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CONSTRUCTION OF SMOOTHING SPLINES BY LINEAR PROGRAMMING METHODS

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The mathematical questions and algorithms for constructing n-th order smoothing splines by means of experimental (kinetic) dependences are elucidated.

1. Let the function $f(x) \in C^Q[X]$, $Q \geq n$ that takes on the approximate values $f(x_1) + \delta_1, \ldots, f(x_N) + \delta_N$ be given discretely with the errors $\delta_1, \ldots, \delta_N$ at the nodes $x_1, \ldots, x_N$ on the segment $X \subset R$. It is required to approximate the function f(x) in each interval $[x_i, x_{i+1})$, $i = \overline{1, N-1}$ by a polynomial of n-th degree, $n \geq 3$:

$$y_i(x) = a_{0i} + a_{1i}x + a_{2i}x^2 + \cdots + a_{ni}x^n, \; x \in [x_i, x_{i+1}) \tag{1}$$

so as to satisfy the requirements [1-6]: I) fusion of the spline derivatives at the mesh nodes $S = \{x_1, \ldots, x_N\}$ up to the (n − 1) order

$$\begin{cases} a_{0i} + a_{1i}x_i + a_{2i}x_i^2 + \cdots + a_{ni}x_i^n = a_{0,i+1}, \\ \cdots\cdots\cdots\cdots \\ (n-1)!\, a_{n-1,i} + n!\, a_{ni}x_i = a_{n-1,i+1}, \; i = \overline{1, N-2}; \end{cases} \tag{2}$$

II) the requirement of minimal variation of the (n − 1)-derivative of $y_i(x)$ (i.e., $\int_{x_1}^{x_N} (y^{(n-1)}(x))^2 dx \underset{a}{\to} \min$), corresponding to condition $|a_{\nu i}| \underset{a}{\to} \min$, $\nu = n-1, n$, $i = \overline{1, N-1}$, in order to avoid oscillating behavior of the graph of the spline; III) location of the spline graph within the error corridor:

$$\begin{cases} |f_\delta(x_i) - a_{0i}| \leqslant \delta_i, \; i = \overline{1, N-1}, \\ |f_\delta(x_N) - a_{0,N-1} - a_{1,N-1}x_N - \cdots - a_{n,N-1}x_N^n| \leqslant \delta_N. \end{cases} \tag{3}$$

2. Conditions I and III yield the search domain for the interval values of the spline approximation coefficients by the system of constraints

$$\begin{cases} a_{0i} \leqslant f_\delta(x_i) + \delta_i, \\ -a_{0i} \leqslant -f_\delta(x_i) + \delta_i, \\ a_{0i} + a_{1i}x_{i+1} + a_{2i}x_{i+1}^2 + \cdots + a_{ni}x_{i+1}^n - a_{0,i+1} = 0, \\ \cdots\cdots\cdots\cdots \\ (n-1)!\, a_{n-1,i} + n!\, a_{ni}x_{i+1} - a_{n-1,i+1} = 0, \; i = \overline{1, N-2}, \\ a_{0,N-1} \leqslant f_\delta(x_{N-1}) + \delta_{N-1}, \end{cases} \tag{4}$$

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$$\begin{cases} -a_{0,N-1} \leqslant -f_\delta(x_{N-1}) + \delta_{N-1}, \\ a_{0,N-1} + a_{1,N-1}x_N + a_{2,N-1}x_N^2 + \cdots + a_{n,N-1}x_N^n \leqslant f_\delta(x_N) + \delta_N, \\ -(a_{0,N-1} + a_{1,N-1}x_N + a_{2,N-1}x_N^2 + \cdots + a_{n,N-1}x_N^n) \leqslant -f_\delta(x_N) + \delta_N. \end{cases} \tag{4}$$

