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EMPLOYMENT OF THE CONJUGATE EQUATIONS OF FIRST AND SECOND ORDER IN EVALUATING THE ERROR OF SOLUTION OF THE HEAT-CONDUCTION EQUATION

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Consideration has been given to the employment of the conjugate problems of first and second orders, which are applied to solution of the inverse problems of heat exchange, to calculate the error of solution of the primal problem from the data on the error of the initial information. It has been shown that the algorithms of solution of the inverse problems of heat exchange in a variational formulation make it possible to directly determine the error of the corresponding primal problems by calculation of the Hessian range.

Introduction. Determination of the error of the result from the error of the initial data is of natural interest in numerical solution of the problems of heat exchange. The methods, in which the sensitivity equations are used, and Monte Carlo methods are best suited to calculate the error. However, algorithms evaluating the error of a calculation result are rather rare in practice, which is caused by the high requirements on the speed of response and memory.

In this work, we have considered the evaluation (economical in terms of computation) of the accuracy of a temperature calculation on the basis of the error of the heat flux. To evaluate the exactness of the solution we employed a Hessian, which is calculated using conjugate equatons applied to solution of the inverse problems of heat conduction.

Evaluation of the Error of Solution with the Use of a Hessian. Let us consider the scheme of evaluating the error with the example of the solution of the one-dimensional equation of heat conduction (primal problem)

$$\rho C \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) = 0 \, . \tag{1}$$

The initial conditions are

$$T(x, 0) = T_0(x) \, ; \quad (x, t) \in (0 < x < X \, ; \; 0 < t < t_k) \, . \tag{2}$$

At one boundary, the heat flux $Q(t)$ containing the error δQ is acting:

$$-\lambda \frac{\partial T}{\partial x}\bigg|_{x=X} = Q(t) + \delta Q \, . \tag{3}$$

The other boundary is heat-insulated. One must determine at it the accuracy of the calculation of the temperature

$$\frac{\partial T}{\partial x}\bigg|_{x=0} = 0 \, . \tag{4}$$

We will solve the problem in a variational formulation formally coincident with the formulation of the inverse boundary-value problem of heat exchange [1, 2]. As a measure of the temperature error at the heat-insulated boundary we take the discrepancy between the exact and noisy (T^{err}) solutions:

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$$\varepsilon(\delta Q(t)) = \int_t (T(0,t) - T^{\text{err}}(t))^2 \, dt \,. \tag{5}$$

The finite-dimensional analog of the discrepancy has the form

$$\varepsilon(\delta Q) = \sum_1^N (T(0,t_i) - T^{\text{err}}(t_i))^2 .$$

This discrepancy is related to the quadratic norm of the temperature error $\varepsilon \sim \|\Delta T\|^2$.

For small values of the error (in the vicinity of the exact solution) the value of ε ($\varepsilon = \delta\varepsilon$) is determined by the value of the Hessian

$$\delta\varepsilon = \frac{1}{2} \frac{\partial^2 \varepsilon}{\partial Q_i \partial Q_j} \delta Q_i \delta Q_j = \frac{1}{2} H_{ij} \delta Q_i \delta Q_j \,, \quad i, j = 1, \ldots, N \,. \tag{6}$$

The average (over δQ) value of the error $\langle \delta\varepsilon \rangle = 0.5 \langle H_{ij} \delta Q_i \delta Q_j \rangle$ will be denoted as $\delta\varepsilon = 0.5 H_{ij} DQ_{ij}$ (DQ_{ij} is the correlation matrix of the error of the heat flux). For an uncorrelated error ($DQ = \text{diag}(\sigma_i^2)$) $\delta\varepsilon = 0.5 H_{ii} \sigma_i^2$. If the error of the data is constant and equal to σ, the error of the result is determined by the spur of the Hessian $\delta\varepsilon = 0.5 H_{ii} \sigma^2$.

Direct numerical differentiation of the discrepancy ε enables one to calculate the Hessian in N^2 recourses to the primal problem, which makes the actual employment of this information difficult. As is well known, solution of the conjugate problem is the most economical method to calculate the gradient. Therefore, it is natural to extend this approach to calculation of the Hessian. The most obvious method of such a calculation is direct numerical differentiation of the gradient obtained from the conjugate problem of first order [1, 2] (a is the differentiation parameter)

$$HdQ = (\text{grad}(Q + adQ) - \text{grad}(Q)) / a \,. \tag{7}$$

It requires solution of $2N$ primal-type problems. There is another approach to calculation of the action of the Hessian; this approach is based on solution of the "conjugate problem of second order" [3]. Here we consider both variants of calculation of the action of the Hessian on the vector and employ as a basis the conjugate equations applied to solution of the inverse problem of heat conduction on determination of the heat flux at one boundary from the measurements of the temperature at the other [1, 2].

