Fitting data in the plane by algebraic curves in parametric representation

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Abstract. *We consider fitting given data points in the plane by an algebraic curve in parametric form. The objective function to be minimized is the sum of squared orthogonal distances (TLS) with an infinite number of equivalent solutions. Some descent algorithm will normally find one of those depending on starting values. Numerical examples are given.*

Key words: *data fitting, TLS, algebraic curves*

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1. The problem

Let data points (x_i, y_i), $i = 1, \ldots, k$ be given in the plane, i.e. neither $x_1 < \ldots < x_k$ nor $y_1 < \ldots < y_k$ is valid. *Figure 1* shows such a set of numbered points for $k = 8$. We will try to find some curve in the plane such that the sum of squared orthogonal distances (TLS) from the points onto the curve will become minimal (Figure 2), i.e. some curve fitting in this sense. Such a curve may be given by a pair.

$$(x(t), y(t)), \quad -\infty \leq t \leq \infty \tag{1}$$

being suitable functions of the curve parameter t. E. g. one could take two cubic spline functions [2].

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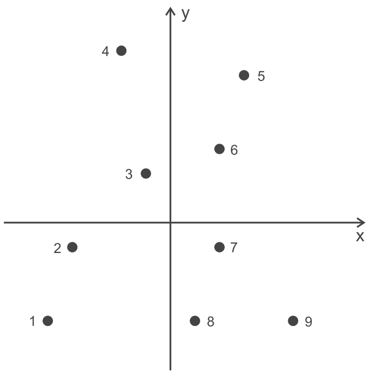

Fig. 1

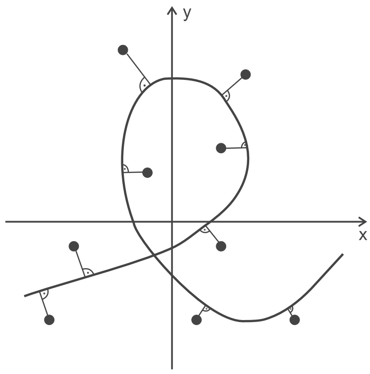

Fig. 2

Here we will discuss the case of

$$x(t) = a_n t^n + a_{n-1} t^{n-1} + \ldots + a_1 t + a_0,$$
$$y(t) = b_m t^m + b_{m-1} t^{m-1} + \ldots + b_1 t + b_0, \tag{2}$$

where $n \geq 1$ and $m \geq 1$. For $n = m = 1$ we have a straight line, for $n = m = 2$ we have some parabola, and for $n, m > 2$ we have some arbitrarily complicated algebraic curve in the plane, see *Examples 2* and *3* later. First we have to determine coefficient vectors

$$\boldsymbol{a} = (a_n, a_{n-1}, \ldots, a_1, a_0)^T, \quad \boldsymbol{b} = (b_m, b_{m-1}, \ldots, b_1, b_0)^T \tag{3}$$

in the above sense, i.e. for each given point (x_i, y_i) we have to find values $t = t_i$, i.e. altogether some vector

$$\boldsymbol{t} = (t_1, \ldots, t_k), \tag{4}$$

such that

$$S(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{t}) = \sum_{k=1}^{n} \min_t \left[(x(t) - x_i)^2 + (y(t) - y_i)^2 \right] \tag{5}$$

is minimized.

2. Nonuniqueness of solutions

Consider as example

$$x(t) = a_2 t^2 + a_1 t + a_0$$

and the transformation

$$t \longrightarrow \alpha t + \beta \quad (\alpha \neq 0)\,. \tag{6}$$

Then we have

$$\begin{aligned} x(\alpha t + \beta) &= a_2(\alpha t + \beta)^2 + a_1(\alpha t + \beta) + a_0 \\ &= a_2 \alpha^2 t^2 + (2 a_2 \alpha \beta + a_1 \alpha) t + (a_2 \beta^2 + a_1 \beta + a_0) \\ &= \widetilde{a}_2 t^2 \qquad\qquad + \widetilde{a}_1 t \qquad\qquad\qquad + \widetilde{a}_0 \\ &= \widetilde{x}(t), \end{aligned} \tag{7}$$

