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Some Algorithms for Quartic Smoothing Splines *

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Abstract

This paper treats quartic splines smoothing mean values. Local representation using the first and the second derivatives in knots is applied. Two algorithms of computing these local parameters are presented for all three types (natural, periodic and complete) of smoothing spline.

Key words: Splines, quartic splines, smoothing mean values.

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1 Quartic spline interpolating mean values

1.1 Statement of the problem

Definition 1.1 Let us have the set of knots

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

The quartic spline $S_{41}(x)$ with defect one on the knot sequence (Δx) is a function with properties:

1. $S_{41}(x)$ is a fourth order polynomial on every interval $[x_i, x_{i+1}]$, $i = 0(1)n$
2. $S_{41} \in C^3[x_0, x_{n+1}]$ (Continuity condition)

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The vector space of functions satisfying these properties will be denoted by $S_{41}(\Delta x)$; it is known that $dim S_{41}(\Delta x) = n + 5$ (see [7]).

Definition 1.2 Let us have given values g_i, $i = 0(1)n$. We say that the quartic spline $S_{41}(x) \in S_{41}(\Delta x)$ interpolates mean values g_i on the knot sequence (Δx) (MVI spline) if the following conditions are satisfied:

$$\int_{x_i}^{x_{i+1}} S_{41}(x)dx = h_i g_i, \quad i = 0(1)n \tag{1}$$

Remark 1 Because $\dim S_{41}(\Delta x) = n + 5$ we need prescribe four conditions besides MVI conditions (for example two boundary conditions at both boundary knots—function and some derivative values, periodicity conditions, more general conditions). Some subclass of such splines will be used in the following.

Definition 1.3 Let us have given values $s_0, m_0, s_{n+1}, m_{n+1}$. We call a MVI spline $S_{41}(x)$

(a) a natural quartic spline if it satisfies boundary conditions

$$S''_{41}(a) = S''_{41}(b) = S^{(3)}_{41}(a) = S^{(3)}_{41}(b) = 0; \tag{2}$$

(b) a periodic quartic spline if it satisfies boundary conditions

$$S^{(j)}_{41}(a) = S^{(j)}_{41}(b), \quad j = 0(1)3; \tag{3}$$

(c) a complete quartic spline if it satisfies boundary conditions

$$S_{41}(a) = s_0, \quad S'_{41}(a) = m_0, \quad S_{41}(b) = s_{n+1}, \quad S'_{41}(b) = m_{n+1}. \tag{4}$$

1.2 Local parameters, continuity conditions

Theorem 1.4 *Let us denote by g_i mean values (1) of $S_{41}(x)$ on $[x_i, x_{i+1}]$, $i = 0(1)n$ and further $m_i = S'_{41}(x_i)$, $M_i = S''_{41}(x_i)$ for $i = 0(1)n + 1$. Then we can write the spline S_{41} on every interval $[x_i, x_{i+1}]$ with these parameters as*

$$\begin{aligned} S_{41}(x) &= g_i + m_i h_i \left(\frac{1}{2}q^4 - q^3 + q - \frac{7}{20}\right) + m_{i+1} h_i \left(-\frac{1}{2}q^4 + q^3 - \frac{3}{20}\right) + \\ &+ M_i h_i^2 \left(\frac{1}{4}q^4 - \frac{2}{3}q^3 + \frac{1}{2}q^2 - \frac{1}{20}\right) + M_{i+1} h_i^2 \left(\frac{1}{4}q^4 - \frac{1}{3}q^3 + \frac{1}{30}\right) \end{aligned} \tag{5}$$

where $q = (x - x_i)/h_i$ is the local parameter, $q \in [0, 1]$.

Remark 2

- The local representation (5) we shall denote (m, M) representation of quartic spline interpolating mean values on the knot sequence (Δx) (for the similar representation of quartic splines interpolating function values see [7]).

- The coefficients (quartic polynomials in variable q) multiplying the parameters g_i, m_i, m_{i+1}, M_i and M_{i+1} are often called basis functions of the MVI problem in (m, M) representation.
- The local representation (5) used for neighbouring intervals ensures implicitly the continuity of $S'_{41}(x)$, $S''_{41}(x)$ in common point.

Theorem 1.5 *The continuity conditions for $S_{41}(x)$ and $S_{41}^{(3)}(x)$ in the knots x_i, $i = 1(1)n$ we can write as recurrence relations:*

$$\frac{3}{20}h_{i-1}m_{i-1} + \frac{7}{20}(h_{i-1} + h_i)m_i + \frac{3}{20}h_i m_{i+1} + \frac{1}{30}h_{i-1}^2 M_{i-1} + \\ + \frac{1}{20}(h_i^2 - h_{i-1}^2)M_i - \frac{1}{30}h_i^2 M_{i+1} = g_i - g_{i-1}, \tag{6}$$

$$m_{i-1} + (p_i^2 - 1)m_i - p_i^2 m_{i+1} + \frac{1}{3}h_{i-1}M_{i-1} + \frac{2}{3}(h_{i-1} + p_i^2 h_i)M_i + \\ + \frac{1}{3}h_i p_i^2 M_{i+1} = 0, \tag{7}$$

where $p_i = h_{i-1}/h_i$, $i = 1(1)n$.