Let us consider the derivation of the conjugate equation to calculate the gradient of discrepancy. We give the corresponding calculations in complete form (although they are widely presented in publications) since they will be required in deriving the conjugate equation of second order. To begin with we combine Eqs. (1) and (5) in a single variational formulation: we write the Lagrangian $L(Q, T, \Psi)$ in the form

$$L(Q(t), T, \Psi) = \int_t (T(0,t) - T^{\text{err}}(t))^2 \, dt + \int\int \rho C \frac{\partial T}{\partial t} \Psi(x,t) \, dt dx - \iint_\Omega \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \Psi(x,t) \, dt dx \,. \tag{8}$$

It is equal to the discrepancy (5) on the solution of Eq. (1) $L(Q(t), T, \Psi) = \varepsilon(\delta Q(t))$.

Problem in Perturbations. Let us perturb the boundary condition ΔQ. Having subtracted the unpertured solution, we obtain the perturbed problem

$$\rho C \frac{\partial \Delta T}{\partial t} - \frac{\partial}{\partial x} \left(\lambda \frac{\partial \Delta T}{\partial x} \right) = 0 \,. \tag{9}$$

The initial conditions are

$$\Delta T(0, x) = 0 \,, \tag{10}$$

the boundary conditions are

$$\left.\frac{\partial \Delta T}{\partial x}\right|_{x=0} = 0\,, \quad -\lambda \left.\frac{\partial \Delta T}{\partial x}\right|_{x=X} = \Delta Q\,(t)\,. \tag{11}$$

In what follows, we will employ Eqs. (9)–(11) to calculate the variations of the Lagrangian (8):

$$\Delta L\,(Q\,(t)) = \int 2\,(T\,(0, t) - T^{\text{err}}\,(t))\,\Delta T dt + \int\int \rho C \frac{\partial \Delta T}{\partial t}\,\Psi\,(x, t)\,dtdx - \iint_{\Omega} \frac{\partial}{\partial x}\left(\lambda \frac{\partial \Delta T}{\partial x}\right)\Psi\,(x, t)\,dtdx\,. \tag{12}$$

Our task is to find a function $\Psi(x, t)$ such that

$$\Delta L = \int_t \Delta Q \text{ grad}\,(\varepsilon)\,dt\,, \tag{13}$$

and all the remaining terms of second order of accuracy vanish. Integration of Eq. (12) by parts with account for the initial and boundary conditions (9)–(11) yields

$$\Delta L\,(Q\,(t)) = \int 2\,(T\,(0, t) - T^{\text{err}}\,(t))\,\Delta T dt + \int\int \rho C \frac{\partial \Psi}{\partial t}\,\Delta T\,(x, t)\,dtdx + \int_X \rho C \Psi\,(x, t)\,\Delta T dx \Big|_{t=0}^{t=t_k} -$$

$$- \int_t \lambda \frac{\partial \Delta T}{\partial x}\,\Psi dt \Big|_{x=0}^{x=X} + \int_t \lambda \frac{\partial \Psi}{\partial x}\,\Delta T dt \Big|_{x=0}^{x=X} - \iint_{\Omega} \frac{\partial}{\partial x}\left(\lambda \frac{\partial \Psi}{\partial x}\right)\Delta T\,(x, t)\,dtdx\,. \tag{14}$$

