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Least squares fitting with elliptic paraboloids

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Abstract. In [4], we discussed the problem of fitting some rotated paraboloid to given measured data in 3-space. A numerical method was developed and numerical examples were given. Recently that method was used to fit some parabolic antenna filter [1]. In this connection the question arises whether this method could be extended for elliptic paraboloids needed for some medical application [2]. We show how this could be done and recommend a numerical method more difficult but similar to that one in [4].

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1. The problem

An elliptic paraboloid with the z-axis as the axis and the origin as the vertex is given by

$$z = d\left(\frac{x^2}{A^2} + \frac{y^2}{B^2}\right), \tag{1}$$

where A and B are the half axes of an ellipse and d is varying. For $A = B = 1$ we would have a rotated paraboloid [4]. Instead of (1), we will better use the canonical parametric form

$$\begin{aligned} x &= Av\cos u \\ y &= Bv\sin u \\ z &= dv^2, \qquad \text{where } u \in [0, 2\pi),\ -\infty < v < \infty, \end{aligned} \tag{2}$$

If $(a, b, c)^T$ is some shifting of the origin and

$$Q(\beta) = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \tag{3}$$

$$P(\gamma) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & -\sin\gamma \\ 0 & \sin\gamma & \cos\gamma \end{pmatrix} \tag{4}$$

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are rotations in the $x-z$ plane and in the $y-z$ plane, then our extended model (2) reads

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = P(\gamma)Q(\beta)\begin{pmatrix} a + Av\cos u \\ b + Bv\sin u \\ c + dv^2 \end{pmatrix} . \tag{5}$$

Remark: A third rotation could be included in the $x-z$ plane [2], but this is omitted due to a larger extent.

If now data points $(x_i, y_i, z_i)^T$ $(i = 1, \ldots, m)$ are given to which model (5) should be fitted in the least square sense, then

$$\frac{1}{2}\sum_{i=1}^{m}\left\|\begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} - P(\gamma)Q(\beta)\begin{pmatrix} a + Av_i\cos u_i \\ b + Bv_i\sin u_i \\ c + dv_i^2 \end{pmatrix}\right\|^2 \tag{6}$$

has to be minimized with respect to the $8 + 2m$ unknowns

$$a, A, b, B, c, d, \beta, \gamma, \boldsymbol{u}, \boldsymbol{v}, \quad \text{where} \quad \boldsymbol{u} = (u_1, \ldots, u_m)^T,\ \boldsymbol{v} = (v_1, \ldots, v_m)^T . \tag{7}$$

It turns out to be somewhat more convenient transforming the given data $(x_i, y_i, z_i)^T$ by

$$\begin{pmatrix} \overline{x_i} \\ \overline{y_i} \\ \overline{z_i} \end{pmatrix} = P(\gamma)^T \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} , \quad \begin{pmatrix} \widetilde{x_i} \\ \widetilde{y_i} \\ \widetilde{z_i} \end{pmatrix} = Q(\beta)^T \begin{pmatrix} \overline{x_i} \\ \overline{y_i} \\ \overline{z_i} \end{pmatrix} . \tag{8}$$

Note that

$$P(\gamma)^{-1} = P(\gamma)^T \qquad \text{and} \qquad Q(\beta)^{-1} = Q(\beta)^T .$$

Now the minimization of (6) is equivalent to the minimization of the following objective

$$\begin{aligned} S(a, A, B, b, c, d, \beta, \gamma, \boldsymbol{u}, \boldsymbol{v}) &= \frac{1}{2}\sum_{i=1}^{m}\left\|\begin{pmatrix} \widetilde{x_i} \\ \widetilde{y_i} \\ \widetilde{z_i} \end{pmatrix} - \begin{pmatrix} a + Av_i\cos u_i \\ b + Bv_i\sin u_i \\ c + dv_i^2 \end{pmatrix}\right\|^2 \\ &= \frac{1}{2}\sum_{i=1}^{m}(\widetilde{x}_i - a - Av_i\cos u_i)^2 + (\widetilde{y}_i - b - Bv_i\sin u_i)^2 + (\widetilde{z}_i - c - dv_i^2)^2 \\ &= \frac{1}{2}\sum_{i=1}^{m} S_i(a, A, b, B, c, d, \beta, \gamma, u_i, v_i) . \end{aligned} \tag{9}$$

2. Necessary conditions for minimum

All $8 + 2m$ partial derivatives of S with respect to the $8 + 2m$ unknowns must become zero. This is a highly nonlinear system of equations that can be solved neither explicitly nor easily numerically (e. g. by NEWTON's method).

Instead we will use a successive minimization method which is generally described in [4] and also realized for rotated paraboloids. But at first we explicitly need all partial derivatives of S. We will list them by the order of variables given in (7).

