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Quartic Smoothing Splines Generalized *

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Abstract

In the variational theory of splines the smoothing splines are constructed on the base of some extremal properties of interpolatory splines on a proper class of more general functions. The spline degree and the form of the minimized functional (the order of the derivative with minimized norm) are strictly connected here. In this article we use spline free parameters to find spline with minimal value of different functionals used for smoothing (with some choice of the derivative order, of the norm used). We use local spline representation and we formulate the corresponding quadratic programming problems for computation of optimal local spline parameters. The problems of function values and mean values smoothing are considered simultaneously here.

Key words: Smoothing splines, generalized quartic smoothing splines.

2000 Mathematics Subject Classification: 41A15, 65D05

1 Introduction

We can find different approaches to the data smoothing generally and also to the smoothing splines. The well known cubic smoothing splines with given smoothing parameter (see [2]) use some extremal property of natural cubic interpolatory splines and give the minimum to the functional which combines a smoothing criterion (the norm of the spline second derivative squared) and

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the least squares criterion (for given data versus smoothed data on the given spline knotset). This idea was generalized to the function values smoothing (FVS) with natural odd degree splines and mean values smoothing (MVS) with even degree splines ([8]), to the splines in general Hilbert spaces ([1], [11], [15]. Some another forms of the smoothing criterion (the norm of jumps in the third derivative) were introduced in [3], [18], [14], a statistical point of view is applied in [16]. In the computational algorithms the local spline parameters (see [2], [18], [14]) or B-spline basis are used ([13], [3]). The connection between the spline degree and the spline derivative degree used in the smoothing part of the functional was slightly relaxed, but still can be found in most of this approaches.

When we narrow the set of functions considered for optimization to the linear space of splines on the given spline knotset and given degree, we can use the spline free parameters for optimization purposes with the type of the functional (the choice of some norm or the derivative order) chosen *independently on the spline degree.* Such approach to the linear, quadratic and cubic smoothing splines is described in [8]. The problems mentioned can be stated in the most cases as some special quadratic programming (QP) problems and they can be solved with standard algorithms of quadratic programming or with some special algorithms (using pseudoinverse, difference equation algorithms).

When we apply similar approach to *the quartic smoothing splines* in some local representation, we have to overcome some technical problems connected with two different types of local parameters used, with computing coefficients of the matrices in the continuity conditions and in quadratic forms of the functionals minimized. This makes more difficult to obtain the results concerning the uniqueness of the minimizer in the case of the general knotset. The aim of this paper is to present the structure of such objects and algorithms for computing local parameters of quartic smoothing splines. The cases of FVS and MVS will be discussed together as similar quadratic programming problems with different input matrices and with similar results.

2 Problem statement

Let us have given the monotone spline knotset on the real axis

$$\mathbf{x} = \{x_i,\ i = 0(1)n+1\} \text{ with stepsizes } h_i = x_{i+1} - x_i$$

and with the points of interpolation $\mathbf{t} = \{t_i,\ x_i < t_i < x_{i+1},\ i = 0(1)n\}$ in the FVS problem. The quartic splines with the defect one on this knotset are piecewise quartic polynomial functions $s(x) \in C^{(3)}$ (with possible jumps in the fourth derivative in spline knots only). The set of quartic splines on the given knotset $\mathbf{x}$ forms linear space $S_4(\mathbf{x})$. Let us consider the problems with errorneous data $\mathbf{p} = \{p_i,\ i = 0(1)n\}$ given as

- the function values $p_i \approx s(t_i)$ in the FVS problem;
- the mean values $p_i \approx \frac{1}{h_i}\int_{x_i}^{x_{i+1}} s(x)dx$ in the MVS problem.

The exact values of function or mean values of the smoothing spline we will denote as $\mathbf{g} = [g_i]$.

Let us now consider some functionals which can be used as some criterion of the spline smoothness evaluated from continuous or discrete form of information (squared norms of derivatives and their generalizations):

$$J_k(s) = \int_{x_0}^{x_{n+1}} [s^{(k)}(x)]^2 dx, \quad J_{kd}(s) = \sum_{j=0}^{k} \sum_{i=0}^{n+1} c_{ji} [s^{(j)}(x_i)]^2, \quad k \in \{0,1,2,3\}. \quad (1)$$

In the following we will discuss the examples where for $k \in \{0,1,2,3\}$ and for special choice of coefficients c_{ji} the functional $J_{kd}(s)$ includes the squared l_2-norms of vectors of one or two local parameters

$$[\mathbf{s}], [\mathbf{m}], [\mathbf{M}], [\mathbf{T}], [\mathbf{m}, \mathbf{M}], [\mathbf{s}, \mathbf{m}], [\mathbf{s}, \mathbf{M}], [\mathbf{s}, \mathbf{T}], [\mathbf{m}, \mathbf{T}], \quad (2)$$

(the notation $\mathbf{s}, \mathbf{m}, \mathbf{M}, \mathbf{T}$ for the vectors of the spline function values, first, second and third spline derivative values in knots x_i is used here—see sections 3.1, 3.2). The least squares (lsq) criterion of the fit of data $\mathbf{p}$ by its approximation $\mathbf{g}$ in the functional minimized can be written as

$$J_{lsq}(s) = \sum_{i=0}^{n} w_i (g_i - p_i)^2 = (\mathbf{g} - \mathbf{p})^T \mathbf{D_w} (\mathbf{g} - \mathbf{p}), \quad \mathbf{D_w} = diag[w_i], \quad w_i \geq 0 \quad (3)$$

with given vector $\mathbf{w} = [w_i]$ of weighting coefficients for the FVS problem and similarly for the MVS problem as

$$J_{lsq}(s) = \sum_{i=0}^{n} w_i h_i^2 (g_i - p_i)^2 = (\mathbf{g} - \mathbf{p})^T \mathbf{D_w^h} (\mathbf{g} - \mathbf{p}), \quad \mathbf{D_w^h} = diag[w_i h_i^2]. \quad (4)$$

