.

The vertical distance between two parallel planes $\pi_i \equiv z = \alpha x + \beta y + \gamma_i$ $(i = 1, 2)$ is $d_v(\pi_1, \pi_2) = |\gamma_1 - \gamma_2|$ and the problem of finding the *vertical width* of a set

$S = \{p_1, \ldots, p_n\} \subset R^3$ is the problem of finding the pair of parallel planes containing S with minimum vertical distance. The problem can be solved in $O(n)$ time because it is a linear programming problem in the variables $(\alpha, \beta, \gamma_1, \gamma_2)$:

$$\left\{ \begin{array}{lll} \text{Minimize} & \gamma_2 - \gamma_1 & \\ \text{subject to} & \alpha x_i + \beta y_i + \gamma_1 \leq z_i \leq \alpha x_i + \beta y_i + \gamma_2 & \text{for } i = 1, \ldots, n \end{array} \right. \tag{VW}$$

If we compare (MA_{LP}) and (VW), we easily realize that:

Remark 1 *Computing the minimum area annulus of a set $S \subset R^2$ is equivalent to computing the vertical width of the set $\hat{S} \subset R^3$ obtained by lifting S to the paraboloid $z = \frac{1}{2}(x^2 + y^2)$.*

In the next result, we give a combinatorial characterization of the solution to the vertical width problem. We consider points in general position (no three points on a vertical plane) but the proof can be easily extended to the general case.

Given two non-vertical parallel planes enclosing S, we denote by $\mathcal{U}$ and $\mathcal{L}$ the sets of points on the upper and lower planes, respectively. Then we have:

Lemma 2 *A pair of non-vertical parallel planes defines the solution of (VW) if, and only if, $\mathcal{U}$ and $\mathcal{L}$ cannot be separated by a vertical plane.*

Proof. Consider a pair of non-vertical parallel planes $z = \alpha x + \beta y + \gamma_i$ $(i = 1, 2)$ enclosing S and denote by (x_i, y_i, z_i) the coordinates of point p_i . Then,

$$\begin{array}{l} \mathcal{L} = \{p_i \in S \,|\, z_i - \alpha x_i - \beta y_i = \gamma_1\} \\ \mathcal{U} = \{p_i \in S \,|\, z_i - \alpha x_i - \beta y_i = \gamma_2\} \end{array}$$

If points in $\mathcal{U}$ and $\mathcal{L}$ can be separated by a vertical plane, there exist $a, b, c \in R$ and $\nu > 0$ such that $a x_i + b y_i + c \geq \nu$ for $p_i \in \mathcal{U}$ while $a x_i + b y_i + c \leq -\nu$ for $p_i \in \mathcal{L}$. Then, for $\varepsilon > 0$ small enough, the planes $\pi_l : z = (\alpha + \varepsilon a)x + (\beta + \varepsilon b)y + \gamma_1 + \varepsilon(c + \nu)$ and $\pi_u : z = (\alpha + \varepsilon a)x + (\beta + \varepsilon b)y + \gamma_2 + \varepsilon(c - \nu)$ contain S and its vertical distance is $\gamma_2 - \gamma_1 - 2\varepsilon\nu$.

Conversely, if the configuration is not the minimum, then there exist a, b, c_1, c_2 such that $a x_i + b y_i + c_1 \leq z_i \leq a x_i + b y_i + c_2$ for all $p \in S$ and $c_2 - c_1 < \gamma_2 - \gamma_1$. In particular, for $p_i \in \mathcal{L}$ we have $(a - \alpha)x_i + (b - \beta)y_i \leq \gamma_1 - c_1$ while for $p_i \in \mathcal{U}$ we have $(a - \alpha)x_i + (b - \beta)y_i \geq \gamma_2 - c_2$. Because $c_2 - c_1 < \gamma_2 - \gamma_1$, we have that $\gamma_1 - c_1 < \gamma_2 - c_2$ and conclude that points of $\mathcal{U}$ and $\mathcal{L}$ can be separated by a vertical plane. $\square$

From this result and Remark 1, we have derived the following combinatorial characterization of the optimal configuration for the minimum area annulus.

