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DESCRIPTIVE SPLINES IN INVERSE HEAT CONDUCTION PROBLEMS: METHOD AND ALGORITHMS

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An algorithm is suggested for generating descriptive splines that permit one to make good use of the available prior information in problems of filtration, approximation, and differentiation of the data of a thermophysical experiment.

When interpreting the data of a thermophysical experiment and, in particular, when solving inverse heat conduction problems, the necessity arises for filtering the noise of measurements, nonparametric representation of the investigated functional relations, and construction of smooth (differentiable) approximations [1]. An effective approach to the solution of the above problems is based on the use of the techniques of smoothing splines [2, 3]. However, when there is a high level of errors in the original data, it is not always possible to obtain a solution that would be appropriate from the viewpoint of both the required accuracy and compliance with certain physical ideas on the process investigated. For example, the appearance of negative values of the first derivative is possible, though it is known that the investigated process is not a time-decreasing one.

The present work considers the construction of a descriptive spline that makes it possible to overcome the above difficulties.

A Descriptive Smoothing Spline and Its Construction. Suppose the investigated function $f(x)$ is represented by the following values measured at the nodes x_i:

$$\tilde{f}_i = f(x_i) + \eta_i, \quad 1 \le i \le n, \tag{1}$$

where η_i is the noise of measurement with zero mean and variance σ_i^2, and the nodes x_i are arranged in increasing order, i.e., $x_1 < x_{i+1}$.

For stable evaluation of $f(x)$ and its derivatives $f'(x)$, $f''(x)$ from the table $\{x_i, \tilde{f}_i\}$, smoothing cubic splines are used [2, 3]. The smoothing cubic spline $S_{n,\alpha}(x)$ is expressed by a third-degree polynomial having a continuous second derivative over the segment (x_1, x_n) and admitting in each interval $[x_i, x_{i+1}]$ the representation

$$S_{n,\alpha}(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3. \tag{2}$$

To ensure the uniqueness of the smoothing spline, at the nodes x_1, x_n the corresponding boundary conditions are assigned [3], determined by the values of $f(x)$ or its derivatives. In the variational approach, the spline $S_{n,\alpha}(x)$ is determined from the minimum of the functional

$$F_\alpha[S, \tilde{f}] = \alpha \int_{x_1}^{x_n} (S''(x))^2 dx + \sum_{i=1}^{n} p_i^{-1} \tilde{f}_i - S_{n,\alpha}(x_i))^2, \tag{3}$$

where α is the smoothing parameter; $p_i > 0$ are the weighting factors. Ultimately a system of algebraic equations for c_i is obtained, from which the coefficients a_i, b_i, and d_i can be found [3]. By selecting the optimal smoothing parameter one succeeds in minimizing the mean square error (MSE) of smoothing [3], defined by the functional

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$$\Delta^2(\alpha) = M\left[\sum_{i=1}^{n}(f(x_i) - S_{n,\alpha}(x_i))^2\right],$$

where $M[\cdot]$ is the expectation operator.

By the descriptive spline $S^*_{n,\alpha}(x)$ we mean a spline that minimizes (3) under the restrictions

$$d_i^{\text{low}} \le D^{l_i} S(x_i) \le d_i^{\text{up}}, \quad i \in I_r, \tag{4}$$

where D^{l_i} is the differentiation operator of the l_i-th order ($l_i = 0, 1, 2$); I_r is a set of N_r indices (N_r is the total number of restrictions); $I_r \subseteq \{1, 2, ..., n\}$, d_i^{low}, d_i^{up} are the lower and upper boundaries. The proposed descriptive spline differs from that on convex sets [4, 5] by two features. First, it permits one to simultaneously take into account prior information about the function $f(x)$ in different forms (including the first and second derivatives and also restrictions of the type of equalities when $d_i^{\text{low}} = d_i^{\text{up}}$). Second, if the number of restrictions is small or if the restrictions are qualitative in character (for example, $S'(x) \ge 0$) and this prior information is not enough to construct an "appropriate" (from the viewpoint of MSE smoothing) spline, the transition to the spline $S^*_{n,\alpha}(x)$ removes this difficulty by a corresponding choice of the smoothing parameter.