To describe the quartic spline on each interval, we can use several local representations (the full description of possible choices is given in [7], some choice will be used in the following sections). *The continuity conditions* (CC) $s^{(j)}(x_i - 0) = s^{(j)}(x_i + 0)$, $j = 1, 2, 3$, for the quartic spline with the defect one can be then described as the underdetermined system of linear equations (recursions) with some free parameters and with the matrix $\mathbf{A}$ consisting e.g. from

— two blocks for unknown values $\mathbf{g}$ and one local parameter;

— six blocks for the unknown values $\mathbf{g}$ and two local parameters used.

The needed detailed description will be given in the corresponding sections (see also [6]). Both smoothing and lsq parts mentioned above can be then expressed as quadratic forms in the local parameters used. The cases of l_2, L_2-norms differ in the coefficients in the (band, diagonal) matrices of such forms only and we can consider them as the problems with similar structure. The final form of the functional minimized can be presented as convex combination (see e.g. [2]) of such two parts or as linear combination (see [3], [16], [18], [17])

$$J_k^\alpha(s) = J_k(s) + \alpha J_{lsq}(s), \quad J_{kd}^\alpha(s) = J_{kd}(s) + \alpha J_{lsq}(s) \quad (5)$$

with the *smoothing parameter* α attached here to the corresponding lsq part, which gives some balance (chosen by the user) between two parts of the functional minimized. In all cases mentioned here the resulting functionals (5) minimized with given value of the smoothing parameter α can be expressed as quadratic forms in the local parameters used. When we denote by $\mathbf{H}, \mathbf{q}$ the symmetric matrix of such form and corresponding vector in the linear part, we can state our problem as the quadratic programming problem with equality constrains, given by the continuity and interpolation conditions:

$$(QP) \qquad \text{Given } \mathbf{H}, \mathbf{q}, \mathbf{A}, \text{ find } \mathbf{c} \text{ with } \min\{\mathbf{c}^T\mathbf{H}\mathbf{c} + \mathbf{q}^T\mathbf{c};\ \mathbf{A}\mathbf{c} = \mathbf{0}\}; \tag{6}$$

here $\mathbf{c}$ denotes the vector of local coefficients used and $\mathbf{A}$ the corresponding matrix from CC. We can use now the results from the optimization theory (see e.g. [4]) to discuss our problem. The existence of some minimizer in all our problems follows from nonnegativity of quadratic forms used and the existence of feasible solutions of underdetermined system of CC. The existence of the strong (unique) minimizer can be characterized by various conditions (see e.g. [5]). For our purposes we shall use the following statement.

Lemma 1 *Let us denote $N(\mathbf{A}), N(\mathbf{H})$ the null spaces of matrices $\mathbf{A}$, $\mathbf{H}$ of the problem QP and let the matrix $\mathbf{A}$ be of full row rank.*

Then the necessary condition for the existence of the strong minimizer is the semidefinitness of $\mathbf{H}$. The sufficient condition for the strong minimizer is

a) positive definitness of the symmetric matrix $\mathbf{H}$ (SPD),

b) or the condition $N(\mathbf{A}) \cap N(\mathbf{H}) = \{0\}$ in case of semidefiniteness of $\mathbf{H}$,

c) or the positive definiteness of the matrix $\mathbf{Z}^\mathbf{T}\mathbf{H}\mathbf{Z}$, where $\mathbf{Z}$ is the matrix of the null space of the matrix $\mathbf{A}$.

Proof of this statement follows from nonnegativity of the matrix $\mathbf{H}$ and uniqueness of the solution of the corresponding unconstrained problem (see [4, pp. 231–232]).

3 Functionals J_{kd}^{α} minimized

3.1 l_2-norms of s, m, M, T as functionals J_{kd}

Let us consider the FVS problem on the *equidistant knotset* $\mathbf{x}$ with points of interpolation $t_i = \frac{1}{2}(x_i + x_{i+1})$ (in this subsection we will consider such a case only). When we want to minimize the l_2-norm of some of the vectors $\mathbf{s}$, $\mathbf{m}$, $\mathbf{M}$, $\mathbf{T}$ of the discrete values of the spline derivative in the knots, then we need to write the CC as recurrences for components of $\mathbf{g}$ and the local parameter chosen (for the nontrivial technique used here see [6])—e.g. with parameters $\{\mathbf{M}, \mathbf{g}\}$ we obtain for $i = 2(1)n-1$ the recursions

$$M_{i-2} + 76M_{i-1} + 230M_i + 76M_{i+1} + M_{i+2} - \frac{384}{2h^2}(g_{i-2} - g_{i-1} - g_i + g_{i+1}) = 0. \tag{7}$$

In the MVS problem on the equidistant knotset with local parameters $\{\mathbf{T}, \mathbf{g}\}$ we obtain recurrences (see [6]) for $i = 2(1)n-1$

$$T_{i-2}+26T_{i-1}+66T_i+26T_{i+1}+T_{i+2}-\frac{120}{h^3}(-g_{i-2}+3g_{i-1}-3g_i+g_{i+1}) = 0. \quad (8)$$

