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ALGORITHMS FOR ESTIMATING OPTIMUM DIMENSIONALITY OF AN APPROXIMATE SOLUTION OF THE CONVERSE THERMAL CONDUCTIVITY PROBLEM

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Algorithms are presented for calculating the optimum dimensionality of an approximate solution, using various *a priori* data on the uncertainty to which the right side of the operator equation is specified.

Formulation of the Problem. Many converse thermal conductivity problems reduce to solution of a type I operator equation [1]

$$K\varphi = f, \tag{1}$$

where $\varphi(x)$, $f(y)$ are functions of the spaces Φ, F; K is a completely continuous operator the null space of which is empty. The right side of $f(y)$ is specified by measurements at a discrete set $\{y_i\}$ of values $\tilde{f}_i = f(y_i) + \xi_i$, $i = 1, 2, \ldots, n$, where ξ_i is the random uncertainty (measurement noise) at the point y_i. It is necessary that we construct a solution of integral equation (1) from the initial data, $\{K, \tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_n\}$. As is well known, such a problem is incorrectly formulated [2], and various stable methods are used for its solution.

In a number of methods, for the approximate solution of Eq. (1) the element $\varphi_N(x)$ of a finite dimensional space Φ_N of dimensionality N is used [3]. The base functions of such a space may be either eigenfunctions of the operator K, or a set of some functions with good approximation properties. With such a construction of the approximate solution, the dimensionality N plays the role of a unique regularization parameter and determines the accuracy of the solution constructed. Choice of "suitable" dimensionality depends on both the level of uncertainty in the measurements, and the differential properties of the unknown solution. With reduced dimensionality the solution $\varphi_N(x)$ will not contain the "fine structure" of the

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function $\varphi(x)$, while with elevated dimensionality oscillations appear in $\varphi_N(x)$, caused by "swinging" in the measurement noise of the right side. Therefore, the problem develops of estimating the optimum (in accordance with some chosen criterion) dimensionality of the finite-dimensional space, the element of which defines the approximate solution of Eq. (1).

Below we will present seven algorithms which permit estimating the optimum dimensionality N_{opt}. For the optimization criterion, we will use the mean-square uncertainty of the right side approximation, defined by the function

$$\Delta^2(N) = M\left[\sum_{i=1}^{n} (f(y_i) - f_N(y_i))^2\right],$$

where $M[\cdot]$ is the mathematical expectancy operator: $f_N(y)$ is the right side of Eq. (1) corresponding to the solution $\varphi_N(x)$.

It is obvious that the spaces Φ_N must be ordered on some scale. We will introduce the discrepancy function

$$\rho(\tilde{f}, f_N) = \sum_{i=1}^{n} w_i (\tilde{f}_i - f_N(y_i))^2, \tag{2}$$

where $w_i > 0$ are weight factors. We denote by m_N the lower boundary of this function, i.e., $m_N = \inf_{\varphi\in\Phi_N} \rho(\tilde{f}, K\varphi)$. We will say that the spaces Φ_N are ordered if the following chain of inequalities is satisfied:

$$m_{N_1} > m_{N_2} > m_{N_3} > \cdots > \inf_{\varphi\in\Phi} \rho(\tilde{f}, K\varphi) \quad \text{for} \quad N_1 < N_2 < N_3 < \cdots \tag{3}$$

Before presenting the algorithm for evaluation of N_{opt}, we will consider the construction of the solution $\varphi_N(x)$ for a specified dimensionality N.

Construction of a Solution in the Space Φ_N. With on loss of generality, we choose as the element $\varphi_N(x)$ the linear combination

$$\varphi_N(x) = \sum_{j=1}^{N} a_j B_j(x),$$

where $B_j(x)$ are base functions of the space Φ_N. We find the vector of the coefficients **a** $= |a_1, a_2, \ldots, a_N|$ from the condition of a minimum in the discrepancy function (2). We note that minimization of Eq. (2) permits calculation of estimates for the vector **a**, which are robust in the class of measurement noise distributions with finite dispersion [4]. For other classes of distributions it is necessary to specify other discrepancy functions.

It can be shown that the vector **a*** which minimizes Eq. (2) can be defined from the system of normal equations

$$\mathbf{B}^T\mathbf{W}\mathbf{B}\mathbf{a} = \mathbf{B}^T\mathbf{W}\tilde{\mathbf{f}}, \tag{4}$$

where $\tilde{\mathbf{f}} = |\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_n|^T$ is the vector of the right side measured values; T is the transportation symbol; **B** is a matrix of dimensions n × N with elements $\{\mathbf{B}\}_{ij} = \Psi_j(y_i)$. The function $\Psi_j(y)$ is an image of the function $B_j(x)$, i.e., $\Psi_j = KB_j$. The diagonal matrix **W** is defined by the expression $\mathbf{W} = \mathrm{diag}\{w_1, w_2, \ldots, w_n\}$. Since the matrix of system (4) is positively defined, then for any vector $\tilde{f}$ there exists a unique coefficient vector **a***, which uniquely defines the approximate solution of Eq. (1) in the space Φ_N.