We now proceed to the presentation of the algorithm for generating the descriptive spline $S^*_{n,\alpha}(x)$. It is shown in the Appendix (see relation (A2)) that $\int (S''(x))^2 dx = s^T Q s$ and then

$$F_\alpha[S, \tilde{f}] = \alpha s^T Q s + (s - \tilde{f})^T P (s - \tilde{f}), \tag{5}$$

where $P = \text{diag}\{p_1, p_2, ..., p_n\}$ is a diagonal matrix; $S = | S_{n,\alpha}(x_1), S_{n,\alpha}(x_2), S_{n,\alpha}(x_n) |^T$ is the vector of the spline values at the nodes x_i; Q is an $n \times n$ matrix determined in the Appendix.

First, we consider one-sided restrictions of the form $D^{l_i}S(x_i) \le d_i^{\text{up}}$, $i \in I_r$, which, with account for relation (A3), can be rewritten as $Ds \le d^{\text{up}}$, where D is an $N_r \times n$ matrix. Taking into account Eq. (5), we arrive at the problem of quadratic programming

$$\min\left\{\frac{1}{2} s^T U_\alpha s + S^T u + \text{const}\right\} \tag{6}$$

under the restrictions

$$Ds \le d^{\text{up}}, \tag{7}$$

here $U_\alpha = 2(\alpha Q + P)$; $u = -2P\tilde{f}$.

We shall examine the existence and uniqueness of the solution of problem (6), (7). The existence of the solution is determined by the consistency of the system of restrictions (7), which is assumed a priori. Hereafter, for any $\alpha > 0$ the matrix U_α is positive-definite, and the minimized functional is strictly convex. The admissible nonempty set of vectors s that satisfy Eq. (7) is a convex set. Therefore, the formulated problem of conventional minimization has a unique solution: s^* [6].

To find s^*, we employ the method of [7]. The Lagrange-dual problem consists in the minimization of the functional

$$\Psi(\mu) = \frac{1}{2}\mu^T D U_\alpha^{-1} D^T \mu + \mu^T (D U_\alpha^{-1} u - d^{\text{up}})$$

with the restriction $\mu \ge 0$, where μ is a vector of dimension N_r. Upon finding the solution of this problem μ^*, the vector s^* is calculated from the matrix relation

$$s^* = s - U_\alpha^{-1} D^T \mu^*,$$

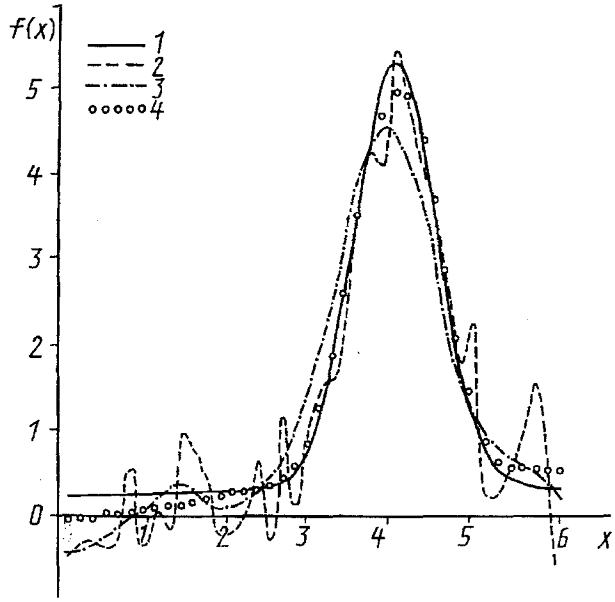

Fig. 1. Approximation of the function $f(x)$: 1) exact function $f(x)$; 2) noisy values; 3) the spline $S_{n,\alpha}(x)$ constructed at $\alpha = \alpha_1$; 4) the spline $S^*_{n,\alpha}(x)$ constructed at $\alpha = \alpha_2$.

where s is the vector that attains the unconditional minimum of functional (6). It is composed of the values of the spline $S_{n,\alpha}(x)$ at the nodes x_i. Thereafter, the system $Am = Hs^*$ with the three-diagonal matrix A is solved, and from the obtained vector m the coefficients b_i, c_i, d_i [3] of the descriptive smoothing spline are determined ($a_1 = \{s^*_\alpha\}_i$).

