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Least Squares Fitting with Cubic Splines

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Abstract

In the paper cubic spline approximation of experimental data by least squares method is considered. An algorithm to construct a cubic spline with mixed-type boundary constraints is derived.

1. Introduction

Curve fitting has found many applications in image processing, computer graphics, pattern recognition and computer-aided geometric design. The least squares method is the most popular tool to approximate experimental data. The best fit in the least squares sense is the instance of the model for which the sum of squared residuals has its least value, a residual being the difference between an observed value and the value given by the model. For this purpose cubic splines are the most frequently used curves. Usually the cubic splines with certain boundary constraints (complete splines, natural splines, etc.) are used. In this paper we consider more general cubic splines with mixed-type boundary constraints and derive a computational algorithm to find the least squares approximation.

2. Construction of a Cubic Spline with Mixed-type Boundary Constraints

Let us consider a partitioning $\Delta : a = t_0 < t_1 < \cdots < t_n = b, \qquad n \geq 1$ (2.1)

of a segment $[a,b]$. Suppose the values v_k at the points t_k, $k = 0,1,\dots,n$ are given. The cubic spline $S(x)$ associated with the partitioning (2.1) is defined as follows (see, for example, [3, 5, 7]):

a) the function $S(x)$ is a cubic polynomial in each segment $[t_k, t_{k+1}]$, $k = 0,1,\dots,n-1$,

b) $S(x) \in C^2[a,b]$,

c) $S(t_k) = v_k$, $k = 0,1,\dots,n$.

The points t_k of the partitioning (2.1) will be referred to as *basic nodes* of the spline. Let us introduce the following notation for spline segments:

$$S(x) = \begin{cases} S_0(x), & x \in [t_0, t_1] \\ S_1(x), & x \in [t_1, t_2] \\ \dots & \dots \\ S_{n-1}(x), & x \in [t_{n-1}, t_n] \end{cases}.$$

Thus, we need to construct cubic polynomials for the values $k = 0,1,\dots,n-1$

$$S_k(x) = a_3^{(k)} x^3 + a_2^{(k)} x^2 + a_1^{(k)} x + a_0^{(k)}, \qquad x \in [t_k, t_{k+1}] \tag{2.2}$$

so that

$$S_k(t_k)=v_k,\ S_k(t_{k+1})=v_{k+1},\quad k=0,1,\dots,n-1,\tag{2.3}$$

$$S_k'(t_k)=S_{k-1}'(t_k),\ S_k''(t_k)=S_{k-1}''(t_k),\quad k=1,2,\dots,n-1.\tag{2.4}$$

To construct the spline, we need to find $4n$ coefficients $a_0^{(k)},a_1^{(k)},a_2^{(k)},a_3^{(k)}$, $k=0,1,\dots,n-1$. The conditions (2.3) and (2.4) provide a system of $4n-2$ linear equations. In order to get a unique solution, we should impose two additional conditions. As a rule, these conditions include first or second order derivatives of the spline at the end points of the segment $[a,b]$ (see, for example, [3, 4, 5]).

In this paper we will consider mixed-type boundary conditions

$$\alpha_1 S''(a)+\alpha_2 S'(a)=d_a,\quad \beta_1 S''(b)+\beta_2 S'(b)=d_b.\tag{2.5}$$

Assume that

$$\alpha_1\ge 0,\ \alpha_2\le 0,\ \alpha_1^2+\alpha_2^2\ne 0,\tag{2.6}$$

$$\beta_1\ge 0,\ \beta_2\ge 0,\ \beta_1^2+\beta_2^2\ne 0.\tag{2.7}$$

As it will be seen below, the conditions (2.6) and (2.7) provide the correctness of the problem, as well as the stability of a numerical algorithm.

