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FUNDAMENTAL QUADRATIC SPLINES AND APPLICATIONS

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Abstract

The paper deals with quadratic splines interpolating function values, first derivative values and with splines smoothing first derivative values. For their representation we use the fundamental quadratic splines which form the basis of the space of the quadratic splines. We employ the fundamental quadratic splines for a discussion of the error propagation and for computation of values of the quadratic spline interpolating the first dertivative values.

Key words: spline function, quadratic spline, smoothing spline, fundamental spline, interpolation, error propagation.

MS Classification: 34A34

1 Introduction. Cubic spline

Let us have a set of knots

$$(\Delta x) = \{x_i : i = 0(1)n+1\}, \qquad a = x_0 < x_1 < \ldots < x_n < x_{n+1} = b.$$

Definition 1 A function $S_{kd}(x)$ is called a spline of order k with the defect d on the set of knots (Δx) if it has the following properties:

a) $S_{kd}(x)$ is a polynomial of degree k on every interval $[x_i, x_{i+1}]$, $i = 0(1)n$;

b) $S_{kd}(x) \in C^{k-d}[a, b]$.

Let us denote $\mathcal{S}_{kd}(\Delta x)$ linear space of the splines of order k with defect d on (Δx) with $\dim \mathcal{S}_{kd}(\Delta x) = k + dn + 1$.

These splines are studied for example in [1], [4]. In case $k = 3$, $d = 1$ we have the classical cubic spline $S_{31}(x) \in \mathcal{S}_{31}(\Delta x)$ which can be written on every interval $[x_i, x_{i+1}]$ by the help of the local parameters $s_i = S_{31}(x_i)$, $M_i = S_1''(x_i)$ as

$$(1) \quad S_{31}(x) = (1-q)s_i + qs_{i+1} - h_i^2 q(1-q)[(2-q)M_i + (1+q)M_{i+1}]/6,$$

where $h_i = x_{i+1} - x_i$, $q = (x - x_i)/h_i$, $i = 0(1)n$.

The continuity conditions yield the following relations between the parameters M_i, s_i

$$(2) \qquad c_i M_{i-1} + 2M_i + a_i M_{i+1} = d_i, \qquad i = 1(1)n$$

with

$$d_i = 3[(s_{i+1} - s_i)/h_i + (s_i + s_{i-1})/h_{i-1}]/(h_i + h_{i-1}),$$
$$a_i = h_i/(h_{i-1} + h_i), \quad c_i = 1 - a_i, \quad i = 1(1)n.$$

If we prescribe function values of the spline

$$S_{31}(x_i) = g_i, \qquad i = 0(1)n+1, \qquad \textit{(interpolating spline)}$$

and two boundary conditions, for example

$$M_0 = g_0'', \qquad M_{n+1} = g_{n+1}'',$$

with given values g_0'', g_{n+1}'', then the conditions (2) form a system of linear equations with the symmetric tridiagonal matrix with a dominating diagonal. The case of $M_0 = 0$, $M_{n+1} = 0$ is known as natural cubic spline.

There are the fundamental natural cubic splines studied in [4] too. These splines f_j are defined for $j = 0(1)n+1$ in this way:

$$f_j(x) \in \mathcal{S}_{31}(\Delta x), \quad f_j(x_i) = \delta_{ji}, \quad i = 0(1)n+1, \quad f_j''(a) = f_j''(b) = 0.$$

The local parameters of the splines $f_j(x)$ can be computed from (2). The natural interpolating cubic spline $S(x)$ can be written in form

$$S_{31}(x) = \sum_{i=0}^{n+1} g_i f_j(x).$$

We shall define fundamental quadratic splines of various types in analogous way in this paper.

2 Quadratic spline. Continuity conditions

If we choose $k = 2,\ d = 1$ in the Definition 1 we obtain the quadratic spline. So the quadratic spline $S(x) = S_{21}(x) \in \mathcal{S}_{21}(\Delta x)$ is the function with properties:

a) $S(x) = a_0^i + a_1^i x + a_2^i x^2, \quad x \in [x_i, x_{i+1}], \quad i = 0(1)n,$

b) $S(x) \in C^1[a, b]$.

Denote $h_i = x_{i+1} - x_i$, $s_i = S(x_i)$, $m_i = S'(x_i)$. The spline $S(x)$ can be written on $[x_i, x_{i+1}]$ as

$$S(x) = s_i + m_i(x - x_i) + (m_{i+1} - m_i)(x - x_i)^2/(2h_i), \tag{3}$$

and the continuity conditions in knots $x_i,\ i = 1(1)n + 1$ yield the following relations between the parameters m_i, s_i (see [3])

$$(m_{i-1} + m_i)/2 = (s_i - s_{i-1})/h_{i-1}, \qquad i = 1(1)n + 1. \tag{4}$$

3 Quadratic spline interpolating given function values

3.1 Formulation and solution of the problem.

Let us have real numbers $m_0, s_i,\ i = 0(1)n + 1$;
we search for a spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ with the properties

$$\begin{aligned} S(x_i) &= s_i, \qquad i = 1(1)n + 1, \\ S'(x_0) &= m_0. \end{aligned} \tag{5}$$

The local parameters $m_i = S'(x_i),\ i = 1(1)n + 1$ can be computed using the recurence relation (4) and function values of this spline we can find using the formula (3). From (3),(4) it follows also that the solution of the problem (5) exists and is unique.

