ON ESTIMATION OF TEMPERATURE UNCERTAINTY USING THE SECOND ORDER ADJOINT PROBLEM

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Running title: On estimation of temperature uncertainty

Abstract

The uncertainty of temperature prediction from the heat flux error is estimated using first and Second Order Adjoint equations. The adjoint codes developed for the inverse heat transfer problems provide the uncertainty estimation for the corresponding forward problems. Numerical tests corroborate the feasibility of fast uncertainty estimation using Hessian maximum eigenvalue obtained via second order adjoint equations.

Nomenclature

H_{ij}-Hessian
Q — heat flux
ΔT — temperature variation
ε -discrepancy
σ- input data error standard deviation
χ - thermal conductivity
λ- eigenvalue
ρ -density
Ψ-first order adjoint variable
$\Delta\Psi$- second order adjoint variable

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Introduction

The estimation of solution uncertainty from the input data error is of interest when heat transfer problems are solved. For this purpose, both Monte-Carlo methods and sensitivity equations are suitable. Nevertheless, algorithms providing both the result and its uncertainty are a rarity in practice due to the high computational burden involved in their solution.

The present paper is concerned with providing a computationally cheap estimation of temperature solution uncertainty from the heat flux error. The uncertainty is estimated from the Hessian spectrum, which is calculated by First Order Adjoint (FOA) equations commonly used for Inverse Heat Transfer problems or by using the Second Order Adjoint (SOA) equations.

Uncertainty Estimation via Hessian Calculation

Consider the uncertainty estimation using the one-dimensional thermal conduction equation (forward problem) as an example.

$$C\rho \frac{\partial T}{\partial t} - \frac{\partial}{\partial X}\left(\chi \frac{\partial T}{\partial X} \right) = 0; \qquad (1)$$

Initial conditions: $T(0,X)=T_0(X);\ (t,X)\in\ (0<t<t_f;\ 0<X<1);$ *(2)*

The boundary ($X=1$) is subjected to the heat flux $Q_w(t)$, which contains the error δQ.

$$\chi \frac{\partial T}{\partial X}\Big|_{X=1} = Q_w(t) + \delta Q \qquad (3)$$

Other boundary is thermally insulated.

$$\frac{\partial T}{\partial X}\Big|_{X=0} = 0; \qquad (4)$$

We search for the uncertainty of temperature prediction $T(t)$ on this boundary.

We pose the problem as an optimization statement formally coinciding with the inverse boundary heat conduction problem [1]. As the measure of uncertainty, we consider the discrepancy between exact and noisy solutions given by :

$$\varepsilon(\delta Q_w(t)) = \int_t \left(T^{exact}_{X=0}(t) - T^{error}_{X=0}(t) \right)^2 dt \qquad (5)$$

The finite dimensional analogue for the discrepancy assumes the form:

$$\varepsilon\left(\delta Q_w(t_i)\right) = \sum_1^N \left(T_{X=0}^{exact}(t_i) - T_{X=0}^{error}(t_i)\right)^2$$

where N is the number of heat flux time nodes (i.e. parameters, containing the error).

For small errors (in vicinity of exact solution) the discrepancy gradient is close to zero and the discrepancy ε is determined by the Hessian.

$$\varepsilon = \frac{1}{2}\frac{\partial^2 \varepsilon}{\partial Q_i \partial Q_j}\delta Q_i \delta Q_j = \frac{1}{2} H_{ij}\delta Q_i \delta Q_j \,;\ i,j=1\ldots N \qquad (6)$$

The averaged (over δQ) error $<\varepsilon>=\frac{1}{2}<H_{ij}\delta Q_i \delta Q_j>$ is determined as $\varepsilon=0.5H_{ij}DQ_{ij}$ (Dq_{ij} is the correlation matrix of the heat flux error). For non-correlated error ($DQ=diag(\sigma_i^2)$) $\varepsilon=0.5H_{ii}\sigma_i^2$. If the data error is constant and equal to σ, the uncertainty of the result is determined by the trace of the Hessian $\varepsilon=0.5H_{ii}\sigma^2$ (here the summation is performed over the repeating index).

The direct differentiation of the discrepancy ε provides the calculation of the Hessian requiring N^2 forward problem runs, which is highly computationally inefficient. It is well known that the adjoint problem provides the most efficient way for carrying out the gradient calculation. So, it is quite natural to extend this approach for Hessian calculation. The straightforward way to proceed is via direct numerical differentiation of the gradient obtained from the first order adjoint problem [1] (where a is the differentiation parameter).

$$HdQ=(grad(Q+adQ)-grad(Q))/a \qquad (7)$$

There exists another approach to Hessian action calculation based on the second order adjoint approach [2],[5]. Here we consider both variants of the Hessian action calculation using adjoint equations from inverse conduction problems [1] as a basis.

