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NATURAL AND SMOOTHING QUADRATIC SPLINE
(An elementary approach)

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Summary. For quadratic spline interpolating local integrals (mean-values) on a given mesh the conditions of existence and uniqueness, construction under various boundary conditions and other properties are studied. The extremal property of such a spline allows us to present an elementary construction and an algorithm for computing needed parameters of such quadratic spline smoothing given mean-values. Examples are given illustrating the results.

Keywords: Spline functions, quadratic spline; interpolation, smoothing by splines: histosplines.

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1. INTRODUCTION. CUBIC SPLINES

Let us have a set of knots $\{x_i;\ i = 0(1)\ n + 1\}$,

$$(\Delta x):\ a = x_0 < x_1 < \ldots < x_n < x_{n+1} = b$$

on the real axis with prescribed values g_i at the knots x_i.

A function $S_3(x) = S_{31}(x)$ is called an interpolating cubic spline on the mesh (Δx) to data $\{g_i;\ i = 0(1)\ n + 1\}$ if it has the following properties:

1° $S_3(x) \in C^2[a, b]$ (*it has defect one*);

2° $S_3(x)$ *is a cubic polynomial on every interval* $[x_i, x_{i+1}]$, $i = 0(1)\ n$;

3° $S_3(x_i) = g_i$, $i = 0(1)\ n + 1$ (*conditions of interpolation*).

The construction of such a function on the set of knots (Δx) under various boundary conditions, the questions of existence and uniqueness and other properties of cubic splines are welldescribed in the literature – e.g. [1], [2], [8], [10].

In the class of cubic splines on (Δx), the so called "natural splines" defined uniquely on the set (Δx) by the conditions of interpolation 3° and by the boundary. conditions

$$S_3''(a) = S_3''(b) = 0,$$

have a minimizing property

$$\text{(1)} \qquad \int_a^b [S_3''(x)]^2 \, dx \leqq \int_a^b [f''(x)]^2 \, dx \quad \text{for all} \quad f \in V,$$
$$V = \{f \in W_2^2[a, b] \; ; \; f(x_i) = g_i \, , \, i = 0(1) \, n + 1\} \, .$$

This property is used in the construction of the cubic smoothing spline, which – in situations, where the values g_i represent some perturbed function values $g(x_i)$ – realizes the minimum of the functional

$$\text{(2)} \qquad J(p) = p \int_a^b [f'']^2 \, dx + \sum_{i=0}^{n+1} [f(x_i) - g_i]^2 \, , \quad f \in V$$

including a regulation parameter p (see [2], [8], [10], for details). Such a cubic smoothing spline yields a compromise between interpolation and smoothness, regulated with the help of the parameter p. We can find analogous minimizing properties at splines of an odd degree described in the literature [1], [4].

For splines of an even degree such a property can be obtained only by a change of the formulation of the problem, as will be shown in the following.

2. INTERPOLATING QUADRATIC SPLINES

It is known that the construction of the interpolating spline of the second (more generally even) order in an analogous way on (Δx) meets with some difficulties (see [2], [3]):

– there is no symmetry in boundary conditions (one free parameter only);

– in some important cases (periodicity) such a spline need not exist in general;

– even if such a spline exists it has some unpleasant properties (an error in boundary conditions or data g_i is transferred over the whole interval without damping).

This difficulties with quadratic (even order) splines can be overcome by separating the meshes of the spline knots and the points of interpolation (which can be important in the applications, too).

Let us have the mesh (see [8]) $(\Delta x \; \Delta t)$:

$(\Delta x \; \Delta t)$ $\quad x_i \, , \quad i = 0(1) \, n + 1$ *knots of the spline,*
$\quad t_i, \quad i = 0(1) \, n$ *points of the interpolation,*
$\quad g_i, \quad i = 0(1) \, n$ *prescribed values in* t_i ;
$$x_0 \leqq a = t_0 < x_1 < t_1 < \ldots < t_{n-1} < x_n < t_n = b \leqq x_{n+1} \, .$$

A function $S_2(x) = S_{21}(x)$ is called an interpolating quadratic spline to the data g_i, if it has the following properties:

1° $S_2(x) \in C^1[a, b]$ *(defect one)*;
2° $S_2(x)$ *is a quadratic polynomial on every interval* $[x_i, x_{i+1}]$, $i = 0(1) \, n$;
3° $S_2(t_i) = g_i \, , \quad i = 0(1) \, n$ *(conditions of interpolation)*.

Theoretical and computational aspects of quadratic splines defined in this way are discussed in [8], [3], [5].

With such a formulation of the interpolation problem, a majority of the above difficulties disappear: such an interpolating spline is uniquely determined by the prescribed values g_i, $i = 0(1)\, n$ and by two other conditions – e.g. by two *boundary conditions* (first, second derivative at boundary, periodicity conditions). The properly chosen parameters of the spline $S_2(x)$ (usually $m_i = S_2'(x_i)$ or $M_i = (S_2''(t_i))$ are computed from a certain tridiagonal system (cyclic tridiagonal in the periodic case) of linear equations with a diagonally dominant matrix of the system. So, we succeeded in giving to quadratic splines construction and local properties analogous to the properties of cubic splines (the localizing properties are even stronger than those of the cubic splines e.g. in case of $t_i = \frac{1}{2}(x_i + x_{i+1})$, which is the most frequently occurring case). We also have new free parameters – the positions of knots – at our disposal; this fact is used frequently in "shape preserving problems".

