Fitting data in space by surfaces in parametric representation with polynomial components

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Abstract. *We consider fitting measured data points in space in the total least squares sense by surfaces in parametric representation with polynomial components in two variables. A well-known descent algorithm is suitably modified. Numerical examples are given.*

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1. The problem

Let data points (x_i, y_i, z_i), $i = 1, \dots, m$ be given in 3-space. We will try to find some special type of surface such that the sum of squared orthogonal distances from the given points onto the surface will become minimal. This surface should be given by some parametric representation

$$\begin{aligned} x &= x(u, v), \\ y &= y(u, v), \\ z &= z(u, v), \end{aligned} \tag{1}$$

$$\begin{aligned} -\infty &\leq \alpha \leq u \leq \beta \leq \infty, \\ -\infty &\leq \gamma \leq v \leq \delta \leq \infty\,. \end{aligned}$$

One example for such a surface is the ellipsoid (see e.g. [2])

$$\begin{aligned} x &= p + a\cos u \cos v, \\ y &= q + b\cos u \sin v, \\ z &= r + c\sin u \end{aligned} \tag{2}$$

in normal position with center (p, q, r) and half axes a, b, and c. The method considered for (2) in [2] and elsewhere will be transcribed here for the case that

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$x(u,v)$, $y(u,v)$, and $z(u,v)$ are polynomials of u and v. If we do no consider planes, the easiest case is

$$\begin{aligned} x &= a_1 + a_2u + a_3v + a_4uv, \\ y &= b_1 + b_2u + b_3v + b_4uv, \\ z &= c_1 + c_2u + c_3v + c_4uv, \\ &-\infty \le u,v \le \infty, \end{aligned} \tag{3}$$

i.e. the case of bilinear functions. Here we will develop the method in full length and give numerical examples. For the biquadratic case

$$\begin{aligned} x &= a_1 + a_2u + a_3v + a_4uv + a_5u^2 + a_6v^2, \\ y &= b_1 + b_2u + b_3v + b_4uv + b_5u^2 + b_6v^2, \\ z &= c_1 + c_2u + c_3v + c_4uv + c_5u^2 + c_6v^2 \end{aligned} \tag{4}$$

it is indicated how to extend the method for higher degree polynomials. Denoting

$$\begin{aligned} \boldsymbol{a} &= (a_1,\dots,a_4)^T, \quad \boldsymbol{b} = (b_1,\dots,b_4)^T, \quad \boldsymbol{c} = (c_1,\dots,c_4)^T \\ \boldsymbol{u} &= (u_1,\dots,u_m)^T, \quad \boldsymbol{v} = (v_1,\dots,v_m)^T \end{aligned} \tag{5}$$

the objective function S to be minimized is

$$S(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c},\boldsymbol{u},\boldsymbol{v}) = \sum_{i=1}^{m} \min_{u,v} \left[(x(u,v)-x_i)^2 + (y(u,v)-y_i)^2 + (z(u,v)-z_i)^2 \right]. \tag{6}$$

There are infinite many equivalent solutions. E.g. with $(a_1,a_2,a_3,a_4,\boldsymbol{u},\boldsymbol{v})$ also $(a_1,-a_2,-a_3,a_4,-\boldsymbol{u},-\boldsymbol{v})$, $(a_1,-a_2,a_3,-a_4,-u,\boldsymbol{v})$, $(a_1,a_2,-a_3,-a_4,u,-\boldsymbol{v})$, and $(a_1,a_3,a_2,a_4,\boldsymbol{v},\boldsymbol{u})$ are parts of the same solution. Similarly to fitting by parametric algebraic curves [3] in the plane, there will be other minima, too, depending on the parametrization as we will also see in examples. Some transformation $u \longrightarrow \alpha u + \beta$, $v \longrightarrow \gamma v + \delta$ will change $\boldsymbol{a}, \boldsymbol{b}$, and $\boldsymbol{c}$ without affecting the minimal value for S.

2. The method for bilinear functions

The necessary conditions for (6) using (3) to become minimal are that altogether $2m+12$ partial derivatives

$$\frac{\partial S}{\partial \boldsymbol{u}}, \frac{\partial S}{\partial \boldsymbol{v}}, \frac{\partial S}{\partial \boldsymbol{a}}, \frac{\partial S}{\partial \boldsymbol{b}}, \frac{\partial S}{\partial \boldsymbol{c}}$$

will vanish. Let us consider

$$\frac{1}{2}\frac{\partial S}{\partial \boldsymbol{a}} = 0\,.$$

(The equation for $\frac{1}{2}\frac{\partial S}{\partial \boldsymbol{b}} = 0$ and $\frac{1}{2}\frac{\partial S}{\partial \boldsymbol{c}} = 0$ will be similar.)

