Least squares fitting with rotated paraboloids*

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Abstract. *In [1] the problem of estimating the parameters of a rotated parabola fitted to measured points in the plane was examined. The corresponding method, also used in [2, 3], is extended here to the case of a rotated paraboloid. Fitting by such a surface occurs in computational metrology e.g. when some parabolic reflector will be checked to be a good one.*

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1. The model

Fitting the given data

$$(x_i, y_i, z_i), \qquad i = 1, \dots, m \tag{1}$$

with some rotated paraboloid e.g. appears in computational metrology when a parabolic reflector is measured. A paraboloid with the z-axis as a rotation axis and the origin as the vertex is given by

$$z = d(x^2 + y^2), \qquad |d| > 0\,. \tag{2}$$

To be able to consider rotations and also for our numerical method it is more convenient to use the parametric form

$$\begin{aligned} x &= v\cos u \\ y &= v\sin u \\ z &= dv^2 \end{aligned} \tag{3}$$

that fulfills (2). Considering a translation of the origin to (a, b, c) and rotations $A(\beta)$ in the $x - z$ plane and $B(\gamma)$ in the $y - z$ plane we finally have

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & -\sin\gamma \\ 0 & \sin\gamma & \cos\gamma \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} a + v\cos u \\ b + v\sin u \\ c + dv^2 \end{pmatrix} \tag{4}$$

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where

$$0 \le v < \infty, \quad 0 \le u < 2\pi \tag{5}$$

and the unknowns are $a, b, c, d, \beta, \gamma$.

Instead of rotating the translated model (2) we prefer to rotate the given data (1). This can be done in two steps by

$$\begin{pmatrix} \overline{x}_i \\ \overline{y}_i \\ \overline{z}_i \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & \sin\gamma \\ 0 & -\sin\gamma & \cos\gamma \end{pmatrix} \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} \qquad (i = 1, \ldots, m) \tag{6}$$

and

$$\begin{pmatrix} \widetilde{x}_i \\ \widetilde{y}_i \\ \widetilde{z}_i \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \overline{x}_i \\ \overline{y}_i \\ \overline{z}_i \end{pmatrix} \qquad (i = 1, \ldots, m)\,. \tag{7}$$

For later purposes we note that

$$\begin{aligned} \widetilde{x}_i' &= -\sin\beta\,\overline{x}_i + \cos\beta\,\overline{z}_i \\ \widetilde{y}_i' &= 0 \\ \widetilde{z}_i' &= -\cos\beta\,\overline{x}_i - \sin\beta\,\overline{z}_i \end{aligned} \tag{8}$$

(Here $'$ means the derivative w.r.t. β.) and

$$\begin{aligned} \widetilde{x}_i' &= \cos\beta\, x_i - \sin\beta(\cos\gamma\, y_i + \sin\gamma\, z_i) \\ \widetilde{y}_i' &= -\sin\gamma\, y_i + \cos\gamma\, z_i \\ \widetilde{z}_i' &= -\sin\beta\, x_i - \cos\beta(\cos\gamma\, y_i + \sin\gamma\, z_i)\,. \end{aligned} \tag{9}$$

(Here $'$ means the derivative w.r.t. γ.)

Now let some point on the paraboloid, i.e. $(a + v_i \cos u_i,\ b + v_i \sin u_i,\ c + dv_i^2)$ with unknown values (u_i, v_i) $(i = 1, \ldots, m)$ correspond to each given and rotated (so far with unknown angles β and γ) data point $(\widetilde{x}_i, \widetilde{y}_i, \widetilde{z}_i)$. Then the minimization of

$$\begin{aligned} &S(a, b, c, d, \beta, \gamma, u_1, \ldots, u_m, v_1, \ldots, v_m) \\ &\qquad = \frac{1}{2}\sum_{i=1}^{m} (\widetilde{x}_i - a - v_i \cos u_i)^2 + (\widetilde{y}_i - b - v_i \sin u_i)^2 + (\widetilde{z}_i - c - dv_i^2)^2 \end{aligned} \tag{10}$$

means to minimize the (half) sum of squared orthogonal distances from the rotated data to the unrotated paraboloid. The equivalent would be to minimize the sum of squared orthogonal distances from the original data to points on the rotated model (4). Anyway, we have introduced a lot of further unknowns, i.e. $2m$, namely $u_1, \ldots, u_m, v_1, \ldots, v_m$. But this will simplify our numerical method to be developed.