Let us consider the question of minimizing properties of quadratic interpolating splines defined on (Δx) or $(\Delta x\ \Delta t)$; we are interested in some analogy with the natural cubic spline with its minimizing property. Yet the facts that – with g_i given –

a) the first order spline $S_1(x)$ (Euler's polygon) minimizes

$$\int_a^b [f'(x)]^2\, \mathrm{d}x \quad (\text{see } [7])\ ;$$

b) the natural cubic spline $S_3(x)$ minimizes

$\int_a^b [f''(x)]^2\, \mathrm{d}x$ (over appropriate clases of functions – see [1], [7] for details)

shows us that there is no place for the direct analogy with interpolating quadratic splines. The usual argument in the proof for odd degree splines makes use of the inequality

$$(3) \qquad 0 \leqq (f^{(m)} - S_{2m-1}^{(m)}, f^{(m)} - S_{2m-1}^{(m)})_2 = (f^{(m)}, f^{(m)})_2 - 2(S_{2m-1}^{(m)}, f^{(m)} - S_{2m-1}^{(m)})_2 - (S_{2m-1}^{(m)}, S_{2m-1}^{(m)})_2\,.$$

Then the minimizing property of S_{2m-1} follows from the orthogonality relation

$$(4) \qquad (S_{2m-1}^{(m)}, f^{(m)} - S_{2m-1}^{(m)})_2 = 0\,,$$

which can be proved using integration by parts (see [1], [7]). But – as we easily see – such orthogonality relations do not hold for quadratic splines – neither on the set (Δx), nor on $(\Delta x\ \Delta t)$! These splines interpolating the values g_i simply have not such a property. To obtain quadratic splines with an analogous property, we have to change formulation of the problem – instead of interpolating the function values, we shall match some mean values of the approximated function over the intervals $[x_i, x_{i+1}]$. Such constructions have appeared originally in data smoothing (approximation of histograms by a smooth function, called histospline – see [2], [6]). The purpose of this paper is to present a simple algorithm for computation of the parameters of such a quadratic spline, to prove its minimizing property and on this basis to present an elementary theory and construction of the quadratic smoothing spline. The general variational theory can be found e.g. in [4], [9].

3. QUADRATIC SPLINES INTERPOLATING MEAN-VALUES (LOCAL INTEGRALS)

3.1 Formulation of the problem

Let us have a set of knots (Δx) with $h_i = x_{i+1} - x_i$, and real numbers g_i, $i = 0(1)\,n$. We search a function $S(x) = S_2(x)$ with the properties

(5)
1° $S(x) \in C^1[a, b]$;

2° $S(x)$ *is a quadratic polynomial on every interval* $[x_i, x_{i+1}]$, $i = 0(1)\,n$;

3° $\int_{x_i}^{x_{i+1}} S(x)\,\mathrm{d}x = h_i g_i$, $\quad i = 0(1)\,n$ $\quad$ (the mean-value interpolation).

Such a function will be called a quadratic spline interpolating the mean-values (local integrals) g_i. According to (5), there are altogether:

$3(n + 1)$ parameters defining $S(x)$;

$n + 1$ conditions of interpolation;

$2n$ continuity conditions at the knots x_i, $i = 1(1)\,n$.

So we have two parameters – for example boundary conditions – for determining the spline.

Let us denote

$$s_i = S(x_i)\,, \quad m_i = S'(x_i)\,; \tag{6}$$

with respect to the property 2°, we use the spline representation

$$\begin{aligned} S(x) &= s_i + m_i(x - x_i) + \frac{1}{2h_i}(m_{i+1} - m_i)(x - x_i)^2 = \\ &= s_{i+1} + m_{i+1}(x - x_{i+1}) + \frac{1}{2h_i}(m_{i+1} - m_i)(x - x_{i+1})^2\,, \\ & x \in [x_i, x_{i+1}]\,. \end{aligned} \tag{7}$$

Integrating by parts over $[x_i, x_{i+1}]$ we obtain

$$\begin{aligned} \int_{x_i}^{x_{i+1}} S(x)\,\mathrm{d}x &= s_i h_i + \tfrac{1}{2} m_i h_i^2 + \frac{1}{6h_i}(m_{i+1} - m_i)\,h_i^3 = \\ &= s_i h_i + \tfrac{1}{6} h_i^2(m_{i+1} + 2m_i) = s_{i+1} h_i - \tfrac{1}{2} m_{i+1} h_i^2 + \frac{1}{6h_i}(m_{i+1} - m_i)\,h_i^3 = \\ &= s_{i+1} h_i + \tfrac{1}{6} h_i^2(-m_i - 2m_{i+1})\,, \quad i = 0(1)\,n\,. \end{aligned} \tag{8}$$

The continuity conditions for $S(x)$ at $x = x_i$, $i = 1(1)\,n$ can be written by virtue of (7) as

$$s_{i-1} + m_{i-1}\,h_{i-1} + \frac{1}{2h_{i-1}}\,(m_i - m_{i-1})\,h_{i-1}^2 = s_i\,;$$

we can write it as a relation between the parameters m_i, s_i

$$\tfrac{1}{2}(m_{i-1} + m_i) = \frac{1}{h_{i-1}}\,(s_i - s_{i-1}) \tag{9}$$

with a simple geometrical meaning.

The continuity conditions for $S'(x)$ are involved implicitly in our notation $m_i = S'(x_i)$, $i = 1(1)\,n$. The conditions of interpolation of mean values can be written – using (8) – as

$$\begin{aligned} &s_i + \tfrac{1}{6}h_i(m_{i+1} + 2m_i) = g_i\,, \quad i = 0(1)\,n\,, \\ &s_{n+1} - \tfrac{1}{6}h_n(m_n + 2m_{n+1}) = g_n\,. \end{aligned} \tag{10}$$

Subtracting relations (10) with indices i, $i - 1$, we obtain

$$s_i - s_{i-1} + \tfrac{1}{6}[h_i(m_{i+1} - m_i) - h_{i-1}(m_i + 2m_{i-1})] = g_i - g_{i-1}\,;$$

dividing by h_{i-1} and using (9) we have

$$\tfrac{1}{2}(m_i + m_{i-1}) + \frac{1}{6h_{i-1}}\,[h_i(m_{i+1} + 2m_i) - h_{i-1}(m_i + 2m_{i-1})] =$$

$$= \frac{1}{h_{i-1}}\,(g_i - g_{i-1})\,.$$

So we can write the interpolation and continuity conditions – after some simple manipulations – as relations between parameters m_i and data g_i, x_i in the form of the three-term recurrence

$$h_{i-1}m_{i-1} + 2(h_{i-1} + h_i)\,m_i + h_im_{i+1} = 6(g_i - g_{i-1})\,, \quad i = 1(1)\,n\,, \tag{11}$$

which has also a simple geometrical meaning.