First let us consider the case, when $n\ge 3$. For the sake of simplicity, we introduce the following notation:

$$h_k=t_{k+1}-t_k,\ k=0,1,\dots,n-1,\tag{2.8}$$

$$m_k=S_k'(t_k),\ k=0,1,\dots,n-1,\quad m_n=S_{n-1}'(t_n),\tag{2.9}$$

$$M_k=S_k''(t_k),\ k=0,1,\dots,n-1,\quad M_n=S_{n-1}''(t_n).\tag{2.10}$$

In the paper [1] it was obtained that the segments of the spline $S(x)$ can be written in the form

$$S_k(x)=v_k+\left(\frac{v_{k+1}-v_k}{h_k}-\frac{2M_k+M_{k+1}}{6}h_k\right)(x-t_k)+\frac{M_k}{2}(x-t_k)^2+\frac{M_{k+1}-M_k}{6h_k}(x-t_k)^3,\tag{2.11}$$

where the quantities M_k, $k=0,1,\dots,n$ are calculated as follows. To find $M=[M_1\ M_2\ \cdots\ M_{n-1}]^T$, first we solve the linear system

$$HM=g\tag{2.12}$$

with the symmetric positive definite matrix

$$H=\begin{bmatrix} d_1 & h_1 & & & \\ h_1 & d_2 & h_2 & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & h_{n-3} & d_{n-2} & h_{n-2} \\ & & & h_{n-2} & d_{n-1}\end{bmatrix},\tag{2.13}$$

where

$$d_1=2h_1+\frac{3h_0(4\alpha_1-\alpha_2h_0)}{2(3\alpha_1-\alpha_2h_0)},\tag{2.14}$$

$$d_k=2(h_{k-1}+h_k),\ k=2,3,\dots,n-2,\tag{2.15}$$

$$d_{n-1}=2h_{n-2}+\frac{3h_{n-1}(4\beta_1+\beta_2h_{n-1})}{2(3\beta_1+\beta_2h_{n-1})},\tag{2.16}$$

And the right-hand side $g=[g_1\ g_2\ \cdots\ g_{n-1}]^T$ is defined by the following formulae:

$$g_1=6\left(\frac{v_2-v_1}{h_1}-\frac{v_1-v_0}{h_0}\right)-\frac{3h_0}{3\alpha_1-\alpha_2h_0}\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right), \tag{2.17}$$

$$g_k=6\left(\frac{v_{k+1}-v_k}{h_k}-\frac{v_k-v_{k-1}}{h_{k-1}}\right),\ k=2,3,\ldots,n-2, \tag{2.18}$$

$$g_{n-1}=6\left(\frac{v_n-v_{n-1}}{h_{n-1}}-\frac{v_{n-1}-v_{n-2}}{h_{n-2}}\right)-\frac{3h_{n-1}}{3\beta_1+\beta_2h_{n-1}}\left(d_b-\beta_2\frac{v_n-v_{n-1}}{h_{n-1}}\right). \tag{2.19}$$

nen

$$M_0=\frac{1}{3\alpha_1-\alpha_2h_0}\left[\frac{\alpha_2h_0}{2}M_1+3\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right)\right], \tag{2.20}$$

$$M_n=\frac{1}{3\beta_1+\beta_2h_{n-1}}\left[-\frac{\beta_2h_{n-1}}{2}M_{n-1}+3\left(d_b-\beta_2\frac{v_n-v_{n-1}}{h_{n-1}}\right)\right]. \tag{2.21}$$

Thus, we have discussed the case, when $n\geq 3$. Now let us consider the cases $n=2$ and $I=1$ separately.

When $n=2$, from the equation (2.21) we get:

$$M_2=\frac{1}{3\beta_1+\beta_2h_1}\left[-\frac{\beta_2h_1}{2}M_1+3\left(d_b-\beta_2\frac{v_2-v_1}{h_1}\right)\right]. \tag{2.22}$$

e quantity M_0 is already defined in (2.20). Inserting the expressions (2.22) and (2.20) into (2.12) yields

$$d_1M_1=g_1, \tag{2.23}$$

here

$$d_1=\frac{3h_0(4\alpha_1-\alpha_2h_0)}{2(3\alpha_1-\alpha_2h_0)}+\frac{3h_1(4\beta_1+\beta_2h_1)}{2(3\beta_1+\beta_2h_1)}, \tag{2.24}$$

$$g_1=6\left(\frac{v_2-v_1}{h_1}-\frac{v_1-v_0}{h_0}\right)-\frac{3h_0}{3\alpha_1-\alpha_2h_0}\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right)-\frac{3h_1}{3\beta_1+\beta_2h_1}\left(d_b-\beta_2\frac{v_2-v_1}{h_1}\right). \tag{2.25}$$