In the case of two-sided restrictions (4), the descriptive spline is generated by the same algorithm after the transition to one-sided restrictions $\tilde{D}s \le \tilde{d}$, where $\tilde{D} = |-D \; \vdots \; D|^T$ is a $2N_r \times n$ matrix; $\tilde{d} = |d^{\text{low}} \; \vdots \; d^{\text{up}}|^T$ is a vector of dimension $2N_r$.

In the above algorithm for generating the descriptive spline the value of the smoothing parameter α exerts a substantial effect on the accuracy. Several approaches can be used for its selection. For example, when selecting α one may ignore the introduced prior information. In this case, to estimate the optimal value α_{opt} algorithms that are based on the optimality criterion and the cross significance method are used [3]. It should be borne in mind that the introduction of the prior information usually exerts a "regularizing" influence, and therefore the obtained value of α can be reduced by one order of magnitude. An alternative approach is the evaluation of α_{opt} by the same algorithms but already with the vector s^* of the values of the descriptive spline computed for each value of α. This substantially (by an order of magnitude or more) increases the expenditure of computer time.

Results of a Computational Experiment. The following are the results of one of the numerous computational experiments dealing with the construction of descriptive smoothing splines. Figure 1 presents a plot of the function $f(x)$ assigned in the interval [0, 6]. Such a function is "difficult"for smoothing and differentiating its noisy values because it contains segments with substantially differing values of the first derivative (Fig. 2). The values of the function measured at 40 nodes x_i were distorted by noise with the relative level δ. These values were used to construct the "ordinary" spline $S_{n,\alpha}(x)$ and the descriptive spline $S^*_{n,\alpha}(x)$ under the restrictions: a) $S(x) \ge 0$, $x \in [0, 6]$; b) $S'(x) \ge 0$, $x \in [0, 3.5]$; c) $S''(x) \ge 0$, $x \in [0, 3.5]$, $x \in [4.5, 6.0]$ and for the smoothing parameter values $\alpha_1 = \alpha_{\text{opt}}$; $\alpha_2 = 0.1\alpha_{\text{opt}}$.

In Figs. 1 and 2 the values of $S_{n,\alpha}(x)$, $S^*_{n,\alpha}(x)$, and its derivatives are given (the noise level $\delta = 10\%$). It is seen that $S^*_{n,\alpha}(x)$ has a higher accuracy and, what is by no means unimportant, that $S^*_{n,\alpha}(x)$ satisfies the physical concepts about the approximated function $f(x)$ and its derivative. We note that the diversity of the prior information used for constructing $S^*_{n,\alpha}(x)$ is due to the intention to demonstrate wide possibilities for the algorithm. In other computational experiments and processings of real experimental data with "poorer" information a substantial increase in the accuracy of the solution of problems with the use of descriptive splines was also observed.

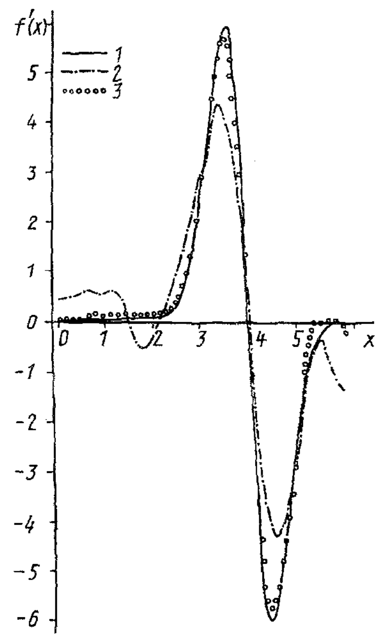

Fig. 2. Approximation of the derivative $f'(x)$: 1) exact derivative $f'(x)$; 2) derivative of the spline $S_{n,\alpha}(x)$; 3) derivative of the spline $S^*_{n,\alpha}(x)$.