Similar recurrences hold in both problems for all couples of local parameters $\{\mathbf{s}, \mathbf{g}\}$, $\{\mathbf{m}, \mathbf{g}\}$, $\{\mathbf{M}, \mathbf{g}\}$, $\{\mathbf{T}, \mathbf{g}\}$ (see [6]). Let us mention that in equidistant case for FVS and MVS problems with different local parameters only the coefficients at $\mathbf{g}$ are different. In both these problems the structure with two blocks and the full row rank of the matrix $\mathbf{A}$ in the CC and corresponding (QP) problem is easily to be seen now. With till unknown values of $\mathbf{g} = [g_j]$ we can write the functional minimized now as

$$J^\alpha_{kd}(s) = \|[s^{(k)}(x_i)]\|_2^2 + \alpha\mathbf{g}^T\mathbf{D}\mathbf{g} - 2\alpha\mathbf{p}^T\mathbf{D}\mathbf{g} + \alpha\mathbf{p}^T\mathbf{D}\mathbf{p} \quad (9)$$

with the matrix $\mathbf{D} = \mathbf{D_w}$ ($\mathbf{D} = \mathbf{D^h_w}$) in FVS (MVS) problem. We can see that in both of this cases the corresponding matrix $\mathbf{H}$ of such a quadratic form is for each $k \in \{0, 1, 2, 3\}$ and any positive value of α the diagonal matrix with positive diagonal elements (special SPD matrix) related to the components g_j, M_j or g_j, T_j. Similar results we obtain for remaining choices of the problem and local parameter.

According to the statement a) of Lemma 1 we have proved in such a way the following theorem.

Theorem 1 *The FVS and MVS problems have on the equidistant knotset for any positive value of the smoothing parameter α and each $k \in \{0, 1, 2, 3\}$ the unique solution with minimal value of the functional $J^\alpha_{kd}(s)$ given in (9).*

Remark 1 Till now, only one from vectors **s, m, M, T** was used in the smoothing part $J_{kd}(s)$.

The optimal values of local parameters used in quadratic form and CC can be computed with QP algorithms (or with generalized pseudoinverse in special cases). The vector of the remaining local parameters have then to be computed from special formulas (see [9]).

The results mentioned in Theorem 1 will be valid also for slightly nonequidistant knotsets or shifted points of interpolation.

Example 1 The results for the MVS problem with given data

$$\mathbf{x} = 0:2:20, \quad \mathbf{p} = [6, 7, 11, 8, 5, 7, 4, 1, 2, 5], \quad \alpha = 0.1, 1, 10, 100$$

we can see plotted on Fig. 1 (the corresponding minimal values of the functional are approximately 5.05, 12.3, 15.0, 15.35).

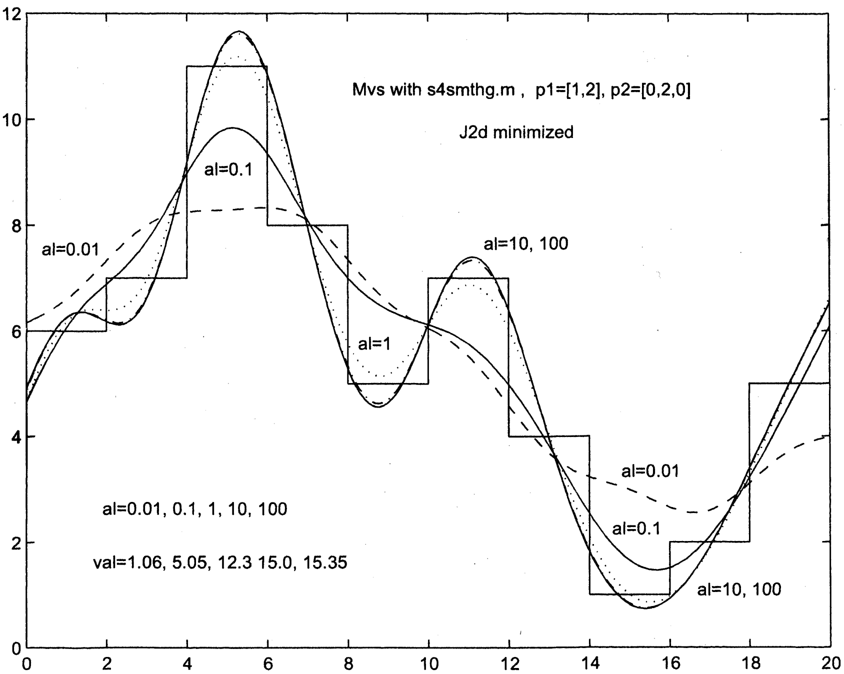

Fig. 1

3.2 Norms of vectors [m,M] etc. as functionals $J_{kd}(s)$

When we are interested to choose as the functional $J_{kd}(s)$ e.g. the squared norm of the vector [**m,M**], we can use the spline local representation with local parameters g_i, m_i, M_i on the interval $[x_i, x_{i+1}]$. It can be written with local variable $u = (x - x_i)/h_i$ and known basis functions—quartic polynomials $\psi, \varphi_0^j, \varphi_1^j$ (see [6] for explicit form of such basis functions for FV and MV problems) as

$$s(x) = \psi(u)g_i + h_i[\varphi_0^1(u)m_i + \varphi_1^1(u)m_{i+1}] + h_i^2[\varphi_0^2(u)M_i + \varphi_1^2(u)M_{i+1}]. \quad (10)$$

The CC can then for the FVS problem on equidistant knotset be written as the system of equations with six blocks structure

$$\begin{aligned} \frac{1}{32}(3m_{i-1} + 26m_i + 3m_{i+1}) + \frac{5}{192}h(M_{i-1} - M_{i+1}) - \frac{1}{h}(g_i - g_{i-1}) = 0, \\ \frac{1}{2h}(m_{i-1} - m_{i+1}) + \frac{1}{6}(M_{i-1} + 4M_i + M_{i+1}) = 0, \qquad i = 1(1)n. \quad (11) \end{aligned}$$