2. The general algorithm

At first we will discuss the algorithm for a more general case. Then we will specify it for our problem. Let the function to be minimized be more generally

$$T = T(w_1, \ldots, w_M) \ge C > -\infty$$

where the M unknowns $w_1, \dots, w_M$ are numbered in some way such that there exist N groups of variables

$$\begin{aligned}
\boldsymbol{w}_1 &= (w_1, \dots, w_{\ell_1}),\\
\boldsymbol{w}_2 &= (w_{\ell_1+1}, \dots, w_{\ell_2}),\\
&\vdots\\
\boldsymbol{w}_N &= (w_{\ell_{N-1}+1}, \dots, w_{\ell_N}),
\end{aligned}$$

of sizes $\ell_L - \ell_{L-1}$ ($L = 1, \dots, N, \ell_0 = 0, \ell_N = M$) with the following property: For $L = 1, \dots, N$ and given

$$\boldsymbol{w}_1^{(t+1)}, \boldsymbol{w}_2^{(t+1)}, \dots, \boldsymbol{w}_{L-1}^{(t+1)}, \boldsymbol{w}_{L+1}^{(t)}, \dots, \boldsymbol{w}_N^{(t)}$$

in the $(t+1)$-th iteration it should be possible to find a *global* minimum $\boldsymbol{w}_L^*$ of the function

$$T(\boldsymbol{w}_L) = T(\boldsymbol{w}_1^{(t+1)}, \dots, \boldsymbol{w}_{L-1}^{(t+1)}, \boldsymbol{w}_L, \boldsymbol{w}_{L+1}^{(t)}, \dots, \boldsymbol{w}_N^{(t)})\,.$$

Then we set $\boldsymbol{w}_L^{(t+1)} = \boldsymbol{w}_L^*$ and proceed. (Necessary conditions for a minimum are $\frac{\partial T}{\partial \boldsymbol{w}_L} = 0$, but we suppose also some means to identify a global minimum.) The above mentioned property would imply

$$\begin{aligned}
&T(\boldsymbol{w}_1^{(t)}, \boldsymbol{w}_2^{(t)}, \boldsymbol{w}_3^{(t)}, \dots, \boldsymbol{w}_N^{(t)})\\
&\quad \geq T(\boldsymbol{w}_1^{(t+1)}, \boldsymbol{w}_2^{(t)}, \boldsymbol{w}_3^{(t)}, \dots, \boldsymbol{w}_N^{(t)})\\
&\quad \geq T(\boldsymbol{w}_1^{(t+1)}, \boldsymbol{w}_2^{(t+1)}, \boldsymbol{w}_3^{(t)}, \dots, \boldsymbol{w}_N^{(t)})\\
&\quad \geq \dots\\
&\quad \geq T(\boldsymbol{w}_1^{(t+1)}, \boldsymbol{w}_2^{(t+1)}, \boldsymbol{w}_3^{(t+1)}, \dots, \boldsymbol{w}_N^{(t+1)})\,.
\end{aligned}$$

Thus we would have a descent when moving from t to $t+1$. For $t = 0$ starting values have to be given. It will depend on these values to which minimum the algorithm will converge.

Now this algorithm will be used for the special objective function S of (10). It will turn out that due to its properties the group sizes are always one and that it will be very easy to find global minima as desired. Just as in the general case it is possible to choose a suitable sequence of $\boldsymbol{w}_1, \dots, \boldsymbol{w}_N$ in order to eventually improve convergence.

3. The algorithm for the rotated paraboloid

Step 0: Let starting values $a, b, c, d, \beta, \gamma$ be given ((u_i, v_i), $i = 1, \dots, m$ will not be needed.)

Step 1: Using β and γ as given we calculate $(\overline{x}_i, \overline{y}_i, \overline{z}_i)$ and $(\widetilde{x}_i, \widetilde{y}_i, \widetilde{z}_i)$ $(i = 1, \dots, m)$ using (6) and (7) in turn.

