MATHEMATICAL COMMUNICATIONS 143
Math. Commun. **18**(2013), 143–150

Fitting conic sections to measured data in 3-space

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Received March 8, 2012; accepted January 5, 2013

Abstract. We consider the problem of fitting given data in 3-space by rotated plane conic sections in the least squares sense. For circles this was done in [4]. For ellipses we will use some details from [2]. Regarding hyperbolas there is a problem using the two branches. However we can follow [2]. Also for parabolas considered for plane data in [1] we can extend the solution method to spatial data. In all cases the use of three rotations (instead of formerly two ones) is discussed and suitably done. All methods will be based on the necessary conditions for a least squares solution. These algorithms are also related to those ones for fitting data in 3-space by paraboloids [5] and elliptic paraboloids [6] with only two out of three possible rotations used here.

AMS subject classifications: 65D10, 65C60

Key words: least squares fitting of spatial data, conic sections

1. Models

At first we will consider nondegenerate conic sections in the $x-y$ plane. In parametic form with center or vertex (parabola) $(0,0,0)^T$ these are:

$$\text{Circle:} \quad \begin{aligned} x(t) &= r\cos t, \\ y(t) &= r\sin t, \\ z(t) &= 0, \qquad 0 \le t \le 2\pi \end{aligned} \tag{1}$$

$$\text{Ellipse:} \quad \begin{aligned} x(t) &= p\cos t, \\ y(t) &= q\sin t, \\ z(t) &= 0, \qquad p \ne q, 0 \le t \le 2\pi \end{aligned} \tag{2}$$

$$\text{Hyperbola:} \quad \begin{aligned} x(t) &= \pm\cosh t, \\ y(t) &= \sinh t, \\ z(t) &= 0, \qquad -\infty \le t \le \infty \\ & (+\text{ right branch}, -\text{left branch}) \end{aligned} \tag{3}$$

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$$\text{Parabola:} \quad x(t) = \frac{1}{2p}t^2 \quad \text{or for } d \neq 0 \quad x(t) = dt^2$$
$$y(t) = t, \tag{4}$$
$$z(t) = 0, \qquad 0 \leq t \leq \infty$$

All these models can be shifted to

$$\boldsymbol{u}(t) = \begin{pmatrix} a + x(t) \\ b + y(t) \\ c \end{pmatrix} \tag{5}$$

and afterwards (or vice versa before) rotated to

$$\boldsymbol{v}(t) = S(\alpha, \beta, \gamma)\boldsymbol{u}(t), \tag{6}$$

where

$$S = S(\alpha, \beta, \gamma) = R(\gamma)Q(\beta)P(\alpha), \tag{7}$$

and where $P(\alpha), Q(\beta), R(\gamma)$ are rotations in the $x-y$, $x-z$, and $y-z$ planes given by

$$P(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{8}$$

$$Q(\beta) = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix}, \tag{9}$$

$$R(\gamma) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & -\sin\gamma \\ 0 & \sin\gamma & \cos\gamma \end{pmatrix}. \tag{10}$$

Now let the given data be

$$\boldsymbol{u}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix}, \qquad i = 1, \ldots, m \tag{11}$$

For later purposes we introduce

$$\overline{\boldsymbol{u}_i} = \begin{pmatrix} \overline{x_i} \\ \overline{y_i} \\ \overline{z_i} \end{pmatrix} = R^T(\gamma)\boldsymbol{u}_i \tag{12}$$

$$\widetilde{\boldsymbol{u}_i} = \begin{pmatrix} \widetilde{x_i} \\ \widetilde{y_i} \\ \widetilde{z_i} \end{pmatrix} = Q^T(\beta)\overline{\boldsymbol{u}_i} = Q^T(\beta)R^T(\gamma)\boldsymbol{u}_i, \tag{13}$$

$$\widehat{\boldsymbol{u}_i} = \begin{pmatrix} \widehat{x_i} \\ \widehat{y_i} \\ \widehat{z_i} \end{pmatrix} \begin{aligned} &= P^T(\alpha)\widetilde{\boldsymbol{u}_i} = P^T(\alpha)Q^T(\beta)\overline{\boldsymbol{u}_i} \\ &= P^T(\alpha)Q^T(\beta)R^T(\gamma)\boldsymbol{u}_i. \end{aligned} \tag{14}$$

2. The ellipse

2.1. The least squares objective function

For some model $\boldsymbol{v} = \boldsymbol{v}(t)$ depending on unknown parameters $(a, b, c, p, q, \alpha, \beta, \gamma)$ (in the case of an ellipse) the function to be minimized is

$$W = \frac{1}{2}\sum_{i=1}^{m} \|\boldsymbol{u}_i - \boldsymbol{v}(t_i)\|^2 . \tag{15}$$

Here $\boldsymbol{u}_i (i = 1, \cdots, m)$ are the given data and $\boldsymbol{t} = (t_1, \ldots t_m)$ are additional unknown values determining points on $\boldsymbol{v} = \boldsymbol{v}(t)$ with the smallest distance to $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m$.