For MVS problem and local parameters g_i, m_i, T_i the CC form on the general knotset the system of equations with similar structure

$$h_{i-1}m_{i-1}+2(h_{i-1}+h_i)m_i+h_im_{i+1}-\frac{1}{60}[7h_{i-1}^3T_{i-1}+8(h_{i-1}^3+h_i^3)T_i+7h_i^3T_{i+1}]$$
$$-(g_i-g_{i-1})/h=0, \qquad i=1(1)n, \tag{12}$$

$$-h_im_{i-1}+(h_{i-1}+h_i)m_i-h_{i-1}m_{i+1}$$
$$+\frac{1}{6}h_{i-1}^2T_{i-1}+\frac{1}{3}h_{i-1}(h_{i-1}+h_i)T_i+\frac{1}{6}h_{i-1}h_iT_{i+1}=0.$$

We can write similarly the CC for all possible local representations (see [7], [6]) and we can prove the full row rank of the corresponding block matrices $\mathbf{A}$ in case of equidistant knotset (for MVS problem even for general knotsets)—e.g. for the mentioned FVS case we can write the system (11) as

$$\mathbf{A}\begin{bmatrix}\mathbf{m}\\ \mathbf{M}\\ \mathbf{g}\end{bmatrix}=\begin{bmatrix}\mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{A}_{13}\\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{A}_{23}\end{bmatrix}\begin{bmatrix}\mathbf{m}\\ \mathbf{M}\\ \mathbf{g}\end{bmatrix}=\mathbf{0}$$

with the block matrix coefficients which can be read from (11). Similar form we can give to CC with parameters $\{\mathbf{g},\mathbf{m},\mathbf{T}\}$ in the MVS problem and all problems mentioned.

The corresponding functionals

$$J_{kd}^{\alpha}(s)=\|[\mathbf{m},\mathbf{M}]\|_2^2+\alpha J_{lsq}$$

to be minimized can all be presented as quadratic forms with diagonal (one block for each local parameter used) SPD matrices $\mathbf{H}$ with positive elements c_{ji}, αw_i (or $\alpha w_i h_i^2$ for MVS). So we can state the following theorem.

Theorem 2 *The FVS problem on equidistant knotset and MVS problem on the general knotset have the unique solution for any positive value of the smoothing parameter α and for functionals $J_{kd}(s)$ corresponding to squared l_2-norms of the vectors* $[\mathbf{s},\mathbf{m}],[\mathbf{s},\mathbf{M}],[\mathbf{s},\mathbf{T}],[\mathbf{m},\mathbf{M}],[\mathbf{m},\mathbf{T}]$.

Remark 2 Similar results will be valid on slightly changed knotsets and for functionals $J_{kd}(s)$ with more general SPD matrix $\mathbf{H}$ (obtained e.g. when we approximate $J_k(s)$ using proper quadrature formulas).

Example 2 The FVS splines from the data

$$\mathbf{x}=-0.5:1:20.5; \quad \mathbf{t}=0:1:20;$$

$$\mathbf{p}=[15,11,4,5,0,-2,-7,-1,6,10,12,16,19,17,13,12,8,6,3,1,0],$$

corresponding to the values of the parameter $\alpha=0.01,0.1,1,10,100$ and with minimal values of the functional equal approximately to 9.6, 70.5, 227.8, 445.2, 622 are plotted on Fig. 2.

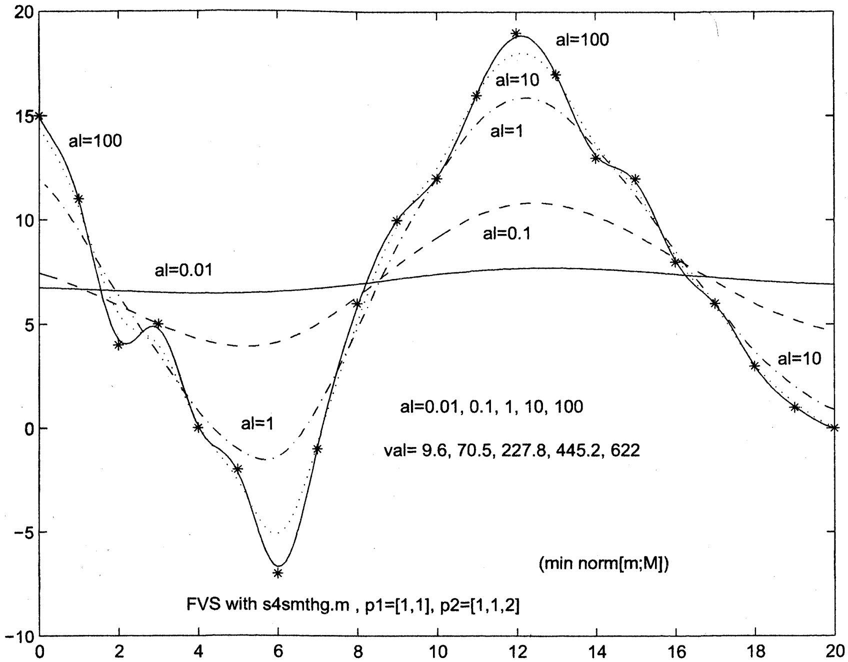

Fig. 2

4 Functionals J_k^α minimized

4.1 Functionals J_0, J_1 with parameters $\{\mathbf{g}, \mathbf{m}, \mathbf{M}\}$

The local representation (10) with parameters $\{\mathbf{g}, \mathbf{m}, \mathbf{M}\}$ for FVS problem can be used to compute the coefficients of quadratic form