In doing so, for $k=0,1$, similar to the expression (2.11), we have:

$$S_k(x)=v_k+\left(\frac{v_{k+1}-v_k}{h_k}-\frac{2M_k+M_{k+1}}{6}h_k\right)(x-t_k)+\frac{M_k}{2}(x-t_k)^2+\frac{M_{k+1}-M_k}{6h_k}(x-t_k)^3. \tag{2.26}$$

Finally, let us discuss the case when $n=1$. Writing the equation (2.21) evaluated for $n=1$, get:

$$M_1=\frac{1}{3\beta_1+\beta_2h_0}\left[-\frac{\beta_2h_0}{2}M_0+3\left(d_b-\beta_2\frac{v_1-v_0}{h_0}\right)\right].$$

…ting the expression (2.20) for M_0 into the last equation, after some rearrangement we obtain

$$M_1=6\,\frac{2(3\alpha_1-\alpha_2h_0)\left(d_b-\beta_2\frac{v_1-v_0}{h_0}\right)-\beta_2h_0\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right)}{4(3\alpha_1-\alpha_2h_0)(3\beta_1+\beta_2h_0)+\alpha_2\beta_2h_0^2}. \tag{2.27}$$

In accordance with the preceding case, we get:

$$S_0(x)=v_0+\left(\frac{v_1-v_0}{h_0}-\frac{2M_0+M_1}{6}h_0\right)(x-t_0)+\frac{M_0}{2}(x-t_0)^2+\frac{M_1-M_0}{6h_0}(x-t_0)^3. \qquad (2.28$$

Thus, the method of constructing interpolation cubic spline with mixed-type boundar constraints is deduced.

3. An Algorithm to Construct a Cubic Spline

Cubic spline fitting is a useful technique to approximate data points due to its stable an smooth characteristics. To this end, a numerical algorithm of constructing a cubic spline wit mixed-type boundary constraints is processed. Assume a set of $m+1$ data points (x_i, y_i) b given:

x	x_0	x_1	$\cdots$	x_m
y	y_0	y_1	$\cdots$	y_m

. (3.1

Consider the following problem: *construct a cubic spline* $S(x)$ *to minimize the expression*

$$E=\sum_{i=0}^{m}\omega_i\left[S(x_i)-y_i\right]^2. \qquad (3.2$$

Here the quantities $\omega_i>0$ are the weights assigned. The value of the expression (3.2) depends on th quantities $v_0, v_1, \cdots, v_n$:.

$$E(v_0,v_1,\ldots,v_n)=\sum_{i=0}^{m}\omega_i\left[S(x_i)-y_i\right]^2. \qquad (3.3$$

As a result, the problem (3.2) takes the following form: *find the quantities* $v_0^*, v_1^*, \ldots, v_n^*$ *such tha*

$$E(v_0^*,v_1^*,\ldots,v_n^*)=\min_{v_0,v_1,\ldots,v_n}E(v_0,v_1,\ldots,v_n). \qquad (3.4$$

The construction of the cubic spline consists of several steps.

Step 1. Definition of quantities M_k, $k=0,1,\ldots,n$.

Cases $n\geq 3$, $n=2$ and $n=1$ are discussed separately.

Case $n\geq 3$

Certainly, we can define the mentioned quantities $M_1, M_2, \ldots, M_{n-1}$ by solving the syste with triadiagonal matrix (2.12). But it is more appropriate to find H^{-1} matrix and get th formula of M as

$$M=H^{-1}g. \qquad (3.5$$

For this, we can get the elements $[\theta_{ij}]_{i,j=1}^{n-1}$ of the matrix H^{-1} by using the method suggested [8]. For $k=1,2,\ldots,n-1$, having in view the equalities (2.17) − (2.19), from (3.5) we get:

$$M_k=\sum_{j=1}^{n-1}\theta_{kj}g_j=\theta_{k1}g_1+\sum_{j=2}^{n-2}\theta_{kj}g_j+\theta_{kn-1}g_{n-1}=$$

$$\theta_{k1}\left[6\left(\frac{v_2-v_1}{h_1}-\frac{v_1-v_0}{h_0}\right)-\frac{3h_0}{3\alpha_1-\alpha_2 h_0}\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right)\right]+$$

$$\sum_{j=2}^{n-2}\theta_{kj}\left[6\left(\frac{v_{j+1}-v_j}{h_j}-\frac{v_j-v_{j-1}}{h_{j-1}}\right)\right]+$$