Algorithms for Estimating Optimum Dimensionality. We will note that direct minimization of the function $\Delta^2(N)$ requires knowledge of the exact right side (or exact solution) of Eq. (1). Such information is as a rule unavailable. We do have the discrepancy vector e(N), the projections of which are defined by expression $e_i(N) = \tilde{f}_i - f_N(y_i)$, i = 1, ..., n. In a number of cases we also have *a priori* information on the correlation matrix $\mathbf{V}_\xi$ of the random measurement noise vector $\xi = |\xi_1, \xi_2, \ldots, \xi_n|^T$. Therefore we will present below seven algorithms for estimating the optimum dimensionality which rely only on available information. It will be assumed that the measurement noise has a zero mean and is not correlated at adjacent measurement points, i.e., $\mathbf{V}_\xi = \mathrm{diag}\{\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2\}$, where σ_i^2 is the noise dispersion at point y_i. Due to the limited size of the study only final results will be presented with appropriate citations to the literature.

Algorithm V. This is a statistical generalization of the discrepancy principle, widely used to select the regularization parameter [5]. We assume that the dispersions $\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2$ are given and introduce the quadratic form

$$V(N) = \mathbf{e}^\mathrm{T}(N)\,\mathbf{V}_\xi^{-1}\mathbf{e}(N) = \sum_{i=1}^{n} e_i^2(N)/\sigma_i^2 .$$

for N_{opt} we take the smallest value of N (denoted by N_V) for which

$$V(N) \in \Theta_{n-N}(\beta) = [\vartheta_{n-N}(\beta/2),\ \vartheta_{n-N}(1-\beta/2)].$$

The boundary points $\vartheta_{n-N}(\beta/2)$, $\vartheta_{n-N}(1-\beta/2)$ of the interval $\Theta_{n-N}(\beta)$ are a quantile of a χ^2-distribution with $n - N$ degrees of freedom for levels $\beta/2$, $1 - \beta/2$, respectively. We recommend that β be taken as 0.05.

Algorithm W. This is based on the criterion of optimal approximation of experimental information of [6]. We assume that the dispersions σ_i^2, $i = 1, 2, \ldots, n$, are specified and introduce the bilinear expression:

$$W(N) = \tilde{f}^\mathrm{T} V_\xi^{-1} e(N) = \sum_{i=1}^{n} \tilde{f}_i e_i(N)/\sigma_i^2 .$$

For N_{opt} we take the smallest value of N (denoted by N_W) for which $W(N) \in \Theta_{n-N}(\beta)$.

Algorithm C. We assume that the measurements of the right side are equally accurate, i.e., $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_n^2 = \sigma^2$. and use the statistics of [7]:

$$C(N) = \sum_{i=1}^{n} e_i^2(N)/\sigma^2 + 2N - n.$$

For N_{opt} we take the largest value of N (denoted by N_C) satisfying the condition $C(N) \leqslant N$.

We will note that the above algorithms require specification of the measurement noise dispersion. When the dispersions are specified inaccurately the dimensionality values obtained may differ significantly from values calculated with accurately specified dispersions. This is a definite shortcoming of algorithms V, W, and C. Therefore, it is desirable to consider algorithms which do not require specification of the noise dispersion.

Algorithm F. We assume that the measurements of the right side are equally accurate and define the statistics [8]:

$$F(N) = \Big(\sum_{i=1}^{n} e_i^2(N-1) - \sum_{i=1}^{n} e_i^2(N)\Big) \Big/ \Big(\sum_{i=1}^{n} e_i^2(N)/(n-N)\Big) .$$

For the optimum dimensionality we take the smallest value of N (denoted by N_F) satisfying the inequalities: $F(N) \geqslant F_\beta(1,\ n-N)$; $F(N+1) \leqslant F_\beta(1,\ n-N-1)$, where $F_\beta(1, n - N)$ is a quantile of level β (β = 0.9-0.95) of a Fisher distribution $\mathcal{F}(1, n - N)$ with degrees of freedom 1, $n - N$.

Algorithm A. This is based on an information criterion used for identification of dynamic systems [9]. We introduce the function

$$A(N) = n \ln\left(\frac{1}{n}\sum_{i=1}^{n} e_i^2(N)\right) + 2N.$$

For N_{opt} we choose the value of N_A which minimizes this function.

