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NUMERICAL EVALUATION OF COEFFICIENTS OF MULTIDIMENSIONAL HEAT EQUATION BY STOCHASTIC DIFFERENTIAL EQUATIONS

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ABSTRACT

A new algorithm of determination of coefficients of multidimensional heat equations on the basis of temperature measurements is proposed. A system of stochastic differential equations (SDE) can be assigned to a linear multidimensional heat equation. The solution of the heat equation can be obtained by solving the corresponding SDE by the method of statistical modeling. The sensitivity analysis is used when solving the considered inverse problem. The method of statistical modeling for evaluation of sensitivity functions is used as well. The application of parallel computers allows a significant increase of the efficiency of the proposed algorithm. The results of numerical calculations are given.

INTRODUCTION

The considered inverse heat transfer problem consists in the definition of unknown coefficients of the heat equation by using the temperature measurements at the given points of an investigated domain. The inverse heat transfer problems arise in many areas of science and engineering, in which there is a necessity for study and design of objects, exposed to the influence of thermal loading. Nowdays the resolution of one-dimensional inverse heat transfer problems is well investigated, and there are many reliable algorithms and programs for their solution. However, this is not the case for higher dimensional problems.

Many problems connected with correctness of statement and solution algorithms arise in connection with the inverse problems solution. In calculations, it is also necessary to take into account high computer costs of algorithms. For example, one reason of the high computer costs is the necessity of solution of a plenty (as a rule) of direct problems when a one inverse problem is solved. Moreover, there are inverse problems (such as multidimensional ones), in which the solution of the direct problem demands high computer costs.

In the present work we attempt to solve a direct problem by Monte Carlo method. First, this approach should create insuperable difficulties, because Monte Carlo method is highly labor-consuming. But it is necessary to take into account the fact that when solving the inverse problem, the solution of the direct problem is required only at those points, where the measurements are made. The Monte Carlo method, as opposed to grid methods, allows us to define a solution of the heat equation only at different given points of the domain. In addition, algorithms of statistical modeling can be easily parallelized, and consequently it is possible to use modern high-efficiency parallel computing systems for the solution of such problems. Eventually we consider a Monter Carlo method not as a one competing with grid methods, but as a one of possible alternatives.

INVERSE HEAT TRANSFER PROBLEM

Let us consider the following boundary value problem for the heat conduction equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\sum_{i,j=1}^{n} b_{ij}(x,p)\frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} f_i(p,x)\frac{\partial u}{\partial x_i},$$

$$
\begin{aligned}
& t \geq 0, x \in G \qquad (1)\\
& u(0,x) = \varphi_0(x), \qquad x \in G, \quad t = 0\\
& u(t,x) = \varphi(t,x), \qquad x \in \partial G,
\end{aligned}
$$

where $B(x,p) = (b_{ij}(x,p))$ is a positive definite symmetric matrix, $G \in R^n$ is a bounded domain with a regular boundary, $p = (p_1, \ldots, p_m)$ is a vector of parameters.

It is required to determine the unknown parameters p, when the temperature measurements are given at some internal points of G .

The boundary value problem (1) can be posed in accordance with the SDE system in the Ito sense (see, for example, (Ventzel, 1975))

$$
y(t,p) = y_0 + \int_0^t f(y(s,p),p)ds + \int_0^t \sigma(y(s,p),p)dw(s), \quad (2)
$$

where $w(\cdot)$ is an n-dimensional standard Wiener process, $y_0 \in R^n$ is the value of $y(t)$ at $t = 0$, $\sigma(y,p)$ is the square matrix, such that $B(y,p) = \sigma(y,p)\sigma(y,p)^T$. Then, according to (Ventzel, 1975) there exists a probabilistic representation of the solution of the boundary value problem (1)

$$
\begin{aligned}
& u(t,y_0,p) = \\
& \langle \varphi_0(y(t,p))\chi(\tau_0 > t) + \varphi(t-\tau_0, y(\tau_0,p))\chi(\tau_0 \leq t) \rangle, \quad (3)
\end{aligned}
$$

where the angular brackets mean the mathematical expectation, τ_0 is the first time moment when the SDE solution (2) reached the boundary of the domain G, $\chi(A)$ is an indicator function of the set A.

