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QUADRATIC SPLINES SMOOTHING THE FIRST DERIVATIVES

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Summary. The extremal property of quadratic splines interpolating the first derivatives is proved. Quadratic spline smoothing the given values of the first derivative, depending on the knot weights w_i and smoothing parameter α, is then studied. The algorithm for computing appropriate parameters of such splines is given and the dependence on the smoothing parameter α is mentioned.

Keywords: splines, quadratic splines, smoothing splines

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1. Introduction

Given knots $(\Delta x) = \{x_i,\ i = 0(1)n+1\}$ of a polynomial spline with prescribed function values $\{g_i\}$, algorithms for computing appropriate parameters of such an interpolating spline as well as answers concerning the questions of existence and various properties of such splines can be found in [1], [2], [3], [9]. The extremal property of polynomial splines of an odd degree $2m-1$ with respect to the functional

$$J(f) = \int_a^b [f^{(m)}]^2 \mathrm{d}x$$

was used to introduce splines smoothing function values, see e.g. [2], [6], [9].

Interpolary splines of an even degree $2m$ does not possess such extremal property with respect to the functional of the above type—even if we interpolate at other points than knots. Such an extremal property can be found, when we interpolate some other appropriate functional instead of the function values. The best known example is the interpolation of mean values on $[x_i, x_{i+1}]$ (or local integrals)—see e.g. [2], [6], [9]. The case of the quadratic spline interpolating mean values (local integrals) is studied in detail in [5]; the extremal property is there used to introduce the quadratic spline smoothing mean values.

In this paper, the results from [4] concerning splines interpolating the first derivatives are used to show that they have a certain extremal property with respect to the functional

$$J(f) = \int_a^b [f'']^2 \mathrm{d}x.$$

This result is used to construct the quadratic spline smoothing the given values of the first derivative.

2. Quadratic spline interpolating the first derivatives

Definition 1. Let us have a set of simple knots (Δx) on $[a, b]$:

$$a = x_0 < x_1 < \ldots < x_n < x_{n+1} = b, \quad h_i = x_{i+1} - x_i.$$

Any function $s(x)$ with the properties

1° $s(x) \in C^1[a, b]$;

2° $s(x)$ is a quadratic polynomial in each interval $[x_i, x_{i+1}]$, $i = 0(1)n$,

is called a quadratic spline on (Δx). Let us denote by $\mathscr{S}(2, \Delta x)$ the linear space of all quadratic splines on (Δx).

Theorem 1 (see [4], [7]). *Let us have a mesh (Δx) and real numbers s_i', $i = 0(1)n + 1$, and one number s_k, $k \in \{0, 1, \ldots, n+1\}$. Then there exists a unique quadratic spline $s \in \mathscr{S}(2, \Delta x)$ such that the conditions*

$$(1) \qquad \begin{aligned} &s'(x_i) = s_i', \quad i = 0(1)n+1 \quad \textit{(conditions of interpolation)},\\ &s(x_k) = s_k \qquad\qquad\qquad\qquad\qquad \textit{(initial condition)} \end{aligned}$$

are fulfilled. Denoting $s_i = s(x_i)$, $t = \dfrac{x - x_i}{h_i}$, we can write

$$(2) \qquad s(x) = (1 - t^2)s_i + t^2 s_{i+1} + h_i t(1-t)s_i' \quad \textit{for } x \in [x_i, x_{i+1}],$$

where the unknown values s_i can be computed from the given s_k, s_i', $i = 0(1)n + 1$ via the recurrence relations

$$(3) \qquad s_i - s_{i-1} = \frac{1}{2} h_{i-1}(s_{i-1}' + s_i'), \quad i = 1(1)n + 1.$$

Example 1. For the data (x_i, m_i), $s_0 = 0$,

x_i	−4	−3	−2	−1	0	1	2	3	4	5	6
m_i	1.0	−0.5	−0.1	−0.8	0.0	7.0	−0.1	−0.1	−0.1	2.0	1.0

the corresponding spline $s \in \mathscr{S}(2, \Delta x)$ is given in Fig. 1.

