Least squares fitting of spheres and ellipsoids using not orthogonal distances

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Abstract. *Berman [1] examined the problem of estimating the parameters of a circle when angular differences between successively measured data points were also measured. Applications were reported. Späth [4] generalized that problem by considering an ellipse. Now we will consider measured data points* (x_k, y_k, z_k) *in space and also associated measured angles* (u_k, v_k) $k = 1, \ldots, n > 8$, *for the canonical parametric representation of a sphere or an ellipsoid. The center and the radius or the three half axes, respectively, and two other parameters will be fitted such that some suitable sum of squared not orthogonal distances between the two measurements is minimized. Numerical examples are given. Generalizations are discussed. Another numerical method was proposed by Watson [5].*

Key words: *least squares, not orthogonal distances, ellipsoid, sphere*

AMS subject classifications: 65D10, 65C60

Received April 8, 2001 Accepted May 14, 2001

1. Introduction

At first we will assume an ellipsoid in a normal position, i.e. without rotations, given by

$$\begin{aligned} x(u,v) &= a + p\,\cos u\,\sin v\,, \\ y(u,v) &= b + q\,\sin u\,\sin v\,, \\ z(u,v) &= c + r\,\cos v\,, \end{aligned} \tag{1}$$

where (a, b, c) is the center, (p, q, r) (not $p = q = r$) are the half axes, and where $0 \le u < 2\pi$, $-\frac{\pi}{2} \le v \le \frac{\pi}{2}$. The sphere will later be a special case of (1), namely for $p = q = r$. Given (x_k, y_k, z_k) and (u_k, v_k), $k = 1, \ldots, n$, it is a very easy linear

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problem to determine (a, b, c, p, q, r) such that

$$\begin{aligned} F(a,b,c,p,q,r) &= \sum_{k=1}^{n}(x_k - a - p\,\cos u_k \sin v_k)^2 \\ &\quad +(y_k - b - q \sin u_k \sin v_k)^2 \\ &\quad +(z_k - c - r\cos v_k)^2 \end{aligned} \tag{2}$$

is minimized. There are no further degrees of freedom to reduce the influence of errors in the measured data. Thus we introduce two unknown angles α and β and try to minimize

$$\begin{aligned} G(a,b,c,p,q,r,\alpha,\beta) &= \sum_{k=1}^{n}(x_k - a - p\,\cos(\alpha+u_k)\sin(\beta+v_k))^2 \\ &\quad +(y_k - b - q\sin(\alpha+u_k)\sin(\beta+v_k))^2 \\ &\quad +(z_k - c - r\cos(\beta+v_k))^2 \end{aligned} \tag{3}$$

As in (2), also in (3) not orthogonal distances are used. Introducing α_k and β_k, $k = 1, \ldots, n$, and defining the unknowns via $s_k = \alpha_k + u_k$, $t_k = \beta_k + v_k$ gives the objective

$$\begin{aligned} H(a,b,c,p,q,r,s_1,\ldots,s_n,t_1,\ldots,t_n) &= \sum_{k=1}^{n}(x_k - a - p\,\cos s_k \sin t_k)^2 \\ &\quad +(y_k - b - q\sin s_k \sin t_k)^2 \\ &\quad +(z_k - c - r\cos t_k)^2 \end{aligned} \tag{4}$$

This is, see Späth [2], the usual objective of total least squares where the unknowns are determined such that the distances are orthogonal. But now the measurements (u_k, v_k) are not used any longer.

2. The ellipsoid

Necessary conditions for G to be minimized are

$$\frac{\partial G}{\partial a} = \frac{\partial G}{\partial p} = 0, \quad \frac{\partial G}{\partial b} = \frac{\partial G}{\partial q} = 0, \quad \frac{\partial G}{\partial c} = \frac{\partial G}{\partial r} = 0, \tag{5}$$

and

$$\frac{\partial G}{\partial \alpha} = \frac{\partial G}{\partial \beta} = 0. \tag{6}$$

