Exact Primitives for Smallest Enclosing Ellipses *

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Introduction

The problem of finding the unique closed ellipsoid of smallest volume enclosing an n-point set P in d-space (known as the *Löwner-John ellipsoid* of P [5]) is an instance of convex programming and can be solved by general methods in time $O(n)$ if the dimension is fixed [12, 6, 3, 1]. The problem-specific parts of these methods are encapsulated in *primitive operations* that deal with subproblems of constant size.

We derive explicit formulae for the primitive operations of Welzl's randomized method [12] in dimension $d = 2$. Compared to previous ones [9, 7, 8], these formulae are simpler and faster to evaluate, and they only contain rational expressions, allowing for an exact solution.

Primitive Operations

For a finite point set P in the plane, not all points on a line, we denote by $\mathrm{ME}(P)$ the smallest enclosing ellipse of P. An inclusion-minimal set $S \subseteq P$ with $\mathrm{ME}(S) = \mathrm{ME}(P)$ is a *support set* of P. Any support set satisfies $|S| \leq 5$ and $\mathrm{ME}(S) = \overline{\mathrm{ME}}(S)$, where $\overline{\mathrm{ME}}(S)$ denotes the smallest ellipse with all points of S on the boundary. In general, if some ellipse exists with a set B on its boundary, then also $\overline{\mathrm{ME}}(B)$ exists and is unique [12].

Given P, Welzl's algorithm computes a support set S of P, provided the following primitive operation is available.

> Given $B \subseteq P$, $3 \leq |B| \leq 5$, such that $\overline{\mathrm{ME}}(B)$ exists, and a query point $q \in P \setminus B$, decide whether q lies inside $\overline{\mathrm{ME}}(B)$.

We call this operation the *in-ellipse test*. As we will see, the case $|B| = 4$ presents the actual difficulty. Our method is based on the concept of *conics*.

Conics

A *conic* $\mathcal{C}$ in *linear form* is the set of points $p = (x, y)^T \in \mathbb{R}^2$ satisfying the quadratic equation

$$\mathcal{C}(p) := rx^2 + sy^2 + 2txy + 2ux + 2vy + w = 0, \qquad (1)$$

r, s, t, u, v, w being real parameters. $\mathcal{C}$ is invariant under scaling the vector (r, s, t, u, v, w) by any nonzero factor. After setting

$$M := \begin{pmatrix} r & t \\ t & s \end{pmatrix}, \quad m := \begin{pmatrix} u \\ v \end{pmatrix}, \qquad (2)$$

the conic assumes the form $\mathcal{C} = \{p^T Mp + 2p^T m + w = 0\}$. If a point $c \in \mathbb{R}^2$ exists such that $Mc = -m$, $\mathcal{C}$ is symmetric about c and can be written in *center form* as

$$\mathcal{C} = \{(p - c)^T M(p - c) - z = 0\}, \qquad (3)$$

where $z = c^T Mc - w$. If $\det(\mathcal{C}) := \det(M) \neq 0$, a center exists and is unique. Conics with $\det(\mathcal{C}) > 0$ define *ellipses*.

By scaling with -1 if necessary, we can w.l.o.g. assume that $\mathcal{C}$ is *normalized*, i.e. $r \geq 0$. If $\mathcal{E}$ is a normalized ellipse, q lies inside $\mathcal{E}$ iff $\mathcal{E}(q) \leq 0$.

If $\mathcal{C}_1, \mathcal{C}_2$ are two conics, the *linear combination*

$$\mathcal{C} := \lambda\mathcal{C}_1 + \mu\mathcal{C}_2, \quad \lambda, \mu \in \mathbb{R}$$

is the conic given by $\mathcal{C}(p) = \lambda\mathcal{C}_1(p) + \mu\mathcal{C}_2(p)$. If p belongs to both $\mathcal{C}_1$ and $\mathcal{C}_2$, p also belongs to $\mathcal{C}$.

Now we are prepared to describe the in-ellipse test, for $|B| = 3, 4, 5$.