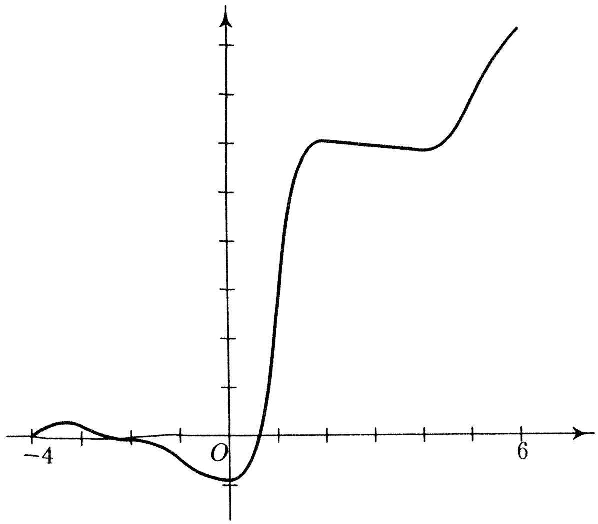

Fig. 1

3. Extremal property

Denote by $W_2^2(\Delta x)$ the linear space of functions f with an absolutely continuous derivative f' on every interval $[x_i, x_{i+1}]$, $i = 0(1)n$, and $f'' \in L^2[a, b]$.

Theorem 2. *Let* $\mathscr{V} = \{f \in W_2^2(\Delta x);\, f'(x_i) = m_i,\ i = 0(1)n+1\}$,

$$J_1(f) = \int_a^b [f''(x)]^2 \mathrm{d}x \qquad (a = x_0,\ b = x_{n+1}). \tag{4}$$

The minimal value of $J_1(f)$ *on the set* $\mathscr{V}$ *is attained for every quadratic spline* $s \in \mathscr{S}(2, \Delta x)$ *with* $s'(x_i) = m_i$, $i = 0(1)n+1$.

Proof. Let f, $s \in \mathscr{V}$, $s \in \mathscr{S}(2, \Delta x)$ and $s'(x_i) = m_i$, $i = 0(1)n+1$. Then

$$\|f'' - s''\|_2^2 = \|f''\|_2^2 - \|s''\|_2^2 - 2(f'' - s'', s'')_2; \tag{5}$$

$$(f'' - s'', s'')_2 = \int_{x_0}^{x_{n+1}} (f'' - s'')s'' \mathrm{d}x = \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} (f'' - s'')s'' \mathrm{d}x =$$

$$= \sum_{i=0}^{n} \left([(f' - s')s'']_{x_i}^{x_{i+1}} - \int_{x_i}^{x_{i+1}} (f' - s')s''' \mathrm{d}x \right) = 0.$$

We can write (5) as

$$\|s''\|_2^2 + \|f'' - s''\|_2^2 = \|f''\|_2^2, \tag{6}$$

from which $\|s''\|_2 \leqslant \|f''\|_2$ follows. □

Let us mention that the extremal spline is not unique—we can add any constant to it (to prescribe any initial condition).

Remark 1. The extremal property just proved is tightly connected to the extremal property of the polygon $s_1(x)$ interpolating the values m_i at x_i $[s_1(x_i) = m_i]$. It is proved in [8], that $s_1(x)$ minimizes the functional $(f', f')_2$ on the set

$$\mathscr{V} = \{f \in W_2^1(\Delta x)\,;\, f(x_i) = m_i,\ i = 0(1)n+1\}.$$

We have $s(x) = \int s_1(x)\,\mathrm{d}x$ in our case.

Remark 2. The extremal property does not hold for splines interpolating the first derivatives at points $t_i \in (x_i, x_{i+1})$—such splines are described in [4], [7].