Because S (6) as a product of orthogonal matrices is also orthogonal, then we have $S^T = S^{-1}$ and thus

$$\begin{aligned} W &= \frac{1}{2}\sum_{i=0}^{m} \|S^T\boldsymbol{u}_i - S^T\boldsymbol{v}(t_i)\|^2 \\ &= \frac{1}{2}\sum_{i=1}^{m} \|\widehat{\boldsymbol{u}}_i - S^T S\boldsymbol{u}(t_i)\|^2 \\ &= \frac{1}{2}\sum_{i=1}^{m} \|\widehat{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)\|^2 \qquad (16) \\ &= \frac{1}{2}\sum_{i=1}^{m} (\widehat{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)^T(\widehat{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)). \qquad (17) \end{aligned}$$

For the ellipse (17) can also be written as

$$W = \frac{1}{2}\sum_{i=1}^{m} (\widehat{x}_i - a - p\cos t_i)^2 + (\widehat{y}_i - b - q\sin t_i)^2 + (\widehat{z}_i - c)^2 . \tag{18}$$

2.2. Necessary conditions for a minimum

The basis for numerical algorithms trying to minimize (16), (18) will be the explicit knowledge of all partial derivatives of (17). In order to fulfill at least the necessary conditions for a minimum of our objective function all of them must be zeroed.

Evidently the conditions

$$\frac{\partial W}{\partial a} = \frac{\partial W}{\partial p} = 0, \qquad \frac{\partial W}{\partial b} = \frac{\partial W}{\partial q} = 0, \qquad \frac{\partial W}{\partial c} = 0$$

give

$$\left.\begin{aligned} am \qquad\qquad + p\sum_{i=1}^{m}\cos t_i &= \sum_{i=1}^{m}\widehat{x}_i \\ a\sum_{i=1}^{m}\cos t_i + p\sum_{i=1}^{m}\cos^2 t_i &= \sum_{i=1}^{m}\widehat{x}_i\cos t_i \end{aligned}\right\} \tag{19}$$

$$
\left.\begin{aligned}
bm \qquad\qquad + q\sum_{i=1}^{m}\sin t_i &= \sum_{i=1}^{m}\widehat{y}_i \\
b\sum_{i=1}^{m}\sin t_i + q\sum_{i=1}^{m}\sin^2 t_i &= \sum_{i=1}^{m}\widehat{y}_i\sin t_i
\end{aligned}\right\} \tag{20}
$$

$$
c = \frac{1}{m}\sum_{i=1}^{m}\widehat{z}_i. \tag{21}
$$

The two systems (19) and (20) will normally have a unique solution (a,p) and (b,q).

Moreover the conditions

$$
\frac{\partial W}{\partial t_i} = 0 \qquad (i = 1,\dots,m)
$$

result in

$$
(q^2 - p^2)\sin t_i\cos t_i + p\,\sin t_i(\widehat{x}_i - a) - q\cos t_i(\widehat{y}_i - b) = 0\,. \tag{22}
$$

Putting $g = \mathrm{tg} t_i$ you will get m polynomial equations of degree four with at least one real solution [2] and thus two or four. Then that one has to be selected that minimizes the i-th part in W (18). Since polynomials of degree four can exactly be solved any numerical methods are not needed here.

Finally we have to care for

$$
\frac{\partial W}{\partial \alpha} = \frac{\partial W}{\partial \beta} = \frac{\partial W}{\partial \gamma} = 0\,.
$$

Using (14) for the first condition we get

$$
\frac{\partial \widehat{\boldsymbol{u}}_i}{\partial \alpha} = \frac{\partial P^T(\alpha)}{\partial \alpha}\widetilde{\boldsymbol{u}}_i \qquad (i = 1,\dots,m)\,.
$$

Applying this to (17) we receive

$$
\begin{aligned}
\frac{\partial W}{\partial \alpha} &= \sum_{i=1}^{m}\left(\frac{\partial \widehat{\boldsymbol{u}}_i}{\partial \alpha}\right)^T(\widetilde{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)) \\
&= \sum_{i=1}^{m}\widetilde{\boldsymbol{u}}_i^T\,\frac{\partial P(\alpha)}{\partial \alpha}\,(\widetilde{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)) \\
&= \sum_{i=1}^{m}\widetilde{\boldsymbol{u}}_i^T\,\frac{\partial P(\alpha)}{\partial \alpha}\,(P^T(\alpha)\widetilde{\boldsymbol{u}}_i - \boldsymbol{u}(t_i)) \\
&= \sum_{i=1}^{m}\widetilde{\boldsymbol{u}}_i^T\,\frac{\partial P(\alpha)}{\partial \alpha}\,P^T(\alpha)\widetilde{\boldsymbol{u}}_i - \widetilde{\boldsymbol{u}}_i^T\,\frac{\partial P(\alpha)}{\partial \alpha}\,\boldsymbol{u}(t_i)\,.
\end{aligned}
$$