Proof The recurrences follow from (m, M) representation when comparing expressions for $S_{41}(x)$, $S_{41}^{(3)}(x)$ at common point x_i of intervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$. Let us mention that the conditions (6), (7) form $2n$ linear equations with $2n + 4$ unknown parameters m_i, M_i. □

1.3 Computing local parameters m, M

For MVI spline on the knot sequence (Δx) we have prescribed the mean values g_i. Let us denote $s_i = S_{41}(x_i)$, $T_i = S_{41}^{(3)}(x_i)$ for $i = 0(1)n + 1$. Unknown local parameters m, M of the spline S_{41} we obtain as the solution of the system of linear equations created by continuity conditions (6) and (7) completed by corresponding boundary conditions.

Let us mention the special cases introduced in the Definition 1.3

(a) *Natural spline ($M_0 = M_{n+1} = T_0 = T_{n+1} = 0$)*
The terms with M_0 and M_{n+1} are left out in (6) and (7) and the whole system is completed by expressions for T_0 and T_{n+1} taken from (m, M) representation:

$$-\frac{6}{h_0^2}m_0 + \frac{6}{h_0^2}m_1 - \frac{2}{h_0}M_1 = 0 \tag{8}$$

$$-\frac{6}{h_n^2}m_{n+1} + \frac{6}{h_n^2}m_n + \frac{2}{h_n}M_n = 0 \tag{9}$$

(b) *Periodic spline ($s_0 = s_{n+1}$, $m_0 = m_{n+1}$, $M_0 = M_{n+1}$, $T_0 = T_{n+1}$)*
Using $m_0 = m_{n+1}$, $M_0 = M_{n+1}$, continuity conditions (6) and (7) in

knot x_1 are rewritten as

$$\frac{3}{20}h_0 m_{n+1} + \frac{7}{20}(h_0 + h_1)m_1 + \frac{3}{20}h_1 m_2 + \frac{1}{30}h_0^2 M_{n+1} + \\ + \frac{1}{20}(h_1^2 - h_0^2)M_1 - \frac{1}{30}h_1^2 M_2 = g_1 - g_0, \tag{10}$$

$$m_{n+1} + (p_1^2 - 1)m_1 - p_1^2 m_2 + \frac{1}{3}h_0 M_{n+1} + \frac{2}{3}(h_0 + p_1^2 h_1)M_1 + \\ + \frac{1}{3}h_1 p_1^2 M_2 = 0. \tag{11}$$

Putting $s_0 = s_{n+1}$, $T_0 = T_{n+1}$, the system (6), (7), (10), (11) is completed by

$$\frac{3}{20}h_n m_n + \frac{7}{20}(h_n + h_0)m_{n+1} + \frac{3}{20}h_0 m_1 + \frac{1}{30}h_n^2 M_n + \\ + \frac{1}{20}(h_0^2 - h_n^2)M_{n+1} - \frac{1}{30}h_0^2 M_1 = g_0 - g_n, \tag{12}$$

$$m_n + (p_{n+1}^2 - 1)m_{n+1} - p_{n+1}^2 m_1 + \frac{1}{3}h_n M_n + \\ + \frac{2}{3}(h_n + p_{n+1}^2 h_0)M_{n+1} + \frac{1}{3}h_0 p_{n+1}^2 M_1 = 0, \tag{13}$$

where $p_{n+1} = h_n/h_0$.

(c) *Complete spline (with prescribed values $s_0, s_{n+1}, m_0, m_{n+1}$)*
The terms with prescribed m_0 and m_{n+1} are transferred to the right sides of (6) and (7) and the whole system is completed by expressions for s_0 and s_{n+1} in (m, M) representation:

$$-\frac{3h_0}{20}m_1 - \frac{h_0^2}{20}M_0 + \frac{h_0^2}{30}M_1 = s_0 - g_0 + \frac{7h_0}{20}m_0 \tag{14}$$

$$\frac{3h_n}{20}m_n - \frac{h_n^2}{20}M_{n+1} + \frac{h_n^2}{30}M_n = s_{n+1} - g_n - \frac{7h_n}{20}m_{n+1} \tag{15}$$

In all three cases the completed system has formally similar form:

$$\begin{pmatrix} \mathbf{A1} & \mathbf{A2} \\ \mathbf{A3} & \mathbf{A4} \end{pmatrix} \begin{pmatrix} m \\ M \end{pmatrix} = \begin{pmatrix} \mathbf{B1} \\ \mathbf{B2} \end{pmatrix} p. \tag{16}$$

The elements of the matrices $\mathbf{A1}, \mathbf{A2}, \mathbf{A3}, \mathbf{A4}$ and $\mathbf{B1}$,$\mathbf{B2}$ are described in continuity conditions (6),(7) and boundary relations (8),(9) (eventually (10) -(13) or (14),(15)). They depend on the geometry of the knot sequence (Δx) only. The matrices $\mathbf{A1}$, $\mathbf{A4}$ are tridiagonal and $\mathbf{A2}$, $\mathbf{A3}$ are band matrices with three nonzero bands (or all matrices are cyclic tridiagonal in case of periodic boundary conditions). We can prove the regularity of the matrix $\begin{pmatrix} \mathbf{A1} & \mathbf{A2} \\ \mathbf{A3} & \mathbf{A4} \end{pmatrix}$ for equidistant knot sequence (Δx) using more detailed concepts of diagonally dominant matrices (given in [2]). In the case of general knot sequence the computations did not show any problems with the regularity, but we have not proved it in general. The vector p contains prescribed mean values (and prescribed boundary conditions in case of complete spline) and m, M are vectors of unknown first and second derivatives in knots.