Step 2: For each $i = 1, \dots, m$ the necessary condition $\frac{\partial S}{\partial u_i} = 0$ results for $v_i \neq 0$ ($v_i = 0$ makes no sense) in

$$\sin u_i(\widetilde{x}_i - a) - \cos u_i(\widetilde{y}_i - b) = 0\,. \tag{11}$$

If
$$\frac{\partial^2 S}{\partial u_i^2} = \cos u_i(\widetilde{x}_i - a) + \sin u_i(\widetilde{y}_i - b) > 0,$$
then the minimum is
$$u_i = \operatorname{atan}\left(\frac{\widetilde{y}_i - b}{\widetilde{x}_i - a}\right), \tag{12}$$
otherwise u_i has to be replaced by $u_i + \pi$ $(i = 1, \ldots, m)$.

Step 3: For each $i = 1, \ldots, m$ the necessary condition $\frac{\partial S}{\partial v_i} = 0$ results (using those u_i from Step 2) in
$$2d^2 v_i^3 + (1 - 2d(\widetilde{z}_i - c))v_i - (\cos u_i(\widetilde{x}_i - a) + \sin u_i(\widetilde{y}_i - b)) = 0\,. \tag{13}$$
As $d \neq 0$, this is a third degree polynomial equation in v_i that has either one real root or three real roots (see also [1]).

In the first case the root must correspond to the unique global minimum because $\lim_{v_i \to \pm\infty} S(v_i) = \infty$. In the second case one has to select that value out of three that minimizes the i-th term of S. (Note that S is separable w.r.t. either u_i or v_i for each $i = 1, \ldots, m$).

Step 4: The necessary condition $\frac{\partial S}{\partial \beta} = 0$ delivers (using (9))
$$H \sin\beta - G \sin\beta = 0, \tag{14}$$
where
$$\begin{aligned} H &= \sum_{i=1}^{n} \overline{x}_i(a + v_i \cos u_i) + \overline{z}_i(c + dv_i^2)\,, \\ G &= \sum_{i=1}^{m} \overline{z}_i(a + v_i \cos u_i) - \overline{x}_i(c + dv_i^2)\,. \end{aligned}$$
If
$$\frac{\partial^2 S}{\partial \beta^2} = H \cos\beta + G \sin\beta > 0,$$
then
$$\beta = \operatorname{atan}\left(\frac{G}{H}\right), \tag{15}$$
else β has to be replaced by $\beta + \pi$.

Step 5: The necessary condition $\frac{\partial S}{\partial \gamma} = 0$ delivers (using (8))
$$U \cos\gamma + V \sin\gamma = 0, \tag{16}$$
where
$$\begin{aligned} U &= \sum_{i=1}^{m} \sin\beta\, y_i(a + v_i \cos u_i) - z_i(b + v \sin u_i) + \cos\beta\, y_i(c + dv_i^2)\,, \\ V &= \sum_{i=1}^{m} \sin\beta\, z_i(a + v_i \cos u_i) - y_i(b + v_i \sin u_i) + \cos\beta\, z_i(c + dv_i^2)\,. \end{aligned}$$

If

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

then

$$\gamma = \operatorname{atan}\left(-\frac{U}{V}\right), \tag{17}$$

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

Step 6: Using the new values for β and γ we now calculate new values for $(\overline{x}_i, \overline{y}_i, \overline{z}_i)$ and $(\widetilde{x}_i, \widetilde{y}_i, \widetilde{z}_i)$ $(i = 1, \ldots, m)$ applying (6) and (7).

Step 7: The necessary conditions $\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial c} = 0$ give in turn

$$a = \frac{1}{m} \sum_{i=1}^{m} (\widetilde{x}_i - v_i \cos u_i), \tag{18}$$

$$b = \frac{1}{m} \sum_{i=1}^{m} (\widetilde{y}_i - v_i \sin u_i), \tag{19}$$

$$c = \frac{1}{m} \sum_{i=1}^{m} (\widetilde{z}_i - d v_i^2). \tag{20}$$

These values (18), (19), and (20) correspond to global minima.