In-ellipse test, $|B| = 3$

It is well-known [11, 7, 8] that $\overline{\mathrm{ME}}(\{p_1, p_2, p_3\})$ is given in center form (3) by

$$c = \frac{1}{3}\sum_{i=1}^{3} p_i, \quad M^{-1} = \frac{1}{3}\sum_{i=1}^{3}(p_i - c)(p_i - c)^T, \quad z = 2.$$

From this, M is easy to compute. Query point q is inside $\overline{\mathrm{ME}}(B)$ iff $(p - c)^T M(p - c) - z \leq 0$.

In-ellipse test, $|B| = 4$

$\overline{\mathrm{ME}}(B)$ is some conic through $B = \{p_1, p_2, p_3, p_4\}$, and any such conic is a linear combination of two special conics $\mathcal{C}_1, \mathcal{C}_2$ through B [10], see Figure 1.

To see that these are indeed conics, consider three points $q_1 = (x_1, y_1), q_2 = (x_2, y_2), q_3 = (x_3, y_3)$ and define

$$[q_1 q_2 q_3] := \det\begin{pmatrix} x_1 - x_3 & x_2 - x_3 \\ y_1 - y_3 & y_2 - y_3 \end{pmatrix}.$$

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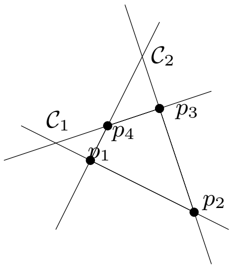

Figure 1: Two special conics through four points

$[q_1q_2q_3]$ records the orientation of the point triple; in particular, if the points are collinear, then $[q_1q_2q_3] = 0$. This implies

$$\mathcal{C}_1(p) = [p_1p_2p][p_3p_4p], \quad \mathcal{C}_2(p) = [p_2p_3p][p_4p_1p],$$

and these turn out to be quadratic expressions as required in the conic equation (1), easily computable from the points in B.

Now, given the query point q, we determine the (unique [10]) conic $\mathcal{C}_0$ through the five points $B \cup \{q\}$. We get $\mathcal{C}_0 = \lambda_0\mathcal{C}_1 + \mu_0\mathcal{C}_2$, with $\lambda_0 = \mathcal{C}_2(q), \mu_0 = -\mathcal{C}_1(q)$. In the sequel we assume that $\mathcal{C}_0$ is normalized.

Case 1. $\det(\mathcal{C}_0) \leq 0$, i.e. $\mathcal{C}_0$ is not an ellipse. Then exactly one of the following statements holds.

(i) q lies inside any ellipse through B.
(ii) q lies outside any ellipse through B.

To prove this, assume there are two ellipses $\mathcal{E}, \mathcal{E}'$ through B, with $\mathcal{E}(q) \leq 0$ and $\mathcal{E}'(q) > 0$. Then we find $\lambda \in [0, 1)$ such that $\mathcal{E}'' := (1-\lambda)\mathcal{E} + \lambda\mathcal{E}'$ satisfies $\mathcal{E}''(q) = 0$, i.e. $\mathcal{E}''$ goes through $B \cup \{q\}$. Hence $\mathcal{E}''$ equals $\mathcal{C}_0$ and is not an ellipse. On the other hand, the convex combination of two ellipses is an ellipse again, a contradiction.

Thus, it suffices to test q against *any* ellipse through the four points to obtain the desired result. Let

$$\alpha = r_1s_1 - t_1^2, \ \beta = r_1s_2 + r_2s_1 - 2t_1t_2, \ \gamma = r_2s_2 - t_2^2,$$

r_i, s_i, t_i the parameters of $\mathcal{C}_i$ in the linear form (1). Then $\mathcal{E} := \lambda\mathcal{C}_1 + \mu\mathcal{C}_2$ with $\lambda = 2\gamma - \beta, \mu = 2\alpha - \beta$ defines such an ellipse. This follows from the fact that

$$\det(\mathcal{E}) = (4\alpha\gamma - \beta^2)(\alpha + \gamma - \beta),$$

and both factors can be shown to have negative sign if the p_i are in convex position (which holds because we know that $\overline{\mathrm{ME}}(B)$ exists) and in (counter)clockwise order (which can be achieved in a preprocessing step)[4].