In the case of regular matrix of the system (16) we can denote

$$\mathbf{S} = \begin{pmatrix} \mathbf{A1} & \mathbf{A2} \\ \mathbf{A3} & \mathbf{A4} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{B1} \\ \mathbf{B2} \end{pmatrix}, \tag{17}$$

and we write the solutions of (16) as

$$\begin{pmatrix} m \\ M \end{pmatrix} = \mathbf{S}p. \tag{18}$$

Remark 3 The (m, M) representation and some other representations of quartic splines interpolating mean values and algorithms for computing unknown parameters of these representations are described in [3], [4] and [9].

1.4 Extremal properties of MVI quartic splines

Let us denote

$$\begin{aligned} V &= \{f \in W_2^2[a,b]; \textstyle\int_{x_i}^{x_{i+1}} f(x)dx = h_i g_i,\ i = 0(1)n\}, \\ V_{per} &= \{f \in V; f \textit{ is periodic with the period } (b-a)\}, \\ V_{com} &= \{f \in V; f(a) = s_0; f'(a) = m_0, f(b) = s_{n+1}, f'(b) = m_{n+1}\} \\ & \qquad \textit{where } s_0, s_{n+1}, m_0, m_{n+1} \textit{ are prescribed numbers,} \end{aligned}$$

and further introduce the functional

$$J_1(f) = \|f''\|_2^2 = \int_a^b [f''(x)]^2 dx \tag{19}$$

$\big(J_1(f)$ can be considered as some measure of smoothness of the curve $f(x)\big)$.

Theorem 1.6 *Functional $J_1(f)$ attains its minimum*

(a) on the set V at some natural spline S_{41};

(b) on the set V_{per} at some periodic spline S_{41};

(c) on the set V_{com} at some complete spline S_{41}.

Proof Assume that $f \in V$ and S_{41} interpolates mean values $g_i = \frac{1}{h_i}\int\limits_{x_i}^{x_{i+1}} f(x)dx$ for $i = 0(1)n$. Using integration by parts we have

$$(S_{41}'', f'' - S_{41}'')_2 = \int_a^b S_{41}''(f - S_{41})''dx = \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} S_{41}''(f - S_{41})''dx =$$

$$= \sum_{i=0}^{n} \{[S''_{41}(f - S_{41})']_{x_i}^{x_{i+1}} - [S'''_{41}(f - S_{41})]_{x_i}^{x_{i+1}} +$$

$$+ \int_{x_i}^{x_{i+1}} S_{41}^{(4)}(f - S_{41})dx\} = [S''_{41}(f' - S'_{41})]_a^b - [S'''_{41}(f - S_{41})]_a^b.$$

Then any from former mentioned boundary conditions

(a) natural conditions $S''_{41}(a) = S''_{41}(b) = S'''_{41}(a) = S'''_{41}(b) = 0$;

(b) periodic conditions $S_{41}^{(j)}(a) = S_{41}^{(j)}(b)$, $j = 0(1)3$;

(c) complete conditions

$$\begin{aligned} S_{41}(a) &= f(a) = s_0, \quad S_{41}(b) = f(b) = s_{n+1}, \\ S'_{41}(a) &= f'(a) = m_0, \quad S'_{41}(b) = f'(b) = m_{n+1}, \end{aligned}$$

imply $(S''_{41}, f'' - S''_{41})_2 = 0$. Using it and writting

$$||f'' - S''_{41}||_2^2 = ||f''||_2^2 - 2(S''_{41}, f'' - S''_{41})_2 - ||S''_{41}||_2^2$$

we obtain $||f''||_2^2 = ||S''_{41}||_2^2 + ||f'' - S''_{41}||_2^2$; therefore the inequality $||f''||_2^2 \geq ||S''_{41}||_2^2$ holds. □

Remark 4

- We say that splines introduced in the previous theorem have the extremal properties mentioned here with respect to the functional J_1.
- The general theorem for spline of even degree is formulated in [6]. (The general theorem for splines of odd degree can be found here, too.)
- Some special theorem of this kind for quartic splines is referred in [5].

2 Quartic smoothing spline

The smoothing splines gives some compromise between an interpolation of prescribed values and a least squares approximation of them. The statement of the general smoothing problem for even (and also odd) degree splines is given e.g in [6]. The algorithms for linear (see [6],[9]), quadratic (see [6],[8]) and cubic splines (see [1],[6],[9]) are often mentioned. The high order splines on equidistant knot sequence are often used too (see [5]). In this section two algorithms for quartic splines on general knot sequence are described.

2.1 The smoothing problem

Let us have given a knot sequence (Δx) with prescribed values $g = (g_0, \dots g_n)^T$, positive weight coefficients $w = (w_0, \dots, w_n)^T$ { in case of complete spline $g = (\bar{m}_0, \bar{s}_0, g_0, g_1, \dots g_n, \bar{s}_{n+1}, \bar{m}_{n+1})^T$ and $w = (w_{-2}, \dots, w_{n+2})^T$ } and some smoothing parameter $\alpha > 0$.
Let us denote:

$$\begin{aligned} V^s &= W_2^2[x_0, x_{n+1}], \\ V^s_{per} &= \{f \in V^s;\ f \text{ is periodic with a period } (b-a)\}, \\ p_i &= \frac{1}{h_i} \int_{x_i}^{x_{i+1}} f(x)dx,\ i = 0(1)n, \end{aligned}$$

and further introduce the functionals

$$J_1(f) = \|f''\|_2^2 = \int_a^b [f''(x)]^2 dx \quad (\textit{ a measure of smoothness }), \tag{20}$$

$$E_1(f) = \sum_{i=0}^{n} w_i(g_i - p_i)^2 \quad (\textit{ a measure of interpolation }), \tag{21}$$

$$\begin{aligned} E_2(f) = {} & w_{-2}(\bar{m}_0 - m_0)^2 + w_{-1}(\bar{s}_0 - s_0)^2 + E_1(f) + \\ & + w_{n+1}(\bar{s}_{n+1} - s_{n+1})^2 + w_{n+2}(\bar{m}_{n+1} - m_{n+1})^2 \\ & (\textit{ boundary conditions acceptance measure included }). \end{aligned} \tag{22}$$