3.2 Boundary conditions s_0, s_{n+1}

We have two free parameters at our disposal; using the boundary conditions $S(x_0) = s_0$, $S(x_{n+1}) = s_{n+1}$ in the first and last relation in (10), we obtain

$$\begin{aligned} &2h_0m_0 + h_0m_1 = 6(g_0 - s_0)\,, \\ &h_nm_n + 2h_nm_{n+1} = 6(s_{n+1} - g_n)\,. \end{aligned} \tag{12}$$

These two equations complete (11) to the system of linear equations

$$
(13) \quad \begin{bmatrix} 2h_0, & h_0, & & & & \\ h_0, & 2(h_0 + h_1), & h_1, & & & \\ & h_1, & 2(h_1 + h_2), & h_2, & & \\ & & \ddots & \ddots & \ddots & \\ & & & h_{n-1}, & 2(h_{n-1} + h_n), & h_n \\ & & & & h_n, & 2h_n \end{bmatrix} \begin{bmatrix} m_0 \\ m_1 \\ m_2 \\ \vdots \\ m_n \\ m_{n+1} \end{bmatrix} = 6 \begin{bmatrix} g_0 - s_0 \\ g_1 - g_0 \\ g_2 - g_1 \\ \vdots \\ g_n - g_{n-1} \\ s_{n+1} - g_n \end{bmatrix}.
$$

The matrix of this system is symmetric, tridiagonal with a dominating diagonal; so we can use effective methods for computing uniquely the parameters $m_i = S'(x_i)$, $i = 0(1)\, n + 1$. Then we can compute the values $s_i = S(x_i)$ using the boundary values s_0 or s_{n+1} and the recurrence relation (9)

$$
(14) \qquad s_i = s_{i-1} + \tfrac{1}{2}h_{i-1}(m_{i-1} + m_i) \quad \text{(we can use (10), too)}\,.
$$

In such a simple way we will have computed all parameters needed for spline representation (7).

Remark. A special case of this problem is mentioned in [2] with the use of another representation of $S(x)$ resulting in a more complicated system of equations with the block structure.

3.3 Boundary conditions m_0, m_{n+1}

When the boundary conditions

$$
(15) \qquad S'(x_0) = m_0\,, \quad S'(x_{n+1}) = m_{n+1}
$$

are given in our problem, we can use this fact for writing (11) as a system of linear equations

(16)

$$
\begin{bmatrix} 2(h_0 + h_1), & h_1, & & \\ h_1, & 2(h_1 + h_2), & h_2, & \\ & \ddots & \ddots & \ddots \\ & & h_{n-1}, & 2(h_{n-1} + h_n) \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \end{bmatrix} = 6 \begin{bmatrix} g_1 - g_0 - \frac{1}{6}h_0 m_0 \\ g_2 - g_1 \\ \vdots \\ g_n - g_{n-1} - \frac{1}{6}h_n m_{n+1} \end{bmatrix}.
$$

The existence and uniqueness of the solution follow from the diagonal dominancy of the symmetric matrix of the system.
The function values s_i can be computed from (14) or (10) as in 3.2.

3.4 Boundary conditions M_0, M_{n+1}

The boundary conditions $S''(x_0 + 0) = M_0$, $S''(x_{n+1} - 0) = M_{n+1}$ can be written in terms of m_i as

$$
(17) \qquad m_0 - m_1 = -h_0 M_0\,, \quad -m_n + m_{n+1} = h_n M_{n+1}\,.
$$

Completing the relations (11) with these two equations, we obtain a system of $n + 2$ equations for parameters m_i, $i = 0(1)\, n + 1$ with a regular matrix of the system.

3.5 Periodicity conditions

To obtain the spline with periodic continuation, we have to prescribe the periodicity conditions

$$s_0 = s_{n+1}\,, \quad m_0 = m_{n+1}\,. \tag{18}$$

Using (10), we can write it as

$$s_0 + \tfrac{1}{6}h_0(m_1 + 2m_{n+1}) = g_0\,, \quad s_{n+1} + \tfrac{1}{6}h_n(-m_n - 2m_{n+1}) = g_n\,.$$

Subtracting again these two relations. we can complete (11) to the system of $n + 1$ linear equations for the parameters m_i, $i = 1(1)\, n + 1$:

(19)

$$\begin{bmatrix} 2(h_0 + h_1), & h_1; & \dots, & & h_0 \\ h_1\,, & 2(h_1 + h_2), & h_2, & & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0, \dots & h_{n-1}, & 2(h_{n-1} + h_n), & h_n & \\ h_0, \dots & & h_n, & & 2(h_0 + h_n) \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \\ m_{n+1} \end{bmatrix} = 6 \begin{bmatrix} g_1 - g_0 \\ g_2 - g_1 \\ \vdots \\ g_n - g_{n-1} \\ g_0 - g_n \end{bmatrix}.$$

The matrix of this system is symmetric, diagonally dominant; we have also uniquely determined parameters m_i for any given data g_i.

3.6 General boundary conditions

It would be possible to consider the more general boundary conditions

$$a_0 m_0 + b_0 m_1 = f_0\,, \quad a_{n+1} m_n + b_{n+1} m_{n+1} = f_{n+1}\,, \tag{20}$$

the special case of which are conditions (12), (15), (17). We can easily state sufficient conditions for existence and uniqueness of the spline $S(x)$ under these conditions. We state the results of 3.1 – 3.5 in the following theorem.

Theorem 1. *With the data $\{x_i, i = 0(1)\, n + 1;\, g_i, i = 0(1)\, n\}$ given, the problem to find a quadratic spline satisfying (5) has a unique solution under the boundary conditions listed below:*

a) $S(x_0) = s_0\,, \quad S(x_{n+1}) = s_{n+1}\,;$

b) $S'(x_0) = m_0\,, \quad S'(x_{n+1}) = m_{n+1}\,;$

c) $S''(x_0) = M_0\,, \quad S''(x_{n+1}) = M_{n+1}\,;$

d) *periodicity conditions* $s_0 = s_{n+1},\, m_0 = m_{n+1}\,;$

e) *general boundary conditions* (20) *with* $|a_0| > |b_0|\,, \quad |b_{n+1}| > |a_{n+1}|\,.$

Remark. We have a symmetric strongly diagonally dominant matrix of the system in cases a), b), d); the boundary values and the mean-values g_i occur on the right-hand side only. It can be shown – using the technique shown in [3] for quadratic splines interpolating function values – that splines interpolating the mean-values share with the cubic splines on (Δx) and with quadratic splines on the mesh $(\Delta x\ \Delta t)$ the localizing property: the errors in boundary values or mean-values have only local influence on the spline and they are damped out with growing distance (this follows from the strong diagonal dominancy of the matrix in (11), completed by boundary conditions).