4. The problem of smoothing the first derivatives

Suppose a set (Δx) of spline knots with weighting parameters $w_i > 0$ and real numbers m_i, $i = 0(1)n+1$, are given. For $f \in W_2^2(\Delta x)$ and a regulating parameter $\alpha > 0$ let us define the functional

$$J_2(f) = \alpha \int_a^b [f''(x)]^2 \mathrm{d}x + \sum_{i=0}^{n+1} w_i [f'(x_i) - m_i]^2. \tag{7}$$

The first part of $J_2(f)$ measures the "mean curvature" of $f(x)$ balanced by the parameter α, the second part the least squares deviation of $f'(x_i)$ from m_i, weighted by the parameters w_i. The function minimizing $J_2(f)$ will represent a certain compromise between straightness and least squares approximation of m_i, balanced by the parameters α, w_i.

Theorem 3. *Let a set of knots (Δx) and parameters α, m_i, $w_i > 0$, $i = 0(1)n+1$ be given.*

Then the functional $J_2(f)$ attains its minimum on $W_2^2(\Delta x)$ for some quadratic spline $s \in \mathscr{S}(2, \Delta x)$.

Proof. Suppose that $J_2(f)$ is minimized on $W_2^2(\Delta x)$ by some $g \in W_2^2(\Delta x)$; let us denote $g'_i = g'(x_i)$. Then for each $s \in \mathscr{S}(2, \Delta x)$ with $s'(x_i) = g'_i$ we have

$$S = \sum_{i=0}^{n+1} w_i (g'_i - m_i)^2 = \sum_{i=0}^{n+1} w_i [s'(x_i) - m_i]^2.$$

The second part of $J_2(f)$ thus takes for g, s the same value S. However, according to (6) and Theorem 2,

$$\int_a^b [s''(x)]^2 \mathrm{d}x \leqslant \int_a^b [g''(x)]^2 \mathrm{d}x \quad \text{for any } g \in W_2^2(\Delta x).$$

This implies $J_2(s) \leqslant J_2(g)$ and proves the theorem. □

Definition 2. A spline $s \in \mathscr{S}(2, \Delta x)$ minimizing $J_2(f)$ is called a quadratic spline smoothing the given first derivatives on (Δx).

Remark. When the parameters α, w_i are not prescribed, we can choose them to achieve some other appropriate properties of $s(x)$.

5. Computation of the parameters of the smoothing spline

Given a knot mesh (Δx), numbers m_i, $w_i > 0$, $i = 0(1)n+1$, and $\alpha > 0$, let us denote by $s_i = s(x_i)$, $s_i' = s'(x_i)$, $i = 0(1)n+1$ the parameters of the spline $s \in \mathscr{S}(2, \Delta x)$ which minimizes $J_2(f)$. The parameters s_i, s_i' are coupled together by the relations (3); $s(x)$ can be then described using the representation (2). For the second derivative we have

$$s''(x) = \frac{s_{i+1}' - s_i'}{h_i} = s_i'' \quad \text{for } x \in (x_i, x_{i+1}). \tag{8}$$

Denote $s' = [s_0', \ldots, s_{n+1}']^T$; then we can write

$$\begin{aligned} J_2(s) &= \alpha \int_a^b [s''(x)]^2 \mathrm{d}x + \sum_{i=0}^{n+1} w_i (s_i' - m_i)^2 = \\ &= \alpha \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} [s''(x)]^2 \mathrm{d}x + \sum_{i=0}^{n+1} w_i (s_i' - m_i)^2 = \\ &= \alpha \sum_{i=0}^{n} \frac{1}{h_i} [s_{i+1}' - s_i']^2 + \sum_{i=0}^{n+1} w_i [s_i' - m_i]^2 = F(s'). \end{aligned} \tag{9}$$