Theorem 4 *A is the annulus of minimum area containing the set S if, and only if, $S \subset A$ and points on the inner circle and points on the outer circle of A cannot be separated by a line.*

This result can be used to show that, under certain conditions, the annulus of minimum area and minimum width are the same and thus the solution to the minimum width problem can be found in $O(n)$ time.

Theorem 5 *Let $S = \{p_1, \ldots, p_n\} \subset R^2$ be a set of points in convex position. If there is an annulus of minimum width containing S with center strictly inside* $\ker S$*, then it can be computed in $O(n)$ time using linear programming.*

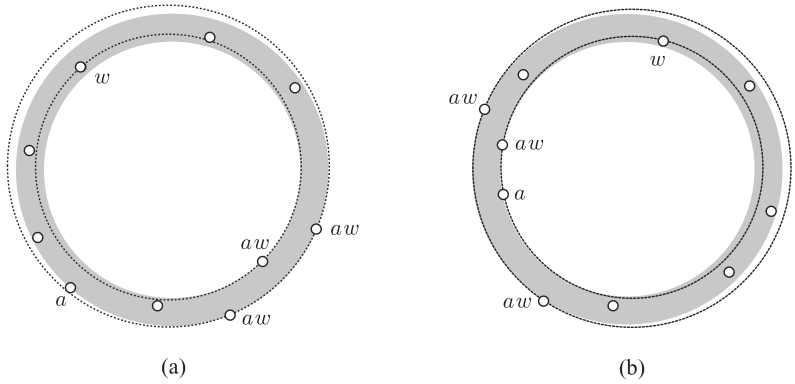

Fig. 3. Examples of local minima configurations.

Proof. We observe that, if S is in convex position, locally minimal configurations for the minimum width problem and for the minimum area problem are the same when the center of the annulus is an interior point of $\ker S$. Therefore, if there is an annulus of minimum width containing S with center strictly inside $\ker S$, then it is also the annulus of minimum area containing S and it can be computed in $O(n)$ time using linear programming. $\square$

In Figure 3 we show two examples where the minimum width annulus and minimum area annulus containing S do not coincide. The minimum area annulus is shaded and points on its boundary are labeled a while the minimum width annulus is drawn with dotted lines and points on its boundary are labeled w (points on the boundary of both annuli are labeled aw).

We conclude the section observing that Theorem 4 can be easily generalized to higher dimensions and, as pointed out by Devillers and Preparata[7], minimizing $R^2 - r^2$ is a very good approximation of minimizing $R - r$ in arbitrary dimension. However, Theorem 5 cannot be generalized to higher dimensions because, as Figure 2 shows, for $d \geq 3$ there is no uniqueness of local minima inside $\operatorname{conv} S$.

5. A Discrete Local Optimization Approach

Consider a point $x_0 \in R^d$ and a unitary vector $\mathbf{v} \in R^d$. We denote by $n_{\mathbf{v}}$ the smallest angle defined by $\mathbf{v}$ and vectors x_0p for $p \in N(x_0)$. Similarly, we denote by $f_{\mathbf{v}}$ the largest angle defined by $\mathbf{v}$ and vectors x_0p for $p \in F(x_0)$. Let p_n and p_f denote, respectively, the points that define $n_{\mathbf{v}}$ and $f_{\mathbf{v}}$ (see Figure 4). It is easy to see that these points are, for $\lambda > 0$ small enough, the nearest and furthest neighbors of $x_0 + \lambda\mathbf{v}$.

Furthermore, from Taylor expansion we have that

$$\mathcal{R}(x_0 + \lambda\mathbf{v}) = d(x_0 + \lambda\mathbf{v}, p_f) - d(x_0 + \lambda\mathbf{v}, p_n) = \mathcal{R}(x_0) + \lambda(\cos n_{\mathbf{v}} - \cos f_{\mathbf{v}}) + o(\lambda).$$

We recall that the roundness diagram of S, denoted by $\mathcal{RD}(S)$, is obtained by merging the closest and furthest-point Voronoi diagram of S. Using this terminol-

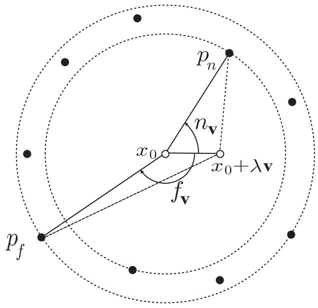

Fig. 4. Illustration for the definitions of Section 5.