4. MINIMIZING PROPERTIES OF QUADRATIC SPLINES

Let us consider quadratic splines $S(x)$, determined on the mesh (Δx) by the mean-value interpolation conditions

$$\int_{x_i}^{x_{i+1}} S(x)\,\mathrm{d}x = h_i g_i\,, \quad i = 0(1)\,n \tag{21}$$

and some of the boundary conditions a)–e) from Theorem 1.

Let us denote $V = \{f \in W_2^1[a, b];\ \int_{x_i}^{x_{i+1}} f(x)\,\mathrm{d}x = h_i g_i,\ i = 0(1)\,n\}$.

Integrating by parts with $f \in V$, we rearrange the inequality

$$0 \leqq \int_a^b (S' - f')^2\,\mathrm{d}x = \int_a^b (f')^2\,\mathrm{d}x - 2\int_a^b (f' - S')\,S'\,\mathrm{d}x - \int_a^b (S')^2\,\mathrm{d}x \tag{22}$$

using

$$\int_{x_i}^{x_{i+1}} (f' - S')\,S'\,\mathrm{d}x = [S'(f - S)]_{x_i}^{x_{i+1}} - S_i'' \int_{x_i}^{x_{i+1}} (f - S)\,\mathrm{d}x\,.$$

The last term vanishes because $f, S \in V$ and we have

$$\begin{aligned}\int_a^b (f' - S')\,S'\,\mathrm{d}x &= \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} (f' - S')\,\mathrm{d}x = \\ &= \sum_{i=0}^{n} [m_{i+1}(f_{i+1} - s_{i+1}) - m_i(f_i - s_i)] = \\ &= m_{n+1}(f_{n+1} - s_{n+1}) - m_0(f_0 - s_0)\,.\end{aligned} \tag{23}$$

It is now easy to see the conditions under which the orthogonality relation $\int_a^b (f' - S')\,S'\,\mathrm{d}x = 0$ holds, from which the minimizing property follows via (22).

Theorem 2. *The functional $J(f) = \int_a^b [f'(x)]^2\,\mathrm{d}x$ is minimized by a quadratic spline $S(x)$ interpolating the mean-values g_i on (Δx):*

a) *over all $f \in V$ by the spline with "natural" boundary conditions $m_0 = m_{n+1} = 0$;*

b) *over all $f \in V$ satisfying the periodicity conditions $f_0 = f_{n+1}$ by the spline with periodic boundary conditions* (18);

c) *over all $f \in V$ satisfying $f_0 = s_0$, $f_{n+1} = s_{n+1}$ by the spline $S(x)$ with the same boundary conditions.*

In all these cases the spline $S(x)$ is *the unique solution of the problem*. Uniqueness of the minima follows by standard arguments of variational calculus: the functional

$F(p) = J(S + pv)$, where $p \in R$ and S is the minimizing spline,

$v \in V$ with

$\int_{x_i}^{x_{i+1}} (v(x) \, dx = 0, i = 0(1)\, n$ has a minimum for $p = 0$ or $v = 0$ only $[(v', S')_2 = 0, \mathrm{d}J/\mathrm{d}p = 2p(v', v')_2; \quad (v', v')_2 = 0$ for $v = 0$ only$]$.

5. APPROXIMATION PROPERTIES OF $S(x)$

Theorem 3. *Let* $g \in C^j[a, b]$, $j \in \{0, 1, 2, 3\}$; $g_i = (1/h_i) \int_{x_i}^{x_{i+1}} g(x)\, dx$, $i = 0(1)\, n$, *and let* $S(x)$ *be the quadratic spline interpolating the mean-values* g_i *on the set* (Δx) *under boundary conditions of the type* $S^{(k)}(x_i) = g^{(k)}(x_i)$, $i = 0, n + 1$; $k \in \{0, 1, 2\}$. *Then*

$$\|S^{(k)} - g^{(k)}\|_C = C_{jk} H^{j-k} \| g^{(j)}\|_C \,, \quad k \leqq j - 1 \,, \quad j = 1, 2, 3 \tag{24}$$

with $H = \max_i \{h_i\}$ *and constants* C_{jk} *given by the scheme*

j/k	0	1	2
1	0,86		
2	4/27	1/27	
3	1/24	1/6	$1/r + r/2$, $\quad r = \max_i \{h_i/h_{i-1}\}$.

Proof. Let us denote

$$f(x) = \int_{x_0}^{x} g(t) \, dt \in C^{j+1}[a, b] \,.$$

a) We have the recurrence relation

$$f_0 = 0 \,, \quad f_{i+1} = f_i + h_i g_i \,, \quad i = 0(1)\, n \quad \text{for the values} \quad f_i = f(x_i) \,.$$

Denote by $S_3(x)$ the cubic spline determined by the conditions of interpolation $S_3(x_i) = f_i$, $i = 0(1)\, n + 1$ and by the boundary conditions $S_3'(x_0) = f'(x_0) = g(x_0)$, $S_3'(x_{n+1}) = f'(x_{n+1}) = g(x_{n+1})$ provided $k = 0$; generally

$$S_3^{(k+1)}(x_0) = g^{(k)}(x_0) \,, \quad S_3^{(k+1)}(x_{n+1}) = g^{(k)}(x_{n+1}) \,, \quad k \in \{0, 1, 2\} \,.$$

Such a spline is determined uniquely by these conditions.

b) The function $S(x) = S_3'(x)$ has the following properties:

1° $S(x)$ is a quadratic spline on (Δx);

2° $\int_{x_i}^{x_{i+1}} S(x) \, dx = \int_{x_i}^{x_{i+1}} S_3'(x) \, dx = [S_3(x)]_{x_i}^{x_{i+1}} = h_i g_i$;

(26) 3° $S(x_i) = g(x_i)$ for $i = 0$, $n + 1$ (generally $S^{(k)}(x_i = g^{(k)}(x_i))$, $k \in \{0, 1, 2\}$; $i = 0$, $n + 1)$.