Case 2. $\det(\mathcal{C}_0) > 0$, i.e. $\mathcal{C}_0$ is an ellipse $\mathcal{E}$. We need to check the position of q relative to $\mathcal{E}^* = \overline{\mathrm{ME}}(B)$, given by

$$\mathcal{E}^* = \lambda^*\mathcal{C}_1 + \mu^*\mathcal{C}_2,$$

with unknown parameters λ^*, μ^*. In the form of (1), $\mathcal{E}$ is determined by $r_0, \ldots, w_0$, where $r_0 = \lambda_0 r_1 + \mu_0 r_2$. By scaling the representation of $\mathcal{E}^*$ accordingly, we can also assume that $r_0 = \lambda^* r_1 + \mu^* r_2$ holds. In other words, $\mathcal{E}^*$ is obtained from $\mathcal{E}$ by varying λ, μ along the line $\{\lambda r_1 + \mu r_2 = r_0\}$. This means,

$$\begin{pmatrix} \lambda^* \\ \mu^* \end{pmatrix} = \begin{pmatrix} \lambda_0 \\ \mu_0 \end{pmatrix} + \tau^* \begin{pmatrix} -r2 \\ r1 \end{pmatrix}. \tag{4}$$

for some $\tau^* \in \mathbb{R}$. Define

$$\mathcal{E}^\tau := (\lambda_0 - \tau r_2)\mathcal{C}_1 + (\mu_0 + \tau r_1)\mathcal{C}_2, \ \tau \in \mathbb{R}.$$

Then $\mathcal{E}^0 = \mathcal{E}, \mathcal{E}^{\tau^*} = \mathcal{E}^*$. The function $g(\tau) = \mathcal{E}^\tau(q)$ is linear, hence we get

$$\mathcal{E}^*(q) = \tau^* \left. \frac{\partial}{\partial\tau}\mathcal{E}^\tau(q)\right|_{\tau=0} = \rho\,\tau^*,$$

where $\rho = \mathcal{C}_2(q)r_1 - \mathcal{C}_1(q)r_2$. Consequently, q lies inside $\overline{\mathrm{ME}}(B)$ iff $\rho\tau^* \leq 0$.

The following Lemma is proved in [2], see also [8].

Lemma *Consider two ellipses $\mathcal{E}_1, \mathcal{E}_2$, and let*

$$\mathcal{E}^\lambda = (1-\lambda)\mathcal{E}_1 + \lambda\mathcal{E}_2$$

be their convex combination, $\lambda \in (0, 1)$. Then $\mathcal{E}^\lambda$ is an ellipse satisfying $\mathrm{Vol}(\mathcal{E}^\lambda) < \max(\mathrm{Vol}(\mathcal{E}_1), \mathrm{Vol}(\mathcal{E}_2))$.

Since $\mathcal{E}^\tau$ is a convex combination of $\mathcal{E}$ and $\mathcal{E}^*$ for τ ranging between 0 and τ^*, the volume of $\mathcal{E}^\tau$ decreases as τ goes from 0 to τ^*, hence

$$\mathrm{sgn}(\tau^*) = -\mathrm{sgn}\left(\left. \frac{\partial}{\partial\tau}\mathrm{Vol}(\mathcal{E}^\tau)\right|_{\tau=0} \right).$$

If $\mathcal{E}^\tau$ is given in center form (3), its area is

$$\mathrm{Vol}(\mathcal{E}^\tau) = \frac{\pi}{\sqrt{\det(M/z)}},$$

as can be seen by choosing the coordinate system according to the principal axes of E, such that M becomes diagonal. Consequently,

$$\mathrm{sgn}\left(\left. \frac{\partial}{\partial\tau}\mathrm{Vol}(\mathcal{E}^\tau)\right|_{\tau=0} \right) = -\mathrm{sgn}\left(\left. \frac{\partial}{\partial\tau}\det(M/z)\right|_{\tau=0} \right).$$

Recall that if M, m collect the parameters of $\mathcal{E}^\tau$ as in (2), $c = M^{-1}m$ being its center, we get $z = c^TMc - w = m^TM^{-1}m - w$, where M, m, w depend on τ (which we omit in the sequel, for the sake of readability). Noting that

$$M^{-1} = \frac{1}{\det(M)} \begin{pmatrix} s & -t \\ -t & r \end{pmatrix},$$

we get

$$z = \frac{1}{\det(M)}(u^2s - 2uvt + v^2r) - w.$$

Let us introduce the following abbreviations.