Since the coefficients a_{ij}, $i = \overline{0, n}$; $j = \overline{1, N-1}$ can have different signs and the standard linear programming problem to which obtaining the interval estimates for a_{ij} reduces has just nonnegative solutions, we set $a_{ij} = a'_{ij} - a''_{ij}$, where $a'_{ij}, a''_{ij} \geqslant 0$. Then condition II results in the requriement of minimum of the absolute value $|a_{\nu j}| = |a'_{\nu j} - a''_{\nu j}|$, $\nu = \overline{n-1, n}$, in each interval $[x_j, x_{j+1})$, $j = \overline{1, N-1}$. Obtaining the interval estimates for a_{ij} with requirements I-III taken into account can be realized by different means, for instance: A) determination of the coefficients $a_{\nu j}$, $\nu = n-1, n$, $j = \overline{1, N-1}$, initially and then all the rest; a_{ij}, $i = \overline{0, n-2}$, $j = \overline{1, N-1}$; B) simultaneous determination of all coefficients by using the multiparameteric regularization method [7] for the components of the solution $a_{\nu j}$, $\nu = n-1, n$, $j = \overline{1, N-1}$.

MODIFICATION A

In each interval $[x_j, x_{j+1})$ we find minimal values of the coefficients $a_{\nu j}{}^0$, $\nu = n-1$, n, $j = \overline{1, N-1}$, in absolute value, for which we solve two problems: Maximize $z_{1\nu j} = a_{\nu j}$ under the constraints (4) and maximize $z_{2\nu j} = -a_{\nu j}$ also under the constraints (4). Then taken as $a_{\nu j}{}^0$, $\nu = n-1$, n, should be the minimal value in absolute value of $\{|z_{1\nu j_{\max}}|, |z_{2\nu j_{\max}}|\}$, i.e., $a^0_{\nu j} = \operatorname{sign} a^0_{\nu j}\,|a^0_{\nu j}|$, where $|a_{\nu j}{}^0| = \min\{|z_{1\nu j_{\max}}|, |z_{2\nu j_{\max}}|\}$, $\nu = n-1$, n. Furthermore, we find the uniformly minimal value $a_{\nu j_{\min}}$, $\nu = n-1$, n, in absolute value in the segment $[x_1, x_N]$ as $a_{\nu j_{\min}} = \alpha a^0_{\nu j}$, where the proportionality factor α is determined from the solution of the problem to maximize $z_3 = -\alpha$ under the constraints (4) but in which all the monomials $a_{\nu j}x_j{}^m$ are replaced by $\alpha a_{\nu j}{}^0 x_j{}^m$, $\nu = n-1$, n, $j = \overline{1, N-1}$, $m = \overline{0, n}$.

Afterwards we proceed to obtain interval estimates for all the other coefficients a_{ij}, $i = \overline{0, n-2}$, $j = \overline{1, N-1}$ for which $\overset{+}{z}_{ij} = a_{ij}$, $i = \overline{0, n-2}$, $j = \overline{1, N-1}$ must be maximized under the constraints (4) but in which all the monomials $a_{\nu j}x_j{}^m$, $\nu = n-1$, n, are replaced by the quantities $z_{3\max} a_{\nu j}{}^0 x_j{}^m$ already known and transposed, respectively, into the right sides of the constraints, and also to maximize $\bar{z}_{ij} = -a_{ij}$ under the same constraints. Then the desired interval estimates for a_{ij}, $i = \overline{0, n-2}$, $j = \overline{1, n-1}$ are determined as

$$a_{ij} = \{\leqslant \overset{+}{z}_{ij_{\max}} \text{ for } \overset{+}{z}_{ij_{\max}} > 0,\ \leqslant \bar{z}_{ij_{\max}} \text{ for } \bar{z}_{ij_{\max}} < 0,\ \geqslant \bar{z}_{ij_{\max}} \text{ for } \bar{z}_{ij_{\max}} > 0,\ \geqslant \overset{+}{z}_{ij_{\max}} \text{ for } \overset{+}{z}_{ij_{\max}} < 0\},\ i = \overline{1, n-2},\ j = \overline{1, N-1}. \tag{5}$$