This means that $S(x)$ is identical with the quadratic spline interpolating the mean-values g_i with the appropriate boundary conditions

$$S^{(k)}(x_i) = g^{(k)}(x_i)\,, \quad i = 0\,, \quad n + 1\,; \quad k \in \{0, 1, 2\}\,.$$

c) It is known in the theory of the cubic interpolating splines that

$$\|S_3^{(k)} - f^{(k)}\|_C \leqq C_{kj}\, H^{m-k} \|f^{(k)}\|_C\,, \quad m \leqq 4\,, \quad k \in \{0, 1, \ldots, m - 1\}$$

with $f \in C^m$ and $S_3^{(k)}(x_i) = f^{(k)}(x_i)$, $i = 0, n + 1$ (see [10], where the constants C_{jk} are also given). But we have $S_3' = S, f' = g$ and the statement of Theorem 3 follows immediately with $j = k - 1$.

6. CUBIC MEAN-VALUES INTERPOLATING SPLINES

Let us consider the question of construction of cubic splines interpolating mean-values instead of function values. It can be shown that for the parameters $s_i = S_3(x_i)$, $m_i = S_3'(x_i)$ of such a spline on the set (Δx) the interpolation and continuity conditions yield the block system of equations with three free parameters, which must be determined by boundary conditions – asymmetry has again appeared. The condition of orthogonality $\int_a^b S_3''(f'' - S'')\,\mathrm{d}x = 0$ cannot be generally fulfilled – there are not minimizing properties. Such properties can again appear if we interpolate the mean-values of the first derivative: $g_i h_i = \int_{x_i}^{x_{i+1}} S_3'(x)\,\mathrm{d}x$. The full discussion of such a problem can be done quite analogous to that in part 4; in this way we can obtain another class of cubic splines minimizing $\int_a^b (f'')^2\,\mathrm{d}x$ over an appropriate set of functions.

7. QUADRATIC SMOOTHING SPLINE

7.1 Relation between natural and smoothing splines

It is well known how to use extremal (minimizing) properties of natural cubic splines to obtain the cubic smoothing spline to the given data (see e.g. [2], [10]). We can quite similarly make use of the minimizing property of quadratic mean-value interpolating splines to construct the quadratic smoothing spline to the given mean values.

Theorem. 4. *Given the values* α; g_i, $i = 0(1)\,n$; $w_i \geqq 0$, $i = 0(1)\,n + 1$ *on the mesh* (Δx) *with* $h_i = x_{i+1} - x_i$, *the functional*

$$J(f) = \int_a^b (f')^2\,\mathrm{d}x + \alpha \sum_{i=0}^{n} w_i [h_i g_i - \int_{x_i}^{x_{i+1}} f(x)\,\mathrm{d}x]^2 \tag{27}$$

is minimized on the class of functions $f \in V = W_2^1[a, b]$ *by some quadratic spline* $S(x)$ *with "natural" boundary conditions* $m_0 = m_{n+1} = 0$.

Proof. Suppose that $J(f)$ assumes its minimum for a function $u(x) \in V$ with the corresponding mean-values $\int_{x_i}^{x_{i+1}} u(x)\,\mathrm{d}x = h_i p_i$, $i = 0(1)\,n$. Then the spline $S(x)$

interpolating the same mean-values p_i, $i = 0(1)\,n$ and obeying the "natural" boundary conditions $m_0 = S'(x_0) = 0$, $m_{n+1} = S'(x_{n+1}) = 0$

– assumes the same value of the second part of $J(u)$;

– assumes a smaller value of the first part of $J(f)$ according to Theorem 2.

The functional (27) represents some interplay between smoothness (the first part of $J(f)$) and interpolation (the second part); we have there free parameters α, w_i at our disposal. The quadratic spline minimizing $J(f)$ will be called *the smoothing spline* to the mean-value data g_i. In its construction we must overcome the problem that we do not know the mean-values of $S(x)$ in advance.

7.2 The algorithm

Let us denote by p_i the mean-values of the spline $S(x)$ we search;

(28) $$\int_{x_i}^{x_{i+1}} S(x)\,\mathrm{d}x = h_i p_i\,, \quad i = 0(1)\,n\,;$$

$m_0 = S'(x_0) = 0$, $m_{n+1} = S'(x_{n+1}) = 0$ according to Theorem 4. The remaining parameters $m_i = S'(x_i)$, $i = 1(1)\,n$, can be calculated according to (16) from the system of equations

(29) $$\begin{bmatrix} 2(h_0 + h_1), & h_1, & & & \\ h_1, & 2(h_1 + h_2), & h_2, & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & h_{n-1} \\ & & & h_{n-1}, & 2(h_{n-1} + h_n) \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_{n-1} \\ m_n \end{bmatrix} = 6 \begin{bmatrix} p_1 - p_0 \\ p_2 - p_1 \\ \vdots \\ p_{n-1} - p_{n-2} \\ p_n - p_{n-1} \end{bmatrix}.$$

The values of $S(x)$ can then be established according to (9), (10) by

(30) $$\begin{aligned} s_0 &= p_0 - \tfrac{1}{6}h_0 m_1\,, \quad s_{n+1} = p_n + \tfrac{1}{6}h_n m_n\,, \\ s_i &= s_{i-1} + \tfrac{1}{2}h_{i-1}(m_{i-1} + m_i)\,, \quad i = 1(1)\,n\,. \end{aligned}$$

Let us write the system (29) in a matrix form

(31) $$\boldsymbol{Rm} = 6\boldsymbol{Qp}$$

with the vectors $\boldsymbol{m} = [m_1, \ldots, m_n]^T$, $\boldsymbol{p} = [p_0, \ldots, p_n]^T$, the square matrix $\boldsymbol{R}$ of the system (29) and the $(n, n + 1)$-matrix $\boldsymbol{Q}$,

$$\boldsymbol{Q} = \begin{bmatrix} -1, & 1, & & & \\ & -1, & 1, & & \\ & & \ddots & \ddots & \\ & & & -1, & 1 \end{bmatrix}.$$