$$\theta_{kn-1}\left[6\left(\frac{v_n-v_{n-1}}{h_{n-1}}-\frac{v_{n-1}-v_{n-2}}{h_{n-2}}\right)-\frac{3h_{n-1}}{3\beta_1+\beta_2 h_{n-1}}\left(d_b-\beta_2\frac{v_n-v_{n-1}}{h_{n-1}}\right)\right]=$$

$$-\theta_{k1}\frac{3h_0}{3\alpha_1-\alpha_2 h_0}\left(d_a-\alpha_2\frac{v_1-v_0}{h_0}\right)-\theta_{kn-1}\frac{3h_{n-1}}{3\beta_1+\beta_2 h_{n-1}}\left(d_b-\beta_2\frac{v_n-v_{n-1}}{h_{n-1}}\right)+$$

$$\sum_{j=1}^{n-1}6\theta_{kj}\left(\frac{v_{j+1}-v_j}{h_j}-\frac{v_j-v_{j-1}}{h_{j-1}}\right).$$

After grouping by quantities v_j, we get:

$$M_k=\sum_{j=0}^{n}\gamma_{kj}v_j+\sigma_k,\quad k=1,2,\dots,n-1, \tag{3.6}$$

where

$$\gamma_{k0}=3\left(\frac{2}{h_0}-\frac{\alpha_2}{3\alpha_1-\alpha_2 h_0}\right)\theta_{k1},$$

$$\gamma_{k1}=3\left(-\frac{2}{h_0}-\frac{2}{h_1}+\frac{\alpha_2}{3\alpha_1-\alpha_2 h_0}\right)\theta_{k1}+\frac{6}{h_1}\theta_{k2}=-\gamma_{k0}+\frac{6}{h_1}(\theta_{k2}-\theta_{k1}),$$

$$\gamma_{kj}=6\left(\frac{1}{h_{j-1}}\theta_{kj-1}-\left(\frac{1}{h_{j-1}}+\frac{1}{h_j}\right)\theta_{kj}+\frac{1}{h_j}\theta_{kj+1}\right),\qquad j=2,3,\dots,n-2,$$

$$\gamma_{kn}=3\left(\frac{2}{h_{n-1}}+\frac{\beta_2}{3\beta_1+\beta_2 h_{n-1}}\right)\theta_{kn-1}, \tag{3.7}$$

$$\gamma_{kn-1}=-3\left(\frac{2}{h_{n-1}}+\frac{2}{h_{n-2}}+\frac{\beta_2}{3\beta_1+\beta_2 h_{n-1}}\right)\theta_{kn-1}+\frac{6}{h_{n-2}}\theta_{kn-2}=-\gamma_{kn}+\frac{6}{h_{n-2}}(\theta_{kn-2}-\theta_{kn-1}),$$

$$\sigma_k=-3\left(\frac{h_0 d_a}{3\alpha_1-\alpha_2 h_0}\theta_{k1}+\frac{h_{n-1}d_b}{3\beta_1+\beta_2 h_{n-1}}\theta_{kn-1}\right).$$

Let us get similar expressions for M_0 and M_n. Substituting into (2.20) the expression for from (3.6) and after some rearrangement we get:

$$M_0=\sum_{j=0}^{n}\gamma_{0j}v_j+\sigma_0, \tag{3.8}$$

where

$$\gamma_{00} = \frac{\alpha_2}{3\alpha_1 - \alpha_2 h_0}\left(\frac{3}{h_0} + \frac{h_0}{2}\gamma_{10}\right),$$
$$\gamma_{01} = \frac{\alpha_2}{3\alpha_1 - \alpha_2 h_0}\left(-\frac{3}{h_0} + \frac{h_0}{2}\gamma_{11}\right),$$
$$\gamma_{0j} = \frac{\alpha_2 h_0}{2(3\alpha_1 - \alpha_2 h_0)}\gamma_{1j}, \quad j = 2,3,\ldots,n, \tag{3.9}$$
$$\sigma_0 = \frac{1}{3\alpha_1 - \alpha_2 h_0}\left(3d_a + \frac{\alpha_2 h_0}{2}\sigma_1\right).$$