Conjugate Problem of First Order. If the function Ψ satisfies the equation

$$\rho C \frac{\partial \Psi}{\partial t} + \lambda \frac{\partial^2 \Psi}{\partial x^2} = 0 \tag{15}$$

with the boundary conditions

$$\lambda \left.\frac{\partial \Psi}{\partial x}\right|_{x=0} = 2\,(T\,(0, t) - T^{\text{err}}\,(t))\,, \tag{16}$$

$$\lambda \left.\frac{\partial \Psi}{\partial x}\right|^{x=X} = 0 \tag{17}$$

and the initial condition

$$\rho C \Psi\,(t, x)\Big|^{t=t_k} = 0\,, \tag{18}$$

then

$$\Delta L = \Delta \varepsilon\,(Q\,(t)) = -\int \lambda \frac{\partial \Delta T}{\partial x}\,\Psi \Bigg|^{x=X} dt = -\int \Delta Q\,(t)\,\Psi\,(X, t)\,dt\,, \tag{19}$$

hence we find the value of the discrepancy gradient

$$\text{grad}\,(\varepsilon) = \Psi\,(X, t)\,. \tag{20}$$

Equations (15)–(18) constitute the conjugate problem of first order. The calculation of the gradient requires a successive solution of the primal and conjugate problems: the conjugate problem is solved in the time-reversed direction. This algorithm makes it possible to calculate the gradient with the expenditure of calculation time which approximately corresponds to two calculations of the heat-conduction equation.

In the presence of the gradient, the action of the Hessian on the vector can be calculated by numerical differentiation with the use of (7); the "cost" of the calculation of the total Hessian will be nearly $2N$ recourses to the solution of the heat-conduction equation. However when the selection of the differentiation parameter a is incorrect the accuracy can be insufficient since in the vicinity of the minimum one has to take the difference of small numbers, which produces a high relative error. The action of the Hessian on the vector can be calculated more accurately using the problem which will be considered below.

Conjugate Problems of Second Order. We consider the perturbation of the conjugate problem (15)–(18) and, in accordance with the terminology of [3], call it the conjugate problem of second order:

$$\rho C \frac{\partial \Delta\Psi}{\partial t} + \lambda \frac{\partial^2 \Delta\Psi}{\partial x^2} = 0 . \tag{21}$$

The boundary conditions are

$$\lambda \frac{\partial \Delta\Psi}{\partial x}\bigg|_{x=0} = 2\Delta T\,(0, t) , \tag{22}$$

$$\lambda \frac{\partial \Delta\Psi}{\partial x}\bigg|^{x=X} = 0 , \tag{23}$$

the initial condition is

$$\Delta\Psi\,(t, x)\,\Big|^{t=t_k} = 0 . \tag{24}$$

Since

$$\Psi\,(Q + \Delta Q) = \Psi\,(Q) + \Delta\Psi \quad \text{and} \quad \nabla\varepsilon Q + \Delta Q = \nabla\varepsilon Q + \nabla^2\,\varepsilon\Delta Q ,$$

taking into account

$$\nabla\varepsilon = \Psi\,(X, t) ,$$

we obtain the action of the Hessian on the prescribed vector ΔQ:

$$\Delta\Psi\,(t, 1) = \nabla^2\varepsilon\Delta Q = H\Delta Q . \tag{25}$$

Thus, to find the action of the Hessian on the prescribed vector ΔQ we solve successively four initial boundary-value problems (of the primal-problem type):

(1) the primal problem, Eqs. (1)–(4) (time increases);

(2) the conjugate problem, Eqs. (15)–(18) (time decreases);

(3) the tangential problem, Eqs. (9)–(11) (time increases);

(4) the conjugate problem of second order, Eqs. (21)–(24) (time decreases).

To find the entire Hessian one must perform the calculation for N unit vectors; thus the "cost" of calculation of the Hessian corresponds to the solution of $4N$ primal-type problems. For linear problems the conjugate equation of second order has a rather simple form, but for nonlinear ones its complexity significantly increases, which can be an obstacle in debugging the program.

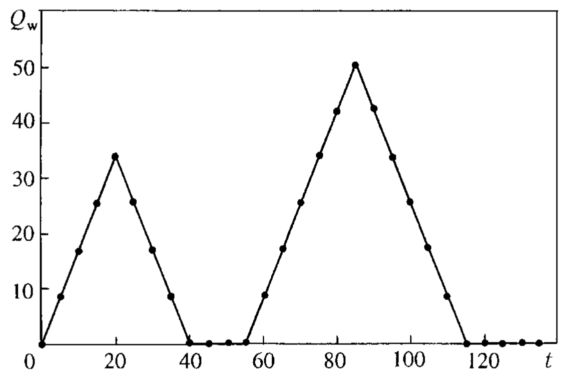

Fig. 1. Change in the heat flux with time. Q_w, kW/m^2; t, sec.