3.2 Fundamental splines.

For the extended set of knots $(\Delta x) = \{x_i : i = -1(1)n + 1\}$ (for example $x_{-1} = x_0 - h_0$) we will construct a basis of the linear space $\mathcal{S}_{21}(\Delta x)$.

Definition 2 *Splines $\bar{H}(x), H_k(x) \in \mathcal{S}_{21}(\Delta x),\ k = 0(1)n + 1$ are called the f-fundamental splines if they have the following properties*

$$\begin{aligned} &H_k(x_i) = \delta_{ki}, \quad i = -1(1)n + 1, \quad H_k'(x_{k-1}) = 0, \\ &\bar{H}(x_i) = 0, \qquad i = -1(1)n + 1, \quad \bar{H}'(x_0) = 1. \end{aligned}$$

Because the extended set of knots is used we can describe all f-fundamental splines $H_k(x)$ by means of simple formulas. The graphs of $H_2(x)$, $\bar{H}(x)$ are plotted in Figure 1 ($h_i = h, n = 5$).

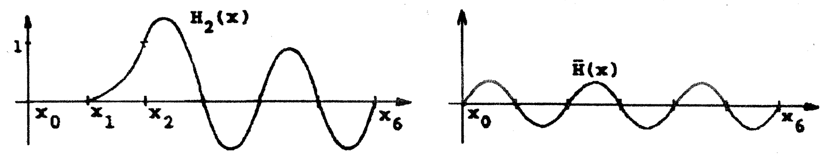

Fig. 1

Lemma 1 *The splines $\bar{H}(x), H_k(x)$, $k = 0(1)n+1$ can be written as*

$$\bar{H}(x) = (-1)^i (x - x_i)(x_{i+1} - x)/h_i, \qquad x_i \le x \le x_{i+1}, \qquad i = 0(1)n.$$

$$H_k(x) = \begin{cases} 0, & x \le x_{k-1}, \\ [(x - x_{k-1})/h_{k-1}]^2, & x_{k-1} \le x \le x_k, \\ (x_{k+1} - x)(x + x_{k+1} - 2x_k)/h_k^2 + 2(x - x_k)(x_{k+1} - x)/(h_k h_{k-1}), & \\ & x_k \le x \le x_{k+1}, \\ (-1)^{j-k}(h_k + h_{k-1})(x_{j+1} - x)(x - x_j)/(h_j h_k h_{k-1}), & \\ & x_j \le x \le x_{j+1}, \quad j = k+1(1)n. \end{cases}$$

Proof It follows from (4) and Definition 2 that

$$\begin{aligned} &H_k'(x_i) = 0, \qquad i = -1(1)k-1, \\ &H_k'(x_k) = 2/h_{k-1}, \\ &H_k'(x_i) = 2(-1)^{i-k}(h_k + h_{k-1})/(h_k h_{k-1}), \qquad i = k+1(1)n+1. \end{aligned}$$

By means of (3) we obtain the formulas for $H_k(x)$. The proof is analogical for $\bar{H}(x)$. □

Lemma 2 *The f-fundamental splines $\bar{H}(x)$, $H_0(x)$, $H_1(x), \ldots, H_{n+1}(x)$ form the basis of the linear space $S_{21}(\Delta x)$.*

Proof Because dim $\mathcal{S}_{21}(\Delta x) = n+3$ (see Def.1) we need to prove a linear independence of these splines only. Let us have

$$\sum_{k=0}^{n+1} a_k H_k(x) + a_{n+2}\bar{H}(x) \equiv 0 \tag{6}$$

and $a_k \neq 0$ for some $k \in \{0, 1, \ldots, n+2\}$. If $a_{n+2} \neq 0$ then derivative of (6) for $x = x_0$ gives contradiction $a_{n+2} = 0$. If $a_i \neq 0$, $i \in \{0, 1, \ldots, n+1\}$, then substituting x_i into (6) we obtain contradiction $a_i = 0$ again. Therefore the splines $\bar{H}(x), H_k(x)$, $k = 0(1)n+1$ are linear independent. □

A solution of the problem (5) can be expressed as

$$S(x) = [m_0 - 2s_0/h_{-1}]\bar{H}(x) + \sum_{i=0}^{n+1} s_i H_i(x). \tag{7}$$

3.3 Error propagation.

Let m_0, s_i be the precise data for spline (7) but we have only disturbed data $\bar{m}_0, \bar{s}_i$ $(i = 0(1)n+1)$ at our disposal. We will study the difference between coresponding splines. Denote

$$\bar{S}(x) = [\bar{m}_0 - 2\bar{s}_0/h_{-1}]\bar{H}(x) + \sum_{i=0}^{n+1} \bar{s}_i H_i(x),$$

$$e(x) = S(x) - \bar{S}(x), \quad e_i = e(x_i), \quad i = 0(1)n+1, \quad e_0' = e'(x_0) = m_0 - \bar{m}_0.$$

Theorem 1 *If* $|e_i| \leq E$, $i = 0(1)n+1$ *then we have for* $x \in [x_j, x_{j+1}]$

$$|e(x)| \leq |e_0'|\, h_j/4 + E \cdot [1 + r(3 + 2(j-1)r)/4], \tag{8}$$

where $r = \max\{\, h_k/h_m;\ k, m = 0(1)n+1\}$ *and* $j \in \{0, \ldots, n\}$.