The derivative $S'(x)$ is a piecewise linear function; let us denote

$S'_{i+1/2} = \frac{1}{2}(m_i + m_{i+1})$. Using then Simpson's formula of numerical integration, we get (exactly!)

$$\int_a^b (S')^2 \, dx = \sum_i \int_{x_i}^{x_{i+1}} (S')^2 \, dx = \sum_i \tfrac{1}{6} h_i (m_i^2 + 4S'^2_{i+1/2} + m_{i+1}^2) =$$

$$= \tfrac{1}{6} \sum_{i=0}^{n} h_i [m_i^2 + (m_i + m_{i+1})^2 + m_{i+1}^2] =$$

$$= \tfrac{1}{3} \sum_{i=0}^{n} h_i (m_i^2 + m_i m_{i+1} + m_{i+1}^2) = \tag{32}$$

$$= \tfrac{1}{6} \sum_{i=1}^{n} m_i [m_{i-1} h_{i-1} + 2(h_{i-1} + h_i) m_i + h_i m_{i+1}] =$$

$$= \tfrac{1}{6} \mathbf{m}^T \mathbf{R} \mathbf{m}; \qquad (m_0 = m_{n+1} = 0).$$

Let us define the functional $F(\mathbf{p})$ by

$$F(\mathbf{p}) = \int_a^b (S')^2 \, dx + \alpha \sum_{i=0}^{n} w_i h_i^2 (g_i - p_i)^2 \tag{33}$$

and denote $\mathbf{D} = \operatorname{diag}[h_i \sqrt{w_i}]_{i=0}^n$ (the diagonal matrix).

Using (32) we can write

$$F(\mathbf{p}) = \tfrac{1}{6} \mathbf{m}^T \mathbf{R} \mathbf{m} + \alpha [\mathbf{D}(\mathbf{g} - \mathbf{p})]^T \mathbf{D}(\mathbf{g} - \mathbf{p}) =$$

$$= \tfrac{1}{6} \mathbf{m}^T \mathbf{R} \mathbf{p} + \alpha (\mathbf{g} - \mathbf{p})^T \mathbf{D}^2 (\mathbf{g} - \mathbf{p})$$

and with $\mathbf{m} = 6\mathbf{R}^{-1}\mathbf{Q}\mathbf{p}$, $\mathbf{R}^T = \mathbf{R}$, $(\mathbf{R}^{-1})^T = \mathbf{R}^{-1}$ we have also

$$F(\mathbf{p}) = 6\mathbf{p}^T \mathbf{Q}^T \mathbf{R}^{-1} \mathbf{Q} \mathbf{p} + \alpha (\mathbf{g} - \mathbf{p})^T \mathbf{D}^2 (\mathbf{g} - \mathbf{p}) . \tag{34}$$

A necessary condition for $\mathbf{p}$ to be the point of an extremum is

$$F'(\mathbf{p}) = 12\mathbf{Q}^T \mathbf{R}^{-1} \mathbf{Q} \mathbf{p} - 2\alpha \mathbf{D}^2 (\mathbf{g} - \mathbf{p}) = \mathbf{O} . \tag{35}$$

With $6\mathbf{R}^{-1}\mathbf{Q}\mathbf{p} = \mathbf{m}$, we can write it as

$$\mathbf{Q}^T \mathbf{m} - \alpha \mathbf{D}^2 (\mathbf{g} - \mathbf{p}) = \mathbf{O} \quad \text{or} \quad \mathbf{D}^2 (\mathbf{g} - \mathbf{p}) = (1/\alpha) \mathbf{Q}^T \mathbf{m} . \tag{36}$$

Multiplying (36) from the left by $6\mathbf{Q}\mathbf{D}^{-2}$ and using (31) we obtain

$$6\mathbf{Q}\mathbf{g} - 6\mathbf{Q}\mathbf{p} = (1/\alpha) 6\mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T \mathbf{m}; \quad \text{rearranging it, we have}$$

$$(\mathbf{R} + (6/\alpha) \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T) \mathbf{m} = 6 \, \mathbf{Q}\mathbf{g} , \tag{37}$$

or

$$(\tfrac{1}{6}\alpha \mathbf{R} + \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T) \mathbf{u} = 6\mathbf{Q}\mathbf{g} \quad \text{with} \quad \mathbf{m} = \tfrac{1}{6}\alpha \mathbf{u} \quad (\text{for small } \alpha \to 0).$$

System (37) can be used to determine the parameters m_i (or u_i) of the spline we search for. The values p_i can be then calculated using (36):

$$\mathbf{p} = \mathbf{g} - (1/\alpha) \mathbf{D}^{-2} \mathbf{Q}^T \mathbf{m} . \tag{38}$$

For the least-square deviation we have $B = (\mathbf{g} - \mathbf{p})^T \mathbf{D}^2(\mathbf{g} - \mathbf{p}) = \|\mathbf{D}(\mathbf{g} - \mathbf{p}\|_2^2 = (1/\alpha^2) \|\mathbf{D}^{-1}\mathbf{Q}^T\mathbf{m}\|_2^2 = \frac{1}{36}\|\mathbf{D}^{-1}\mathbf{Q}^T\mathbf{u}\|_2^2$, and finally $F(\mathbf{p}) = \frac{1}{6}\mathbf{m}^T\mathbf{R}\mathbf{m} + \alpha B$.
The function values of $S(x)$ can be obtained using (30). We can see from (37) that for $\alpha \to \infty$, $S(x)$ converges to the spline interpolating the mean-values g_i; for $\alpha \to 0$, the vector $\mathbf{u}$ becomes independent of $\mathbf{R}$ and $\mathbf{m} \to \mathbf{O}$; $S(x)$ then converges to a constant function (the least-square approximation of g_i).