$$J_0(s) = \int_{x_0}^{x_{n+1}} [s(x)]^2\, dx = \sum_{i=0}^{n} h_i g_i^2 + \frac{9}{80} \sum_{i=0}^{n} h_i^2 g_i (m_{i+1} - m_i)$$

$$- \frac{7}{480} \sum_{i=0}^{n} h_i^3 g_i (M_i + M_{i+1}) + \frac{1}{322560} \sum_{i=0}^{n} h_i^3 (8483 m_i^2 + 9914 m_i m_{i+1} + 8483 m_{i+1}^2)$$

$$+ \frac{1}{258048} \sum_{i=0}^{n} h_i^5 \Big(239 M_i^2 - \frac{1962}{5} M_i M_{i+1} + 239 M_{i+1}^2 \Big)$$

$$+ \frac{1}{322560} \sum_{i=0}^{n} h_i^4 (3119 m_i M_i - 2257 m_i M_{i+1} + 2257 m_{i+1} M_i - 3119 m_{i+1} M_{i+1}).$$

The functional $J_0^\alpha(s)$ we can then write in the matrix form as

$$J_0^\alpha(s) = \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix}^T \begin{bmatrix} \mathbf{D} & \mathbf{R_{12}} & \mathbf{R_{13}} \\ \mathbf{R_{12}^T} & \mathbf{R_{22}} & \mathbf{R_{23}} \\ \mathbf{R_{13}^T} & \mathbf{R_{23}^T} & \mathbf{R_{33}} \end{bmatrix} \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix} - 2\alpha \begin{bmatrix} \mathbf{p_w} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}^T \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix} + \alpha \mathbf{p_w^T p} \quad (13)$$

with the diagonal matrix $\mathbf{D} = \mathrm{diag}[\mathbf{h} + \alpha\mathbf{w}]$, vector $\mathbf{p_w} = \mathrm{diag}[\mathbf{w}]\mathbf{p}$, bidiagonal matrices $\mathbf{R_{12}}, \mathbf{R_{13}}$ and tridiagonal matrices $\mathbf{R_{22}}, \mathbf{R_{23}}, \mathbf{R_{33}}$, the coefficients of which can be recognized from explicit expression written above. We can compute the functional $J_0^\alpha(s)$ for the MVS problem with the same local parameters (for $J_0(s)$ see [9]) and we obtain as the result the quadratic form with similar matrix structure (but with different, more simple coefficients and with the vector $\mathbf{p_w^h} = \mathrm{diag}[w_i h_i^2]\mathbf{p}$ and with the matrix $\mathbf{D} = \mathbf{D_w^h} = \mathrm{diag}[h_i + \alpha h_i^2 w_i]$).

The functional $J_1(s)$ (the L_2-norm of the spline first derivative squared) of the FVS spline on the equidistant knotset (equal zero for constant $s(x)$ only) computed from the same local representation gives more simple quadratic form

$$J_1(s) = \int_{x_0}^{x_{n+1}} [s'(x)]^2\, dx = \frac{1}{210} \begin{bmatrix} \mathbf{m} \\ \mathbf{M} \end{bmatrix}^T \begin{bmatrix} \mathbf{R_1} & \frac{1}{2}\mathbf{Q} \\ \frac{1}{2}\mathbf{Q}^T & \frac{1}{2}\mathbf{R_2} \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \mathbf{M} \end{bmatrix} =$$

$$= \sum_{i=0}^{n} \frac{h_i}{210} [78m_i^2 + 54m_i m_{i+1} + 78m_{i+1}^2 + h_i^2(2M_i^2 - 3M_i M_{i+1} + 2M_{i+1}^2)$$
$$+ h_i(22m_i M_i - 13m_i M_{i+1} + 13m_{i+1} M_i - 22m_{i+1} M_{i+1}] \quad (14)$$

with $(n+1,\ n+1)$ SPD matrices $\mathbf{R_1}, \mathbf{R_2}$; on the equidistant knotset these matrices are

$$\mathbf{R_1} = h \begin{bmatrix} 78 & 27 & & & \\ 27 & 156 & 27 & & \\ & \ddots & \ddots & \ddots & \\ & & 27 & 156 & 27 \\ & & & 27 & 78 \end{bmatrix}, \quad \mathbf{R_2} = h^3 \begin{bmatrix} 4 & -3 & & & \\ -3 & 8 & -3 & & \\ & \ddots & \ddots & \ddots & \\ & & -3 & 8 & -3 \\ & & & -3 & 4 \end{bmatrix},$$

$$\mathbf{Q} = h^2 \begin{bmatrix} 22 & -13 & & & \\ 13 & 0 & -13 & & \\ & \ddots & \ddots & \ddots & \\ & & 13 & 0 & -13 \\ & & & 13 & -22 \end{bmatrix}.$$

Let us mention that we obtain identical expression for $J_1(s)$ in case of MVS problem (the explanation see in [9]).

The functional $J_1^\alpha(s)$ we can then write in the matrix form as

$$J_1^\alpha(s) = \frac{1}{210} \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix}^T \begin{bmatrix} \mathbf{D} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{R_1} & \frac{1}{2}\mathbf{Q} \\ \mathbf{0} & \frac{1}{2}\mathbf{Q}^T & \frac{1}{2}\mathbf{R_2} \end{bmatrix} \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix} - 2\alpha \begin{bmatrix} \mathbf{p_w} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}^T \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{M} \end{bmatrix} + \alpha \mathbf{p_w^T p} \quad (15)$$

with $\mathbf{D} = 210\alpha\mathbf{D_w}$ and vector $\mathbf{p_w}$ introduced above. We obtain the same form for the functional $J_1^\alpha(s)$ in the MVS problem (but with the vector $\mathbf{p_w^h}$ and matrix $\mathbf{D} = \mathbf{D_w^h}$ described above).