Theorem 2.1 *Let the knot sequence (Δx), values g and coefficients w, α be given. Then the functional*

$$J_2(f) = J_1(f) + \alpha E_1(f) \tag{23}$$

attains its minimum

(a) on the set V^s at some natural spline S_{41};

(b) on the set V^s_{per} at some periodic spline S_{41}.

The functional

$$J_3(f) = J_1(f) + \alpha E_2(f) \tag{24}$$

is minimized on the set V^s by some complete spline S_{41}. (Let us mention that in all cases the extremal spline interpolates some unknown mean values p_i.)

Proof

(a) Assume that $f \in V^s$ gives a minimum to J_2 on V^s and that p_i are corresponding mean values of $f(x)$ and that natural spline $S_{41}(x) \in V^s$ interpolates these mean values. Then $E_1(f) = E_1(S_{41})$ and extremal properties of S_{41} from Theorem 1.6 imply $J_1(S_{41}) \leq J_1(f)$; we have therefore $J_2(S_{41}) \leq J_2(f),\ \forall f \in V^s$.

(b) In case of periodic spline the proof is similar.

(c) Assume that $f \in V^s$ gives a minimum to J_3 on V^s and that p_i are corresponding mean values of $f(x)$. Let $S_{41}(x) \in V^s$ interpolate mean values p_i and satisfy boundary conditions $s_0 = f(x_0), s_{n+1} = f(x_{n+1}), m_0 = f'(x_0), m_{n+1} = f'(x_{n+1})$. Then $E_2(f) = E_2(S_{41})$ and extremal properties of S_{41} imply $J_1(S_{41}) \le J_1(f)$; we have therefore $J_3(S_{41}) \le J_3(f), \forall f \in V^s$.

□

Remark 5 The minimization problems (23) and (24) in Theorem 2.1 are often called the *smoothing problems.*

2.2 Functionals J_1, E_1 and E_2 in m, M terms

We give the more detailed descriptions of functionals to be minimized in terms of (m, M) local representation here.

Theorem 2.2 *If $S_{41}(x)$ is MVI quartic spline then we can express functional $J_1(S_{41})$ as a function of the first and the second derivatives of S_{41} in knots x_i as follows:*

$$J_1(S_{41}) = \sum_{i=0}^{n}\Big(\tfrac{6}{5h_i}m_i^2 + \tfrac{6}{5h_i}m_{i+1}^2 + \tfrac{2h_i}{15}M_i^2 + \tfrac{2h_i}{15}M_{i+1}^2 + 2(-\tfrac{6}{5h_i}m_im_{i+1} + \\ + \tfrac{1}{10}m_iM_i + \tfrac{1}{10}m_iM_{i+1} - \tfrac{1}{10}m_{i+1}M_i - \tfrac{1}{10}m_{i+1}M_{i+1} - \tfrac{h_i}{30}M_iM_{i+1})\Big) \tag{25}$$

Proof Differentiating twice the (m, M) representation we obtain

$$S_{41}''(x) = A_i(q)m_i + B_i(q)m_{i+1} + C_i(q)M_i + D_i(q)M_{i+1}$$

with

$$\begin{aligned} A_i(q) &= 6(q^2 - q)/h_i, & B_i(q) &= -A_i(q), \\ C_i(q) &= 3q^2 - 4q + 1, & D_i(q) &= 3q^2 - 2q. \end{aligned}$$

Using the identity $\int_{x_i}^{x_{i+1}} (S_{41}''(x))^2 dx = h_i \int_0^1 (S_{41}''(q))^2 dq$ we can compute:

$$\begin{aligned} h_i \int_0^1 A_i^2(q)dq &= 6/(5h_i); & h_i \int_0^1 C_i^2(q)dq &= 2h_i/15; \\ h_i \int_0^1 D_i^2(q)dq &= 2h_i/15; & h_i \int_0^1 A_i(q)C_i(q)dq &= 1/10; \\ h_i \int_0^1 A_i(q)D_i(q)dq &= 1/10; & h_i \int_0^1 C_i(q)D_i(q)dq &= -h_i/30. \end{aligned}$$

Substituting these results into $J_1(S_{41}) = \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} (S_{41}''(x))^2 dx$ we obtain (25). □