Condition (5) gives in turn

$$\begin{pmatrix} n & \sum\limits_{k=1}^{n} \cos(\alpha+u_k)\sin(\beta+v_k) \\ \sum\limits_{k=1}^{n} \cos(\alpha+u_k)\sin(\beta+v_k) & \sum\limits_{k=1}^{n} \cos^2(\alpha+u_k)\sin^2(\beta+v_k) \end{pmatrix} \begin{pmatrix} a \\ p \end{pmatrix} = \begin{pmatrix} \sum\limits_{k=1}^{n} x_k \\ \sum\limits_{k=1}^{n} x_k \cos(\alpha+u_k)\sin(\beta+v_k) \end{pmatrix} \tag{7}$$

$$\begin{pmatrix} n & \sum\limits_{k=1}^{n} \cos(\alpha+u_k)\sin(\beta+v_k) \\ \sum\limits_{k=1}^{n} \cos(\alpha+u_k)\sin(\beta+v_k) & \sum\limits_{k=1}^{n} \cos^2(\alpha+u_k)\sin^2(\beta+v_k) \end{pmatrix} \begin{pmatrix} b \\ q \end{pmatrix} = \begin{pmatrix} \sum\limits_{k=1}^{n} y_k \\ \sum\limits_{k=1}^{n} y_k \sin(\alpha+u_k)\sin(\beta+v_k) \end{pmatrix} \tag{8}$$

$$\begin{pmatrix} n & \sum\limits_{k=1}^{n} \cos(\beta+v_k) \\ \sum\limits_{k=1}^{n} \cos(\beta+v_k) & \sum\limits_{k=1}^{n} \cos^2(\beta+v_k) \end{pmatrix} \begin{pmatrix} c \\ r \end{pmatrix} = \begin{pmatrix} \sum\limits_{k=1}^{n} z_k \\ \sum\limits_{k=1}^{n} z_k \cos(\beta+v_k) \end{pmatrix} \tag{9}$$

These three linear 2×2 systems are such that for given α and β they will have a unique solution if at least two of the u_k and two of the v_k are different (normally fulfilled). (For $\alpha = \beta = 0$ (7), (8), and (9) give the unique minimum of (2) when replacing G by F in (5)). For arbitrary α and β now consider (6). We have

$$\begin{aligned} \frac{1}{2}\frac{\partial G}{\partial \alpha} &= (q^2-p^2)\sum_{k=1}^{n} \cos(\alpha+u_k)\sin(\alpha+u_k)\sin^2(\beta+v_k) \\ &\quad + \sum_{k=1}^{n} [(x_k-a)p\sin(\alpha+u_k) - (y_k-b)q\cos(\alpha+u_k)]\sin(\beta+v_k), \end{aligned} \tag{10}$$

$$
\begin{aligned}
\frac{1}{2}\frac{\partial G}{\partial \beta} &= \sum_{k=1}^{n}[p^2\cos^2(\alpha+u_k)+q^2\sin^2(\alpha+u_k)-r^2]\sin(\beta+v_k)\cos(\beta+v_k) \\
&\quad -\sum_{k=1}^{n}[(x_k-a)p\cos(\alpha+u_k)+(y_k-b)q\sin(\alpha+u_k)]\cos(\beta+v_k) \\
&\quad +\sum_{k=1}^{n}(z_k-c)r\sin(\beta-v_k).
\end{aligned} \tag{11}
$$

Given some approximations for (a,b,c,p,q,r) we may use the Newton's method (perhaps for just one or for several steps) to improve an approximate solution to (6), i.e. performing

$$
\begin{pmatrix} \alpha^{(t+1)} \\ \beta^{(t+1)} \end{pmatrix} = \begin{pmatrix} \alpha^{(t)} \\ \beta^{(t)} \end{pmatrix} - \begin{pmatrix} \frac{\partial^2 G}{\partial \alpha^2} & \frac{\partial^2 G}{\partial \alpha \partial \beta} \\ \frac{\partial^2 G}{\partial \alpha \partial \beta} & \frac{\partial^2 G}{\partial \beta^2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial G}{\partial \alpha} \\ \frac{\partial G}{\partial \beta} \end{pmatrix}, \tag{12}
$$

where within the second term on the right-hand side the expressions have to be evaluated at $(\alpha^{(t)},\beta^{(t)})$. This is not very difficult because we explicitly have

$$
\begin{aligned}
\frac{1}{2}\frac{\partial^2 G}{\partial \alpha^2} &= (q^2-p^2)\sum_{k=1}^{n}[\cos^2(\alpha+u_k)-\sin^2(\alpha+u_k)]\sin^2(\beta+v_k) \\
&\quad +\sum_{k=1}^{n}[(x_k-a)p\cos(\alpha+u_k)+(y_k-b)q\sin(\alpha+u_k)]\sin(\beta+v_k),
\end{aligned} \tag{13}
$$