Following [2], we can introduce another functional

$$F_1(\mathbf{p}) = (1 - \alpha) \int_a^b (S')^2 \, dx + \alpha \sum_{i=0}^{n} w_i h_i^2 (g_i - p_i)^2 \,, \quad \alpha \in [0, 1] \,, \tag{40}$$

which is also minimized by the natural quadratic spline $S(x)$. Proceeding in an analogous manner, from $F_1'(\mathbf{p}) = \mathbf{O}$ we obtain the system of equations

$$[6(1 - \alpha)\, \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T + \alpha\mathbf{R}]\, \mathbf{m} = 6\alpha\mathbf{Q}\mathbf{g} \,, \quad \text{or, with} \quad \mathbf{m} = 6\alpha\mathbf{u} \,, \tag{41}$$

$$[6(1 - \alpha)\, \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T + \alpha\mathbf{R}]\, \mathbf{u} = \mathbf{Q}\mathbf{g} \,, \tag{42}$$

$$\mathbf{p} = \mathbf{g} - 6(1 - \alpha)\, \mathbf{D}^{-2}\mathbf{Q}^T\mathbf{u} \,, \tag{43}$$

$$B = (\mathbf{g} - \mathbf{p})\, \mathbf{D}^2(\mathbf{g} - \mathbf{p}) = \|\mathbf{D}(\mathbf{g} - \mathbf{p})\|_2^2 = \|6(1 - \alpha)\, \mathbf{D}^{-1}\mathbf{Q}^T\mathbf{u}\|_2^2 \,. \tag{44}$$

The system of equations (41), (42) for $\alpha = 1$ gives the interpolating spline, for $\alpha \to 0$ we have $m_i \to 0$ (constants least-square approximation). Algorithmically the system (42) is easier to handle than the system (37).
In both systems – (37), (41) or (42) – we can see that
- the matrix $\mathbf{R}$ is symmetric and tridiagonal (see (20));
- the matrix $\mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T$ is symmetric and tridiagonal, too:

$$\mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T = \begin{bmatrix} d_0 + d_1, & -d_1, & & & \\ -d_1, & d_1 + d_2, & -d_2, & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -d_{n-1} \\ & & & -d_{n-1}, & d_{n-1} + d_n \end{bmatrix},$$

$$\mathbf{D}^{-2} = \operatorname{diag}[\mathrm{d}_i] \,.$$

These facts imply that the matrices

$$\mathbf{R} + (6/\alpha)\, \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T \,, \quad 6(1 - \alpha)\, \mathbf{Q}\mathbf{D}^{-2}\mathbf{Q}^T + \alpha\mathbf{R}$$

are symmetric and tridiagonal, too.

Both matrices are diagonally dominant and so we have a unique solution of the systems (37) or (41) for any data α, $\mathbf{g}$, $\mathbf{w}$.

Theorem 5. *There is a unique quadratic smoothing spline $S(x)$ to any data x_i, g_i, w_i, α under consideration.*

8.1 The approximation properties of the mean-value interpolating or smoothing spline $S(x)$ to the function $f(x) = x\,e^{-x}$, $x \in [0, 5]$ are demonstrated in Example 1. We have written the values S, S' for
a) interpolating splines related to boundary conditions

$$s_0 = f(x_0)\,, \quad s_{n+1} = f(x_{n+1})\,;$$
$$m_0 = m_{n+1} = 0\,;$$

periodic boundary conditions (Table I, Fig. 1);

Table I (Example 1; interpolation; results rounded to 3—4 decimals).

x_i	$f(x_i)$	$f'(x_i)$	g_i	s_i	m_i	s_i	m_i	s_i	m_i
0·0	0	1	0·1539	$\underline{0}$	0·964	0·109	$\underline{0}$	0·098	0·097
0·4	0·268	0·402	0·3142	0·269	0·381	0·244	0·673	0·246	0·644
0·7	0·348	0·148	0·3615	0·348	0·142	0·354	0·064	0·354	0·072
1·0	0·368	0	0·3645	0·368	−0·006	0·366	0·017	0·367	0·015
1·25	0·358	−0·072	0·3472	0·358	−0·073	0·359	−0·079	0·359	−0·077
1·5	0·335	−0·112	0·3036	0·335	−0·115	0·334	−0·115	0·334	−0·119
2·0	0·271	−0·135	0·2069	0·270	−0·142	0·271	−0·140	0·272	−0·128
3·0	0·149	−0·100	0·0794	0·151	−0·097	0·149	−0·104	0·139	−0·193
5·0	0·034	−0·027		$\underline{0{\cdot}034}$	−0·020	0·045	$\underline{0}$	0·098	0·097
				s_0, s_8		$m_0 = m_8 = 0$		periodic	

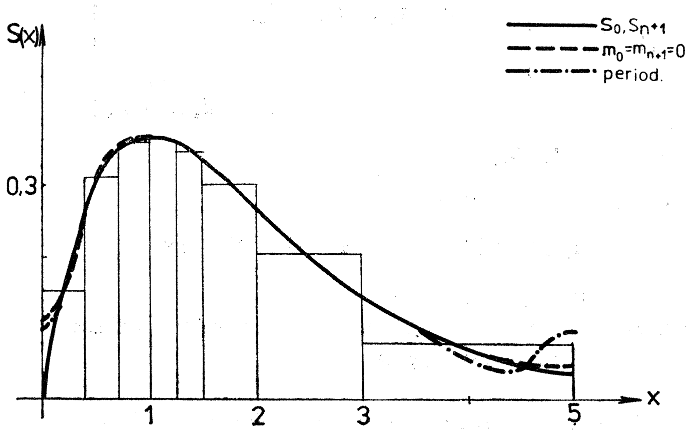

Fig. 1

b) smoothing splines with parameter α and weight coefficients

$$\alpha = 10\,, \quad \text{all} \quad w_i = 1\,;$$

$$\alpha = 10\,, \quad w_i = \{1, 1, 5, 10, 6, 3, 2, 1, 1\} \quad \text{(Table II, Fig. 2)}\,.$$

Table II (Example 1; smoothing).

x_i	s_i	m_i	s_i	m_i
0·0	0·226	0	0·243	0
0·4	0·251	0·128	0·275	0·160
0·7	0·284	0·087	0·321	0·146
1·0	0·301	0·026	0·348	0·037
1·25	0·302	−0·013	0·346	−0·058
1·5	0·295	−0·043	0·326	−0·097
2·0	0·259	−0·103	0·269	−0·131
3·0	0·154	−0·107	0·152	−0·104
5·0	0·046	0	0·047	0
	$\alpha = 10$, $B = 0{\cdot}002$	$w_i = 1$	$\alpha = 10$, $w_i = 1, 1, 5, 10, 6, 3, 2, 1, 1$	$B = 0{\cdot}002$