Similarly, from the formula (2.21) we get:

$$M_n = \sum_{j=0}^{n}\gamma_{nj}v_j + \sigma_n, \tag{3.10}$$

where

$$\gamma_{nj} = -\frac{\beta_2 h_{n-1}}{2(3\beta_1 + \beta_2 h_{n-1})}\gamma_{n-1j}, \quad j = 0,1,\ldots,n-2,$$
$$\gamma_{n\,n-1} = \frac{\beta_2}{3\beta_1 + \beta_2 h_{n-1}}\left(\frac{3}{h_{n-1}} - \frac{h_{n-1}}{2}\gamma_{n-1\,n-1}\right),$$
$$\gamma_{nn} = -\frac{\beta_2}{3\beta_1 + \beta_2 h_{n-1}}\left(\frac{3}{h_{n-1}} + \frac{h_{n-1}}{2}\gamma_{n-1\,n}\right), \tag{3.11}$$
$$\sigma_n = \frac{1}{3\beta_1 + \beta_2 h_{n-1}}\left(3d_b - \frac{\beta_2 h_{n-1}}{2}\sigma_{n-1}\right).$$

After inputting the vectors

$$\hat{M} = [M_0\ M_1 \cdots M_{n-1}\ M_n]^T, \qquad v = [v_0\ v_1\ v_{n-1}\ v_n]^T \tag{3.12}$$

and summing up the expressions (3.6), (3.8) and (3.10), we can write:

$$\hat{M} = \Gamma v + \sigma, \tag{3.13}$$

where

$$\Gamma = \begin{bmatrix} \gamma_{00} & \gamma_{01} & \cdots & \gamma_{0n-1} & \gamma_{0n} \\ \gamma_{10} & \gamma_{11} & \cdots & \gamma_{1n-1} & \gamma_{1n} \\ \vdots & \vdots & & \vdots & \vdots \\ \gamma_{n-10} & \gamma_{n-11} & \cdots & \gamma_{n-1n-1} & \gamma_{n-1n} \\ \gamma_{n0} & \gamma_{n1} & \cdots & \gamma_{nn-1} & \gamma_{nn} \end{bmatrix}, \quad \sigma = \begin{bmatrix} \sigma_0 \\ \sigma_1 \\ \vdots \\ \sigma_{n-1} \\ \sigma_n \end{bmatrix}. \tag{3.14}$$

Case $n = 2$

In this case, we have quantities M_0, M_1 and M_2. From the equality (2.23) we have:

$$M_1 = \frac{g_1}{d_1}. \tag{3.15}$$

Let us substitute the expression (2.25) instead of g_1. Now we can rearrange and regroup th equality (3.15) as follows:

$$M_1 = \sum_{j=0}^{2}\gamma_{1j}v_j + \sigma_1, \tag{3.16}$$

where

$$\begin{aligned}
\gamma_{10} &= \frac{1}{d_1}\left(\frac{6}{h_0} - \frac{3\alpha_2}{3\alpha_1 - \alpha_2 h_0}\right),\\
\gamma_{11} &= \frac{3}{d_1}\left(-\frac{2}{h_0} - \frac{2}{h_1} + \frac{\alpha_2}{3\alpha_1 - \alpha_2 h_0} - \frac{\beta_2}{3\beta_1 + \beta_2 h_1}\right),\\
\gamma_{12} &= \frac{3}{d_1}\left(\frac{2}{h_1} + \frac{\beta_2}{3\beta_1 + \beta_2 h_1}\right),\\
\sigma_1 &= -\frac{3}{d_1}\left(\frac{h_0 d_a}{3\alpha_1 - \alpha_2 h_0} + \frac{3h_1 d_b}{3\beta_1 + \beta_2 h_1}\right).
\end{aligned} \tag{3.17}$$

Note that d_1 is defined in formula (2.24). Similar to the case $n \geq 3$, for the quantity M_0 we get:

$$M_0 = \sum_{j=0}^{2} \gamma_{0j} v_j + \sigma_0 . \tag{3.18}$$

Then inserting the expression (3.16) instead of M_1, from (2.22) yields

$$M_2 = \sum_{j=0}^{2} \gamma_{2j} v_j + \sigma_2 , \tag{3.19}$$

where

$$\begin{aligned}
\gamma_{20} &= -\frac{\beta_2 h_1}{2(3\beta_1 + \beta_2 h_1)}\gamma_{10},\\
\gamma_{21} &= \frac{\beta_2}{3\beta_1 + \beta_2 h_1}\left(\frac{3}{h_1} - \frac{h_1}{2}\gamma_{11}\right),\\
\gamma_{22} &= -\frac{\beta_2}{3\beta_1 + \beta_2 h_1}\left(\frac{3}{h_1} + \frac{h_1}{2}\gamma_{12}\right),\\
\sigma_2 &= \frac{1}{3\beta_1 + \beta_2 h_1}\left(3d_b - \frac{\beta_2 h_1}{2}\sigma_1\right).
\end{aligned} \tag{3.20}$$

Summing up (3.16), (3.18) and (3.19), we get the formula (3.13) for $n = 2$.