We have

$$\frac{\partial S}{\partial a}=0 \iff \sum_{i=1}^{m} a+Av_i\cos u_i=\sum_{i=1}^{m}\widetilde{x_i}\ , \tag{10}$$

$$\frac{\partial S}{\partial A}=0 \iff \sum_{i=1}^{m} av_i\cos u_i+Av_i^2\cos^2 u_i=\sum_{i=1}^{m}v_i\cos u_i\ , \tag{11}$$

$$\frac{\partial S}{\partial b}=0 \iff \sum_{i=1}^{m} b+Bv_i\sin u_i=\sum_{i=1}^{m}\widetilde{y_i}\ , \tag{12}$$

$$\frac{\partial S}{\partial B}=0 \iff \sum_{i=1}^{m} bv_i\sin u_i+Bv_i^2\sin^2 u_i=\sum_{i=1}^{m}v_i\sin u_i \tag{13}$$

$$\frac{\partial S}{\partial c}=0 \iff \sum_{i=1}^{m} c+dv_i^2=\sum_{i=1}^{m}\widetilde{z_i} \tag{14}$$

$$\frac{\partial S}{\partial d}=0 \iff \sum_{i=1}^{m} cv_i^2+dv_i^4=\sum_{i=1}^{m}\widetilde{z_i}v_i^2. \tag{15}$$

Further,

$$\begin{aligned}\frac{\partial S}{\partial \beta}=0 \iff & \sum_{i=1}^{m}\frac{\partial\widetilde{x_i}}{\partial\beta}(\widetilde{x_i}-a-Av_i\cos u_i)+\sum_{i=1}^{m}\frac{\partial\widetilde{y_i}}{\partial\beta}(\widetilde{y_i}-b-Av_i\sin u_i)\\ &+\sum_{i=1}^{m}\frac{\partial\widetilde{z_i}}{\partial\beta}(\widetilde{z_i}-c-dv_i^2)=0.\end{aligned} \tag{16}$$

Here corresponding to (8) we have

$$\begin{pmatrix}\widetilde{x_i}\\ \widetilde{y_i}\\ \widetilde{z_i}\end{pmatrix}=Q(\beta)^TP(\gamma)^T\begin{pmatrix}x_i\\ y_i\\ z_i\end{pmatrix} \tag{17}$$

and also

$$\begin{pmatrix}\dfrac{\partial\widetilde{x_i}}{\partial\beta}\\ \dfrac{\partial\widetilde{y_i}}{\partial\beta}\\ \dfrac{\partial\widetilde{z_i}}{\partial\beta}\end{pmatrix}=\frac{\partial Q(\beta)^T}{\partial\beta}\begin{pmatrix}\overline{x_i}\\ \overline{y_i}\\ \overline{z_i}\end{pmatrix}\ . \tag{18}$$

Inserting (17) and (18) into (16) we receive

$$\frac{\partial S}{\partial\beta}=0 \iff H\sin\beta-G\cos\beta=0, \tag{19}$$

where

$$H = \sum_{i=1}^{m} \overline{x}_i(a + Av_i \cos u_i) + \overline{z}_i(c + dv_i^2)$$
$$G = \sum_{i=1}^{m} \overline{z}_i(a + Av_i \cos u_i) + \overline{x}_i(c + dv_i^2) \ .$$

For a minimum we must have

$$\frac{\partial^2 S}{\partial \beta^2} = H \cos\beta + G \sin\beta > 0 \ .$$

In this case

$$\beta = \operatorname{atan}\left(\frac{G}{H}\right), \tag{20}$$

else this value has to be replaced by $\beta + \pi$. Using (8) the variable β also depends on γ.

Similarly to (16)-(20) we have

$$\begin{aligned}\frac{\partial S}{\partial \gamma} = 0 \iff & \sum_{i=1}^{m} \frac{\partial \widetilde{x}_i}{\partial \gamma}(\widetilde{x}_i - a - Av_i \cos u_i) + \sum_{i=1}^{m} \frac{\partial \widetilde{y}_i}{\partial \gamma}(\widetilde{y}_i - b - Bv_i \sin u_i) \\ & + \sum_{i=1}^{m} \frac{\partial \widetilde{z}_i}{\partial \gamma}(\widetilde{z}_i - c - dv_i^2) = 0. \end{aligned} \tag{21}$$

Using (8) we have

$$\begin{pmatrix} \dfrac{\partial \widetilde{x}_i}{\partial \gamma} \\ \dfrac{\partial \widetilde{y}_i}{\partial \gamma} \\ \dfrac{\partial \widetilde{z}_i}{\partial \gamma} \end{pmatrix} = Q(\beta)^T \ \frac{\partial P(\gamma)^T}{\partial \gamma} \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} . \tag{22}$$

Putting (17) and (22) into (21) after lengthy calculations we get

$$\frac{\partial S}{\partial \gamma} = 0 \iff U \cos\gamma + V \sin\gamma = 0, \tag{23}$$

where

$$U = \sum_{i=1}^{m} \sin\beta y_i(a + Av_i \cos u_i) - z_i(b + Bv_i \sin u_i) + \cos\beta y_i(c + dv_i^2),$$
$$V = \sum_{i=1}^{m} \sin\beta z_i(a + Av_i \cos u_i) + y_i(b + Bv_i \sin u_i) + \cos\beta z_i(c + dv_i^2) \ .$$

For a minimum we must have

$$\frac{\partial^2 S}{\partial \gamma^2} = -U \sin\gamma + V \cos\gamma > 0\ .$$

In this case

$$\gamma = -\left(\frac{U}{V}\right) \tag{24}$$

else this value has to be replaced by $\gamma + \pi$.