TABLE 1. Eigenvalues Calculated Using the Problem of First and Second Orders

j	1	2	3	4	5	6	7	8	9	10	11–17	18	19–28
H_1	5590	644	217	100	54.8	30.4	19.6	11.3	6.6	4.5	...	0	~0
H_2	6060	640	212	97.2	51.7	30.1	18.2	11.3	7.6	5.1	...	0.2	~0

TABLE 2. Evaluation of the Error Using Different Methods

Problem of first order H_1	Problem of second order H_2	μ_{max}	Result of averaging over 200 calculations
0.354	0.345	0.32	0.326

Calculation Results. We have calculated the Hessian by differentiation of the conjugate problem of first order and by solution of the conjugate problem of second order. The same finite-difference algorithm (integro-interpolation method) has been applied to solution of all the problems in question. The model problem contained 28 time nodes of the heat flux (with an interval of 5 sec) (see Fig. 1). The thermal conductivity of the material was $\lambda = 10^{-4}$ kW/(m·K), the volumetric heat capacity was $\rho C = 500$ kJ/(m^3·K), and the thickness was 3 mm; there were 20 cells over the thickness. The comparison of the calculations of the Hessian has shown that the numerical differentiation (problem of first order) yields a greater violation of the Hessian symmetry than the problem of second order. The eigenvalues calculated with the use of the conjugate problem of first order (H_1) and second order (H_2) (formulas (3) and (25) respectively) are given in Table 1.

The problem in question has nonnegative eigenvalues by virtue of the singleness of the inverse boundary-value problem of heat exchange [1]; part of the eigenvalues must be close to zero by virtue of incorrectness. In numerical calculations in the vicinity of zero, both methods yield a certain number of small negative eigenvalues; however the conjugate problem yields much fewer of them, which confirms its higher accuracy. From the viewpoint of evaluating the error it is precisely large eigenvalues that are of greatest interest, and in the region of these eigenvalues the coincidence of both methods is good. The spur of the Hessian H_{ij} is 7073 for the problem of first order and 6952 for the problem of second order.

We must note a rapid decrease in the eigenvalues in order (Table 1). Therefore, we can get by with the contribution of the maximum eigenvalues of the Hessian $\delta\varepsilon \approx \mu_{max}\sigma^2$ to evaluate the error in this problem. Calculation of the maximum eigenvalue μ_{max} by iterations can require a much smaller number of recourses to a system of partial differential equations than the calculation of the entire Hessian. To find the maximum eigenvalue one employs the iteration method in the form $X_{m+1} = HX_m$; $\mu = \max (X_m + 1)/\max (X_m)$, where $\max (X_m)$ denotes the maximum component of the vector X_m. For the problem in question the iteration method yields a maximum eigenvalue of 6423 in seven iterations (calculation using the Hessian H_{ij} yields $\mu_{max} = 5590$ for the problem of first order and $\mu_{max} =$ 6060 for the problem of second order).

The estimates of the error ε for a normally distributed error of the initial data with a variance of 0.01 using the spur of the Hessian, calculated with the use of the conjugate problem of first and second orders ($\delta\varepsilon = 0.5H_{ii}\sigma^2$), using the maximum eigenvalue ($0.5\mu_{max}\sigma^2$), and using averaging over 200 calculations are given in Table 2.

It should be noted that all four estimates of Table 2 are rather close in value.

Discussion. Complete information on the errors in this problem (variance of the temperature at any point x) can be calculated (in the linear case) by employing the sensitivity coefficients $\langle \delta T^2 \rangle = S_{ik} \langle dQ_k dQ_l \rangle S_{il}$, $S_{ik} = \dfrac{\partial T(t_i, x)}{\partial Q(\tau_k)}$.

The sensitivity function $S(t, x, \tau) = \dfrac{\partial T(t, x)}{\partial Q(\tau)}$ [2] satisfies the equations

$$\rho C \frac{\partial S}{\partial t} + \lambda \frac{\partial^2 S}{\partial x^2} = 0 . \tag{26}$$