2.2.1 Natural spline

Under natural boundary conditions (2) we can write (25) in the following matrix form

$$J_1(S_{41}) = (m^T, M^T) \begin{pmatrix} \mathbf{G1} & \mathbf{G2} \\ \mathbf{G2}^T & \mathbf{G4} \end{pmatrix} \begin{pmatrix} m \\ M \end{pmatrix} \quad , \tag{26}$$

where we use the vector and matrix notation: $m = (m_0, \ldots m_{n+1})^T \in R^{n+2}$,

$$M = (M_1, \ldots M_n)^T \in R^n, \quad \mathbf{G1} \in R^{(n+2)\times(n+2)},$$

$$\mathbf{G1} = \begin{pmatrix} \frac{6}{5h_0} & -\frac{6}{5h_0} & & & \\ -\frac{6}{5h_0} & \frac{6}{5h_0} + \frac{6}{5h_1} & -\frac{6}{5h_1} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{6}{5h_{n-1}} & \frac{6}{5h_{n-1}} + \frac{6}{5h_n} & -\frac{6}{5h_n} \\ & & & -\frac{6}{5h_n} & \frac{6}{5h_n} \end{pmatrix},$$

$$\mathbf{G2} = \begin{pmatrix} \frac{1}{10} & & & & \\ 0 & \frac{1}{10} & & & \\ -\frac{1}{10} & 0 & \frac{1}{10} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{10} & 0 & \frac{1}{10} \\ & & & -\frac{1}{10} & 0 \\ & & & & -\frac{1}{10} \end{pmatrix} \in R^{(n+2)\times n},$$

$$\mathbf{G4} \in R^{n\times n},$$

$$\mathbf{G4} = \begin{pmatrix} \frac{2(h_0+h_1)}{15} & -\frac{h_1}{30} & & & \\ -\frac{h_1}{30} & \frac{2(h_1+h_2)}{15} & -\frac{h_2}{30} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{h_{n-2}}{30} & \frac{2(h_{n-2}+h_{n-1})}{15} & -\frac{h_{n-1}}{30} \\ & & & -\frac{h_{n-1}}{30} & \frac{2(h_{n-1}+h_n)}{15} \end{pmatrix}$$

(tridiagonal matrices; elements not described are equal zero).

2.2.2 Periodic spline

Under periodic boundary conditions (3) we can write (25) in the following matrix form

$$J_1(S_{41}) = (m^T, M^T) \begin{pmatrix} \mathbf{G1} & \mathbf{G2} \\ \mathbf{G2}^T & \mathbf{G4} \end{pmatrix} \begin{pmatrix} m \\ M \end{pmatrix} \quad , \tag{27}$$

where we use the notation: $m = (m_1, \ldots m_{n+1})^T \in R^{n+1}$,

$$M = (M_1, \ldots M_{n+1})^T \in R^{n+1}, \quad \mathbf{G1} \in R^{(n+1)\times(n+1)},$$

$$\mathbf{G1} = \begin{pmatrix} \frac{6}{5h_0}+\frac{6}{5h_1} & \frac{-6}{5h_1} & & & \frac{-6}{5h_0} \\ \frac{-6}{5h_1} & \frac{6}{5h_1}+\frac{6}{5h_2} & \frac{-6}{5h_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{-6}{5h_{n-1}} & \frac{6}{5h_{n-1}}+\frac{6}{5h_n} & \frac{-6}{5h_n} \\ \frac{-6}{5h_0} & & & \frac{-6}{5h_n} & \frac{6}{5h_n}+\frac{6}{5h_0} \end{pmatrix},$$

$$\mathbf{G2} = \begin{pmatrix} 0 & \frac{1}{10} & & & -\frac{1}{10} \\ -\frac{1}{10} & 0 & \frac{1}{10} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{10} & 0 & \frac{1}{10} \\ \frac{1}{10} & & & -\frac{1}{10} & 0 \end{pmatrix} \in R^{(n+1)\times(n+1)},$$

$$\mathbf{G4} \in R^{(n+1)\times(n+1)},$$

$$\mathbf{G4} = \begin{pmatrix} \frac{2(h_0+h_1)}{15} & -\frac{h_1}{30} & & & -\frac{h_0}{30} \\ -\frac{h_1}{30} & \frac{2(h_1+h_2)}{15} & -\frac{h_2}{30} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{h_{n-1}}{30} & \frac{2(h_{n-1}+h_n)}{15} & -\frac{h_n}{30} \\ -\frac{h_0}{30} & & & -\frac{h_n}{30} & \frac{2(h_n+h_0)}{15} \end{pmatrix}$$

(cyclic tridiagonal matrices).

2.2.3 Complete spline

Under complete boundary conditions (4) we can write (25) in the following matrix form

$$\begin{aligned} J_1(S_{41}) &= (m^T, M^T)\begin{pmatrix} \mathbf{G1} & \mathbf{G2} \\ \mathbf{G2}^T & \mathbf{G4} \end{pmatrix}\begin{pmatrix} m \\ M \end{pmatrix} + (m^T, M^T)\begin{pmatrix} \mathbf{H1} \\ \mathbf{H2} \end{pmatrix} p + \\ &+ p^T(\mathbf{H1}^T, \mathbf{H2}^T)\begin{pmatrix} m \\ M \end{pmatrix} + p^T\mathbf{K}p \quad , \end{aligned} \tag{28}$$

where we use the notation: $p = \left(m_0, s_0, p_0, p_1 \ldots, p_n, s_{n+1}, m_{n+1}\right)^T \in R^{n+5}$,

$$m = (m_1, \ldots m_n)^T \in R^n, \quad M = (M_0, \ldots M_{n+1})^T \in R^{n+2}, \quad \mathbf{G1} \in R^{n\times n},$$

$$\mathbf{G1} = \begin{pmatrix} \frac{6}{5h_0}+\frac{6}{5h_1} & \frac{-6}{5h_1} & & & \\ \frac{6}{5h_1} & \frac{6}{5h_1}+\frac{6}{5h_2} & \frac{-6}{5h_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{-6}{5h_{n-2}} & \frac{6}{5h_{n-2}}+\frac{6}{5h_{n-1}} & \frac{-6}{5h_{n-1}} \\ & & & \frac{-6}{5h_{n-1}} & \frac{6}{5h_{n-1}}+\frac{6}{5h_n} \end{pmatrix},$$