Proof The function $e(x)$ is the spline from the space $\mathcal{S}_{21}(\Delta x)$:

$$e(x) = [e_0' - 2e_0/h_{-1}]\bar{H}(x) + \sum_{i=0}^{n+1} e_i H_i(x).$$

Therefore

$$|e(x)| \leq (2|e_0/h_{-1}| + |e_0'|)K_1 + EK_2, \tag{9}$$

where

$$K_1 = \max\{|\bar{H}(t)|,\ t \in [x_j, x_{j+1}]\}, \qquad K_2 = \max\{\sum_{i=0}^{n+1} |H_i(t)|,\ t \in [x_j, x_{j+1}]\}$$

From the Lemma 1 and the necessary conditions of a maximum it follows for $j \neq 0$ that

$$\begin{aligned}
K_1 &= (-1)^j \bar{H}((x_{j+1}+x_j)/2) = h_j/4 \\
K_2 &= H_{j+1}((x_{j+1}+x_j)/2) + H_j((x_{j+1}+x_j)/2) + \\
&\quad + \sum_{i=0}^{j-1}(-1)^{j-i} H_i((x_{j+1}+x_j)/2) = \\
&= 1 + \frac{1}{4}[2h_j/h_{j-1} + \sum_{i=0}^{j-1} h_j(h_i+h_{i-1})/(h_i h_{i-1})].
\end{aligned}$$

Let us substitute these results into (9). For $1 \leq j \leq n$ we obtain

$$|e(x)| \leq 3Eh_j/(4h_{-1}) + h_j|e_0'|/4 + EC$$

where

$$C = [1 + (2h_j/h_{j-1} + h_j/h_0 + \sum_{i=1}^{j-1} h_j(h_i+h_{i-1})/(h_i h_{i-1}))/4].$$

Because the spline $e(x)$ is determined uniquely by the set of knots (Δx) and by the values e_0', e_i, $i = 0(1)n+1$, so it is independent of h_{-1} on $[x_0, x_{n+1}]$. Hence,

$$\lim_{h_{-1}\to\infty} |e(x)| = |e(x)| \quad \text{holds for} \quad x \in [x_0, x_{n+1}].$$

Considering $h_{-1} \to \infty$ in the last inequality and using $h_k/h_m \leq r$ we obtain (8) (for $j = 0$ analogically). □

We see that the spline (7) has unsatisfactory error propagation features. The best case occurs if $h_i = h$ (so $r = 1$; usually $e_0' = 0$ too). Under this conditions we obtain from (8)

$$|e(x)| \leq E \cdot (5+2j)/4 = E_j$$

This simple formula can be used for computation of the estimation of error on interval $[x_j, x_{j+1}]$ (see example 1).

4 Quadratic spline interpolating given values of the derivative

4.1 Formulation and solution of the problem.

Let us have real numbers s_0, m_i, $i = 0(1)n+1$;
we search for a spline $S(x) \in \mathbb{S}_{21}(\Delta x)$ with the properties

$$\begin{aligned}
S'(x_i) &= m_i, \qquad i = 1(1)n+1, \\
S(x_0) &= s_0.
\end{aligned} \tag{10}$$

The local parameters $s_i = S(x_i)$, $i = 1(1)n + 1$ can be computed using the recurence relation (4) and function values of this spline we can find using the formula (3). From (3),(4) it follows also that the solution of the problem (5) exists and is unique.

4.2 Fundamental splines.

We will construct another basis of the linear space $\mathcal{S}_{21}(\Delta x)$ suitable for interpolation of the first derivative values.

Definition 3 Splines $\bar{F}(x), F_k(x) \in \mathcal{S}_{21}(\Delta x)$, $k = 0(1)n + 1$ are called the Df-fundamental splines if they have the following properties

$$\begin{aligned} &F_k'(x_i) = \delta_{ki}, \quad i = 0(1)n + 1, \\ &F_k(x_0) = 0, \\ &\bar{F}(x) = 1, \qquad x \in [x_0, x_{n+1}]. \end{aligned}$$

The Lemma 3 gives the exact description of the splines $F_k(x)$, $k = 0(1)n+1$ (see Fig. 2; $h_i = h$).