and also

$$\widetilde{x}\left(\frac{t-\beta}{\alpha}\right) = x(t) \tag{8}$$

As both

$$S(\widetilde{\boldsymbol{a}}, \widetilde{\boldsymbol{b}}, t_1, \ldots, t_k) = S(\boldsymbol{a}, \boldsymbol{b}, \alpha t_1 + \beta, \ldots, \alpha t_k + \beta) \tag{9}$$

and

$$S(\boldsymbol{a}, \boldsymbol{b}, t_1, \ldots, t_k) = S\left(\widetilde{\boldsymbol{a}}, \widetilde{\boldsymbol{b}}, \frac{t_1-\beta}{\alpha}, \ldots, \frac{t_k-\beta}{\alpha}\right) \tag{10}$$

are valid, we will have an infinite number of equivalent solutions.

3. Necessary conditions for some solution

If we denote by t_i the minimal value of t in the i-th term in (5), then we can write

$$\begin{aligned} S(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{t}) = \sum_{i=k}^{k} \big[& \big(a_n t_i^n + a_{n-1} t_i^{n-1} + \ldots + a_1 t_i + a_0 - x_i\big)^2 \\ & + \big(b_m t_i^m + b_{m-1} t_i^{m-1} + \ldots + b_1 t_1 + b_0 - y_i\big)^2 \big]. \end{aligned} \tag{11}$$

The necessary conditions for the t_i are

$$\begin{aligned} \frac{1}{2}\frac{\partial S}{\partial t_i} = & (n a_n t_i^{n-1} + \ldots + a_1)(a_n t_i^n + \ldots + a_0 - x_i) \\ & + (m b_m t_i^{m-1} + \ldots + b_1)(b_m t_i^m + \ldots + b_0 - y_i) = 0 \\ & (i = 1, \ldots, k) \end{aligned} \tag{12}$$

These are polynomial equations with odd degree $max(2n-1, 2m-1)$. If there are several real zeroes, then that one is to choose for each i that gives the smallest value in the i-th term of (5). For a numerical solution the subroutine RPOLY [1] is strongly recommended.

The further necessary conditions are

$$\frac{1}{2}\frac{\partial S}{\partial a_j} = \sum_{i=1}^{k} t_i^j (a_n t_i^n + \ldots + a_0 - x_i) = 0 \qquad (j = 0, \ldots, n), \tag{13}$$

$$\frac{1}{2}\frac{\partial S}{\partial b_j} = \sum_{i=1}^{k} t_i^j (b_m t_i^m + \ldots + b_0 - y_i) = 0 \qquad (j = 0, \ldots, m), \tag{14}$$

Denoting

$$\begin{aligned} &\boldsymbol{x} = (x_1, \ldots, x_k)^T, && \boldsymbol{y} = (y_1, \ldots, y_k)^T \\ &C = (c_{ij}) = t_i^{n+1-j} && (i = 1, \ldots, k;\ j = 1, \ldots, n+1), \\ &D = (d_{ij}) = t_i^{m+1-j} && (i = 1, \ldots, k;\ j = 1, \ldots, m+1), \end{aligned} \tag{15}$$

we see that (13) and (14) are the normal equations of the two minimization problems

$$\begin{aligned} \|C\boldsymbol{a}-\boldsymbol{x}\|_2^2 &\longrightarrow \min, \\ \|D\boldsymbol{b}-\boldsymbol{y}\|_2^2 &\longrightarrow \min, \end{aligned} \tag{16}$$

where $\boldsymbol{a}$ and $\boldsymbol{b}$ are the unknown vectors (3). For given values $t_1, \ldots, t_k$ the two problems (16) can easily be solved by the modified Gram-Schmidt method, see e.g. subroutine MGS from [3]. To avoid terms 0^0 we require $t_i \neq 0$ $(i = 1, \ldots, k)$.