$$\mathbf{G2} = \begin{pmatrix} -\frac{1}{10} & 0 & \frac{1}{10} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{10} & 0 & \frac{1}{10} \end{pmatrix} \in R^{n\times(n+2)},$$

$$\mathbf{G4} = \begin{pmatrix} \frac{2h_0}{15} & -\frac{h_0}{30} & & & \\ -\frac{h_0}{30} & \frac{2(h_0+h_1)}{15} & -\frac{h_1}{30} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{h_{n-1}}{30} & \frac{2(h_{n-1}+h_n)}{15} & -\frac{h_n}{30} \\ & & & -\frac{h_n}{30} & \frac{2h_n}{15} \end{pmatrix} \in R^{(n+2)\times(n+2)},$$

$$\mathbf{H1} \in R^{n\times(n+5)}, \quad \mathbf{H2} \in R^{(n+2)\times(n+5)}, \quad \mathbf{K} \in R^{(n+5)\times(n+5)},$$

$$(\mathbf{H1})_{ij} = \begin{cases} -6/(5h_0) & i = j = 1 \\ -6/(5h_n) & i = n, \quad j = n+5 \\ 0 & others \end{cases}$$

$$(\mathbf{H2})_{ij} = \begin{cases} 1/10 & i = 1,2; j = 1 \\ -1/10 & i = n+1, n+2; \quad j = n+5 \\ 0 & others \end{cases}, \qquad \mathbf{H} = \begin{pmatrix} \mathbf{H1} \\ \mathbf{H2} \end{pmatrix},$$

$$(\mathbf{K})_{ij} = \begin{cases} 6/(5h_0) & i = j = 1 \\ 6/(5h_n) & i = j = n+5 \\ 0 & others. \end{cases}$$

We shall use the matrix notations also for functionals E_1, E_2 in all cases of boundary conditions mentioned. When we denote the diagonal matrices of weight coefficients

$$\mathbf{D}_1 = \text{diag}[w_i]_{i=0}^{n} \quad , \mathbf{D}_2 = \text{diag}[w_i]_{i=-2}^{n+2}$$

then the matrix forms of functionals E_1 (defined by (21)) and E_2 (defined by (22)) are:

$$E_1 = (g-p)^T \mathbf{D}_1 (g-p), \tag{29}$$

$$E_2 = (g-p)^T \mathbf{D}_2 (g-p). \tag{30}$$

2.3 Computing local parameters of the smoothing spline

Let us denote

$$\mathbf{G} = \begin{pmatrix} \mathbf{G1} & \mathbf{G2} \\ \mathbf{G2}^T & \mathbf{G4} \end{pmatrix}$$

where $\mathbf{G1}, \mathbf{G2}, \mathbf{G3}, \mathbf{G4}$ are matrices given by (26) (eventually (27) or (28)). Let us have the matrices $\mathbf{S}$ (defined by (17)), $\mathbf{G}$, $\mathbf{D}_1$, $\mathbf{D}_2$, $\mathbf{H}$, $\mathbf{K}$ (described in (28)) and vector g. The algorithm for computing local parameters of quartic splines smoothing given values g can be described in special cases mentioned as follows:

(a) *Natural (or periodic) spline*
Substituting (29), (18) and (26) (or (27)) into functional J_2 defined by (23) we obtain the value of $J_2(S_{41})$ as the function of p (with the same notation) given as

$$J_2(S_{41}) = J_2(p) = p^T \mathbf{S}^T \mathbf{G} \mathbf{S} p + \alpha (g-p)^T \mathbf{D}_1 (g-p).$$

From necessary conditions of minima

$$J_2'(p) = 2\mathbf{S}^T\mathbf{G}\mathbf{S}p - 2\alpha\mathbf{D}_1(g-p) = 0$$

we obtain the system of linear equations for computing unknown mean values p:

$$(\mathbf{S}^T\mathbf{G}\mathbf{S} + \alpha\mathbf{D}_1)p = \alpha\mathbf{D}_1 g \tag{31}$$

Finally we compute unknown parameters m and M using computed p and (18).

(b) *Complete spline*
Substituting (29), (28) and (18) into J_3 (defined in (24)) we obtain

$$J_3(p) = p^T\mathbf{S}^T\mathbf{G}\mathbf{S}p + p^T\mathbf{S}^T\mathbf{H}p + p^T\mathbf{H}^T\mathbf{S}p + p^T\mathbf{K}p + \alpha(g-p)^T\mathbf{D}_2(g-p).$$

The necessary conditions of minima

$$J_3'(p) = 2(\mathbf{S}^T\mathbf{G}\mathbf{S} + \mathbf{S}^T\mathbf{H} + \mathbf{H}^T\mathbf{S} + \mathbf{K})p - 2\alpha\mathbf{D}_2(g-p) = 0$$

produce the system of linear equations for computing unknown values p:

$$(\mathbf{S}^T\mathbf{G}\mathbf{S} + \mathbf{S}^T\mathbf{H} + \mathbf{H}^T\mathbf{S} + \mathbf{K} + \alpha\mathbf{D}_2)p = \alpha\mathbf{D}_2 g \tag{32}$$

Then we again compute unknown parameters m and M using (18).