Case $n = 1$

From the expression (2.27) we have:

$$M_1 = \sum_{j=0}^{1} \gamma_{1j} v_j + \sigma_1 , \tag{3.21}$$

where

$$\begin{aligned}
\gamma_{10} &= \frac{6}{h_0} \cdot \frac{2\beta_2(3\alpha_1 - \alpha_2 h_0) - \alpha_2\beta_2 h_0}{4(3\alpha_1 - \alpha_2 h_0)(3\beta_1 + \beta_2 h_0) + \alpha_2\beta_2 h_0^2},\\
\gamma_{11} &= \frac{6}{h_0} \cdot \frac{-2\beta_2(3\alpha_1 - \alpha_2 h_0) + \alpha_2\beta_2 h_0}{4(3\alpha_1 - \alpha_2 h_0)(3\beta_1 + \beta_2 h_0) + \alpha_2\beta_2 h_0^2},\\
\sigma_1 &= 6\,\frac{2(3\alpha_1 - \alpha_2 h_0)d_b - \beta_2 h_0 d_a}{4(3\alpha_1 - \alpha_2 h_0)(3\beta_1 + \beta_2 h_0) + \alpha_2\beta_2 h_0^2}.
\end{aligned} \tag{3.22}$$

Similar to the case $n \geq 3$, for M_0 we have

$$M_0 = \sum_{j=0}^{0} \gamma_{0j} v_j + \sigma_0 . \qquad (3.23)$$

Summing up the expressions (3.21) and (3.23), we get the formula (3.13) for $n = 1$. Thus,

$$M_k = \sum_{j=0}^{n} \gamma_{kj} v_j + \sigma_k , \quad k = 1,2,\ldots,n-1, \qquad (3.24)$$

where the coefficients γ_{kj} and the quantities σ_k are defined in the corresponding formulae, depending on the value of n.

Step 2. Definition of the values $S(x_i)$, for $i = 0,1,\ldots,m$.

First let us obtain the formula for the value $S(\xi)$, $\xi \in [a,b]$ through the quantities $v_0, v_1, \ldots, v_n$. Assume $\xi \in [t_k, t_{k+1}]$, $0 \le k \le n-1$. In this case, from the expression (2.26) we have

$$S(\xi) = S_k(\xi) = v_k + \left(\frac{v_{k+1} - v_k}{h_k} - \frac{2M_k + M_{k+1}}{6} h_k \right)(\xi - t_k) + \frac{M_k}{2}(\xi - t_k)^2 + \frac{M_{k+1} - M_k}{6h_k}(\xi - t_k)^3 \qquad (3.25)$$

(see also the formulae (2.26) and (2.28)). After substituting the expression (3.24) instead of M_k, we get:

$$S(\xi) = \sum_{j=0}^{n} \mu_{kj}(\xi) v_j + \delta_k(\xi) . \qquad (3.26)$$

Let

$$\hat{\mu}_{kj}(\xi) = \frac{\xi - t_k}{6h_k}\left[\left(-2h_k^2 + 3h_k(\xi - t_k) - (\xi - t_k)^2\right)\gamma_{kj} + \left(-h_k^2 + (\xi - t_k)^2\right)\gamma_{k+1j}\right], \qquad (3.27)$$

for $j = 0,1,\ldots,n$. Then, define the following quantities:

$$\mu_{kj}(\xi) = \hat{\mu}_{kj}(\xi), \quad j \ne k, k+1, \qquad (3.28)$$

$$\mu_{kk}(\xi) = \hat{\mu}_{kk}(\xi) + 1 - \frac{\xi - t_k}{h_k}, \qquad (3.29)$$

$$\mu_{kk+1}(\xi) = \hat{\mu}_{kk+1}(\xi) + \frac{\xi - t_k}{h_k}, \qquad (3.30)$$

$$\delta_k(\xi) = \frac{\xi - t_k}{6h_k}\left[\left(-2h_k^2 + 3h_k(\xi - t_k) - (\xi - t_k)^2\right)\sigma_k + \left(-h_k^2 + (\xi - t_k)^2\right)\sigma_{k+1}\right]. \qquad (3.31)$$