Let u^*_{ij} be the temperature measurements at the given points of the domain G x_i $(i = 1, \ldots, l)$ at the times t_j $(j = 1, \ldots, k)$. Then the problem of an estimation of parameters can be reduced to minimization of the following functional

$$
\min_p F(p) = \sum_{i,j} (u^*_{ij} - u(t_j, x_i, p))^2 \qquad (4)
$$

Application of the gradient type methods for minimization of (4) requires calculation of derivatives $\partial u/\partial p$, which can be obtained by differentiation of (3) with respect to p. Here the derivatives of the kind $\partial y_i/\partial p_j$ appear, which express the sensitivity of the solution of (2) to the variation of the parameters p. It is shown (Gikhman, 1968), that with fulfilment of the existence and uniqueness conditions of the SDE solution, and with allowance for the fact that there exist sufficiently smooth and limited derivatives of $f(t,p)$, $\sigma(t,p)$, the solution of the SDE system (2) is differentiable with respect to the parameters p. The parametric derivatives satisfy the system, that can be obtained from (2) as a result of its differentiation with respect to parameters, i.e., from the system

$$
\begin{aligned}
y_p(t,p) = y_p(0) + \int_0^t (\frac{\partial f}{\partial y} y_p(s,p) + \frac{\partial f}{\partial p})ds + \\
\int_0^t (\frac{\partial \sigma}{\partial y} y_p(s,p) + \frac{\partial \sigma}{\partial p})dw(s), \qquad (5)
\end{aligned}
$$

where $y_p = (\partial y_i/\partial p_j)$ is a parametric derivatives matrix. Thus, the problem of determination of coefficients of equation (1) is reduced to minimization of functional (4). In this case the calculation of values of functional (4) is done on the basis of statistical modeling of trajectories of the stochastic process determined by the SDE system (2). And the calculation of values of the derivatives of (4) is carried out on the basis of statistical modeling of trajectories of the stochastic process determined by system (2), (5).

The simulation of trajectories of solutions of the SDE systems (2) and (2), (5) was done by the generalized Euler method with a constant integration step

$$
y_{n+1} = y_n + hf(t_n, y_n) + \sqrt{h}\sigma(t_n, y_n)\zeta_n, \qquad (6)
$$

where y_n is a value of a trajectory of the stochastic process at the time t_n, h is an integration step, ζ_n is a sequence of independent among themselves normal random vectors with independent components, having zero mathematical expectation and unit dispersion. In numerical calculations the vectors ζ_n are obtained by a random number generator.

Solution of the equation (1) by the method of statistical modeling is a computationally labor intensive process. However, this approach can be justified by the following: when the given inverse problem is solved, it is sufficient to know the solution of the direct problem only at those points of the domain G, at which the measurement of temperature is made. The Monte Carlo permits to calculate the value of temperature at anyone point of the domain G without grid.

In this paper, we show the capacity of this method by solving a model three-dimensional problem which has exact solution.

SOLUTION OF A MODEL PROBLEM

As a model problem we shall consider the determination of the factors p_1, p_2, p_3 in a thermophysical experiment of a three-dimensional ball cooling , when the temperature at its center is higher than at any other point. The corresponding heat equation boundary value problem is the following

$$\begin{aligned} &\frac{\partial u}{\partial t} = \frac{1}{2}(p_1\frac{\partial^2 u}{\partial x_1^2} + p_2\frac{\partial^2 u}{\partial x_2^2} + p_3\frac{\partial^2 u}{\partial x_3^2}), \\ &\quad t \in (0,T), \quad \|x\|^2 < 1, \\ &u(0,x) = u_0(1-r), \quad r = (x_1^2 + x_2^2 + x_3^2)^{\frac{1}{2}}, \\ &u(t,x) = 0, \qquad \|x\|^2 = 1, \end{aligned} \tag{7}$$

where u_0 is the initial temperature at the center of the ball, $p_i > 0$, $i = 1,2,3$. The inverse problem of determination of p_1, p_2, p_3 satisfies the uniqueness conditions if the temperature measurements at the center of the ball are known (Volkov, 1984). In addition, for the purpose of stability of calculations we took the temperature measurements at other internal points of the ball.

In the case when p_1, p_2, p_3 fulfil the condition $p_1 = p_2 = p_3 = 2p$, the exact solution of the boundary value problem (7) can be written down as the following expansion

$$u(t,x) = \sum_{n=1}^{\infty} \beta_n \exp^{-n^2\pi^2 pt} \frac{\sin(\pi n r)}{r}, \tag{8}$$

where

$$\beta_n = 2\int_0^1 u_0 x(1-x)\sin(\pi n x)dx$$

In the model problem the "measurements" of temperature were calculated using formula (8) with $p_1 = p_2 = p_3 = 1$.