For $s(x) \not\equiv 0$ we have $J_0(s) > 0$ and the symmetric matrix $\mathbf{H}$ of the quadratic form $J_0^\alpha(s)$ is positive definite. For the data $\mathbf{p}$ different from constant vector (in such a case we have the solution $\mathbf{g} = \mathbf{p}$, $\mathbf{m} = \mathbf{M} = \mathbf{0}$) we have also $J_1(s) > 0$. The matrix $\mathbf{H}$ is then again positive definite.

The results obtained we can state in the following theorem.

Theorem 3 *The FVS problems on equidistant mesh and MVS problems on general mesh with functionals $J_0^\alpha(s), J_1^\alpha(s)$ have the unique minimizer for data $\mathbf{p}$ different from vector with $p_i = const.$*

Example 3 The results of computing MVS spline with input data

$$\mathbf{x} = 0:2:20; \quad \mathbf{p} = [6,7,11,8,5,7,4,1,2,5], \quad k = 0, \quad \alpha = 0.1, 1, 10, 100$$

are plotted in Fig. 3. The minimal values of the functional $J_0^\alpha(s)$ are approximately 15, 142, 1231, 11771.

When we try to compute the quadratic forms $J_2^\alpha(s)$, $J_3^\alpha(s)$ with local parameters $\{\mathbf{g}, \mathbf{m}, \mathbf{M}\}$, we obtain singular matrix $\mathbf{H}$. To obtain more simple structure of such matrix, we will use another local spline representation.

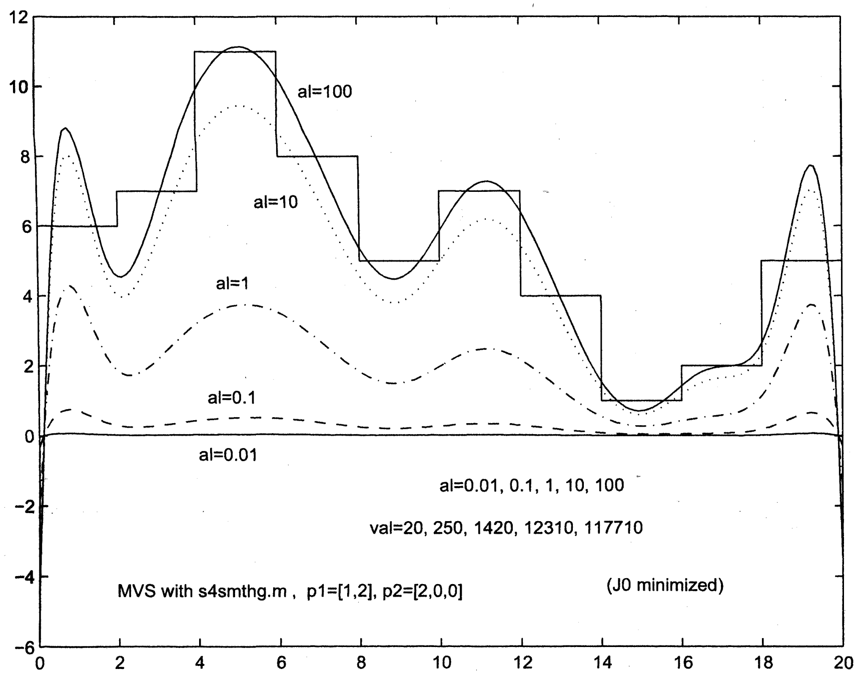

Fig. 3

4.2 Functionals J_2^α, J_3^α with parameters $\{\mathbf{g}, \mathbf{m}, \mathbf{T}\}$

When we use this local spline representation (see [6] for the description of basis functions used here)

$$s(x) = \psi(u)g_i + h_i[\varphi_0^1(u)m_i + \varphi_1^1(u)m_{i+1}] + h_i^3[\varphi_0^2(u)T_i + \varphi_1^2(u)T_{i+1}] \quad (16)$$

then the computation of expressions for functionals J_k with $k = 2, 3$ gives for FVS and MVS problems the identical results

$$J_2(s) = \sum_{i=0}^{n} \left[\frac{1}{h_i}(m_i^2 - 2m_i m_{i+1} + m_{i+1}^2) + \frac{h_i^3}{180}(4T_i^2 + 7T_i T_{i+1} + 4T_{i+1}^2) \right],$$

$$J_3(s) = \frac{1}{3}\sum_{i=0}^{n} h_i(T_i^2 + T_i T_{i+1} + T_{i+1}^2). \quad (17)$$

We can see here the block diagonal structure in the matrices of forms

$$J_2(s) = \begin{bmatrix} \mathbf{m} \\ \mathbf{T} \end{bmatrix}^T \begin{bmatrix} \mathbf{R_1} & \\ & \mathbf{R_2} \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \mathbf{T} \end{bmatrix}; \quad J_3(s) = \begin{bmatrix} \mathbf{m} \\ \mathbf{T} \end{bmatrix}^T \begin{bmatrix} \mathbf{0} & \\ & \mathbf{R_2} \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \mathbf{T} \end{bmatrix} \quad (18)$$

with SPD matrix $\mathbf{R_2}$ and symmetric semidefinite matrix $\mathbf{R_1}$ (different for functionals J_2, J_3)—their components we can read from (17).