$$
\begin{aligned}
\frac{1}{2}\frac{\partial^2 G}{\partial \beta \partial \alpha} &= 2(q^2-p^2)\sum_{k=1}^{n}\cos(\alpha+u_k)\sin(\alpha+u_k)\sin(\beta+v_k)\cos(\beta+v_k) \\
&\quad +\sum_{k=1}^{n}[(x_k-a)p\sin(\alpha+u_k)-(y_k-b)q\cos(\alpha+u_k)]\cos(\beta+v_k),
\end{aligned} \tag{14}
$$

$$
\begin{aligned}
\frac{1}{2}\frac{\partial^2 G}{\partial \beta^2} &= \sum_{k=1}^{n}[p^2\cos^2(\alpha+u_k)+q^2\sin^2(\alpha+u_k)-r^2] \\
&\qquad (\cos^2(\beta+v_k)-\sin^2(\beta+v_k)) \\
&\quad +\sum_{k=1}^{n}[(x_k-a)p\cos(\alpha+u_k)+(y_k-b)q\sin(\alpha+u_k)]\sin(\beta+v_k) \\
&\quad +\sum_{k=1}^{n}(z_k-c)r\cos(\beta+v_k).
\end{aligned} \tag{15}
$$

Similarly to the case of an ellipse, see Späth [4], we propose the following descent method (assuming that the Newton step or steps is or are forced – possibly by damping – to give a descent):

Step 1: Let be given starting value $\alpha^{(0)}$ and $\beta^{(0)}$ for α and β, e.g. $\alpha^{(0)} = \beta^{(0)} = 0$ (the solution of (2)), and set $t = 0$.

Step 2: Solve (7), (8), and (9) with $\alpha = \alpha^{(t)}$ and $\beta = \beta^{(t)}$ to receive $(a^{(t+1)}, b^{(t+1)}, c^{(t+1)}, p^{(t+1)}, q^{(t+1)}, r^{(t+1)}) = (a, b, c, p, q, r)$.

Step 3: For those values do one or several Newton steps (perhaps controlling the step size in order to get a descent) to get $(\alpha^{(t+1)}, \beta^{(t+1)})$ as new estimates for (α, β). If no overall convergence has occurred, then set $t := t + 1$ and return to Step 2 if t has not become too large.

To test our algorithm we generated test data sets in the following way. Starting with $(a, b, c) = (0, 1, 2)$ and $(p, q, r) = (3, 5, 8)$ we randomly generated values (u_k, v_k), $k = 1, \dots, n = 25$ with $0 \leq u_k \leq 2\pi$, $-\pi/2 \leq v_k \leq \pi/2$. Then we calculated via (1) the corresponding values (x_k, y_k, z_k), $k = 1, \dots, n = 25$. Afterwards all the values $(u_k, v_k, x_k, y_k, z_k)$, $k = 1, \dots, n = 25$ were disturbed by multiplying them with $1 + h/100$ where h was randomly chosen from the interval $[-g, g]$ for $g = 0, 2, 5, 10$ in turn and the results were rounded in each case to two decimals after the floating point. Thus for $g = 0$ we expect the objective function value (3) near zero and increasing with g. For the starting value $(\alpha, \beta) = (0, 0)$ *Table 1* contains the results. The number of iterations to get four significant decimals after the floating point is denoted by it; F means $G(\dots, 0, 0)$.

	$g = 0$	$g = 2$	$g = 5$	$g = 10$
it	3	4	4	4
F	.007369	.611507	3.432712	13.493775
G	.007312	.599595	3.372981	13.346126
a	-.0009	.0054	.0111	.0179
b	1.0016	.9846	.9848	.9090
c	1.9986	2.0839	2.1531	2.3552
p	2.9983	2.9869	2.9733	2.9343
q	5.0007	4.9618	4.8895	4.7355
r	8.0014	7.9441	7.9250	7.7878
α	.000637	-.007807	-.012852	-.021395
β	-.000131	-.002420	-.007361	-.011776

Table 1.

Just to try it, we also used $(\alpha, \beta) = (1, 2)$ and $(\alpha, \beta) = (4, 2)$, as starting values. Though the values of $G(\dots, \alpha, \beta)$ were significantly larger in this case we got the same minima as before but needed some more iterations. However, we had to realize that minima are not unique because changing α to $\alpha + k\pi$ and for β to $\beta + j\pi$ will give the same objective function value when the signs of p and q are correspondingly adapted.

For the mentioned three starting values we used just one Newton iteration without any step control and evidently received the global minimum. Because of the relation between F and G $(\alpha,\beta)=(0,0)$ seems to be canonical as a starting value. For other ones it might occur that some step control is necessary or that even convergence of some other minimum will happen.