If we denote by (u_i, v_i) the minimum of the i-th term in (6) with respect to (u, v) we have

$$\begin{aligned}
\frac{1}{2}\frac{\partial S}{\partial a_1} &= \sum_{i=1}^{m}(a_1 + a_2u_i + a_3v_i + a_4u_iv_i - x_i) = 0,\\
\frac{1}{2}\frac{\partial S}{\partial a_2} &= \sum_{i=1}^{m}u_i(a_1 + a_2u_i + a_3v_i + a_4u_iv_i - x_i) = 0,\\
\frac{1}{2}\frac{\partial S}{\partial a_3} &= \sum_{i=1}^{m}v_i(a_1 + a_2u_i + a_3v_i + a_4u_iv_i - x_i) = 0,\\
\frac{1}{2}\frac{\partial S}{\partial a_4} &= \sum_{i=1}^{m}u_iv_i(u_1 + a_2u_i + a_3v_i - a_4u_iv_i - x_i) = 0.
\end{aligned} \tag{7}$$

Defining the $m \times 4$ matrix A by

$$A = \begin{pmatrix} 1 & u_1 & v_1 & u_1v_1 \\ 1 & u_2 & v_2 & u_2v_2 \\ 1 & u_2 & v_3 & u_3v_3 \\ \vdots & & & \\ 1 & u_m & v_m & u_mv_m \end{pmatrix} \tag{8}$$

the coefficient matrix of (a_1, a_2, a_3, a_4) in (7) is A^TA and the right-hand side is $A^T\boldsymbol{x}$ where $\boldsymbol{x} = (x_1, \dots, x_m)^T$, i.e. (7) can be written as

$$A^TA\boldsymbol{a} = A^T\boldsymbol{x}\,. \tag{9}$$

These are the normal equations for the problem

$$\|A\boldsymbol{a} - \boldsymbol{x}\|_2^2 \longrightarrow \min\,. \tag{10}$$

Similarly, for $\boldsymbol{a}$ und $\boldsymbol{c}$ we get

$$\|A\boldsymbol{b} - \boldsymbol{y}\|_2^2 \longrightarrow \min, \tag{11}$$

$$\|A\boldsymbol{c} - \boldsymbol{z}\|_2^2 \longrightarrow \min \tag{12}$$

where $\boldsymbol{y} = (y_1, \dots, y_m)^T$ and $\boldsymbol{z} = (z_1, \dots, z_m)^T$. That means that equations (7) can be solved by solving (10) for $\boldsymbol{a}$ and similarly (11) for $\boldsymbol{b}$ and (12) for $\boldsymbol{c}$ where $\boldsymbol{u}$ and $\boldsymbol{v}$ are given. Note that the coefficient matrix in (10), (11) and (12) is always the same. Thus you just need one orthogonalization (subroutine MGS [3]) of the columns of A.

Now consider the minimization of the i-th term in (6) with respect to (u, v). The equations

$$\frac{1}{2}\frac{\partial S}{\partial u} = 0, \quad \frac{1}{2}\frac{\partial S}{\partial v} = 0$$

give

$$
\begin{aligned}
(a_2 + a_4 v)(a_1 + a_2 u + a_3 v + a_4 uv - x_i) &= 0,\\
(b_2 + b_4 v)(a_1 + a_2 u + a_3 v + a_4 uv - y_i) &= 0,\\
(c_2 + c_4 v)(a_1 + a_2 u + a_3 v + a_4 uv - z_i) &= 0,
\end{aligned}
\tag{13}
$$

and

$$
\begin{aligned}
(a_3 + a_4 u)(a_1 + a_2 u + a_3 v + a_4 uv - x_i) &= 0,\\
(b_3 + b_4 u)(a_1 + a_2 u + a_3 v + a_4 uv - y_i) &= 0,\\
(c_3 + c_4 u)(a_1 + a_2 u + a_3 v + a_4 uv - z_i) &= 0.
\end{aligned}
\tag{14}
$$