Necessary conditions for s' to minimize $F(s')$ are

$$\begin{gathered} \left[\frac{\partial F}{\partial s_0'}\right] = \frac{-2\alpha(s_1' - s_0')}{h_0} + 2w_0(s_0' - m_0) = 0, \\ \left[\frac{\partial F}{\partial s_k'}\right] = \frac{-2\alpha(s_{k+1}' - s_k')}{h_k} + \frac{2\alpha(s_k' - s_{k-1}')}{h_{k-1}} + 2w_k(s_k' - m_k) = 0, \quad k = 1(1)n, \\ \left[\frac{\partial F}{\partial s_{n+1}'}\right] = \frac{2\alpha(s_{n+1}' - s_n')}{h_n} + 2w_{n+1}(s_{n+1}' - m_{n+1}) = 0. \end{gathered} \tag{10}$$

Rearranging them, we obtain a tridiagonal system of equations (with $p_i = \dfrac{\alpha}{h_i}$, $i = 0(1)n$)

$$\begin{gathered} [w_0 + p_0]s_0' - p_0 s_1' = w_0 m_0 \\ -p_{k-1}s_{k-1}' + [w_k + (p_{k-1} + p_k)]s_k' - p_k s_{k+1}' = w_k m_k, \quad k = 1(1)n, \\ -p_n s_n' + (p_n + w_{n+1})s_{n+1}' = w_{n+1} m_{n+1} \end{gathered} \tag{11}$$

for the unknown values s'_i, $i = 0(1)n+1$. The matrix of this system is diagonally dominant and thus regular.

Theorem 4. *Given a knot set (Δx), numbers m_i, $w_i > 0$, $i = 0(1)n+1$, and $\alpha > 0$, then there exists a unique solution s' of the system (11). Choosing one index $k \in \{0, \ldots, n+1\}$ and a number $s_k = s(x_k)$ arbitrarily, we can uniquely determine the values s_j, $j \neq k$ using the recurrence relation (3).*

The corresponding smoothing spline $s \in \mathscr{S}(2, \Delta x)$ can be then written in the form (2).

Remark 1. The value of $J_2(s)$ depends also on the chosen value of $\alpha > 0$. If this value is not prescribed, we can search for its optimal value via the minimization of J_2 using known minimization algorithms.

Remark 2. It can be seen from the coefficients of the system (11) that with $\alpha \to 0+$ the smoothing spline tends to be the spline interpolating the values of the derivatives m_i (e.g. $s'(x_i) \to m_i$); with $\alpha \to \infty$ the spline $s(x)$ tends to the straight line with

$$s'_i = \text{const} = \Big(\sum_{i=0}^{n+1} w_i\Big)^{-1} \sum_{i=0}^{n+1} w_i m_i$$

(the weighted arithmetic mean). This follows from (11) [when we sum all equations] and from the fact of minimization of the functional $J_2(s)$.

Remark 3. It is possible to place the regulating parameter α into the second part of the functional. When we define (as some authors do) the functional

$$J_3(f) = \int_a^b [f''(x)]^2 \mathrm{d}x + \alpha \sum_{i=0}^{n+1} w_i [f'(x_i) - m_i]^2,$$

then in the same way as before we obtain for the parameters s'_i of the minimizing spline a system of equations

$$\begin{aligned} (p_0 + \alpha w_0)s'_0 - p_0 s'_1 &= \alpha w_0 m_0, \quad p_i = \frac{1}{h_i}, \\ -p_{k-1}s'_{k-1} + (p_{k-1} + p_k + \alpha w_k)s'_k - p_k s'_{k+1} &= \alpha w_k m_k, \quad k = 1(1)n, \\ -p_n s'_n + (p_n + \alpha w_{n+1})s'_{n+1} &= \alpha w_{n+1} m_{n+1}. \end{aligned} \tag{12}$$

The two limiting cases from Remark 2 will interchange their places now.