ogy, Theorem 1 can be restated as follows: x_0 is a local minimum of $\mathcal{R}(x)$ if, and only if, x_0 is a vertex of $\mathcal{RD}(S)$ such that, for every $\mathbf{v} \in \mathcal{S}^{d-1}$ it holds

$$\cos n_{\mathbf{v}} - \cos f_{\mathbf{v}} > 0. \tag{1}$$

Of course, this quantity is just the directional derivative of $\mathcal{R}(x)$ if the function is smooth, but our plan is to travel along the edges of $\mathcal{RD}(S)$, where directional derivatives of $\mathcal{R}(x)$ do not exist. Therefore, we define the *lateral directional derivative*

$$D_{\mathbf{v}^+}\mathcal{R}(x_0) = \lim_{\lambda \to 0+} \frac{\mathcal{R}(x_0 + \lambda \mathbf{v}) - \mathcal{R}(x_0)}{\lambda} = \cos n_{\mathbf{v}} - \cos f_{\mathbf{v}}.$$

The algorithm follows the idea of local optimization but, instead of moving along the direction of steepest descent of the function, we move along the edge of $\mathcal{RD}(S)$ which minimizes $D_{\mathbf{v}^+}\mathcal{R}$ until a new vertex of the roundness diagram is reached. Because we do not compute $\mathcal{RD}(S)$ explicitly, in each step we have to compute the edges of the diagram starting at the given vertex and the derivative of the function in the direction of each edge. We shall see that if x_0 is a local minimum of the roundness function, $D_{\mathbf{v}^+}\mathcal{R}$ is minimized when $\mathbf{v}$ is the direction of an edge of $\mathcal{RD}(S)$ (in this case, the minimum is bigger than zero), but this is not necessarily the case if x_0 is not a local minimum. Therefore, instead of choosing the direction of steepest descent and proceeding along a direction which is not an edge of $\mathcal{RD}(S)$, we prefer to keep traveling on the diagram and take advantage of the *discrete* nature of the problem. In this way, in each step we advance "as much as we can" and the value of the function always decreases. Although the algorithm works for arbitrary dimensions, in the rest of the paper we concentrate on $d = 2$ and $d = 3$, which are the cases of practical interest in tolerancing metrology applications.

The algorithm is extremely simple and can be described as follows:

Input A set of points S and a nominal center c.

Output A local minimum of $\mathcal{R}(x)$.

begin

Step 1 From c, move to a vertex of $\mathcal{RD}(S)$.

General step While the vertex is not a local minimum, compute the incident edge of $\mathcal{RD}(S)$ which minimizes $D_{\mathbf{v}^+}\mathcal{R}$ and move to the other incident vertex.

end

Step 1 can be trivially performed in $O(n)$ time and, because we do not compute any Voronoi diagram, each iteration of the General step also takes linear time. Therefore, the worst case complexity of the algorithm is $O(Kn)$, where K is the number of vertices of the roundness diagram that are visited during the process. For $d = 2$, $K = \theta(n^2)$, leading to a cubic algorithm, and the complexity is bigger for $d = 3$. However, in the experiments that will be presented in the next section we can see that K grows very slowly with n and thus the complexity of the algorithm "in practice" is close to linear.

In the rest of this section, we study conditions that guarantee that the local minimum that we reach with the algorithm is the global minimum of the function. We are going to look more closely at the local minimum configurations to show that cases that allow another nearby local minimum are very unlikely to be encountered in practice. More importantly, the conditions can be checked once the local minimum has been reached in order to guarantee that we have found the global minimum of the problem.

We are going to make two assumptions on the input:

(A1) $S \subset \mathcal{A}(O, 1-\delta, 1+\delta)$ for $\delta = 0.05$.

(A2) There is at least one point of S inside any cone with apex at O and angle $\beta = \pi/5$.