Finally,

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

must be examined. First we consider

$$\begin{aligned} \frac{\partial S}{\partial v_i} = \frac{\partial S_i}{\partial v_i} = 0 \iff & A \cos u_i (\widetilde{x}_i - a - A v_i \cos u_i) \\ & +\ B \sin u_i (\widetilde{y}_i - b - B v_i \sin u_i) \\ & +\ 2 d v_i (\widetilde{z}_i - c - d v_i^2) = 0 \\ \iff & 2 d^2 v_i^3 (A^2 \cos^2 u_i + B^2 \sin^2 u_i - 2d(\widetilde{z}_i - c)) v_i \\ & - [A \cos u_i (\widetilde{x}_i - a) + B \sin u_i (\widetilde{y}_i - b)] = 0. \end{aligned} \tag{25}$$

These are m polynomial equations of degree three, each with one or three real solutions. If there are three real roots, then the one with the smallest value for S_i $(i = 1, \dots, m)$ must be selected.

Analogously, we have to look for

$$\begin{aligned} \frac{\partial S}{\partial u_i} = \frac{\partial S_i}{\partial u_i} = 0 \iff & A v_i \sin u_i (\widetilde{x}_i - a - A v_i \cos u_i) \\ & -\ B v_i \cos u_i (\widetilde{y}_i - b - B v_i \sin u_i) = 0 \\ \iff & (B^2 - A^2) v_i^2 \sin u_i \cos u_i \\ & +\ A v_i \sin u_i (\widetilde{x}_i - a) - B v_i \cos u_i (\widetilde{y}_i - b) = 0. \end{aligned} \tag{26}$$

Putting

$$u = u_i, \quad w = (B^2 - A^2) v_i^2, \quad p = A v_i (\widetilde{x}_i - a), \quad q = B v_i (\widetilde{y}_i - b)$$

for (26) we get

$$w \sin u \cos u + p \sin u - q \cos u = 0. \tag{27}$$

Substituting

$$r = \mathrm{tg} u$$

for (27) we receive again a polynomial equation but now of degree four. It can be shown that it has at least one real root [3]. This means that there exist two or four real solutions. Again for each $i = 1 \dots, m$ this one with the smallest value of S_i has to be chosen. Note that polynomial equations of degree three and four can be solved exactly, i.e. without some iterative numerical method.

3. Numerical algorithms

There are many possible sequences of the following series of necessary conditions (10) through (15), (18,23), and (25,26) for $i = 1, \dots, m$ to be always fulfilled during the minimization process. We will describe two possible sequences. All values of unknows newly calculated in previous steps ought to be used within Steps 1 – 4.

Method I

Step 0: Let starting values for $\beta, \gamma, \boldsymbol{u}$ and $\boldsymbol{v}$ be given (e.g. $u_i = \frac{2\pi i}{m}$, v_i equidistant within the interval $[\min_k z_k, \max_k z_k]$ for $k = 1 \dots, m$).

Step 1: Calculate (a, A), (b, B), and (c, d) using in each case the corresponding two linear equations (10,11), (12,13), and (14,15). Those will always have a unique solution corresponding to an absolute minimum.

Step 2: Calculate $\beta = \beta(a, A, c, d, \gamma)$ by (19) and also $\gamma = \gamma(a, A, b, B, c, d, \beta)$ by (23) as described.

Step 3: Calculate all real zeroes (1 or 3) for $v_i = v_i(u_i)$ via (25,26) and also those (2 or 4) for $u_i = u_i(v_i)$ $(i = 1, \dots, m)$ and select in each case the one with the smallest value of S_i.

Step 4: Calculate S. If it has decreased again, then go back to Step 1, else STOP. Check for some minimum of S, i.e. if at least all necessary conditions are fulfilled.

Method II

Step 0: Let $a, A, b, B, c, d, \beta, \gamma$ and $\boldsymbol{u}$ *or* $\boldsymbol{v}$ be given as starting values.

Step 1: Calculate $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{v})$ or $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{u})$ for given $\boldsymbol{v}$ *or* $\boldsymbol{u}$ in Step 1 similarly to Step 3 of Method I. Select the zeroes such that S_i is minimal.

Step 2: Calculate $\beta = \beta(\gamma)$ *and* $\gamma = \gamma(\beta)$ by (19) and (23) as in Step 2 of Method I.

Step 3: Calculate (a, A), (b, B), and (c, d) as in Step 1 of Method I.

Step 4: As decribed in Method I.

There may be other sequences for the variables resulting in other methods, too. But it does not seem possible to select some *best* sequence in the sense that its success does not depend on the given data $(x_i, y_i, z_i)^T$ $(i = 1, \dots, m)$ and with *best* convergence properties. There is also no convergence proof for any method. But as was indicated by numerical experiments for $A = B = 1$ [4], Method II perfectly worked and so we recommend it here, too.

References

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