De Boor in [2] uses (more suitably from the computational point of view, when we want to minimize J_3 with respect to α) the regualating parameter α in the form of a convex combination

$$J_4(f) = \alpha \int_a^b [f''(x)]^2 \mathrm{d}x + (1 - \alpha) \sum_{i=0}^{n+1} w_i [f'(x_i) - m_i]^2.$$

In that case the system for the required parameters s_i' reads

$$\begin{aligned} (13) \qquad & [p_0 + (1-\alpha)w_0]s_0' - p_0 s_1' = (1-\alpha)w_0 m_0, \quad p_i = \frac{\alpha}{h_i}, \\ -p_{k-1}s_{k-1}' + {} & [p_{k-1} + p_k + (1-\alpha)w_k]s_k' - p_k s_{k+1}' = (1-\alpha)w_k m_k, \quad k = 1(1)n, \\ & -p_n s_n' + [p_n + (1-\alpha)w_{n+1}]s_{n+1}' = (1-\alpha)w_{n+1}m_{n+1}. \end{aligned}$$

Example 2. For the data (x_i, m_i) from Example 1 with weighting coefficients $w_i = 1$ and $\alpha = 0,\ 2,\ 20,\ 10^6$ the corresponding smoothing splines are plotted in Fig. 2.

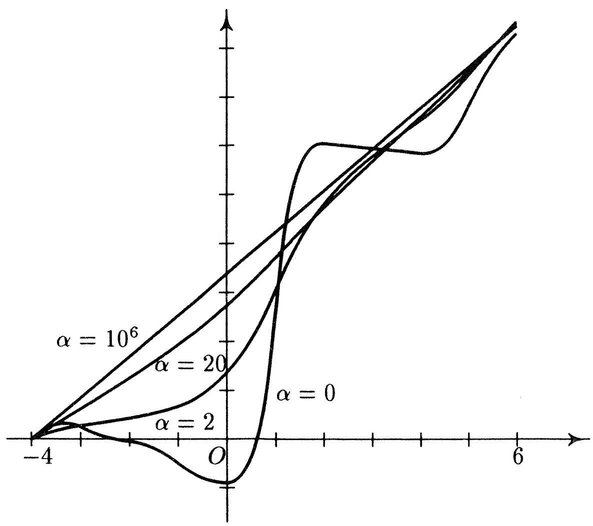

Fig. 2

References

[1] *Ahlberg J.H., Nilson E.N., Walsh J.L.*: The Theory of Splines and Their Aplications, Academic Press, N.Y., 1967.

[2] *de Boor C.*: A Practical Guide to Splines, Springer Verlag, N.Y., 1978.

[3] *Kobza J.*: An algorithm for parabolic splines, Acta UPO, FRN *88* (1987), 169–185.

[4] *Kobza J.*: Quadratic splines interpolating the first derivatives, Acta UPO, FRN *100* (1991), 219–233.

[5] *Kobza J. and Zápalka D.*: Natural and smoothing quadratic spline, Applications of Mathematics *36* no. 3 (1991), 187–204.

[6] *Laurent P.-J.*: Approximation et Optimization, Hermann, Paris, 1972.

[7] *Sallam S. and Tarazi M.N.*: Quadratic spline interpolation on uniform meshes, In Splines in Numerical Analysis (Schmidt J.W., Spaeth H., eds.), Akademie-Verlag, Berlin, 1989, pp. 145–150.

[8] *Schultz M.*: Spline Analysis, Prentice-Hall, Englewood Cliffs, N.Y., 1973.
[9] *Vasilenko V.A.*: Spline Functions: Theory, Algorithms, Programs, Nauka, SO, Novosibirsk, 1983. (In Russian.)

Souhrn

KVADRATICKÉ SPLAJNY VYHLAZUJÍCÍ PRVNÍ DERIVACE

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V práci je dokázána jistá extremální vlastnost kvadratických splajnů interpolujících zadané hodnoty prvních derivací (Věta 1). Pak je definován splajn vyhlazující zadané hodnoty derivací pomocí funkcionálu $J_2(f)$ s parametrem α a váhovými koeficienty w_i (Věta 3, Definice 2). Je odvozen algoritmus výpočtu parametrů vyhlazujícího splajnu (Věta 4).

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