Because

$$\frac{\partial P(\alpha)}{\partial \alpha}\, P^T(\alpha) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = A$$

and

$$\widetilde{\boldsymbol{u}}_i^T A \widetilde{\boldsymbol{u}}_i = 0$$

we finally get

$$0 = \frac{\partial W}{\partial \alpha} = -\sum_{i=1}^{m} \widetilde{\boldsymbol{u}}_i^T \begin{pmatrix} -\sin\alpha & -\cos\alpha & 0 \\ \cos\alpha & -\sin\alpha & 0 \\ 0 & 0 & 0 \end{pmatrix} \boldsymbol{u}(t_i)$$

$$= \sum_{i=1}^{m} (\widetilde{x}_i, \widetilde{y}_i, \widetilde{z}_i) \begin{pmatrix} \sin\alpha(a + x(t_i) + \cos\alpha(b + y(t_i)) \\ -\cos\alpha(a + x(t_i) + \sin\alpha(b + y(t_i)) \\ 0 \end{pmatrix} .$$

This gives

$$G \sin\alpha + H \cos\alpha = 0, \tag{23}$$

where

$$G = \sum_{i=1}^{m} \widetilde{x}_i(a + x(t_i)) + \widetilde{y}_i(b + y(t_i)), \tag{24}$$

$$H = \sum_{i=1}^{m} \widetilde{x}_i(b + y(t_i)) - \widetilde{y}_i(a + x(t_i)). \tag{25}$$

The condition (23) gives

$$\operatorname{tg}\alpha = -\frac{H}{G}\,. \tag{26}$$

If

$$\frac{\partial^2 W}{\partial \alpha^2} = G\cos\alpha - H\sin\alpha > 0\,,$$

then

$$\alpha = \operatorname{arctg}\left(-\frac{H}{G}\right), \tag{27}$$

otherwise we must use

$$\alpha := \alpha + \pi \tag{28}$$

to get the minimum.

Now similarly we have

$$\frac{\partial W}{\partial \beta} = \sum_{i=1}^{m} \overline{\boldsymbol{u}}_i^T \frac{\partial Q(\beta)}{\partial \beta}\, Q^T(\beta) \overline{\boldsymbol{u}}_i - \sum_{i=1}^{m} \overline{\boldsymbol{u}}_i^T \frac{\partial Q(\beta)}{\partial \beta}\, P(\alpha) \boldsymbol{u}(t_i), \tag{29}$$

$$\frac{\partial W}{\partial \gamma} = \sum_{i=1}^{m} \overline{\boldsymbol{u}}_i^T \frac{\partial R(\gamma)}{\partial \gamma}\, R^T(\gamma) \boldsymbol{u}_i - \sum_{i=1}^{m} \boldsymbol{u}_i^T \frac{\partial R(\gamma)}{\partial \gamma}\, Q(\beta) P(\alpha) \boldsymbol{u}(t_i) \tag{30}$$

to be zeroed. In both expressions the first terms vanish as before and the second ones give equations like (23) for tgβ and tgγ.

2.3. Numerical algorithms

The principal algorithm used below is described in abstract form in [4] and it was realized for the problems treated there and elsewhere. We propose realizations for our function W (17), (18) in two different ways. The main idea is to fix all but one variable or some group of variables, to globally minimize the corresponding W w.r.t. the rest, then to fix this variable or these ones, and to globally minimize w.r.t. some other variable or some other ones and so on. Applying this to our problem we first have to notice the dependences:

a, b, p, q	depend on	$\alpha, \beta, \gamma, \boldsymbol{t}$	(19), (20),
c	depends on	α, β, γ	(21),
$\boldsymbol{t}$	depends on	$a, b, p, q, \alpha, \beta, \gamma$	(22),
α, β, γ	depend on	$a, b, \boldsymbol{t}, \alpha, \beta, \gamma$	(29), (30).

The announced two successive minimization algorithms for W are:

Algorithm A:

Step 0: Let $\alpha, \beta, \gamma, \boldsymbol{t}$ be given as starting values, e.g. by

$$\alpha = \beta = \gamma = 0, t_i = \frac{2\pi(i-1)}{m} \qquad (i = 1, \ldots, m).$$

Step 1: Use the necessary conditions (19),(20), (21) to calculate unique global minima for a, b, c, p, q using the current values for $a, \beta, \gamma, \boldsymbol{t}$.