2.4 Existence and uniqueness

Theorem 2.3 *Let us have given the knot sequence* (Δx) *with prescribed values* $g = (g_0, \dots g_n)^T$, *weight coefficients* $w = (w_0, \dots, w_n)^T$ { *in case of complete spline* $g = (\bar{m}_0, \bar{s}_0, g_0, g_1, \dots g_n, \bar{s}_{n+1}, \bar{m}_{n+1})^T$ *and* $w = (w_{-2}, \dots, w_{n+2})^T$ } *and the smoothing parameter* $\alpha > 0$. *If the matrix of system (16) is regular, then the natural, periodic and complete smoothing quartic spline exist and they are determined uniquely for all* $\alpha > 0$.

Proof The definition of functional J_1 implies $J_1 \geq 0$. The matrices $\mathbf{D}_1$ and $\mathbf{D}_2$ are positive definite (i.e. $u^T\mathbf{D}_i u > 0$, $\forall u \neq 0$, $i = 1, 2$) because $\mathbf{D}_1$ and $\mathbf{D}_2$ are diagonal with positive factors on the diagonal. Then

(a) $0 < J_1(u) + \alpha u^T\mathbf{D}_1 u = u^T(\mathbf{S}^T\mathbf{G}\mathbf{S} + \alpha\mathbf{D}_1)u$, $\forall u \neq 0$ for natural and periodic splines.

(b) $0 < J_1(u) + \alpha u^T\mathbf{D}_2 u = u^T(\mathbf{S}^T\mathbf{G}\mathbf{S} + \mathbf{S}^T\mathbf{H} + \mathbf{H}^T\mathbf{S} + \mathbf{K} + \alpha\mathbf{D}_2)u$, $\forall u \neq 0$ for complete spline.

These relations imply that matrices $(\mathbf{S}^T\mathbf{G}\mathbf{S} + \mathbf{S}^T\mathbf{H} + \mathbf{H}^T\mathbf{S} + \mathbf{K} + \alpha\mathbf{D}_2)$ and $(\mathbf{S}^T\mathbf{G}\mathbf{S} + \alpha\mathbf{D}_1)$ are regular and therefore systems (31) and (32) have only one solution p. The parameters m, M are then uniquely determined from (18). □

2.5 Computing local parameters by optimization techniques

The smoothing problem (23) for natural and periodic spline has the following form of quadratic programming problem (relations (16), (29), (26) or (27) used):

$$\textit{Minimize} \qquad (m^T, M^T, p^T) \begin{pmatrix} \mathbf{G1} & \mathbf{G2} & \mathbf{0} \\ \mathbf{G2}^T & \mathbf{G4} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \alpha\mathbf{D}_1 \end{pmatrix} \begin{pmatrix} m \\ M \\ p \end{pmatrix} +$$

$$+ (m^T, M^T, p^T) \begin{pmatrix} 0 \\ 0 \\ -2\alpha\mathbf{D}_1 g \end{pmatrix} + \alpha g^T \mathbf{D}_1 g$$

$$\textit{under conditions} \quad \begin{pmatrix} \mathbf{A1} & \mathbf{A2} & -\mathbf{B1} \\ \mathbf{A3} & \mathbf{A4} & -\mathbf{B2} \end{pmatrix} \begin{pmatrix} m \\ M \\ p \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

The smoothing problem (24) for complete spline has the following form of the quadratic programming problem (using (16), (28) and (30)):

$$\textit{Minimize} \qquad (m^T, M^T, p^T) \begin{pmatrix} \mathbf{G1} & \mathbf{G2} & \mathbf{H1} \\ \mathbf{G2}^T & \mathbf{G4} & \mathbf{H2} \\ \mathbf{H1}^T & \mathbf{H2}^T & \mathbf{K} + \alpha\mathbf{D}_2 \end{pmatrix} \begin{pmatrix} m \\ M \\ p \end{pmatrix} +$$

$$+ (m^T, M^T, p^T) \begin{pmatrix} 0 \\ 0 \\ -2\alpha\mathbf{D}_2 g \end{pmatrix} + \alpha g^T \mathbf{D}_2 g$$

$$\textit{under conditions} \quad \begin{pmatrix} \mathbf{A1} & \mathbf{A2} & -\mathbf{B1} \\ \mathbf{A3} & \mathbf{A4} & -\mathbf{B2} \end{pmatrix} \begin{pmatrix} m \\ M \\ p \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Remark 6 These quadratic programming problems are equivalent to solving the Kuhn–Tucker conditions as the systems of linear equations with sparse matrix.

2.6 Numerical examples

The algorithms in sections 2.3 (Alg. 2.3) and 2.5 (Alg. 2.5) were realized in MATLAB. Both algorithms give identical results.

Example 1 The smoothed values are obtained as sum of mean values of function $f(x)$ and randomly (with uniform distribution) generated error values. This values are smoothed for different parameters α.

(a) Natural smoothing spline:
function $f(x) = 3x^2 \exp^{-x}$, knot sequence $x = [-1 : 0.1 : 4]$ (see Fig. 1).

(b) Periodic smoothing spline:
function $f(x) = \sin(2\pi x)$, knot sequence $x = [0 : 0.02 : 1]$ (see Fig. 2).

(c) Complete smoothing spline:
function $f(x) = (x^2 - 25)^2/100$, knot sequence $x = [-5 : 0.1 : 5]$ (see Fig. 3).