Assumption (A1) is analogous to (C1) for the Restricted Roundness Problem and assumption (A2) is similar to (C2) and prevents "big holes" in the set S. By using the same ideas as in the proof of Lemma 1, it can be shown that the local minimum found by the algorithm is inside $\mathcal{B}(O, 0.1)$. If we identify $\mathcal{S}^{d-1}$ with the set of unitary vectors in R^d, a sufficient condition for the local minimum found by the algorithm to be the global minimum of the problem can be stated in the following way:

Theorem 6 *Let $x_0 \in \mathcal{B}(O, 0.1)$ be a local minimum of $\mathcal{R}(x)$ and denote $\mathcal{R}(x_0) = \gamma$. We define*

$$m = \min_{\mathbf{v} \in \mathcal{S}^{d-1}} D_{\mathbf{v}^+}\mathcal{R}(x_0) = \min_{\mathbf{v} \in \mathcal{S}^{d-1}} (\cos n_{\mathbf{v}} - \cos f_{\mathbf{v}}).$$

If $m > \gamma^2$, then x_0 is the global minimum of $\mathcal{R}(x)$.

Proof. We observe that from the characterization of the local minima of the roundness function, we have $m > 0$. Furthermore, $\mathcal{R}(x_0 + \lambda\mathbf{v}) > \mathcal{R}(x_0)$ for $\lambda > 0$ small enough. We are going to show that this inequality holds for any $\lambda > 0$ if $m > \gamma^2$.

Let p_n and p_f be, respectively, the nearest and furthest neighbors of x_0 determining the angles $n_\mathbf{v}$ and $f_\mathbf{v}$ with $\mathbf{v}$ and consider $\mathcal{R}^*(x_0 + \lambda\mathbf{v}) = d(x_0 + \lambda\mathbf{v}, p_f) - d(x_0 + \lambda\mathbf{v}, p_n)$. We observe that $\mathcal{R}(x_0 + \lambda\mathbf{v}) \geq \mathcal{R}^*(x_0 + \lambda\mathbf{v})$.

If we denote by r the inner radius of the annulus, the non-zero solution of the equation

$$\mathcal{R}^*(x_0 + \lambda\mathbf{v}) = \mathcal{R}(x_0)$$

is

$$\lambda_0 = \frac{2\,r\,\gamma(r+\gamma)(\cos n_\mathbf{v} - \cos f_\mathbf{v})}{\gamma^2 - (\gamma\cos f_\mathbf{v} - r(\cos n_\mathbf{v} - \cos f_\mathbf{v}))^2}. \tag{2}$$

Because the numerator of (2) is always positive we have that, if λ_0 is positive,

$$\lambda_0 \geq \frac{2\,r(r+\gamma)}{\gamma}(\cos n_\mathbf{v} - \cos f_\mathbf{v}) \geq 2\,r\big(1 + \frac{r}{\gamma}\big)m > 2r\gamma(r+\gamma). \tag{3}$$

Therefore, we have

$$\mathcal{R}(x_0 + \lambda\mathbf{v}) \geq \mathcal{R}^*(x_0 + \lambda\mathbf{v}) > \gamma = \mathcal{R}(x_0) \quad \text{if} \quad 0 < \lambda \leq 2r\gamma(r+\gamma).$$

On the other hand, from assumption (A2) and following the same idea as in the proof of Lemma 1, if we denote $K = \cos(\pi/10)$ then we can write

$$\mathcal{R}(x_0 + \lambda\mathbf{v}) \geq \sqrt{r^2 + \lambda^2 + 2\lambda rK} - \sqrt{(r+\gamma)^2 + \lambda^2 - 2\lambda rK}.$$

Therefore,

$$\frac{(\mathcal{R}(x_0 + \lambda\mathbf{v}))^2 - \gamma^2}{2} \geq A - B$$

where

$$A = r^2 + \lambda^2 + \gamma r$$
$$B = \big((r^2 + \lambda^2)^2 - 4\lambda^2 r^2 K^2 + \gamma(2r+\gamma)(r^2 + \lambda^2 + 2\lambda rK)\big)^{1/2}.$$

A straightforward computation shows that

$$A^2 - B^2 \geq \lambda\big((\frac{7r^2}{2} - \gamma^2)\lambda - (4r + 2\gamma)\gamma r\big) = \lambda E_1(\lambda).$$