Step 8: Finally $\frac{\partial S}{\partial d} = 0$ gives (using (20)) the global minimum

$$d = \frac{\sum_{i=1}^{m} v_i^2 (\widetilde{z}_i - c)}{\sum_{i=1}^{m} v_i^4} \tag{21}$$

w.r.t. d.

Step 9: Calculate the current value of S to compare it with the one in the next iteration and compare also the values of the unknowns in two successive iterations (e.g. relative error less than given ε). If accuracy is not sufficient, then go back to Step 2. Otherwise calculate the residuals of the fit, i.e.

$$\begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} - B(\gamma) A(\beta) \begin{pmatrix} a + v_i \cos u_i \\ b + v_i \sin u_i \\ c + d v_i^2 \end{pmatrix} \qquad (i = 1, \ldots, m), \tag{22}$$

and also the translation for the original data by

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} := B(\gamma) A(\beta) \begin{pmatrix} a \\ b \\ c \end{pmatrix}. \tag{23}$$

4. Numerical examples

At first we produced data points (x_i, y_i, z_i), $i = 1, \ldots, m = 20$ on an unrotated paraboloid by defining

$$x_i = 5r_1,\ y_i = 5r_2,\ z_i = .5(x_i^2 + y_i^2),$$

where r_1 and r_2 are different and equally distributed pseudorandom numbers in $[-1, 1]$ for each new i. These data were rotated by $A(.5)$ and $B(-.5)$ and afterwards translated by $(a, b, c) = (1, 2, 3)$ to give the first data set. Four further data sets were derived similarly by adding $g{*}r$ to the new x_i, y_i, z_i where again $r \in [-1, 1]$ was pseudo-randomly varying with each component and with each $i = 1, \ldots, m = 20$. The number g was 0 for the first data set and $g = .1, .25, .6, 1$ for the four other ones, respectively. The data of all five data sets were rounded to three digits after the decimal point before using them. For a global minimum of S we thus would expect $S \approx 0$ for $g = 0$ and S increasing with g.

To test our algorithm we used ten different starting values for $(a, b, c, d, \beta, \gamma)$, namely $(r_1, r_2, r_3, r_4, r_5, r_6)$, where r_k $(k = 1, \ldots, 6)$ were different pseudorandom numbers equally distributed in $[0, 1]$, different for each of the five data sets and also different for each of the ten sets. The results are found in *Table 1*.

g	a	b	c	d	β	γ	S	it	ri
0	1.0002	2.0002	3.0001	.5000	.5000	-.5000	.00000124	1285	$450 - 2400$
.1	.9774	1.9922	2.9793	.5044	.4978	-.5005	.07953690	870	$700 - 1200$
.25	.8283	2.0519	3.0584	.4861	.4967	-.5023	.21590963	1570	$975 - 2300$
.6	2.7480	1.9731	1.3587	.6586	.5733	-.4020	.53725064	1810	$1575 - 2100$
1.	1.3638	1.4461	2.2132	.5974	.4831	-.5242	3.12157106	910	$600 - 1175$

Table 1.

Astonishingly for each value of $g = 0, .1, .25, .6, 1$ we received for each of the ten starting values the same value for S (thus most probably the global minimum) and also for the unknowns $a, b, c, d, \beta, \gamma, u_1, \ldots, u_m, v_1, \ldots, v_m$. The range of the number of iterations ri to get four exact digits after the decimal point for all unknowns and also the corresponding average number it of iterations seem rather high at first glance. But on the other hand, the overall computing time for all five data sets and each time ten starting values was about one minute on a PC and thus remarkably low. Considering the value of S this one normally was very fast decreasing during the first few iterations and then it took a very large number of iterations to receive the attended four digits accuracy.

5. Conclusions

The described algorithm to fit the measured data with a rotated paraboloid can be implemented easily and it seems to behave well with arbitrary starting values, though a global minimum cannot be guaranteed. The same situation is with the GAUSS-NEWTON (see [4]) or the NEWTON method where you need the Jacobian and/or the Hessian matrix, too.) Our algorithm can also be realized in a similar way e.g. for spheres [2], for ellipsoids [3], cylinders, and half cones.

References

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