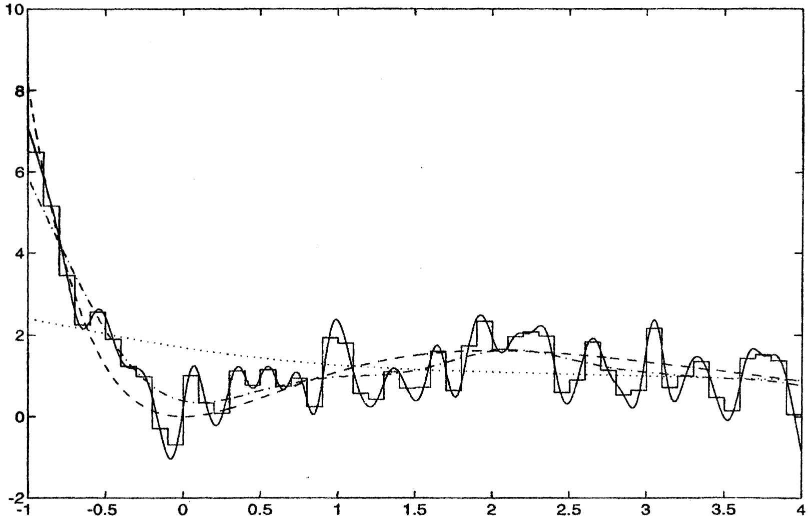

Figure 1: Natural quartic smoothing splines for $\alpha = 0.05$ (dotted), $\alpha = 20$ (dashdot), $\alpha = 1E6$ (solid) and original function (dashed).

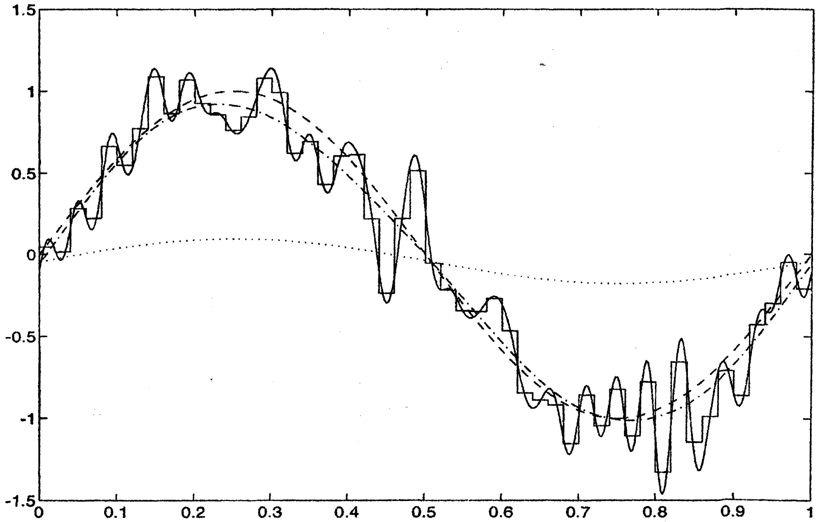

Figure 2: Periodic quartic smoothing splines for $\alpha = 5$ (dotted), $\alpha = 100$ (dashdot), $\alpha = 1E9$ (solid) and original function (dashed).

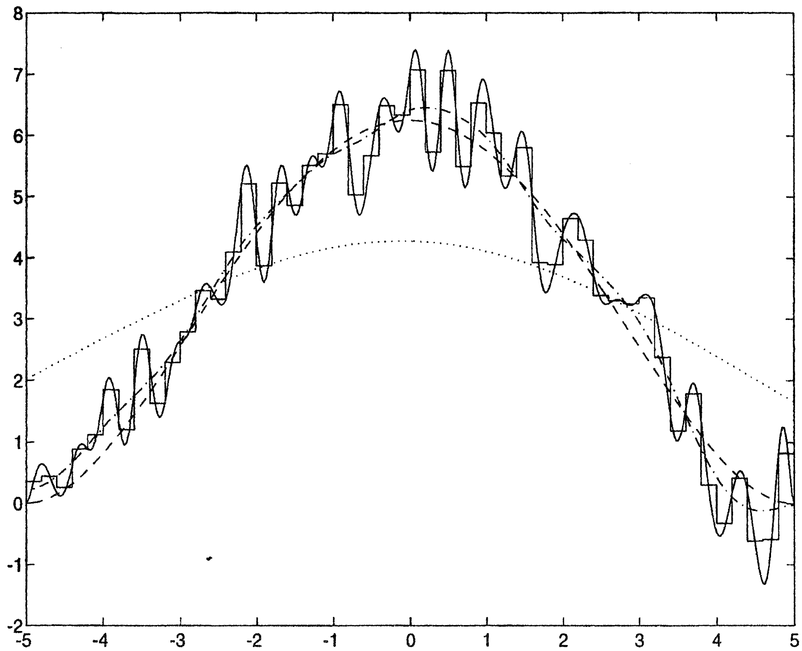

Figure 3: Complete quartic smoothing splines for $\alpha = 0.005$ (dotted), $\alpha = 20$ (dashdot), $\alpha = 1E6$ (solid) and original function (dashed).

Example 2 This example gives a comparison of "computing time" (measured by Matlab function `cputime`) with respect to density of knot sequence (Δx). The function is identical as in example 1.a and $\alpha = 1000$ is used. The results are summarized in following table:

n	10	20	50	100	200	500	1000
alg. 2.3	0.22	0.5	4.28	32.69	270.62	-	-
alg. 2.5	0.44	0.6	1.1	2.25	5.38	28.56	39.27

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