Algorithm U. This technique realizes the cross-validation method of [6, 10]. For the optimum dimensionality we take the value of N_U which minimizes the function

$$U(N) = \frac{1}{n}\sum_{i=1}^{n} e_i^2(N)/[1 - N/n]^2.$$

Algorithm R. This is based on ordered minimization of empirical risk [4]. For N_{opt} we choose the value of N_R which minimizes the function

$$R(N) = \frac{1}{n}\sum_{i=1}^{n} e_i^2(N) \Big/ \left[1 - \left(\frac{N(\ln n/N+1) - \ln\eta}{n}\right)^{1/2}\right]_\infty,$$

where

$$[z]_\infty = \begin{cases} z, & z \geqslant 0; \\ \infty, & z < 0, \end{cases} \quad \eta = 0{,}02 - 0{,}05.$$

We will note a characteristic feature of these last three algorithms. The values of the minimizing functions are determined by two quantities. The first (of the form $\sum_{i=1}^{n} e_i^2(N)/n$) decreases with increase in N, while the second (the term 2N or the dividend in U(N), R(N)), which reflects the "complexity" of the solution constructed, increases. Determining a compromise between the values of these two quantities is the basis of the last three algorithms.

Evaluation of Numerical Experiment Results. To study the properties of the optimum dimensionality estimates obtained by the algorithms presented above, a numerical experiment was performed (described in [11]) to construct a solution of a type I Fredholm integral equation. Cubic B-splines [11] were used as base functions. Statistical modeling for various noise levels was used to find N_{opt} and error values $\Delta^2(N)$ for various estimates of N_{opt}. The volume of samples taken was 50.

Analysis of these results revealed that for known dispersions of measurement noise algorithm W evaluates N_{opt} with satisfactory accuracy. Algorithms V and C, as a rule, give lowered dimensionality values, corresponding to an "oversmoothed" solution. If the noise dispersion is not known, then for values of $N_{opt}/n < 0.3$ it is desirable to use algorithm U for calculating N_{opt}, while for values $N_{opt}/n \geqslant 0.3$ algorithm R is suitable. It should be noted that in case of correlated measurement noise (the correlation coefficient at adjacent points being set equal to 0.2) algorithm U leads to elevated dimensionality values and insufficient smoothing of measurement noise.

NOTATION

$\varphi(x)$, unknown solution of the operator equation; f(y), exact right-hand side of equation; $\tilde{f}_i$, measured values of right-hand side; N, dimensionality of finite-dimensional space Φ_N; $\varphi_N(x)$, approximate solution of integral equation of dimensionality N; $f_N(y)$, right-hand side of equation corresponding to $\varphi_N(x)$; $B_j(x)$, base functions; ξ_i, measurement noise; V_ξ, measurement noise correlation function; σ_i^2, measurement noise dispersion; $e_i(N)$, discrepancy of i-th measurement; e(N), $\vartheta_{n-N}(\beta/2)$ iscrepancy vector; e(n), quantile of χ^2-distribution with n − N degrees of freedom of level β/2; $F_\beta(1, n-N)$, quantile of Fisher distribution of level β with degrees of freedom 1, n − N; V(N), W(N), C(N), F(N), A(N), U(N), R(N), functionals used to find optimum dimensionality estimates; N_{opt}, optimum dimensionality.

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NUMERICAL SOLUTION OF THE INVERSE PROBLEM OF HEAT CONDUCTION BY USING REGULARIZED DIFFERENCE SCHEMES

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The stability of difference schemes is investigated for the approximate solution of a multidimensional incorrect heat-conduction problem with inverse time.

Among the inverse problems of heat transfer [1], the problem with inverse time for the heat-conduction equation that belongs to the A. N. Tikhonov conditionally correct class attracts a great deal of attention. The general approach to the solution of unstable problems is formulated in [2] on the basis of the method of regularization. The method of quasiinversion [3] which consists in perturbing the initial equation has received wide propagation for differential equations. Of the later modifications of this method we note that described in [4] where a "pseudoparabolic" perturbation of the original equation as well as a "hyperbolic" modification are examined [1]. The stability of appropriate difference schemes of the quasi-inversion method is investigated in [5, 6].

Regularization of difference schemes is achieved in this paper by selecting a negative weight in the usual scheme with weights [7]. Economical difference schemes analogous to the locally one-dimensional schemes [7] in solving the direct heat conduction problem, are proposed in the multidimensional case. General results of the A. A. Samarskii [8] theory of stability of difference schemes are used in investigating the stability.

FORMULATION OF THE PROBLEM

Let Ω denote a n-dimensional parallelepiped: $\Omega=\{x|x=(x_1,\ x_2,\ \ldots,\ x_n),\ 0<x_k<l_k,\ k=1,\ 2,\ \ldots,\ n\}$.

For $x\in\Omega$ let us determine the uniform elliptical operator L:

$$Lu=\sum_{k=1}^{n}L_k u=\sum_{k=1}^{n}\frac{\partial}{\partial x_k}a_k(x_k)\frac{\partial u}{\partial x_k}$$

with sufficiently smooth coefficients $a_k(x_k)\geqslant a_0>0,\ k=1,\ 2,\ \ldots,\ n$. The function u(x, t) satisfies the heat-conduction equation with inverse time

$$\frac{\partial u}{\partial t}+Lu=0,\ x\in\Omega,\ t\in S=(0,\ T),\ T>0, \tag{1}$$

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