MODIFICATION B

To find the interval estimates by the method of linear programming with the requirements I-III taken into account, we apply multiparametric regularization to obtain solutions with minimal projection norm in the solution subspace defined by the coefficients $a_{\nu j}$, $\nu = n-1$, n, $j = \overline{1, N-1}$. Seeking the solution $a_{(r)} \in R^p$ with minimal projection norm in the subspace R^r, $r \leq p$ (norm of the vector $(\mathbf{a}_{(r)})^T = (a_{k+1}, \ldots, a_{k+r})$, $0 \leqslant k \leqslant p$, $1 \leqslant r \leqslant p-k$), by the multiparametric regularization method for the linear systems $\mathbf{X}_{(N\ p)}\mathbf{a}_{(p\ 1)} = \mathbf{y}_{(N\ 1)}$ or the linear programming problem $\max_{\mathbf{a}} \mathbf{Ca}$ under the constraints $\mathbf{Xa} \leqslant \mathbf{y}$ (the dimensionalities of $\mathbf{X}$, $\mathbf{a}$ and $\mathbf{y}$ are the same) reduces by analogy with [7] to the solution, respectively, of systems $\mathbf{XW}_{(r)}\mathbf{u} = \mathbf{y}$ or $\max_{u} \mathbf{CW}_{(r)}\mathbf{u}$ under the constraints $\mathbf{XW}_{(r)}\mathbf{u} \leqslant \mathbf{y}$, where $\mathbf{W}_{(r)}$ is the matrix, $0 \leq k \leq p$, $1 \leq r \leq p-k$, of form

$$\mathbf{W}_{(r)} = \left(\begin{array}{c|c|c} \mathbf{E}_{(k)} & \multicolumn{2}{c}{\mathbf{0}_{(k\times(\max\{N,p\}-k))}} \\ \hline \multicolumn{2}{c|}{\mathbf{X}_{k+1,k+r\,(r\times N)}} & \mathbf{0}_{(r\times(p-N)_+)} \\ \hline \mathbf{0}_{(p-k-r)\times(k+r)} & \mathbf{E}_{(p-k-r)} & \mathbf{0}_{(p-k-r)\times(p-N)_+} \end{array}\right), \tag{6}$$

where $\mathbf{X}_{k+1,k+r} = \begin{pmatrix} x_{1,k+1} \cdots x_{N,k+1} \\ x_{1,k+r} \cdots x_{N,k+r} \end{pmatrix}$; $(p - N)_+ = \{p - N$ for $p > N$ and 0 for $p < N\}$; $\mathbf{E}(\cdot)$ is the unit matrix of dimensionality $(\cdot)$. Then the solution with the minimal projection in the solution subspace is $\mathbf{a}_{(r)} = \mathbf{W}_{(r)}\mathbf{u}$. For $k = 0$, $r = n$ the matrix is $\mathbf{W}_{(n)} = \mathbf{X}^T$ [7]. In matrix form the system (4) is

$$\mathbf{X}\mathbf{a} \leqslant \mathbf{y}, \tag{7}$$

where

$$\mathbf{X} = \begin{pmatrix} \boxed{1} & \boxed{-1} & & & & \mathbf{0} \\ & \boxed{2} & \boxed{-1} & & & \\ & & \ddots & \ddots & & \\ & & & \boxed{j} & \boxed{-1} & \\ \mathbf{0} & & & & & \begin{matrix} 1 & 0 & \cdots & 0 \\ -1 & 0 & \cdots & 0 \\ 1 & x_N & \cdots & x_N^n \\ -1 & -x_N & \cdots & -x_N^n \end{matrix} \end{pmatrix},$$

$$\boxed{j} = \begin{pmatrix} 1 & 0 & \cdots & & & 0 \\ -1 & 0 & \cdots & & & 0 \\ 1 & x_j & \cdots & & x_j^{n-1} & x_j^n \\ 0 & 1 & 2x_j & \cdots & (n-1)x_j^{n-2} & nx_j^{n-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & 0 & (n-1)! & n!x_j \end{pmatrix},$$

$$\boxed{-1} = \begin{pmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \\ -1 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & -1 \end{pmatrix}, \quad j = \overline{1, N-2}.$$