4. A descent method

The two problems (15) and the k equations (12) will now be interatively solved such that the objective function (11) will decrease at each step. Convergence to some minimum or even to some global minimum is not guaranteed. But empirically that method works pretty well if not counting an often large number of iterations.

Step 1: For the iteration index ℓ with $\ell = 0$ let $\boldsymbol{t}^{(0)}$ be given with $t_i^{(0)} \neq 0$ $(i = 1, \ldots, k)$, e.g. $t_i^{(0)} = i$ or some other values with $t_1^{(0)} < t_2^{(0)} < \ldots < t_k^{(0)}$, if the given points ought to be ordered in this way. Set $S^{(0)}$ equal to a big number.

Step 2: Put $\boldsymbol{t}^{(\ell)}$ into (15) and solve the two problems (16) for $\boldsymbol{a}^{(\ell+1)} = \boldsymbol{a}$ and $\boldsymbol{b}^{(\ell+1)} = \boldsymbol{b}$. As $\boldsymbol{a}$ and $\boldsymbol{b}$ are linear, S is reduced by this way.

Step 3: Determine $\boldsymbol{t}^{(\ell+1)}$ by calculating for each $i = 1, \ldots, k$ all real zeroes of (12) and by selecting that one that minimizes the i-th term within (11). Calculate $S^{(\ell+1)} = S(\boldsymbol{a}^{(\ell+1)}, \boldsymbol{b}^{(\ell+1)}, \boldsymbol{t}^{(\ell+1)})$. S is reduced again.

Step 4: If some maximal number of iterations (to be given) is not reached and if $S^{(\ell+1)} < S^{(\ell)}$, then set $\ell := \ell + 1$, $S^{(\ell+1)} := S^{(\ell+2)}$, and go back to Step 2.

5. Examples

We consider one set of data for different values of n and m. Those given data points $(k = 12)$ are

x	−1	−3	−5	−6	−5	−2	0	3	5	4	2	−1
y	−7	−5	−4	−2	0	1	0	−2	−1	2	3	4

and the starting vector $\boldsymbol{t}^{(0)}$ in each case was

$$\boldsymbol{t}^{(0)} = (1.25, 1.75, 3.25, 3.75, 5.25, 5.75, 7.25, 7.75, 9.25, 9.75, 11.25, 11.75)^T.$$

Example 1. $n = m = 2$. *The coefficients of* (12) *are*

$$\begin{aligned} t^3 &: 2a_2^2 + 2b_2^2, \\ t^2 &: 3a_1a_2 + 3b_1b_2, \\ t &: 2a_2(a_0 - x_i) + 2b_2(b_0 - y_i), \\ 1 &: a_1(a_0 - x_i) + b_1(b_0 - y_i). \end{aligned}$$

We ended up with

$$\boldsymbol{t} = (.96, 1.65, 2.19, 2.89, 3.36, 10.05, 10.78, 11.75, 12.02, 11.45, 10.86, 9.90)^T,$$
$$S = 22.31 \quad (S^{(0)} = 89.27),$$
$$\boldsymbol{a} = (.283, -3.089, 1.234)^T,$$
$$\boldsymbol{b} = (-.263, 3.981, -10.91)^T.$$

The corresponding parabola together with the given points can be seen in Figure 3.