The CC with parameters **g, m, T** in both problems we can write as (see [6])

$$\begin{aligned} \mathbf{Bg} + \mathbf{A_{11}m} + \mathbf{A_{12}T} &= \mathbf{0} \\ \mathbf{A_{21}m} + \mathbf{A_{22}T} &= \mathbf{0} \end{aligned} \quad (19)$$

with full row rank matrices $\mathbf{A_{ij}}$ and bidiagonal (*n, n+1*)- matrix

$$\mathbf{B} = \frac{1}{h}\begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \end{bmatrix}.$$

The complete functional minimized $J_2^\alpha(s)$ we can write then for $k = 2$ and FVS problem in the matrix form with $\mathbf{p_w}, \mathbf{D_w}$ described above as

$$J_2^\alpha(s) = \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{T} \end{bmatrix}^T \begin{bmatrix} \alpha\mathbf{D_w} & & \\ & \mathbf{R_1} & \\ & & \mathbf{R_2} \end{bmatrix} \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{T} \end{bmatrix} - 2\alpha \begin{bmatrix} \mathbf{p_w} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}^T \begin{bmatrix} \mathbf{g} \\ \mathbf{m} \\ \mathbf{T} \end{bmatrix} + \alpha\mathbf{p_w^T p}. \quad (20)$$

We obtain similar result for MVS problem with the above mentioned objects $\mathbf{D_w^h}, \mathbf{p_w^h}$. The same structure of the matrix of the quadratic form, but with the matrix $\mathbf{R_1} = \mathbf{0}$ we can find for the functionals $J_3^\alpha(s)$ in the FVS and MVS problems.

Theorem 4 *The FVS and MVS problems on the general knotset with functionals $J_2^\alpha(s)$, $J_3^\alpha(s)$ have the unique minimizer for any data $\mathbf{p}, \mathbf{w} > \mathbf{0}$, and for each $\alpha > 0$.*

Proof We will use the criterion given in the Lemma 1 to the QP problem with corresponding matrices $\mathbf{H}$ of the quadratic form and full row rank matrix $\mathbf{A}$ of the continuity conditions with the structure described in (19) for both functionals in FVS and MVS problems.

1) The functional $J_2^\alpha(s)$ we have written as quadratic form in parameters $\{\mathbf{g}, \mathbf{m}, \mathbf{T}\}$ with the block diagonal matrix $\mathbf{H} = \mathrm{diag}[\alpha \mathbf{D_w}, \mathbf{R_1}, \mathbf{R_2}]$. Let us suppose that $[\mathbf{g}; \mathbf{m}; \mathbf{T}] \in N(\mathbf{H})$. Then from regularity of matrices $\mathbf{D_w}, \mathbf{R_2}$ the identities $\mathbf{g} \equiv \mathbf{0}$, $\mathbf{T} \equiv \mathbf{0}$ follow. The remaining equality $\mathbf{R_1 m} = \mathbf{0}$ is fulfilled by the vector with constant components only. But the rest of CC constrains $\mathbf{A_{11} m} = \mathbf{0}$, $\mathbf{A_{21} m} = \mathbf{0}$ can be then fulfilled with the vector $\mathbf{m} \equiv \mathbf{0}$ only. So the sufficient condition b) from Lemma 1 is fulfilled for the problem with the functional $J_2^\alpha(s)$.

2) For the functional $J_3^\alpha(s)$ we have the matrix $\mathbf{H} = \mathrm{diag}[\alpha \mathbf{D_w}, \mathbf{O}, \mathbf{R_2}]$. Let us again consider the vector $[\mathbf{g}; \mathbf{m}; \mathbf{T}] \in N(\mathbf{H})$. The regularity of matrices $\mathbf{D_w}, \mathbf{R_2}$ implies then $\mathbf{g} \equiv \mathbf{0}, \mathbf{T} \equiv \mathbf{0}$. The overdetermined system from the remaining CC system $\mathbf{A_{11} m} = \mathbf{0}$, $\mathbf{A_{21} m} = \mathbf{0}$ has the trivial solution $\mathbf{m} \equiv \mathbf{0}$ only, because the corresponding homogeneous difference equations with different coefficients have in both cases common the trivial solutions only. So the matrices $\mathbf{H}$, $\mathbf{A}$ have only null vector common in their nullspaces.

Quite similarly we can consider the MVS problem (with the matrix $\mathbf{D_w^h}$ instead od $\mathbf{D_w}$). □