Then the desired interval estimates of the spline coefficients are obtained from the solutions of two problems: Maximize $\overset{+}{z}_i = a_i$, $i = \overline{1, (n + 1)(N - 1)}$ under the constraints

$$\mathbf{X}\mathbf{W}_{(n-1,n)}\mathbf{u} \leqslant \mathbf{y}, \tag{8}$$

where $\mathbf{W}_{(n-1,n)}$ is the matrix $(n + 1)N \times \max\{N, p\}$, whose submatrix $\mathbf{X}_{(n-1,n)}$ rows consist of columns of the matrix $\mathbf{X}$, corresponding to the coefficients

$$a_{\nu j},\ \nu = n-1,\ n;\ (a_i,\ i = \overline{1,\ (n+1)(N-1)}) \equiv \mathbf{a} \equiv \mathbf{W}_{(n-1,n)}\mathbf{u};$$

$$\mathbf{y}^T = (f_\delta(x_1) + \delta_1,\ -f_\delta(x_1) + \delta_1,\ 0,\ \ldots,\ 0,\ f_\delta(x_{N-2}) + \delta_{N-2}, -f_\delta(x_{N-2}) + \\ + \delta_{N-2},\ 0,\ \ldots,\ 0,\ f_\delta(x_{N-1}) + \delta_{N-1},\ -f_\delta(x_{N-1}) + \delta_{N-1},\ f_\delta(x_N) + \delta_N, \\ - f_\delta(x_N) + \delta_N),$$

and also maximize $\bar{z}_i = -a_i$ under the constraints (8). Then the desired interval estimates are determined as

$$a_i = \{\leqslant \overset{+}{z}_{i\max} \text{ for } \overset{+}{z}_{i\max} > 0,\ \leqslant \bar{z}_{i\max} \text{ for } \bar{z}_{i\max} < 0,\ \geqslant \bar{z}_{i\max} \text{ for } \\ \bar{z}_{i\max} > 0,\ \geqslant \overset{+}{z}_{i\max} \text{ for } \overset{+}{z}_{i\max} < 0\},\ i = \overline{1,\ (n+1)\ (N-1)}. \tag{9}$$

As in modification A the values a_i can here be estimated as $a_i = (a_{i_{\max}} + a_{i_{\min}})/2$.

3. It is required to determine the contribution of each node x_j with the value $f_\delta(x_j) + \delta_j$ from the network of nodes S as well as the errors δ_j, $j = \overline{1, N}$ in the values of the upper and lower bounds of the interval estimates of the coefficients a_{ij} in order to construct the optimal network $S^* \subset [x_1, x_N]$ from the condition of minimum length of the interval estimate $\Delta a_l = |a_{l_{\max}} - a_{l_{\min}}|$ of the given coefficient a_l, $l = \overline{1, (n+1)(N-1)}$, i.e.,

$$\Delta a_l \underset{S}{\rightarrow} \min, \tag{10}$$

or from the condition of minimum sum of the lengths of the interval estimates for several or all the coefficients $\sum_{l=l}^{l+q} \Delta a_l$, $l \geqslant 1$, $l + q \leqslant (n+1)(N-1)$, i.e.,

$$\sum_{l=l}^{l+q} \Delta a_l \underset{S}{\rightarrow} \min. \tag{11}$$

To estimate these contributions as well as the contributions of the conditions for fusion of the derivatives (2) on the boundaries of the interval estimates for a_{ij} it is required to solve problems dual to (4) and (5) (modification A) or to (8) and (9) (modification B).

<u>Modification A</u>. We obtain the contributions mentioned from solutions of the problem: Minimize $\overset{+}{z}_l = \mathbf{y}^T\mathbf{B}_l$, where

$$\mathbf{y}^T\mathbf{B}_l = (f_\delta(x_1) + \delta_1)\overset{+}{b}{}_1^l - (f_\delta(x_1) - \delta_1)\bar{b}_1^l - (a_{n-1,1}x_2^{n-1} + a_{n1}x_2^n)b_{01}^l - ((n-1)a_{n-1,1}x_2^{n-2} + na_{n1}x_2^{n-1})b_{11}^l + \dots +$$

$$+ (a_{n-1,2} - (n-1)!a_{n-1,1} - n!a_{n1}x_2)b_{n-1,1}^l + \dots + (f_\delta(x_{N-2}) + \delta_{N-2})\overset{+}{b}{}_{N-2}^l - (f_\delta(x_{N-2}) - \delta_{N-2})\bar{b}_{N-2}^l -$$