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APPENDIX

We introduce the vector of the second derivatives $m = |S''_{n,\alpha}(x_1), \ldots, S''_{n,\alpha}(x_n)|^T$, which is related to the vector $s = |S_{n,\alpha}(x_1), \ldots, S_{n,\alpha}(x_n)|^T$ by the matrix relation [3]

$$Am = Hs. \tag{A1}$$

The elements of the three-diagonal matrices A and H are defined by the boundary conditions used [3]. Here, we restrict ourselves to the "natural" boundary conditions $S''_{n,\alpha}(x_1) = S''_{n,\alpha}(x_n) = 0$. Then $m = |S''_{n,\alpha}(x_2), \ldots, S''_{n,\alpha}(x_{n-1})|^T$, and the elements of the $(n-2) \times (n-2)$ matrix A are defined as $A_{i,i} = (h_i + h_{i+1})/3$, $1 \le i \le n-2$, $A_{i,i+1} = A_{i+1,i} = h_{i+1}/6$, $1 \le i \le n-3$, where $h_i = x_{i+1} - x_i$. The $(n-2) \times n$ matrix H has the elements $H_{i,i} = 1/h_i$; $H_{i,i+1} = -(1/h_i + 1/h_{i+1})$; $H_{i,i+2} = 1/h_{i+1}$, $1 \le i \le n-2$. Then, using the vector m, the functional $F[S] = \int (S''(x))^2 dx$ can be rewritten in the form $F[S] = m^T A m$ or (taking into account Eq. (A1)) as

$$F[S] = s^T H^T A^{-1} Hs = s^T Qs. \tag{A2}$$

The vectors a, b, and c, composed of the spline coefficients a_i, b_i, and c_i, are connected with the vector s by the following matrix relations: $a = D_0 s$, $b = D_1 s$, $c = D_2 s$, where $D_0 = I$ is the unit matrix, D_1, D_2 are $(n \times n)$ and $(n\text{-}2) \times n$ matrices;

$$D_1 = L + TA^{-1}H; \quad D_2 = \frac{1}{2} A^{-1} H.$$

The matrix L has the dimensions $(n \times n)$ and the elements $L_{i,i} = -1/h_i$, $L_{i,i+1} = 1/h_i$, $L_{n,n-1} = -1/h_{n-1}$, $L_{n,n} = 1/h_{n-1}$, and T is an $n \times [n-2]$ matrix that is defined as $T_{i,i} = -h_i/6$, $T_{i+1,i} = -h_{i+1}/3$, $T_{n,n-2} = h_{n-1}/6$.

Having denoted the i-th line of the matrices D_0, D_1, and D_2 by $D_{0,i}$, $D_{1,i}$, $D_{2,i}$, the l_i-th derivative of restrictions (4) can be rewritten in the form

$$D^{l_i} S_{n,\alpha}(x_i) = \begin{cases} D_{0,i}\, s, & \text{if } l_i = 0; \\ D_{1,i}\, s, & \text{if } l_i = 1; \\ D_{2,i}\, s, & \text{if } l_i = 2. \end{cases}$$

Then the system of restrictions (4) can be represented in the form of the matrix inequality

$$d^{\text{low}} \leq Ds \leq d^{\text{up}}, \tag{A3}$$

in which D is an $N_r \times n$ matrix composed of the lines $D_{l,i}$, $1 \leq i \leq N_r$.

NOTATION

$f(x)$, investigated function; $\widetilde{f}_i$, measured values; $S_{n,\alpha}(x)$, smoothing spline; a_i, b_i, c_i, d_i, coefficients of the spline; $S^*_{n,\alpha}(x)$, descriptive spline; α, smoothing parameter; p_i, weighting factors; d_i^{low}, d_i^{up}, lower and upper boundaries of admissible values for the derivative $D_i^{l_i} S(x_i)$ at the node x_i; s, vector of spline values at the nodes.

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