Given $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ and $v = v_i$ (13) can be solved for $u_i = u$ giving

$$
\begin{aligned}
u = -\big[&(a_2 + a_4 v)(a_1 + a_3 v - x_i) + (b_2 + b_4 v)(b_1 + b_3 v - y_i)\\
&+ (c_2 + c_4 v)(c_1 + c_3 v - z_i)\big] \Big/ \big[(a_2 + a_4 v)^2 + (b_2 + b_4 v)^2 + (c_2 + c_4 v)^2\big]
\end{aligned}
\tag{15}
$$

and given $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ and $u = u_i$ (14) can be solved for $v_i = v$ giving

$$
\begin{aligned}
v = -\big[&(a_3 + a_4 u)(a_1 + a_2 u - x_i) + (b_3 + b_4 u)(b_1 + b_2 u - y_i)\\
&+ (c_3 + c_4 u)(c_1 + c_2 u - z_i)\big] \Big/ \big[(a_3 + a_4 u)^2 + (b_3 + b_4 u)^2 + (c_3 + c_4 u)^2\big].
\end{aligned}
\tag{16}
$$

The formulas (10), (11), (12), (15), (16) suggest the following alternating descent algorithm:

Step 1: Choose some suitable starting values for $(u_i^{(0)}, v_i^{(0)})$, $i = 1, \ldots, m$. They must be such that rank$(A) = 4$ for the matrix (8). (E.g. $u_i, v_i = u_i + \varphi$ (φ constant) is not suitable.) Otherwise problems (10) to (12) would not have unique solutions. Set iteration index $t = 0$.

Step 2: Put $(u_i^{(t)}, v_i^{(t)})$, $1, \ldots, m$ into (8) and solve (10) to (12) for $\boldsymbol{a}^{(t)} = \boldsymbol{a}$, $\boldsymbol{b}^{(t)} = \boldsymbol{b}$, $\boldsymbol{c}^{(t)} = \boldsymbol{c}$. S decreases.

Step 3: Put $v_i^{(t)}$ into (15) and solve for $u_i^{(t+1)} = u$; put $u_i^{(t+1)}$ for u into (16) and solve for $v_i^{(t+1)} = v$. S decreases.

Step 4: If S still decreases and a maximal number of iterations is not yet performed, then set $t = t + 1$ and go back to Step 2, otherwise STOP.

3. A numerical example for bilinear functions

Using

$$
\boldsymbol{a} = (1, -2, 3, 1)^T,\ \boldsymbol{b} = (-1, 4, 1, -1)^T,\ \boldsymbol{c} = (3, 1, -1, -.5)^T \tag{17}
$$

and parameter values

$$
u_i = (i + 2) * .1,\ v_i = ((i - 4) * .2)^2, \quad i = 1, \ldots, 16 \tag{18}
$$

and considering (3) we produced points (x_i, y_i, z_i), $i = 1, \dots, 16$ lying on the corresponding surface. This gives the first data set and is for control purposes. The second data set was derived by deleting all but one decimal digit after the decimal point and the third one was received by rounding x_i, y_i and z_i to integers. In both cases the points do no longer lie on the defined surface above. The third set is

x	2	1	0	0	0	0	1	2	3	5	7	9	13	16	20	25
y	0	1	1	1	2	2	3	3	3	4	4	4	3	3	2	2
z	3	3	3	4	4	4	3	3	3	2	1	0	-1	-3	-4	-6

Using the above values (18) for (u_i, v_i), $i = 1, \dots, 16$ as starting values we got (as expected) after one iteration $S = 0$ and (17) back. For the second data set we got after 500 iterations $S = .0108$ and

$$\begin{aligned} \boldsymbol{a} &= (.9859, -2.0022, 3.0389, .9759)^T, \\ \boldsymbol{b} &= (-1.0847, 4.1792, .8122, -.9223)^T, \\ \boldsymbol{c} &= (3.0039, 1.015, -.9994, -.5009)^T. \end{aligned}$$

Because of small pertubations of the data we got (as expected) a small value for S and only slightly changed values for $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ as against (18).