Step 2: Calculate $\boldsymbol{t}$ by (22) using the current values for $a, b, p, q, \alpha, \beta, \gamma$. Hereby select t_i such that this value minimizes the i-th term of W.

Step 3: Calculate α, β, γ as functions of the current values of $a, b, \alpha, \beta, \gamma, \boldsymbol{t}$ always using the latest values, i.e. for β use the new α, for γ use the new values of α, β.

Step 4: Calculate W. If it has no longer decreased or if some maximum number of iterations has exeeded, then STOP. Else go back to Step 2.

Algorithm B:

Step 0: Let $a, b, c, p, q, \alpha, \beta, \gamma$ be given as starting values, e.g. a, b, c as the means of x_i, y_i, z_i $(i = 1, \ldots, m)$, p, q arbitrary, and $\alpha = \beta = \gamma = 0$.

Step 1: Use Step 2 of Algorithm A.

Step 2: Use Step 3 of Algorithm A.

Step 3: Use Step 1 of Algorithm A.

Step 4: Use Step 4 of Algorithm A.

The numerical results for real world data with a slightly modified version of Algorithm B in the case of the circle are given in Chapter 3.

3. The circle

The easiest way of getting A and B for the circle from those for the ellipse is to use $p = q = r$ in (2), and to replace

$$\frac{\partial W}{\partial p} = \frac{\partial W}{\partial q} = 0 \qquad \text{by} \quad \frac{\partial W}{\partial r} = 0$$

and, as the circle (1) must not be rotated in the $x - y$ plane, is to set $\alpha = 0$ or $P(\alpha) = I$ and finally to ignore $\frac{\partial W}{\partial \alpha} = 0$, respectively.

A second idea is to start with a cylinder of infinite length as model [3] and to develop algorithms similar to A and B. Afterwards the length of that cylinder can be reduced to zero resulting in a circle [4] and the former algorithms can be adapted, see [4]. We used them for some real life example [4]. The $m = 9$ data were measured in some constructed subway tunnel. They were

x_i	y_i	z_i
21302.986	22912.496	22.928
21304.370	22915.276	23.079
21304.845	22916.347	25.817
21302.375	22911.485	26.589 ·
21302.448	22911.462	24.205
21303.049	22912.764	28.050
21304.012	22914.706	28.082
21304.567	22915.054	27.141

In order to verify whether some cross-section is a good circle or not we fitted the data by some circle and got really sufficient results:

$$\begin{aligned} a &= 21303.5852 \\ b &= 22913.7068 \\ c &= 25.3418 \\ r &= 2.8095 \\ \beta &= 1.0875 \\ \gamma &= -1.5681\,. \end{aligned}$$

4. The hyperbola

Considering the right branch (3) you simply have to replace $(\sin, \cos)$ by $(\sinh, \cosh)$ in (18) and in derived formulas for the ellipse. In the case of the left branch (3) $(\sin, \cos)$ have to be replaced by $(\sinh, -\cosh)$. Some further smaller changes are needed as described in [2].

If you would like to use the two branches simultaneously as a model, then the best you can do is to associate each $\boldsymbol{u}_i$ $(i = 1, \ldots, m)$ with either the right or the left branch of the hyperbola and to modify W correspondingly [2].

5. The parabola

We consider our model (4) in the form

$$x(t) = dt^2,\ d \neq 0, \qquad y(t) = t, \quad z(t) = 0$$

The objective function V corresponding to W (18)is then

$$\begin{aligned} V &= V(a, b, c, d, \alpha, \beta, \gamma, \boldsymbol{t}) \\ &= \frac{1}{2}\sum_{i=1}^{m}(\widehat{x}_i - a - dt_i^2)^2 + (\widehat{y}_i - b - t_i)^2 + (\widehat{z}_i - c)^2 \,. \end{aligned}$$

The partial derivatives w.r.t. $a, b, c, d, \alpha, \beta, \gamma$ are very similar to those for the ellipse. The main difference is

$$\frac{\partial V}{\partial t_i} = 2d^2 t_i^3 - t_i(2d\,(\widehat{x}_i - a) - 1) - (\widehat{y}_i - b) \qquad (i = 1, \ldots, m)$$

which have to be zeroed. These are m polynomials of degree 3 with one or three real zeroes instead of those of degree 4 for the ellipse or for the hyperbola. The details for the model without α, β, γ in 3-space but with just one angle φ for some parabola in the plane can be found in [1] and could easily be adjusted in the case of the above V.

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