3. The sphere

Some parametric version of a sphere is received by putting $p=q=r$ into (1). The objective G (2) is modified correspondingly. Conditions (5) are reduced to

$$\frac{\partial G}{\partial a}=\frac{\partial G}{\partial b}=\frac{\partial G}{\partial c}=\frac{\partial G}{\partial r}=0 \tag{16}$$

i.e. explicitly collapse to

$$\begin{pmatrix} n & 0 & 0 & \sum_{k=1}^{n} cu_k\, sv_k \\ 0 & n & 0 & \sum_{k=1}^{n} su_k\, sv_k \\ 0 & 0 & n & \sum_{k=1}^{n} cv_k \\ \sum_{k=1}^{n} cu_k\, sv_k & \sum_{k=1}^{n} su_k\, sv_k & \sum_{k=1}^{n} cv_k & n \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ r \end{pmatrix} \tag{17}$$

$$= \begin{pmatrix} \sum_{k=1}^{n} x_k \\ \sum_{k=1}^{n} y_k \\ \sum_{k=1}^{n} z_k \\ \sum_{k=1}^{n} x_k\, cu_k\, sv_k + y_k\, su_k\, sv_k + z_k\, cv_k \end{pmatrix},$$

where

$$\begin{aligned} cu_k &= \cos(\alpha+u_k), \\ su_k &= \sin(\alpha+u_k), \\ cv_k &= \cos(\beta+v_k), \\ sv_k &= \sin(\beta+v_k). \end{aligned}$$

The necessary conditions (6) as well as the Hessian (10), (11), and (12) will be received by simply setting $p=q=r$ in those formulae. Thus within the algorithm from *Section 2* we have only to replace Step 2 by

Step 2′: Solve (17) with $\alpha=\alpha^{(t)}$, $\beta=\beta^{(t)}$ to get $(a^{(t+1)},b^{(t+1)},c^{(t+1)},r^{(t+1)})=(a,b,c,r)$.

For the sphere the test data were similarly produced as for the ellipsoid. We set $r=5$ $(=p=q)$. For $(\alpha,\beta)=(0,0)$ as starting values the results are given in *Table 2*.

	$g=0$	$g=2$	$g=5$	$g=10$
it	3	3	3	3
F	.007064	.503849	2.822914	11.154648
G	.006843	.478991	2.726410	10.815996
a	.0000	.0077	.0159	.0241
b	1.0019	.9820	.9489	.8952
c	1.9992	2.0563	2.1334	2.2933
r	5.0007	4.9642	4.9133	4.7930
α	.000216	-.010807	-.021074	-.041410
β	-.000614	-.000925	-.003125	-.002317

Table 2.

For $g = 2$ the starting values $(\alpha, \beta) = (1, 2), (4, 2)$ we had convergence to a local minimum given in both cases by $a = -.4763$, $b = .6202$, $c = 5.7933$, $r = .3575$, $\alpha = 4.3826$, $\beta = 1.730$ and $G = 272.68$. Step size control by damping succeeded in making no progress at all. Thus $(\alpha, \beta) = (0, 0)$ as the starting value is strongly recommended.

4. Generalizations

To improve the fit with G would mean to introduce more degrees of freedom, i.e. further parameters additional to α and β. Instead of $(\alpha + u_k, \beta + v_k)$ one could choose e.g. $(\alpha + su_k, \beta + tv_k)$, where α and β are angles as before and where $s, t \in \mathbb{R}$; even $(\alpha + s_1u_k + t_1v_k, \beta + s_2u_k + t_2v_k)$ is possible, see Späth [3] for a corresponding numerical method. Also, rotated ellipsoids with those choices could similarly be treated by introducing unknown elementary rotations.

Further, instead of (1) we could consider a general surface model

$$\begin{aligned} x &= x(u, v, \mathbf{a}), \\ y &= y(u, v, \mathbf{b}), \\ z &= z(u, v, \mathbf{c}), \end{aligned} \tag{18}$$

where $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are parameters vectors of (perhaps different) lengths n_a, n_b, n_c. If we assume that the components of those vectors do linearly appear in (18), then we can proceed as with the ellipsoid. Instead of 2×2 the sizes of the linear systems will be $n_a \times n_a$, $n_b \times n_b$, and $n_c \times n_c$. If $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ would have common components, some of those systems will collapse similar by to the sphere. Additionally, generalizations to higher dimensions are obvious.

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