In the third case after 500 iterations we had $S = 1.1056$ and

$$\begin{aligned} \boldsymbol{a} &= (1.0451, -1.9181, 4.5886, -.1234)^T, \\ \boldsymbol{b} &= (-.7100, 3.5654, .2807, -.4858)^T, \\ \boldsymbol{c} &= (2.9602, 1.9090, -1.1177, -.4729)^T. \end{aligned}$$

Then we used

$$u_i = (i - 7) * .25, \quad v_i = ((i + 1) * .25)^2, \ i = 1, \dots, 16 \tag{19}$$

instead of (18) as starting values for the same three data sets as before. In case 1 we had again after one iteration $S = 0$, but different values for the coefficients of (3), namely

$$\begin{aligned} \boldsymbol{a} &= (-6.8200, -5.3600, 1.8560, .2560)^T, \\ \boldsymbol{b} &= (-.1800, -.2480, .7040, -.2560)^T, \\ \boldsymbol{c} &= (5.8100, 1.8800, -.6080, -.1280)^T. \end{aligned}$$

For the second and the third case we received after about five hundred iterations $S = .0142$ and $S = .9115$ and again similar values for the coefficients as before. The slightly different values of S for (18) as against (19) ought to be due to the fact of not being a sufficient number of iterations or due to different minima.

4. The method for biquadratic and higher degree functions

In the case of (4) the objective function is

$$S(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c},\boldsymbol{u},\boldsymbol{v}) = \sum_{i=1}^{m} \min_{u,v} \big[(a_1 + a_2u + a_3v + a_4uv + a_5u^2 + a_6v^2 - x_i)^2$$
$$+ (b_1 + b_2u + b_3v + b_4uv + b_5u^2 + b_6v^2 - y_i)^2 \qquad (20)$$
$$+(c_1 + c_2u + c_3v + c_4uv + c_5u^2 + c_6v^2 - z)^2\big]$$

where $\boldsymbol{a} = (a_1,\dots,a_6)^T$, $\boldsymbol{b} = (b_1,\dots,b_6)^T$, $\boldsymbol{c} = (c_1,\dots,c_6)^T$. The problems (10) to (12) are the same as before but with A changed into

$$A = \begin{pmatrix} 1 & u_1 & v_1 & u_1v_1 & u_1^2 & v_1^2 \\ 1 & u_2 & v_2 & u_2v_2 & u_2^2 & v_2^2 \\ 1 & u_3 & v_3 & u_3v_3 & u_3^2 & v_3^2 \\ \vdots & \vdots & & & & \\ 1 & u_m & v_m & u_mv_m & u_m^2 & u_m^2 \end{pmatrix} \qquad (21)$$

Thus Steps 1 and 2 are as before if $A, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ are modified. Step 4 is indentical. For Step 3 we need the equations

$$\frac{1}{2}\frac{\partial S}{\partial u} = \frac{1}{2}\frac{\partial S}{\partial v} = 0$$

for $(u,v) = (u_i,v_i)$, $i = 1,\dots,m$. These are

$$\begin{aligned} &(a_2 + a_4v + 2a_5u)\,(a_1 + a_2u + a_3v + a_4uv + a_5u^2 + a_6v^2 - x_i) \\ &+ (b_2 + b_4v + 2b_5u)\,(b_1 + b_2u + b_3v + b_4uv + b_5u^2 + b_6v^2 - y_i) \\ &+ (c_2 + c_4v + 2c_5u)\,(c_1 + c_2u + c_3v + c_4uv + c_5u^2 + c_6v^2 - z_i) = 0\,. \end{aligned} \qquad (22)$$

and

$$\begin{aligned} &(a_3 + a_4v + 2a_6u)\,(a_1 + a_2u + a_3v + a_4uv + a_5u^2 + a_6v^2 - x_i) \\ &+ (b_3 + b_4v + 2b_6u)\,(b_1 + b_2u + b_3v + b_4uv + b_5u^2 + b_6v^2 - y_i) \\ &+ (c_3 + c_4v + 2c_6u)\,(c_1 + c_2u + c_3v + c_4uv + c_5u^2 + c_6v^2 - z_i) = 0\,. \end{aligned} \qquad (23)$$

Both equations (22) and (23) have maximal degree three for both variables u and v. Thus fixing u and v in one of these equations results in getting a polynomial equation of degree three in v and u, respectively. There will be always one or three real roots to be inserted in the other equations. From the altogether maximal sixteen possible combinations we have to select that one with the minimal value of the i-th term in (20). Thus Step 3 reads:

Step 3′: Put $v_i^{(t)}$ into (22) and solve for one or three real solutions $u_i^{(t+1)} = u$; put those $u_i^{(t+1)}$ for u into (23) and solve for one or three real solutions $v_i^{(t+1)} = v$. If the right combination is selected, S will again decrease.

For higher degree functions the procedure is similar. But the degree of the polynomial equations will become higher and also the number of combinations to be checked.

References

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