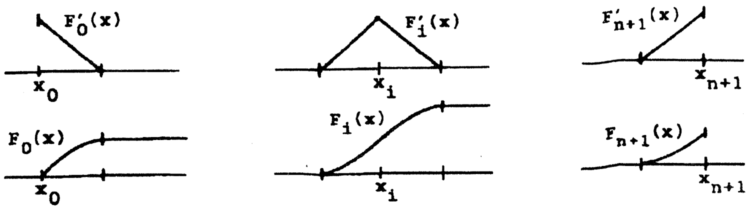

Fig. 2

Lemma 3 *The splines $F_k(x)$, $k = 0(1)n + 1$ can be written as*

$$F_0(x) = \begin{cases} (x - x_0) - (x - x_0)^2/(2h_0), & x \in [x_0, x_1], \\ h_0/2, & x \in [x_1, x_{n+1}]. \end{cases}$$

$$F_k(x) = \begin{cases} 0, & x \in [x_0, x_{k-1}], \\ (x - x_{k-1})^2/(2h_{k-1}), & x \in [x_{k-1}, x_k], \\ h_{k-1}/2 + (x - x_k) - (x - x_k)^2/(2h_k), & x \in [x_k, x_{k+1}], \\ (h_k + h_{k-1})/2, & x \in [x_{k+1}, x_{n+1}]. \end{cases}$$

$$F_{n+1}(x) = \begin{cases} 0, & x \in [x_0, x_n], \\ (x - x_n)^2/(2h_n), & x \in [x_n, x_{n+1}]. \end{cases}$$

Proof It follows from (4) and Definition 3 that

$$F_k(x_i) = \begin{cases} 0, & i = 0(1)k-1, \\ h_{k-1}/2, & i = k, \\ (h_{k-1}+h_k)/2, & i = k+1(1)n+1, \end{cases} \tag{11}$$

where $k = 0(1)n+1$, $h_{-1} = 0$. Substituting this results together with the postulates from Definition 3 into formula (3) (on every interval $[x_i, x_{i+1}]$) we obtain the formulas for Df-fundamental splines. □

Lemma 4 *The Df-fundamental splines $\bar{F}(x), F_0(x), F_1(x), \ldots, F_{n+1}(x)$ form the basis of the linear space $\mathcal{S}_{21}(\Delta x)$.*

This Lemma can be proved in an analogous way as Lemma 2. The solution of the problem (10) can be expressed in this way

$$S(x) = s_0 + \sum_{i=0}^{n+1} m_i F_i(x). \tag{12}$$

4.3 Error propagation.

Let s_0, m_i be the exact data for the spline (12) but we have only disturbed data $\bar{s}_0, \bar{m}_i$ $(i = 0(1)n+1)$. We will study the difference between coresponding splines. Denote

$$\bar{S}(x) = \bar{s}_0 + \sum_{i=0}^{n+1} \bar{m}_i F_i(x),$$

$$e(x) = S(x) - \bar{S}(x),\ e_i' = e'(x_i),\ i = 0(1)n+1,\ e_0 = e(x_0) = s_0 - \bar{s}_0.$$

Theorem 2 *If $|e_i'| \le E$, $i = 0(1)n+1$ then for $x \in [x_0, x_{n+1}]$ we have*

$$|e(x)| \le |e_0| + E \cdot (x - x_0).$$

Proof Because $e(x) \in \mathcal{S}_{21}(\Delta x)$ and $F_i(x) \ge 0$ (see Lemma 3) we obtain

$$|e(x)| = |e_0 + \sum_{i=0}^{n+1} e_i' F_i(x)| \le |e_0| + \sum_{i=0}^{n+1} E F_i(x).$$

The expression on the right hand side is the quadratic spline interpolating the values $m_i = E$, $i = 0(1)n+1$ of derivative, $s_0 = |e_0|$ — but it is the straight line $p(x) = |e_0| + E \cdot (x - x_0)$. □

4.4 An algorithm using the Df-fundamental splines.

Let us have a set of knots (Δx) with $h_i = x_{i+1} - x_i$ and real numbers s_0, m_i, $i = 0(1)n+1$. The spline interpolating the values of the first derivative can be written in the form (12). If we want to compute a value of this spline for $x' \in [x_k, x_{k+1}]$ $(0 \le k \le n)$ we can use the formula (12), the Lemma 3 and (11). Then

$$
\begin{aligned}
S(x') &= s_0 + \sum_{i=0}^{k+1} m_i F_i(x') = \\
&= s_0 + \frac{1}{2} m_0 h_0 + \sum_{i=1}^{k-1} m_i F_i(x') + m_k F_k(x') + m_{k+1} F_{k+1}(x') = \\
&= s_0 + \frac{1}{2}[m_0 h_0 + \sum_{i=1}^{k-1} m_i (h_{i-1} + h_i)] + m_k F_k(x') + m_{k+1} F_{k+1}(x').
\end{aligned}
$$

Thus

$$
S(x') = r + m_k(x' - x_k) + (m_{k+1} - m_k)(x' - x_k)^2/(2h_k), \tag{13}
$$

where

$$
r = \begin{cases} s_0, & k = 0, \\ s_0 + \dfrac{1}{2}[m_0 h_0 + m_k h_k + \displaystyle\sum_{i=1}^{k-1} m_i (h_{i-1} + h_i)], & (1 \le k \le n). \end{cases} \tag{14}
$$

In that way the calculation of $S(x')$ can be described by the following

Algorithm DF:

1° Find index k such that $x' \in [x_k, x_{k+1}]$;
2° Compute r using (14);
3° Compute $S(x')$ using (13).