$$- (a_{n-1,N-2}x_{N-1}^{n-1} + a_{n,N-2}x_{N-1}^n)b_{0,N-2}^l - ((n-1)a_{n-1,N-2}x_{N-1}^{n-2} + na_{n,N-2}x_{N-1}^{n-1})b_{1,N-2}^l + \dots +$$

$$+ (a_{n-1,N-1} - (n-1)!a_{n-1,N-2} - n!a_{n,N-2}x_{N-1})b_{n-1,N-2}^l + (f_\delta(x_{N-1}) + \delta_{N-1})\overset{+}{b}{}_{N-1}^l - (f_\delta(x_{N-1}) - \delta_{N-1})\bar{b}_{N-1}^l +$$

$$+ (f_\delta(x_N) + \delta_N - a_{n-1,N-1}x_N^{n-1} - a_{n,N-1}x_N^n)\overset{+}{b}{}_N^l - (f_\delta(x_N) - \delta_N - a_{n-1,N-1}x_N^{n-1} - a_{n,N-1}x_N^n)\bar{b}_N^l,$$

under the constraints

$$(\mathbf{X}_{(\urcorner n-1,n)})^T\mathbf{B}_l \geqslant \mathbf{e}_l,\ l = \overline{1, (n-1)(N-1)}, \tag{12}$$

where $\mathbf{B}_l^T = (\overset{+}{b}{}_1^l, \bar{b}_1^l, b_{01}^l, \dots, \overset{+}{b}{}_N^l, \bar{b}_N^l)$ is the vector of the contributions, $\mathbf{e}_l^T = (\overbrace{0\dots01}^{l}0\dots0)$; $\mathbf{X}_{(\urcorner n-1,n)}$ denotes the matrix X without columns corresponding to the coefficients $a_{\nu j}$, $\nu = n-1, n$, $j = \overline{1, N-1}$. Then the components of the vector $\hat{\mathbf{B}}_{l_{\min}}: \hat{\overset{+}{b}}{}_{l_{\min}}^l, \hat{\bar{b}}{}_{\min}^l$ are contributions of the quantities $f_\delta(x_j) + \delta_j$ and $f_\delta(x_j) - \delta_j$ at the upper bound of values of the component $a_{\ell_{\max}}$ of the coefficient vector $\mathbf{a}$ (the coefficients $a_{n-1,1}, a_{n1}, \dots, a_{n-1,N-1}, a_{n,N-1}$ are not components of) and $\hat{b}_{ij}^l$ is the contribution of the condition for fusion of the i-th derivative at the j-th node of the network S. Hence, the contribution $f_\delta(x_j)$ to $a_{\ell_{\max}}$ is determined as $(\overset{+}{b}{}_{j_{\min}}^l + \bar{b}_{j_{\min}}^l)/2$, while the values of the errors δ_j are as $(\overset{+}{b}{}_{j_{\min}}^l - \bar{b}_{j_{\min}}^l)/2$. The contributions of these same quantities are estimated analogously at the lower bound of the component $a_{\ell_{\min}}$ of the coefficients vector of the spline $\mathbf{a}$: Minimize $\bar{z}_l = \mathbf{y}^T\mathbf{B}_l$ under the constraints

$$(\mathbf{X}_{(\urcorner n-1,n)})^T\mathbf{B}_l \geqslant -\mathbf{e}_l,\ l = \overline{1, (n-1)(N-1)}. \tag{13}$$

Then the components of the vector of the solution $\check{\mathbf{B}}_{l_{\min}}: \check{\overset{+}{b}}{}_{j_{\min}}^l, \check{\bar{b}}{}_{j_{\min}}^l, \check{b}_{ij_{\min}}^l$, $l = \overline{1, (n-1)(N-1)}$, $i = \overline{0, n-1}$, $j = \overline{1, N}$, are contributions, respectively, of $f_\delta(x_j) + \delta_j$, $f_\delta(x_j) - \delta_j$ and the fusion condition for the i-derivative at the j-node of the mesh S at the lower value of the component $a_{\ell_{\min}}$ of the coefficients vector of the spline $\mathbf{a}$. Then the contributions of the quantities $f_\delta(x_j)$, δ_j to value $a_{\ell_{\min}}$ are determined as $(\check{\overset{+}{b}}{}_{j_{\min}}^l + \check{\bar{b}}{}_{j_{\min}}^l)/2$ and $(\check{\overset{+}{b}}{}_{j_{\min}}^l - \check{\bar{b}}{}_{j_{\min}}^l)/2$ respectively.