For each data point x_i, $i = 0,1,\ldots,m$, after determining the segment $[t_k, t_{k+1}]$ the point belongs to, from (3.26) we have:

$$S(x_i) = \sum_{j=0}^{n} a_{ij} v_j + \rho_i , \qquad (3.32)$$

where

$$a_{ij} = \mu_{kj}(x_i), \quad i = 0,1,\ldots,m, \quad j = 0,1,\ldots,n , \qquad (3.33)$$

$$\rho_i = \delta_k(x_i), \quad i = 0,1,\ldots,m . \qquad (3.34)$$

Let us introduce the vectors

$$S = [S(x_0)\ S(x_1) \cdots S(x_m)]^T, \quad v = [v_0\ v_1 \cdots v_n]^T . \qquad (3.35)$$

From (3.32) we have:

$$S = Av + \rho , \qquad (3.36)$$

where

$$A=\begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0n} \\ a_{10} & a_{11} & \cdots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m0} & a_{m1} & \cdots & a_{mn} \end{bmatrix}, \quad \rho=\begin{bmatrix} \rho_0 \\ \rho_1 \\ \vdots \\ \rho_m \end{bmatrix}. \tag{3.37}$$

Step 3. Definition of the quantities $v_0, v_1, \dots, v_n$.

We have already found the expressions of the spline $S(x_i)$ in the form of equation (3.32) depending on the quantities $v_0, v_1, \dots, v_n$. Substituting these expressions into minimand (3.3) yields

$$E(v_0,v_1,\dots,v_n)=\sum_{i=0}^{m}\omega_i[S(x_i)-y_i]^2=\sum_{i=0}^{m}\omega_i\left[\sum_{j=0}^{n}a_{ij}v_j+\rho_i-y_i\right]^2=$$

$$\sum_{i=0}^{m}\omega_i\left[\sum_{j,l=0}^{n}a_{ij}a_{il}v_jv_l-2\sum_{j=0}^{n}a_{ij}(y_i-\rho_i)v_j+(y_i-\rho_i)^2\right]=$$

$$\sum_{j,l=0}^{n}\left(\sum_{i=0}^{m}a_{ij}\omega_ia_{il}\right)v_jv_l-2\sum_{j=0}^{n}\left(\sum_{i=0}^{m}a_{ij}\omega_i(y_i-\rho_i)\right)v_j+\sum_{i=0}^{m}\omega_i(y_i-\rho_i)^2.$$

By taking partial derivatives of E equal to zero, we get a system of linear algebraic equations (*normal system*):

$$\sum_{l=0}^{n}\left(\sum_{i=0}^{m}a_{ij}\omega_ia_{il}\right)v_l=\sum_{i=0}^{m}a_{ij}\omega_i(y_i-\rho_i), \quad j=0,1,\dots,n. \tag{3.38}$$

After inserting a diagonal matrix

$$\Omega=\begin{bmatrix} \omega_0 & & & \\ & \omega_1 & 0 & \\ & 0 & \ddots & \\ & & & \omega_m \end{bmatrix}$$

and a vector of the data

$$y=[y_0\ y_1\ \cdots\ y_m]^T,$$

we can write the normal system (3.38) in the form

$$A^T\Omega Av=A^T\Omega(y-\rho), \tag{3.39}$$

where the matrix A is defined in (3.37), while the vectors v and ρ are defined in (3.35) and (3.37), respectively.

Let us sum up the steps above. By solving the normal system (3.39), we get the optimal values $v_0^*, v_1^*, \dots, v_n^*$ of the quantities $v_0, v_1, \cdots, v_n$, which are solutions of (3.4). Then the cubic spline $S(x)$ is constructed by the method, given in Section 2.

Finally, let us define some properties of the matrix $A^T\Omega A$, particularly, the conditions of being a nonsingular matrix.