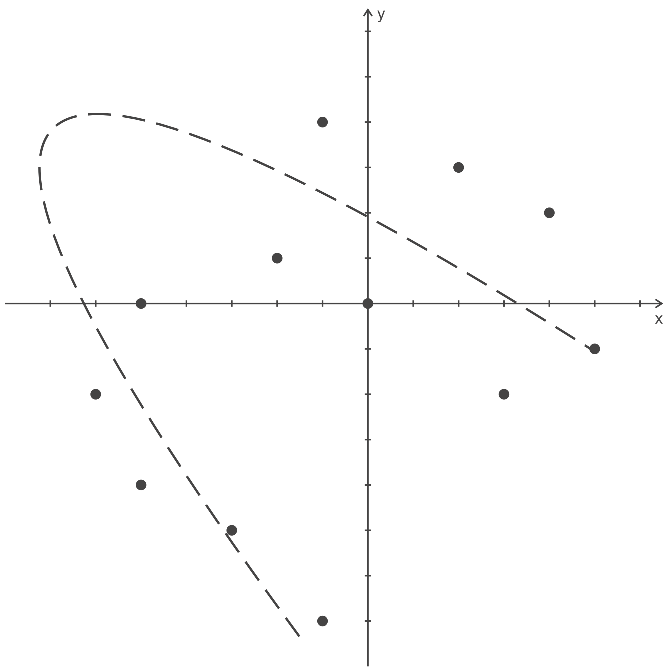

Fig. 3

Example 2. $n = m = 3$. *The coefficients of* (12) *are*

$$\begin{aligned}
t^5 &: 3a_3^2 + 3b_3^2,\\
t^4 &: 5a_2a_3 + 5b_2b_3,\\
t^3 &: 4a_1a_3 + 2a_2^2 + 4b_1b_2 + 2b_2^2,\\
t^2 &: 3a_3(a_0 - x_i) + 3a_1a_2 + 3b_3(b_0 - y_i) + 3b_1b_3,\\
t &: 2a_2(a_0 - x_i) + a_1^2 + 2b_2(b_0 - y_i) + b_1^2,\\
1 &: a_1(a_0 - x_i) + b_1(b_0 - y_i).
\end{aligned}$$

Here we ended up with

$$\boldsymbol{t} = (1.53, 1.90, 2.26, 2.76, 4.70, 5.61, 6.17, 7.03, 7.51, 11.11, 11.41, 11.75)^T,$$
$$S = 2.749 \quad (S^{(0)} = 8.849),$$
$$\boldsymbol{a} = (-.15, 2.82, -14.19, 14.63)^T,$$
$$\boldsymbol{b} = (.07, -1.52, 9.41, -18.09)^T.$$

In this case $t_1 < t_2 < \ldots < t_{12}$ *was not changed as against to* Example 1. *The resulting curve can be seen in* Figure 4.

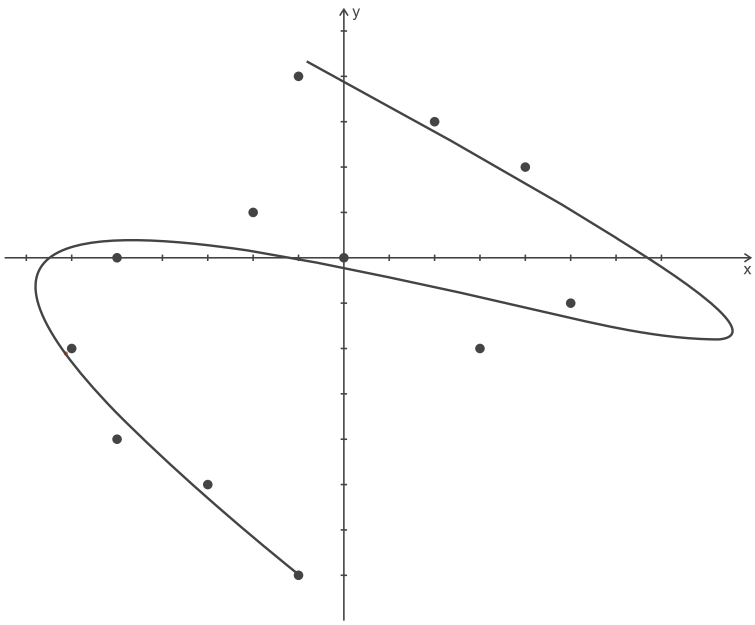

Fig. 4

Example 3. $n = 3,\ m = 4$. *This time the coefficients of* (12) *are not symmetric with respect to* $\boldsymbol{a}$ *and* $\boldsymbol{b}$ *and they are*