Because $E_1(\lambda)$ increases with λ, in order to show that $A - B \geq 0$ if $\lambda > 2r^2\gamma$, it is enough to see that

$$E_1(2r^2\gamma) = r\gamma\big(7r^3 - (4 + 2\gamma^2)r - 2\gamma\big) = r\gamma E_2(\gamma) \geq 0,$$

and this follows from the facts that $E_2(\gamma)$ decreases with γ and that

$$E_2(0.1) = 7r^3 - 4.02r - 2 \geq 0$$

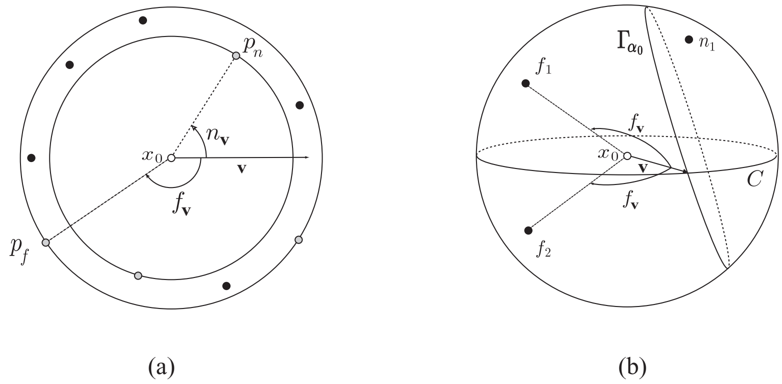

Fig. 5. Illustration for the proof of Proposition 1.

because $r > 0.85$. $\square$

In order to get a geometric interpretation of $\min_{\mathbf{v}\in\mathcal{S}^{d-1}} D_{\mathbf{v}^+}\mathcal{R}(x_0)$ (and to compute it easily), we prove the following:

Proposition 1 *If x_0 is a local minimum of $\mathcal{R}(x)$, then* $\min_{\mathbf{v}\in\mathcal{S}^{d-1}} D_{\mathbf{v}^+}\mathcal{R}(x_0)$ *is achieved when* $\mathbf{v}$ *is the direction of an edge of the roundness diagram of S incident to x_0.*

Proof. Without loss of generality, we can assume that x_0 is the origin of the coordinate system. First, we consider the case $d = 2$. If $\mathbf{v}$ is not parallel to an edge of the roundness diagram incident to x_0, then there is a unique point $p_n \in N(x_0)$ determining an angle $n_{\mathbf{v}}$ with $\mathbf{v}$ (as in Figure 5.a) and analogously for p_f and $f_{\mathbf{v}}$. Therefore, we can slightly move $\mathbf{v}$ towards $p_n p_f$ thus decreasing $\cos n_{\mathbf{v}} - \cos f_{\mathbf{v}}$.

For $d = 3$, if $\mathbf{v}$ is not parallel to a face of the roundness diagram incident to x_0, then we can repeat the argument of the previous paragraph. Finally, assume that $\mathbf{v}$ is parallel to a face but not to an edge of the roundness diagram incident to x_0. Then, either $\mathbf{v}$ is parallel to the bisector plane of the points in $F(x_0)$ and is not parallel to the bisector plane of the points in $N(x_0)$, or the opposite. Assume that we are in the former situation, the latter one can be handled in an analogous way.

In this situation, there are two points $p_{f1}, p_{f2} \in F(x_0)$ determining an angle $f_{\mathbf{v}}$ with $\mathbf{v}$ and one point $p_n \in N(x_0)$ determining an angle $n_{\mathbf{v}}$ with $\mathbf{v}$. Let f_1, f_2 and n_1 be the projections of p_{f1}, p_{f2} and p_n, respectively, on the unit sphere centered at x_0 (see Figure 5.b). Then, $\mathbf{v}$ is constrained to the maximal circle C defined by the intersection of the plane $\mathbf{x} \cdot f_1 f_2 = 0$ with the unit sphere. Let Γ_α denote the circle intersection of the plane

$$\mathbf{x} \cdot f_1 c_1 = \alpha$$

with the unit sphere. Because x_0 is a local minimum,

$$\cos n_{\mathbf{v}} - \cos f_{\mathbf{v}} = \mathbf{v} \cdot f_1 c_1 = \alpha_0 > 0$$

and furthermore Γ_{α_0} intersects (or is tangent to) C and grows when α_0 diminishes, we can conclude that $\mathbf{v}$ is not a local minimum of $D_{\mathbf{v}^+}\mathcal{R}(x_0)$. $\square$