For any vector v, we have:

$$(A^T\Omega Av,v)=(\Omega Av,Av)=\sum_{i=0}^{m}\omega_i\left(\sum_{j=0}^{n}a_{ij}v_j\right)^2. \tag{3.40}$$

Hence,

$$(A^T\Omega A v, v) \ge 0 \quad \forall v.$$

The latter means that $A^T\Omega A$ is a positive semidefinite matrix.

Under some additional conditions, $A^T\Omega A$ becomes a positive definite matrix.

Condition 3.1: Assume $m > 3n$ *and partitioning (2.1) of the segment* $[a,b]$ *is such that each interval* (t_k, t_{k+1}), $0 \le k \le n-1$ *includes at least three points from data (3.1).*

Theorem 3.1: If condition 3.1 is satisfied then $A^T\Omega A$ is a positive definite matrix.

Proof. Consider the following intervals of partitioning (2.1):

$$\Delta_0 = [t_0, t_1),\ \Delta_1 = [t_1, t_2), \dots, \Delta_{n-2} = [t_{n-2}, t_{n-1}),\ \Delta_{n-1} = [t_{n-1}, t_n].$$

Having in view the notation (3.33), the equality (3.40) can be rewritten as follows:

$$(A^T\Omega A v, v) = \sum_{x_i \in \Delta_0} \omega_i \left(\sum_{j=0}^{n} \mu_{0j}(x_i) v_j \right)^2 + \sum_{x_i \in \Delta_1} \omega_i \left(\sum_{j=0}^{n} \mu_{1j}(x_i) v_j \right)^2 + \dots + \sum_{x_i \in \Delta_{n-1}} \omega_i \left(\sum_{j=0}^{n} \mu_{n-1,j}(x_i) v_j \right)^2 =$$

$$= \sum_{k=0}^{n-1} \sum_{x_i \in \Delta_k} \omega_i \left(\sum_{j=0}^{n} \mu_{kj}(x_i) v_j \right)^2.$$

Let

$$B_k(x) = \sum_{j=0}^{n} \mu_{kj}(x) v_j, \quad x \in [t_k, t_{k+1}], \quad k = 0,1,\dots n-1 \tag{3.41}$$

As follows from (3.27) ÷ (3.30), the function $B_k(x)$ is a cubic polynomial and

$$B_k(t_k) = v_k, \quad B_k(t_{k+1}) = v_{k+1}. \tag{3.42}$$

Thus,

$$(A^T\Omega A v, v) = \sum_{k=0}^{n-1} \sum_{x_i \in \Delta_k} \omega_i B_k^2(x_i). \tag{3.43}$$

Assume $v = [v_0\ v_1 \cdots v_n]^T \ne 0$. Now let us discuss two possible cases.

a) The vector v has a zero component. In this case, there exists a segment $[t_m, t_{m+1}]$, $0 \le m \le n-1$ such that $v_m = 0, v_{m+1} \ne 0$ or $v_m \ne 0, v_{m+1} = 0$. Since $B_m(x)$ is a cubic polynomial with the property (3.42), it can have no more than two roots in (t_m, t_{m+1}). Thus, from the condition 3.1 we get:

$$\sum_{x_i \in \Delta_m} \omega_i B_m^2(x_i) > 0,$$

and from (3.43) we can write, that $(A^T\Omega A v, v) > 0$.

b) The vector v does not have a zero component. In this case the polynomial $B_k(x)$ can have no more than three roots in (t_k, t_{k+1}). Since $m > 3n$ (condition 3.1), then from (3.43) obviously follows that $(A^T\Omega A v, v) > 0$.

The theorem is proved.

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Խորանարդային սպլայններով մոտարկումը փոքրագույն քառակուսիների մեթոդով

Մ. Խաչատրյան

Ամփոփում

ոդվածում դիտարկվում է փորձարարական տվյալների մոտարկումը խորանարդային լայններով՝ փոքրագույն քառակուսիների մեթոդով: Արտածվում է խառը տիպի եզրային մանափակումներով խորանարդային սպլայնների կառուցման ալգորիթմը:

ппроксимация кубическими сплайнами по методу наименьших квадратов

М. Хачатрян

Аннотация

В статье рассматривается аппроксимация экспериментальных данных методом еньших квадратов с помощью кубических сплайнов. Выводится алгоритм построения рполяционных кубических сплайнов с краевыми ограничениями смешанного типа.