Modification B. We obtain estimates of the desired contributions from the solutions of the problems dual to (8) and (9): minimize $\overset{+}{z}_l = \mathbf{y}^T \mathbf{B}_l$ under the constraints

$$\mathbf{W}^T_{(n-1,n)}\mathbf{X}^T\mathbf{B}_l \geqslant \mathbf{W}^T_{(n-1,n)}\mathbf{C}_l, \ \mathbf{C}_l = (\overbrace{0\ldots0}^{l}10\ldots0), \ l = \overline{1, \ (n+1)(N-1)}, \tag{14}$$

and also minimize $\overline{z}_\ell = y^T B_\ell$ under the constraints

$$\mathbf{W}^T_{(n-1,n)}\mathbf{X}^T\mathbf{B}_l \geqslant - \mathbf{W}^T_{(n-1,n)}\mathbf{C}_l, \ l = \overline{1, \ (n+1)(N-1)}. \tag{15}$$

Let $\hat{\mathbf{B}}_{\ell\min}$ and $\check{\mathbf{B}}_{\ell\min}$ denote the solutions of the problems (14) and (15). Then the desired contributions of the nodes of the network S, the errors δ_j, and the conditions for fusion of the derivatives at the boundaries of the interval estimates for the spline coefficients, including the coefficients $a_{n-1,j}$, $j = \overline{1, N-1}$ in this case, are determined by the components of the vectors $\hat{\mathbf{B}}_{\ell\min}$ and $\check{\mathbf{B}}_{\ell\min}$.

In conclusion, we note that the algorithms considered are general in nature and can be applied for the construction of splines of different orders and defects on the basis of other basis functions; questions of the existence and uniqueness of the appropriate splines do not here enter within the framework of this report.

NOTATION

δ_i, error of giving a function at the i-node; x_i, coordinate of the argument at the i-node; $X = [x_1, x_N]$, segment on which the function is given discretely; R, a one-dimensional axis; $f(x) \in C^Q[X]$, a Q times differentiable function in the segment X; $f(x_i) + \delta_i$, $f_\delta(x_i)$, values of the function in the i-node aggravated by errors; n, order of the polynomial spline; $y_i(x)$, running value of the approximating polynomial between two nodes; a_{ij}, $i = \overline{0, n}$, $j = \overline{1, N-1}$, $a_{\nu j}$, coefficients of the approximating polynomial between two nodes; S, node network; a'_{ij}, a''_{ij}, terms of the difference representation of the spline coefficients; $a_{\nu j}{}^0$, minimal value, in absolute value, of the coefficients $a_{\nu j}$; $z_{1\nu j}$, $z_{2\nu j}$, $\overset{+}{z}_{ij}$, $\overset{-}{z}_{ij}$, $z_{3\max}$, $\overset{+}{z}_i$, $\overset{-}{z}_i$, $\overset{+}{z}_l$, $\overset{-}{z}_l$ are target functions of the appropriate linear programming problems; α, constant factor; $a_{\nu j\min}$, uniformily minimal, in absolute value, values of the coefficients $a_{\nu j}$ in the coefficients X; R^p, R^r, Euclidean spaces of dimensionality p and r; X, matrix of the left side of the system of linear algebraic equations; a, vector of the desired unknowns of the system of linear equations; y, vector of the free terms (the right sides) of the system of linear equation; $W_{(r)}$, matrix of the mapping of the space of solutions of the system of linear equations into control space in the multiparametric regularization procedure; u, vector of the control (regularization) parameters; $B_l = \{\hat{B}_l, \check{B}_l\}$, vector of contributions of the quantities $f_\delta(x_i) + \delta_i$, $f_\delta(x_i) - \delta_i$ and fusion conditions for derivatives in the interval estimates (their upper and lower bounds) of the smoothing spline coefficients.

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