$$d := \det(M), \quad Z := u^2s - 2uvt + v^2r.$$

With primes (d', Z' etc.) we denote derivatives w.r.t. τ. Now we can write

$$\frac{\partial}{\partial\tau}\det(M/z) = (d/z^2)' = \frac{d'z - 2dz'}{z^3}. \tag{5}$$

Since $d(0), z(0) > 0$ (recall that $\mathcal{E}$ is a normalized ellipse), this is equal in sign to

$$\delta := d(d'z - 2dz'),$$

at least when evaluated for $\tau = 0$, which is the value we are interested in. Furthermore, we have

$$\begin{aligned} d'z &= d'(\frac{1}{d}Z - w) = \frac{d'}{d}Z - d'w, \\ dz' &= d(\frac{Z'd - Zd'}{d^2} - w') = \frac{Z'd - Zd'}{d} - dw'. \end{aligned}$$

Hence

$$\begin{aligned} \delta &= d'Z - dd'w - 2(Z'd - Zd' - d^2w') \\ &= 3d'Z + d(2dw' - d'w - 2Z'). \end{aligned}$$

Rewriting Z as $u(us - vt) + v(vr - ut) = uZ_1 + vZ_2$, we get

$$\begin{aligned} d &= rs - t^2, & Z_1' &= u's + us' - v't - vt', \\ d' &= r's + rs' - 2tt', & Z_2' &= v'r + vr' - u't - ut', \end{aligned}$$

$$Z' = u'Z_1 + uZ_1' + v'Z_2 + vZ_2'.$$

For $\tau = 0$, all these values can be computed directly from $r(0), \ldots, w(0)$ (the defining values of $\mathcal{E}$) and their corresponding primed values $r'(0), \ldots w'(0)$. For the latter we get $r'(0) = 0, s'(0) = r_1s_2 - r_2s_1, \ldots, w'(0) = r_1w_2 - r_2w_1$. We obtain that q lies inside $\overline{\mathrm{ME}}(B)$ iff $\mathrm{sgn}\,(\rho\ \delta(0)) \le 0$.

In-ellipse test, $|B| = 5$

In Welzl's algorithm, B attains cardinality 5 only if before, a test 'p inside $\overline{\mathrm{ME}}(B \setminus \{p\})$?' has been performed (with a negative result), for some $p \in B$. In the process of doing this test, the unique conic (which we know is an ellipse $\mathcal{E}$) through the points in B has already been computed, see previous section. Now we just 'recyle' $\mathcal{E}$ to conclude that q lies inside $\overline{\mathrm{ME}}(B)$ iff $\mathcal{E}(q) \le 0$.

Implementation

We have implemented the in-ellipse tests as subroutines of Welzl's method with move-to-front heuristic [12], without any tuning.[1] On a Sun SPARC-station 20, using rational arithmetic over integers of arbitrary length provided by LEDA[2], the algorithm takes 220 seconds to compute $\mathrm{ME}(P)$, P a set of 10,000 points with random 32-bit integer coordinates. Under floating-point arithmetic, the computing time drops to 2 seconds, but the result might be incorrect. This gap (suggesting successful usage of floating-point filters and other techniques to combine fast arithmetic with exact computation) is explained by the fact that numbers get large under rational arithmetic. If the input coordinates are k-bit integers, an exact evaluation of $\delta(0)$ in case of $|B| = 4$ (which is the most expensive operation) requires $30k + O(1)$ bits of precision in the worst case.

The output of the algorithm is a support set S. In addition, for $|S| \ne 4$, our method determines $\mathrm{ME}(P) = \mathrm{ME}(S) = \overline{\mathrm{ME}}(S)$ explicitly. For $|S| = 4$, the value τ^* defining $\overline{\mathrm{ME}}(S)$ via (4) appears among the roots of (5); a careful analysis [7, 8] reduces this to a cubic polynomial in τ, thus an exact symbolic representation or a floating-point approximation of τ^* and $\overline{\mathrm{ME}}(S)$ can be computed in a postprocessing step.

[1] A tuned version will become part of the CGAL library, see http://www.cs.ruu.nl/CGAL/

[2] See http://www.mpi-sb.mpg.de/LEDA/leda.html

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