This algorithm can be used instead of the algorithm based on the continuity conditions (4) and the formula (3). We use it if we want to economize a working storage capacity because we needn't know all local parameters s_i. This ignorance must be compensated by step 2°. So we do $2(k+1)$ algebraic operatios in the course of step 2° and for computation of local parameters s_i we need $6(n+1)$ algebraic operations $(0 \le k \le n)$. Therefore we use the algorithm DF if we want to know a few values of the spline only. A reduction of a working storage is more expressive for biquadratic splines of the tensor product type.

5 Quadratic splines smoothing given values of derivative

5.1 Smoothing cubic spline.

It is well-known (see [1],[4]) that the natural interpolating cubic spline minimizes the functional

$$J(f) = \int_a^b [f''(x)]^2 dx \quad \text{on} \quad \bar{V} = \{f | f \in W_2^2[a,b],\ f(x_i) = g_i,\ i = 0(1)n+1\}.$$

This property was used in the construction of the smoothing cubic spline, which minimizes the functional

$$\bar{J}(f) = \alpha \int_a^b [f''(x)]^2 dx + \sum_{i=0}^{n+1} w_i [f(x_i) - g_i]^2 \quad \text{on} \quad W_2^2[a,b],$$

where $\alpha > 0$, $w_i > 0$. The smoothing cubic spline can be represented by means of the fundamental smoothing cubic splines $\phi_k(x)$ as

$$S_{31}(x) = \sum_{k=0}^{n+1} g_k \phi_k(x),$$

where $\phi_k(x) \in \mathcal{S}_{31}(\Delta x)$, $k = 0(1)n+1$ are defined by (see [4])

$$\phi_k(x_i) + \alpha[\phi_k^{(3)}(x_i+) - \phi_k^{(3)}(x_i-)] = \delta_{ik}, \quad i = 0(1)n+1.$$

We will show analogical construction of the smoothing quadratic splines.

5.2 Smoothing quadratic splines.

The quadratic splines interpolating the first derivative values have extremal properties analogous to extermal properties of the cubic natural interpolating splines.

Theorem 3 (see [3]) *Let us have a set of knots* (Δx) *and real numbers* m_i, $i = 0(1)n+1$. *Denote*

$$J_1(f) = \int_a^b [f''(x)]^2 dx, \quad V = \{f | f \in W_2^2[a,b],\ f'(x_i) = m_i,\ i = 0(1)n+1\}.$$

Functional $J_1(f)$ *is minimized on* V *by every spline* $S(x) \in \mathcal{S}_{21}(\Delta x)$, *which interpolates the values of the first derivatives* m_i, $i = 0(1)n+1$. □

We will use this Theorem to the construction of the smoothing quadratic splines.

Theorem 4 (see [3]) *Let us have a set of knots (Δx), real numbers m_i, $w_i > 0$, $i = 0(1)n+1$ and a regulation parametr $\alpha > 0$. Denote*

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

Functional $J_2(f)$ is minimized on $W_2^2[a,b]$ by some spline $S(x) \in \mathcal{S}_{21}(\Delta x)$. First derivatives $s_i' = s'(x_i)$ of this spline fulfil the system of linear equations

$$(15)\quad \begin{aligned} &(w_0 + \alpha/h_0)s_0' - (\alpha/h_0)s_1' = w_0 m_0, \\ &-(\alpha/h_{k-1})s_{k-1}' + (w_k + \alpha/h_{k-1} + \alpha/h_k)s_k' - (\alpha/h_k)s_{k+1}' = w_k m_k, \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad k = 1(1)n, \\ &-(\alpha/h_n)s_n' + (w_{n+1} + \alpha/h_n)s_{n+1}' = w_{n+1} m_{n+1}. \end{aligned} \qquad \square$$

The matrix of the system of linear equations (15) is tridiagonal, symmetric and diagonally dominating. So we have unique solution of the system (15) and one free parameter for determining of the corresponding spline (we can choose for example $S(x_0) = s_0$). The quadratic spline minimizing $J_2(f)$ is called the *smoothing spline.*

5.3 Another type of necessary and sufficient conditions.

In the following lemmas we will use the notation

$$f(x_i+) = \lim_{x \to x_i+} f(x), \qquad f(x_i-) = \lim_{x \to x_i-} f(x).$$

Lemma 5 *A spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ minimizes the functional $J_2(f)$ if and only if*

$$(16)\qquad S'(x_k) + \alpha D_k / w_k = m_k, \qquad k = 0(1)n+1,$$

where $\quad D_k = S''(x_k-) - S''(x_k+), \quad S''(x_0-) = S''(x_{n+1}+) = 0.$

Proof a) First we prove that the conditions (16) are necessary. Let us consider a quadratic spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ which minimizes the functional $J_2(f)$. Denote $S_1(x) = S(x) + tF_k(x)$, where t is an arbitrary real number and $F_k(x)$ the spline from the Definition 3 ($0 \le k \le n+1$). Then