A stochastic process corresponding to the boundary value problem (7) is determined only by the diffusion term. This process is described by the following system of three stochastic differential equations

$$y_i(t,p) = y_i(0) + p_i^{1/2}\int_0^t dw_i(s), \quad i = 1,2,3 \tag{9}$$

The sensitivities of solution of the SDE system (9) to parameters variations are determined by the SDE system

$$\frac{\partial y_i}{\partial p_i}(t,p) = \frac{\partial y_i}{\partial p_i}(0) + \frac{1}{2p_i^{1/2}}\int_0^t dw_i(s), \quad i = 1,2,3 \tag{10}$$

The measurements of temperature were simulated with the use of formula (8) at the following seven points: $\bar{x}_1 = (0,0,0)$, $\bar{x}_2 = (0.3,0,0)$, $\bar{x}_3 = (0,0.3,0)$, $\bar{x}_4 = (0,0,0.3)$, $\bar{x}_5 = (-0.3,0,0)$, $\bar{x}_6 = (0,-0.3,0)$, $\bar{x}_7 = (0,0,-0.3)$.

At each of these seven points 40 values of temperature were calculated using formula (8) with the time interval $\Delta t = 0.2$ starting with $t_0 = 0.2$. As the initial values of parameters the vector $p^0 = (1.4; 0.6; 1.4)$ was taken.

The following estimates of parameters $\tilde{p} = (0.95; 1.03; 1.08)$ were computated as a result of the minimization of functional (4) with the sample volume of 20,000 .

The modeling of trajectories of stochastic processes, defined by the SDE's (9) and (10) was carried out using formula (6) with the step $h = 0.001$.

For minimization of (4) one version of r-algorithm was used. This method is based on stretching the space in the direction of a difference of two consecutive gradients (Shor, 1979) and is intended for minimization of rough functions.

As is seen from the description of the soluble problem, the main problem in calculations is the modeling of trajectories of stochastic processes, determined by equations (9), (10).

In our calculations, the number of trajectories should be of order 10^4 — 10^5 for the reduction of influence of a statistical error on estimations of the parameters.

The statistical modeling of each trajectory in calculation of the value of functional (4) and its derivatives is made independently of any other trajectory. Therefore this part of the program can be easily parallelized by splitting the common number of simulated trajectories on the parallel working processors.

Application of parallel computing machinery

In order to realize the given program, the parallel computing system MVS-100 of eight parallel processors Intel860 was used.

The general structure of the parallel program consists in the following. The processor with the number 0 plays a key role in the solution of the problem. It inputs the initial data, makes minimization of the objective function and outputs results of calculations. The other processors are connected with calculation of the objective function and its gradient.

Processors with numbers $1, 2, \ldots, 7$ input the initial data for modeling of the number of trajectories, and each

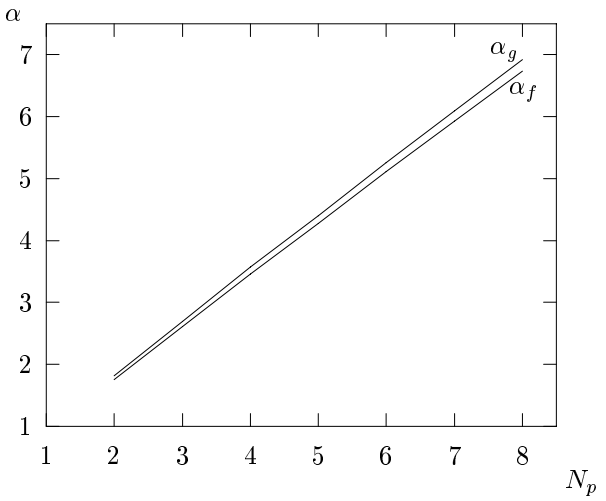

Figure 1. The speed-up of computation of the objective function and its gradient; α_f - the speed-up with calculation of the objective function; α_g - the speed-up with calculation of the gradient; N_p - the number of processors.

of them outputs the calculated contributions into the objective function and its gradient. As the common number of simulated trajectories is very high, the greater part of computer time is spent on modeling of trajectories, while expenses for data transfer are rather insignificant. Therefore, it is possible to expect that the speed-up will be close to a linear function of the number of processors with a large number of trajectories.

Fig. 1 demonstrates the obtained values of the speed-up for the calculation of the objective function and its gradient. The speed-up here is the ratio between the computational time for one processor and computational time for i $(i = 2, \ldots, 8)$ processors.

It is required more CPU-time for the calculation of the gradient, while the expenses needed for data transfer are less than those for the evaluation of the function. Therefore, the speed-up for the computation of the gradient is greater than that for the computation of the objective function.

CONCLUSION

The method of estimation of coefficients of a multidimensional equation by statistical modeling was proposed. The evaluation of both the solution of the direct problem and the sensitivity functions is made by solving special SDE systems, connected with the initial boundary value problem. The numerical experiment has shown a good agreement with the exact data. The considered algorithm can be easily parallelized, and the multiprocessor computer systems allow a considerable increase of its efficiency.

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