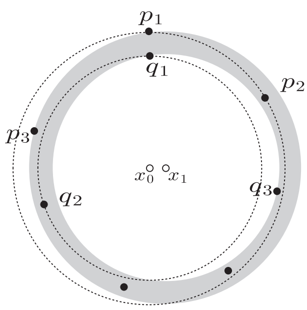

Fig. 6. x_0 is a local minimum but the global minimum is x_1.

It is worth noting that this result is not true if x_0 is not a local minimum. In these cases, the minimum of $D_{\mathbf{v}^+}\mathcal{R}(x_0)$ can be determined by only two points. Therefore, the direction of steepest descent of the function does not always coincide with an edge of the roundness diagram, and the proposed algorithm is not equivalent to the classical local optimization approach.

We can see now why local minima of the roundness function of almost round sets which are not the global minima are unlikely to be encountered in practice. If x_0 is a local minimum of the roundness function and the set is almost round, Theorem 6 and Proposition 1 state that x_0 can only fail to be the global minimum of the function if there exists an edge of the roundness diagram incident to x_0 with direction $\mathbf{v}$ and such that $n_{\mathbf{v}} \simeq f_{\mathbf{v}}$. Then, it is necessary that:

- For $d = 2$ we have three out of the four points defining the local minimum near the boundary of a cone and, therefore, two points of the local minimum configuration are "almost collinear" with x_0. In Figure 6, x_0 is a local minimum with points p_1, p_2, q_1 and q_2 on the boundary of the annulus (they alternate angularly) but the global minimum is x_1 and points on the boundary of the globally optimal annulus are p_1, p_3, q_1 and q_3.
- For $d = 3$ we have four out of the five points defining the local minimum near the boundary of a cone and, therefore, there are four "almost coplanar" points in the configuration defining the local minimum.

6. Experimental Results

We have done experiments with two kinds of input data:

- For $d = 2$, with some data provided by the National Institute of Standards and Technology (NIST) which imitates a variety of error patterns that occur in practice.

Set	w_n	w	$(w_n - w)/w$	it.	w_a	$(w_a - w)/w$
S_1	0.017888	0.017811	0.00429	1	0.017929	0.00663
S_2	0.017744	0.017644	0.00567	1	0.017717	0.00418
S_3	0.001990	0.001975	0.00754	1	0.001986	0.00602
S_4	0.009976	0.009945	0.00317	2	0.010088	0.01443
S_5	0.006985	0.006666	0.04776	2	0.006933	0.04006
S_6	0.006959	0.006720	0.03557	6	0.006752	0.00477
S_7	0.017870	0.002009	7.89088	10	0.002114	0.05236

Table 1. Results on data simulating frequent error patterns in metrology applications. Starting at the second column we have the nominal width, the real width, the relative error, the number of iterations performed by the algorithm, the algebraic width of the set (defined below) and the relative error between algebraic width and real width.

– Both for $d = 2$ and $d = 3$ with data randomly generated inside the annulus $\mathcal{A}(O, 1 - e, 1 + e)$ for $e = 10^{-i}$ and $i = 1, 2, 3, 4$.

Table 1 shows the results of the first experiment. $S_1, \ldots, S_7$ are samples of 800 points with nominal center at the origin and nominal radius 1. In the second column we have the nominal width, i.e. $w_n = \mathcal{R}(O)$, and in the third column the local minimum obtained for the algorithm starting at the nominal center. In all these cases, the computed local minimum can be guaranteed to be the global minimum of the function by a direct application of Theorem 6. The fourth column shows the relative improvement over the nominal width and the fifth the number of iterations of the algorithm (i.e. the number of vertices of the roundness diagram that are visited during the procedure). If a good choice of the nominal center has been made $(S_1, \ldots, S_4)$, then already the first or the second vertex of the roundness diagram is the solution to the problem. Only when a very poor choice of the nominal center is made (S_7) the number of iterations grows a little bit. Finally, the sixth column shows the *algebraic width* of the set, which is an alternative measure used in industry. For computing the algebraic width, we minimize

$$\sum_{i=1}^{n}((d(X, p_i))^2 - r^2)$$

in the variables $(X = (x, y), r)$, which can be transformed into a linear least squares fit. Now, if X_a is the *algebraic center* (solution to the problem), the algebraic width is $w_a = \mathcal{R}(X_a)$. We can see in the table how poor this solution can be (in some cases, even worst than the nominal width). Finally, it is worth noting that, in all these cases, the minimum area annulus is exactly the same as the minimum width annulus.