$$J_2(S_1) = \alpha J_1(S_1) + t^2 w_k + 2tw_k[S'(x_k) - m_k] + \sum_{i=0}^{n+1} w_i [S'(x_i) - m_i]^2,$$

$$J_2(S_1) - J_2(S) = a_k t^2 + 2b_k t,$$

where

$$a_k = w_k + \alpha \int_a^b [F_k''(x)]^2 dx > 0,$$

$$b_k = \alpha \int_a^b F_k''(x) S''(x) dx + w_k [S'(x_k) - m_k].$$

If $b_k \neq 0$ then we will get contradiction because we can choose $t \in R$ such that $|t| < 2|b_k|/a_k$, $\mathrm{sgn}(t) = \mathrm{sgn}(b_k)$ and obtain $J_2(S_1) < J_2(S)$. Therefore we have

$$0 = b_k = \alpha \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} F_k''(x) S''(x) dx + w_k [S'(x_k) - m_k]. \tag{17}$$

We rearrange the integrals in (17) using integration by parts and the identity $S^{(3)}(x) \equiv 0$ on $[x_i, x_{i+1}]$. Then we obtain

$$\sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} F_k''(x) S''(x) dx \quad = \quad \begin{cases} -S''(x_0+) = D_0, & k = 0; \\ S''(x_k-) - S''(x_k+) = D_k, & k = 1(1)n; \\ S''(x_{n+1}-) = D_{n+1}, & k = n+1. \end{cases}$$

Substituting this results into (17) we obtain (16).

b) We prove that the conditions (16) are sufficient.

Let us have $f(x) \in W_2^2[a, b]$ and let the spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ comply with (16). Denote

$$\bar{J}_2(f - S) = \alpha \int_a^b [f''(x) - S''(x)]^2 dx + \sum_{i=0}^{n+1} w_i [f'(x_i) - S'(x_i)]^2.$$

Thus

$$\bar{J}_2(f - S) \geq 0. \tag{18}$$

This functional can be rewritten also as

$$\begin{aligned} \bar{J}_2(f - S) &= J_2(f) - J_2(S) - \\ &- 2[\alpha I + \textstyle\sum_{i=0}^{n+1} w_i (f'(x_i) - S'(x_i))(S'(x_i) - m_i)], \end{aligned} \tag{19}$$

where

$$I = \int_a^b [f''(x) - S''(x)] S''(x) dx.$$

Let us rearrange the functional I using integration by parts, the identity

$$S^{(3)}(x) \equiv 0 \quad \text{on} \quad [x_i, x_{i+1}]$$

and the conditions (16):

$$I=\sum_{i=0}^{n}\int_{x_i}^{x_{i+1}}[f''(x)-S''(x)]S''(x)dx=$$

$$=\sum_{i=0}^{n}[(f'(x)-S'(x))S''(x)|_{x_i+}^{x_{i+1}}-\int_{x_i}^{x_{i+1}}(f'(x)-S'(x))S^{(3)}(x)dx]=$$

$$=\sum_{i=0}^{n+1}[f'(x_i)-S'(x_i)][S''(x_i-)-S''(x_i+)]=$$

$$=\sum_{i=0}^{n+1}w_i[f'(x_i)-S'(x_i)][m_i-S'(x_i)]/\alpha.$$

Hence, it follows from (19) that $\bar{J}_2(f-S)=J_2(f)-J_2(S)$ and from (18) we obtain $J_2(S)\leq J_2(f)$. □

Remark 1 The conditions (16) can be used for the formation of the system of the linear equations (15) too (substituting $S''(x_k-)=(s'_k-s'_{k-1})/h_{k-1}$, $S''(x_k+)=(s'_{k+1}-s'_k)/h_k$).

5.4 Fundamental splines for smoothing.

Now we shall use the conditions (16) for construction of another basis of the space $\mathcal{S}_{21}(\Delta x)$ suitable for representation of the smoothing splines.

Definition 4 Let us have a set of knots (Δx) and real numbers $\alpha>0$, $w_i>0$, $i=0(1)n+1$. Splines $\bar{\Phi}(x)$, $\Phi_k(x)\in\mathcal{S}_{21}(\Delta x)$, $k=0(1)n+1$ are called the S_α-fundamental splines if they have the following properties

$$\Phi'_k(x_i)+\alpha[\Phi''_k(x_i-)-\Phi''_k(x_i+)]/w_i=\delta_{ki},\quad i=0(1)n+1,\quad \Phi_k(x_0)=0,$$

$$\bar{\Phi}(x)=1,\quad x\in[a,b].$$

According to the Theorem 4 and Lemma 5 we know that S_α-fundamental splines exist because these are the smoothing splines for data $m_i=\delta_{ik}$, $i=$ $=0(1)n+1$. The examples of splines $\Phi_3(x)$ for various α are given in Figure 3 $(h_i=h,n=5)$.