$$\begin{aligned}
&t^7 : 4b_4^2,\\
&t^6 : 7b_3b_4,\\
&t^5 : 3a_3^2 + 6b_2b_4 + 3b_3^2,\\
&t^4 : 5a_2a_3 + 5b_1b_4 + 5b_2b_3,\\
&t^3 : 4a_1a_3 + 2a_2^2 + 4b_4(b_0 - y_i) + 4b_1b_3 + 2b_2^2,\\
&t^2 : 3a_3(a_0 - x_i) + 3a_1a_2 + 3b_3(b_0 - y_i) + 3b_1b_3,\\
&t\ \ : 2a_2(a_0 - x_i) + a_1^2 + 2b_2(b_0 - y_i) + b_1^2,\\
&1\ \ : a_1(a_0 - x_i) + b_1(b_0 - y_i).
\end{aligned}$$

Here we got

$$\begin{aligned}
\boldsymbol{t} &= (1.54, 1.89, 2.21, 2.64, 4.92, 5.76, 6.31, 7.16, 7.66, 11.07, 11.39, 11.76)^T,\\
S &= 2.727 \quad (S^{(0)} = 8.546),\\
\boldsymbol{a} &= (-.106, 2.074, -10.65, 10.05)^T,\\
\boldsymbol{b} &= (.002, .0084, -.7713, 6.288, -14.26)^T.
\end{aligned}$$

The corresponding curve is in Figure 5. *Because of the small value for* b_5, *both the final* S *(though a little bit smaller) and the curves from* Example 2 *and* 3 *do not differ very much.*

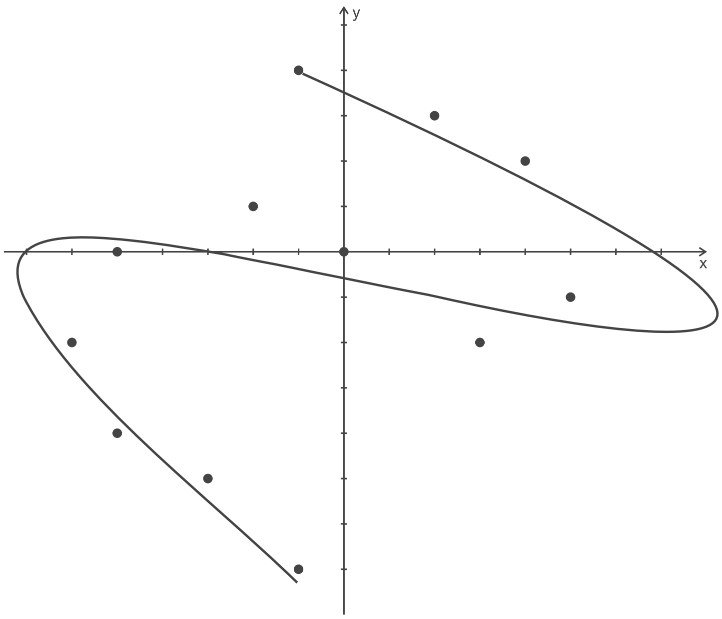

Fig. 5

The calculations for the three examples were repeated with $t_i^{(0)} = i$ *and* $t_i^{(0)} = i/2 + .5$ *. We got the same values for the final* S *and of course not for* $\boldsymbol{a}$ *and* $\boldsymbol{b}$ *with different numbers of iterations (between 100 and 200).*

References

[1] RPOLY: *FORTRAN Subroutine zur Berechnung der Nullstellen von Polynomen: Collected Algorithms of the ACM*, Nr. 493.

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[3] H. Späth, *Numerik*, Vieweg, 1994.