For the randomly generated data, we have computed the average of 20 iterations of the algorithm for sets of $500, 1000, 2000, \ldots, 10000$ points. As a starting point for the algorithm, we have chosen a random point $x \in \mathcal{B}(O, 0.1)$ with the aim of measuring the complexity of the roundness diagram in a neighborhood of the solution (if the origin is chosen as a starting point, the number of the iterations

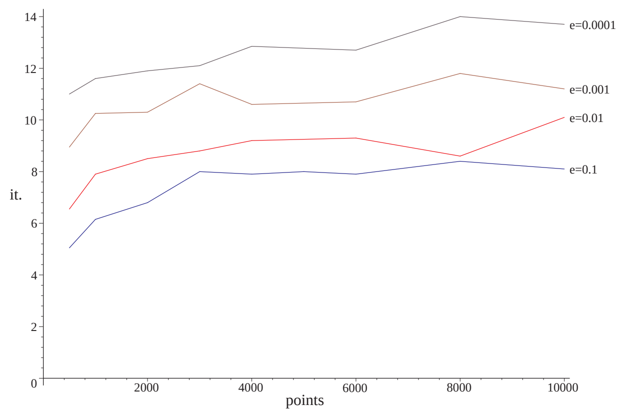

Fig. 7. Number of iterations for randomly generated data (d=2).

does not seem to grow with n). The results are shown in Figure 7 and Figure 8 for $d = 2$ and $d = 3$ respectively.

As should be expected, the number of iterations grows with the dimension and also if the nominal width of the sample diminishes. However, the behavior is clearly sublinear and, therefore, the performance of the algorithm in practice is subquadratic.

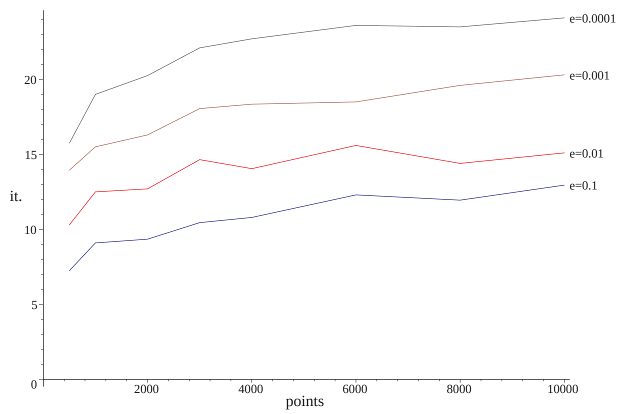

Fig. 8. Number of iterations for randomly generated data (d=3).

7. Final Remarks

We conclude with some directions of research suggested by the work:

- The techniques used in this paper could be extended to deal with sets in the shape of a circular arc or a spherical cap.
- The main drawback of the minimum width annulus is that it is very sensitive to

errors in the data. Therefore, it would be very interesting to try to generalize this work to compute the thinnest annulus containing all but k of the points, where k is small, in the same way that it has been done in[13] for LP-type problems.

- If we take into account some uncertainty in the measurements, the objective is to compute the thinnest annulus containing a given set of disks. If the radius of the disks are small compared with the width of the annulus and they do not intersect, the approach proposed in the paper should also be useful.
- Try to generalize this approach to other problems in Tolerancing Metrology, like measuring flatness of almost flat sets, collinearity of almost collinear points or circularity of almost circular sets in the space.

Acknowledgements

We would like to thank Dr. C. Shakarji from NIST, who kindly provided numerical data for the experiments of Section 6. We also want to thank the anonymous referees who carefully read the paper and whose comments improved the quality of this work.

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