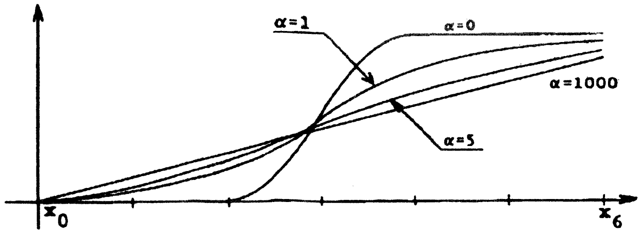

Fig. 3

We should have to write $\Phi_k(x;\alpha)$ instead of $\Phi_k(x)$. Because it would lead to complicated formulas we shall not use this notation. In the following text we will suppose that α is a fixed positive parameter.

Lemma 6 *Every spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ which minimizes $J_2(f)$ for data m_k, $w_k > 0$, $k = 0(1)n+1$, $\alpha > 0$ can be expressed by means of S_α-fundamental splines as*

$$S(x) = S(x_0) + \sum_{k=0}^{n+1} m_k \Phi_k(x).$$

Proof
Define $\Phi_k''(x) = S''(x) = 0$ for $x \notin [a,b]$. Let us have the spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ which minimizes $J_2(f)$. Denote

$$S_1(x) = S(x_0) + \sum_{k=0}^{n+1} m_k \Phi_k(x).$$

This spline satisfies the conditions (16) because of

$$\begin{aligned} &S_1'(x_i) + \alpha[S_1''(x_i-) - S_1''(x_i+)]/w_i = \\ &\quad = \sum_{k=0}^{n+1} m_k\{\Phi_k'(x_i) + \alpha[\Phi_k''(x_i-) - \Phi_k''(x_i+)]/w_i\} = \sum_{k=0}^{n+1} m_k \delta_{ki} = m_i. \end{aligned}$$

So the spline $S_1(x)$ also minimizes the functional $J_2(f)$, from the Theorem 4 it follows that $S_1'(x_i) = S'(x_i)$, $i = 0(1)n+1$. Because of $S_1(x_0) = S(x_0)$ we obtain from 4.1 that $S_1(x) \equiv S(x)$ on $[a,b]$. □

Lemma 7 *The S_α-fundamental splines $\ddot{\Phi}(x), \Phi_0(x), \Phi_1(x), \ldots, \Phi_{n+1}(x)$ form the basis of the linear space $\mathcal{S}_{21}(\Delta x)$.*

Proof We prove that every spline $S(x) \in \mathcal{S}_{21}(\Delta x)$ can be described with some $a_i \in R$ as

$$S(x) = a_{n+2} + \sum_{i=0}^{n+1} a_i \Phi_i(x). \tag{20}$$

Denote

$$a_i = S'(x_i) + \alpha[S''(x_i-) - S''(x_i+)]/w_i, \quad i = 0(1)n+1, \quad a_{n+2} = S(x_0),$$

where $S(x) \in \mathcal{S}_{21}(\Delta x)$ is an arbitrary spline.
If we substitute $m_i = a_i$, $i = 0(1)n+1$ into $J_2(f)$ then the spline $S(x)$ minimizes the functional $J_2(f)$ and we can describe it according to Lemma 6 in the form (20). Because dim $\mathcal{S}_{21}(\Delta x) = n + 3$, the S_α-fundamental splines constitute the basis of the linear space $\mathcal{S}_{21}(\Delta x)$. □

The smoothing spline from the Theorem 4 can be expressed as

$$S(x) = s_0 + \sum_{i=0}^{n+1} m_k \Phi_k(x).$$

Remark 2 The fundamental cubic splines were used in [4] in the construction of the bicubic splines of the tensor product type. We have the same opportunity in case of the qudratic splines.

6 Examples

6.1 We will demonstrate error propagation in the quadratic spline interpolating the function values. Let the data x_i, $s_i = S(x_i)$ and disturbed data $\bar{s}_i$ are given in the following table ($m_0 = \bar{m}_0 = 1$).

i	0	1	2	3	4	5	6	7	8
x_i	0	1	2	3	4	5	6	7	8
s_i	-0.5	0.3	0.5	0.2	-0.2	-0.6	-0.2	0.1	0.6
$\bar{s}_i$	-0.4	0.2	0.55	0.18	-0.27	-0.55	-0.12	0.2	0.58

Thus the estimation of the error in the knots x_i is

$$E = max\{|s_i - \bar{s}_i|, \ i = 0(1)n+1\} = 0.1 \ .$$

On the Fig.4 we can see the spline $S(x)$, disturbed spline $\bar{S}(x)$ and functions $E_l(x) = S(x) - |e(x)|$, $E_u(x) = S(x) + |e(x)|$; the bound of the error $e(x)$ is computed by means of the Theorem 1.