The boundary conditions are

$$\lambda \left. \frac{\partial S}{\partial X} \right|_{x=X} = \delta\, (t - \tau) , \tag{27}$$

$$\left. \frac{\partial S}{\partial X} \right|_{x=0} = 0 , \tag{28}$$

The initial condition is

$$S\,(t = 0) = 0 . \tag{29}$$

Calculation of the sensitivity function implies solution of a system of higher order than the primal problem and storage of multidimensional calculation results. For low values of the error the Fisher information matrix $\sum\limits_i \dfrac{\partial T_i}{\partial Q_j} \dfrac{\partial T_i}{\partial Q_k}$ obtained from the sensitivity functions approximates the Hessian, which ensures the consistency of the methods in question:

$$H_{jk} = \frac{\partial^2 \varepsilon}{\partial Q_j \partial Q_k} = 2 \sum_i \frac{\partial T_i}{\partial Q_j} \frac{\partial T_i}{\partial Q_k} - 2 \sum_i (T_i - T_i^{\mathrm{err}}) \frac{\partial^2 T_i}{\partial Q_j \partial Q_k} .$$

If we are interested in the time-averaged temperature at a certain point (or any other temperature functional), the conjugate equations can be more efficient from the viewpoint of computer memory. Therefore, the approach to calculation of the error of the results which is based on solution of the conjugate problems appears quite justified, especially in the cases where it enables one to employ the existing set of algorithms to solve the inverse problems [1, 2].

In evaluating the error, differentiation of the conjugate problem of first order is more preferable than solution of the problem of second order since it is simpler algorithmically though it ensures close accuracy for large eigenvalues. Solution of the problem of second order is more preferable in problems where an accurate calculation of the Hessian is required (for example, in analysis of the uniqueness of the solution).

The numerical experiments confirm the heuristic considerations that an approximate evaluation of the accuracy using the maximum eigenvalue of the Hessian is possible. Since the action of the Hessian on the vector can be calculated in 2–4 recourses to a primal-type problem, one can rapidly calculate the maximum eigenvalue by iterations. The expenditure of time weakly depends on the dimensions of the initial data and is much lower than the expenditure of time on calculating the entire Hessian.

It is possible that the information of second order can also be of interest in the problems of experiment design. The approach to experiment design on the basis of the information matrix of Fisher has been described in [2]. The minimum eigenvalue $\mu_{\min}$ and the condition number and the determinant are considered as the condition number of the problem and of the quality of measurements.

TABLE 3. Number of "Large" Eigenvalues as a Function of Thickness

X/X_0	1	2	4	6	8	10	12
M	22	17	13	8	4	1	0

The presence of nearly zero quantities μ_{min} is typical of ill-posed problems; therefore, the relative error of μ_{min} is inevitably very high. It is possible that the number of eigenvalues which are larger than the data error can be used as the alternative criterion. In this connection, we have calculated the Hessian range for different thicknesses of the material using the conjugate problem of second order. The number of small eigenvalues increases with thickness, which is demonstrated in Table 3, where M is the number of eigenvalues which are larger than 10^{-4}. The parameters of the problem have been described above; the initial thickness is X_0 = 2.5 mm. Thus, the effective range of the Hessian can be used as the indicator of the degree of correctness of the problem and of the volume of information contained in the initial data.

Conclusions. The exactness of the solution of the heat-conduction equation can be evaluated by the data on the error of the initial data using the conjugate equations of first order, which are employed in solving the inverse problems, and using the conjugate equations of second order. The expenditure of time, evaluated as the number of recourses to solution of the primal problem, linearly depends on the dimensions of the initial data with a coefficient of 2 or 4. The numerical evaluation of the accuracy of a temperature calculation by the data on the error of the heat flux confirmed the suitability of the equations of first and second order.

The numerical experiments confirm the possibility of a rapid approximate evaluation of the error using the maximum eigenvalue of the Hessian calculated by iterations.

The algorithms of solution of the inverse problems of heat exchange make it possible to directly determine the error of the corresponding primal problems.

NOTATION

C, heat capacity, kJ/(kg·K); T, temperature, K; T^{err}, temperature in the presence of the error; x, coordinate; X thickness of the sample, m; t, time, sec; t_k, duration of the process, sec; Q, heat flux, kJ/m^2; H_{ij}, Hessian; L, Lagrangian; N, number of nodes of approximation of the heat flux with respect to time; S, sensitivity function; λ, thermal-conductivity coefficient, kJ/(m·K); δQ, error of the heat flux; $\delta(t - \tau)$, Dirac delta function; ρ, density, kg/m^3; ε, discrepancy; σ, variance of the error of the initial data; Ψ, conjugate variable of first order; $\Delta\Psi$, conjugate variable of second order; ΔT, increment in the temperature; μ, eigenvalues of the Hessian. Subscripts: min, minimum value; max, maximum value.

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