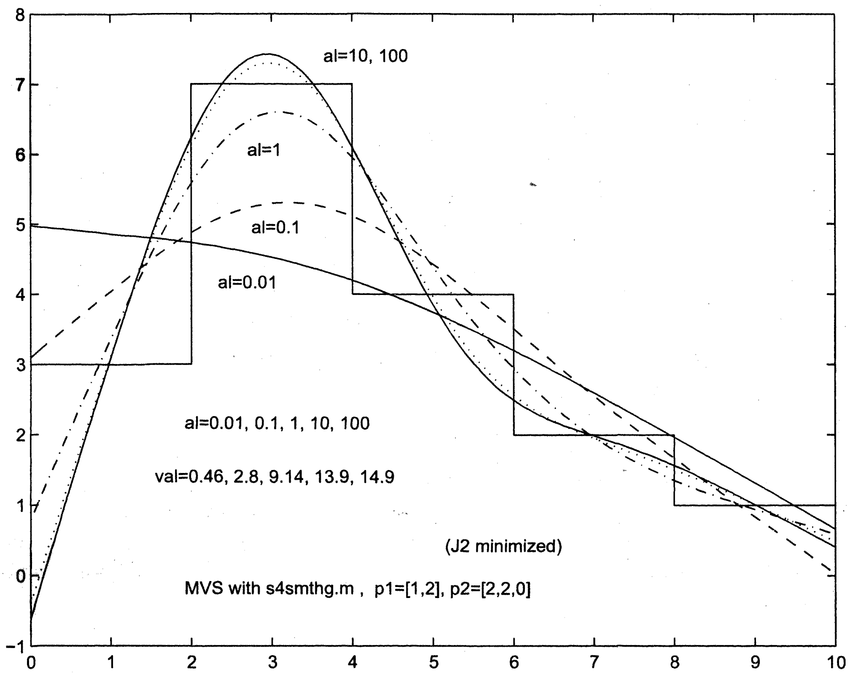

Fig. 4

Example 4 The MVS splines with input data

$$\mathbf{x} = 0:2:10; \quad \mathbf{p} = [3,7,4,2,1]; \quad k = 2,3; \quad \alpha = 0.1, 1, 10, 100$$

are plotted on Figs 4, 5; the corresponding minimal values of J_k^α are for $k = 2$: $[2.8, 9.1, 13.9, 14.9]$; for $k = 3$: $[1.24, 3.28, 5.15, 5.54]$.

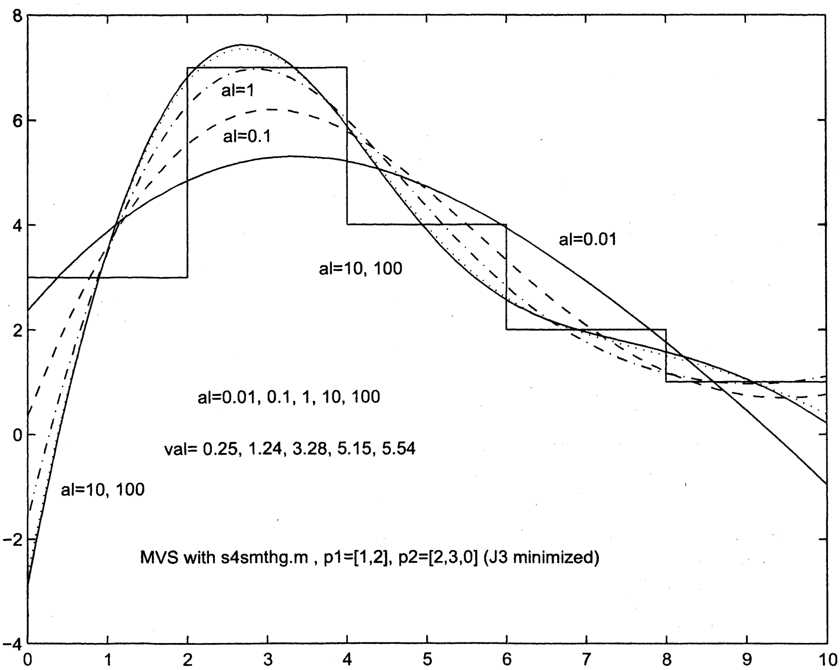

Fig. 5

Remark 3 In all examples given above we can find the similar common features of the smoothing procedure:
— the monotone increasing character of the functional with α growing;
— the convergence to the spline with zero value of the first part $J_k(s)$ for $\alpha \to 0$;
— the convergence to interpolatory spline for $\alpha \to \infty$;
— we can observe special oscilatory trends in case $k = 0$.

5 Algorithms, M-file s4smthg.m

As we have shown in the foregoing sections, we can use pseudoinverse matrix solution of the system of CC for computing optimal spline parameters in some simple cases. For linear, quadratic or cubic smoothing splines we can sometimes eliminate some parameters from CC and use the unconstrained minimization technique (see [2], [3], [8]). The general problems were stated here as problems of quadratic programming with equality constrains. The Matlab function (M-file) `s4smthg.m` was worked out by the author for the purpose of computing local parameters of the quartic smoothing spline (the function values for visualisation and another purposes can be then computed with another function `spl4hodn.m` or `s4smg.m`).

The syntax of this function is

```
function [pr1,pr2,g,val]=s4smthg(x,t,p,p1,p2,w,al),
```

with *input arguments*
x ... the vector of spline knots (equidistant or general),
t ... the vector of interpolation points—interval midpoints for FVS, empty for MVS
p ... the vector of the values to be smoothed (FV, MV),
p1=[1,1], [1,2] ... equidistant knotset used for FVS, MVS,
p1=([2,1]), [2,2] ... general knotset used for (FVS), MVS;
p2=[i,k,j] ... the code of the functional minimized:
[0,k,0], k=0:3 ... J^{α}_{kd},
[0,k,1], k=0:3 ... approximation of J_k with trapezoidal rule;
[1,k,j], k=0,1; j=1,2,3 (j>k) ... vector of [k,j]-th derivative;
[2,k,0], k=0:3 ... $J_k(s)$ in [g,m,M] local representation:
[3,k,0], k=2,3 ... $J_k(s)$ in [g,m,T] local representation:
w ... positive weighting coefficients in the lsq part;
al ... nonnegative value of the smoothing parameter α.
Output parameters **[pr1,pr2,g,val]**:
pr1, pr2 ... vectors of the optimal spline local parameters (ordered according to user's choice of [i,j,k]);
g ... the vector of smoothing spline function values in knots or mean values;
val ... minimal value of the functional optimized.

The algorithm computes from input data the components of the matrices and vectors in equality constrains and quadratic form. The pseudoinverse approach or the **qp**-function from Matlab is used in `s4smthg.m` for computing optimal spline local parameters.

The algorithms and M-files for computing with MVS quartic splines with natural, periodic or complete boundary conditions can be found also in [10].

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