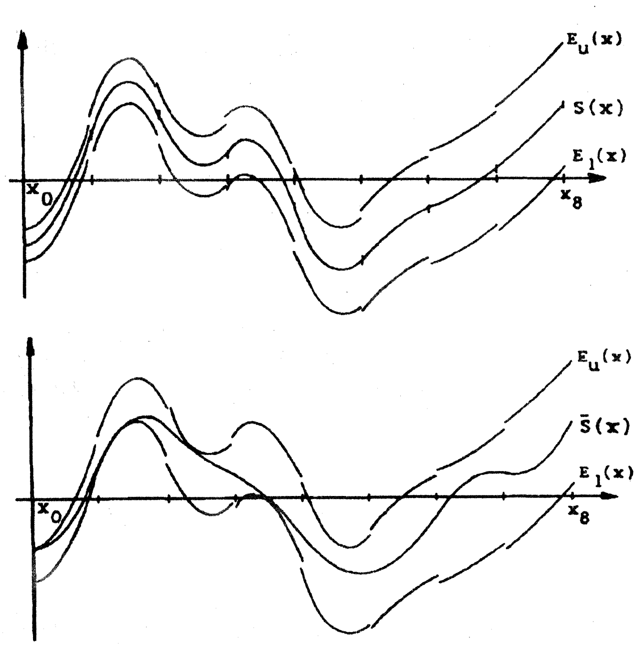

Fig. 4

6.2 As in Example 6.1 we will demonstrate error propagation in the quadratic spline interpolating the values of the first derivative. Let us have the data x_i, $m_i = S'(x_i)$ and disturbed data $\bar{m}_i$ given by the table ($s_0 = \bar{s}_0 = 0$).

i	0	1	2	3	4	5	6	7	8	9	10
x_i	−4	−3	−2	−1	0	1	2	3	4	5	6
m_i	1	−0.5	−0.1	−0.8	0	7	−0.1	−0.1	−0.1	2	1
$\bar{m}_i$	1.5	−1	−0.5	−1	0.5	6.6	0	0.3	0.4	2.5	1.4

Thus the estimation of the error of the derivative values in the knots x_i is

$$E = max\{|m_i - \bar{m}_i|,\ i = 0(1)n+1\} = 0.5 \ .$$

On the Fig.5 we can see (as in Example 6.1) the spline $S(x)$, disturbed spline $\bar{S}(x)$ and splines $E_l(x) = S(x) - |e(x)|$, $E_u(x) = S(x) + |e(x)|$; in this case the bound of the error $|e(x)|$ is computed by means of the Theorem 2 and $E_l(x)$, $E_u(x) \in \mathbb{S}_{21}(\Delta x)$.

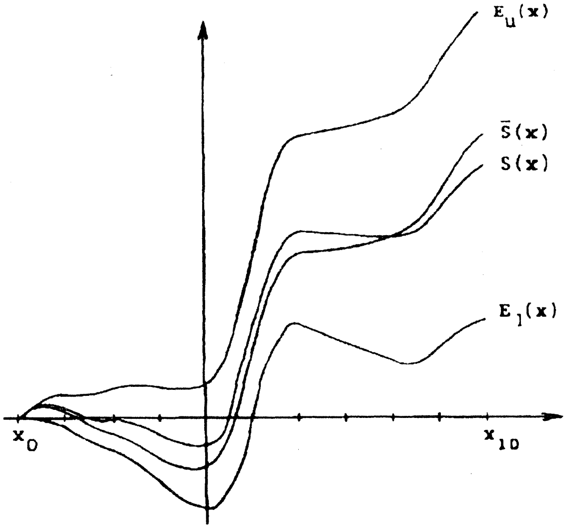

Fig. 5

6.3 Now we show some example of the quadratic spline smoothing the values of the first derivative. The data x_i, w_i, m_i are given in the following table ($s_0 = 0$).

i	0	1	2	3	4	5	6	7	8	9	10
x_i	-4.7	-2.1	-0.2	1	2.3	4.1	5	6	7.3	8.4	10
w_i	0.1	0.1	0.18	1	0.1	0.5	1.5	0.1	0.1	0.5	0.1
m_i	-1	-0.2	-0.5	0	2	2.1	0.1	-0.1	0.3	0	2

For the values $\alpha = 0; 0.3; 2; 1000$ we obtain the splines $S(x;\alpha)$ shown on the Fig 6. For $\alpha \to 0$ this spline tends to the spline interpolating the derivatives, for $\alpha \to \infty$ to the straight line $S(x;\infty) = k(x - x_0) + s_0$, where

$$k = \frac{\sum_{i=0}^{n+1} w_i m_i}{\sum_{i=0}^{n+1} w_i}. \tag{21}$$

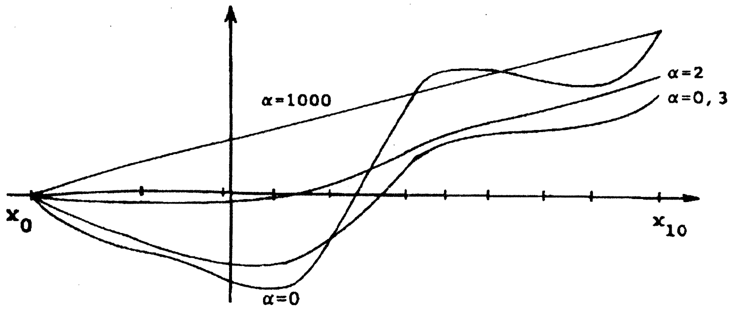

Fig. 6

The parameters w_i were choosen by means of formula (21) such that

$$S(x_0;\infty) = S(x_0;0), \qquad S(x_{n+1};\infty) = S(x_{n+1};0)$$

holds.

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