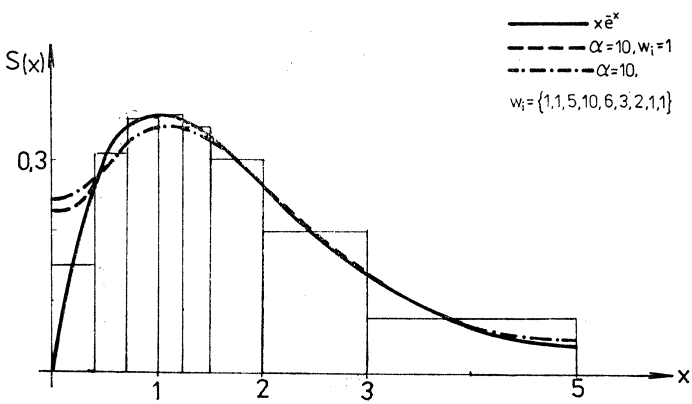

Fig. 2

8.2 Interpolation and smoothing to given data g_i are demonstrated in Example 2:

c) interpolation with respect to boundary conditions

$$m_0 = m_7 = 0\,,$$

$$s_0 = s_7 = 0\,,$$

periodicity conditions (Table III, Fig. 3);

Table III (Example 2; interpolation)

x_i	g_i	s_i	m_i	s_i	m_i	s_i	m_i
1	1	−0·451	0	0	− 1·52	2·20	− 8·96
2	5	3·901	8·70	3·761	9·04	3·082	10·73
3·5	−1	0·669	−13·01	0·694	−13·13	0·79	−13·78
4	2	−1·085	5·998	−1·104	5·94	−1·134	6·09
5	6	5·171	6·51	5·235	6·73	5·224	6·63
7	0	1·146	−10·54	0·796	−11·17	0·927	−10·92
7·5	4	0·341	7·32	1·202	12·80	0·878	10·73
9		5·829	0	−0·768	−14·40	2·20	− 8·96
		$m_0 = m_7 = 0$		$s_0 = s_7 = 0$		periodicity	

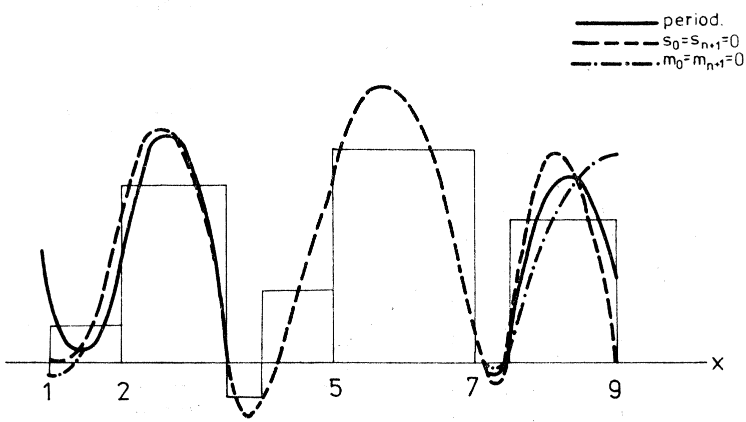

Fig. 3

d) smoothing with parameters

$\alpha = 10$, all $w_i = 1$,

$\alpha = 50$, all $w_i = 1$,

$\alpha = 10$, $w_i = \{1, 5, 1, 5, 10, 20, 1, 5\}$ (Table IV, Fig. 4).

Table IV (Example 2; smoothing).

x_i	g_i	s_i	m_i	s_i	m_i	s_i	m_i
1	1	0·640	0	−0·105	0	0·597	0
2	5	3·337	5·39	3·663	7·54	3·619	6·04
3·5	−1	2·734	−6·20	1·544	−10·36	2·881	− 7·03
4	2	1·361	0·70	−0·161	3·54	1·044	− 7·03
5	6	4·221	5·02	4·712	6·21	4·529	7·29
7	0	3·753	−5·48	2·146	− 8·77	1·520	−10·30
7·5	4	2·891	2·04	1·286	5·33	0·536	6·36
9		4·419	0	5·286	0	5·308	0
		$\alpha = 10$		$\alpha = 50$		$\alpha = 10$	
		$w_i = 1$		$w_i = 1$		$w_i = 1, 5, 1, 5, 10, 20, 1, 5$	

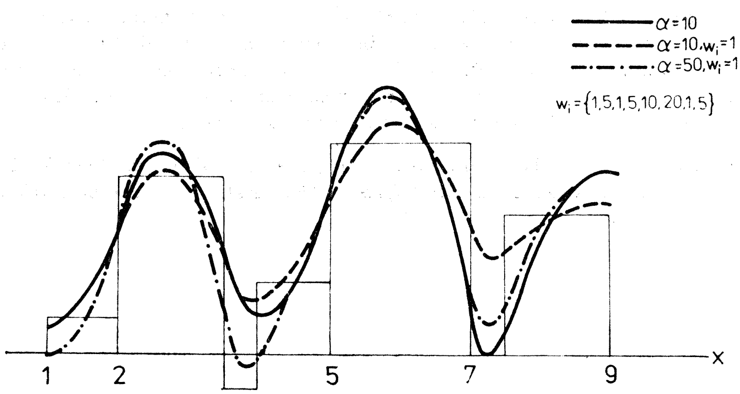

Fig. 4

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Souhrn

PŘIROZENÝ A VYHLAZUJÍCÍ KVADRATICKÝ SPLAJN

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V práci se studují podmínky existence, konstrukce a vlastnosti kvadratického splajnu, interpolujícího lokální integrály (střední hodnoty) na zadané síti uzlů. Jsou uvedeny soustavy rovnic pro výpočet parametrů takového splajnu za různých okrajových podmínek, tvrzení o existenci a jednoznačnosti takových splajnů (Věta 1), jejich extremální vlastnosti (Věta 2), věta o jejich aproximačních vlastnostech (Věta 3). Dále je ukázána konstrukce kvadratického splajnu, vyhlazujícího zadané střední hodnoty; příslušný minimalizovaný funkcionál obsahuje další volitelné parametry (Věta 4, Věta 5). Výsledky jsou ilustrovány na příkladech.

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