Let us consider the adjoint problem for discrepancy gradient calculation in some detail (although the derivation may be found elsewhere in Alekseev and Navon [4]) since these transformations will turn out to be useful for deriving the second order adjoint statements. First, we form the Lagrangian $L(Q_w,T,\Psi)$

$$L(Q_w(t),T,\Psi) = \int_t \left(T^{exact}(t,0) - T^{error}(t,0)\right)^2 dt +$$

$$+\iint \rho C \frac{\partial T}{\partial t}\Psi(x,t)dtdx -$$

$$-\iint_\Omega \frac{\partial}{\partial X}\left(\chi \frac{\partial T}{\partial X}\right)\Psi(x,t)dtdx; \qquad (8)$$

This Lagrangian is equal to discrepancy (5) on a solution of Eq. (1): $L(Q_w(t),T,\Psi) = \varepsilon(\delta Q_w(t)$.

Tangent linear problem

Second, we perturb the boundary condition by ΔQ_w. By subtracting the undisturbed solution we obtain the tangent linear problem.

$$C\rho \frac{\partial \Delta T}{\partial t} - \frac{\partial}{\partial X}\left(\chi \frac{\partial \Delta T}{\partial X} \right) = 0; \qquad (9)$$

With initial conditions:

$$\Delta T(0,X)=0;$$

and boundary conditions

$$\frac{\partial \Delta T}{\partial X}\Big|_{X=0} = 0; \qquad (10)$$

$$\chi \frac{\partial \Delta T}{\partial X}\Big|_{X=1} = \Delta Q_w(t); \qquad (11)$$

Further, we use Eqs. (9-11) for the calculation of the Lagrangian (8) variation.

$$\Delta L(Q_w(t)) = \int 2\left(T^{exact}(0,t) - T^{error}(0,t)\right)\Delta T dt +$$

$$+\iint \rho C \frac{\partial \Delta T}{\partial t} \Psi(x,t) dt dx -$$

$$-\iint_{\Omega} \frac{\partial}{\partial X}\left(\chi \frac{\partial \Delta T}{\partial X} \right)\Psi(x,t) dt dx; \qquad (12)$$

Our purpose is to find $\Psi(t,x)$ such that

$$\Delta L = \int_t \Delta Q_w grad(\varepsilon) dt;$$

while all other first order terms are equal to zero. Integrating Eq. (12) by parts and taking into account the initial and boundary conditions (9-11) gives

$$\Delta L(Q_w(t)) = \int 2\left(T^{exact}(0,t) - T^{error}(0,t)\right)\Delta T dt +$$

$$-\iint \rho C \frac{\partial \Psi}{\partial t} \Delta T(x,t) dt dx + \int_X \rho C \Psi(X,t) \Delta T dX \Big|_{t=0}^{t=t_f} -$$

$$-\int_t \chi \frac{\partial \Delta T}{\partial x} \Psi dt \Big|_{x=0}^{x=1} + \int_t \chi \frac{\partial \Psi}{\partial x} \Delta T dt \Big|_{x=0}^{x=1} - \iint_{\Omega} \frac{\partial}{\partial X}\left(\chi \frac{\partial \Psi}{\partial X} \right)\Delta T(x,t) dt dx; \qquad (13)$$

First Order Adjoint problem

If the function Ψ satisfies the following equation

$$\rho C \frac{\partial \Psi}{\partial t} + \chi \frac{\partial^2 \Psi}{\partial X^2} = 0; \qquad (14)$$

with boundary conditions:

$$\chi \frac{\partial \Psi}{\partial X}\Big|_{X=0} = -2\left(T^{exact}(0,t) - T^{error}(0,t)\right) \qquad (15)$$

$$\chi \frac{\partial \Psi}{\partial X}\Big|^{X=1} = 0; \qquad (16)$$

and final condition:

$$\rho C \Psi(t,x)\Big|^{t=t_f} = 0; \qquad (17)$$

then

$$\Delta L = \Delta \varepsilon(Q_w(t)) = -\int \chi \frac{\partial \Delta T}{\partial X} \Psi\Big|^{X=1} dt = -\int \Delta Q_w(t) \Psi(t,1) dt \qquad (18)$$

The discrepancy gradient may be obtained from the above expression:

$$grad(\varepsilon) = -\Psi(t,1); \qquad (19)$$

Equations (14-17) form the First Order Adjoint problem. The gradient is calculated by the solution of the forward and adjoint problems. The adjoint problem is solved backward in the time direction. This algorithm provides the gradient for an approximate computational cost of about double that of the solution of the heat conduction equation (the relative cost equals 2).

Having the gradient available at our disposal, the Hessian action may be computed by numerical differences using Eq. (7), then the Hessian relative computational cost is *2N*. However, if the parameter of differentiation *a* is poorly chosen, a low Hessian accuracy may result due to computing the difference between two small values. The Hessian may be computed more accurately via the alternative approach that we discuss below.

Second Order Adjoint Problem

Let us form the problem tangent to adjoint one (14-17) and, according to [2], denote it as the Second Order Adjoint problem:

$$\rho C \frac{\partial \Delta \Psi}{\partial t} + \chi \frac{\partial^2 \Delta \Psi}{\partial X^2} = 0; \qquad (20)$$

With boundary conditions:

$$\chi \frac{\partial \Delta \Psi}{\partial X}\Big|_{X=0} = 2\Delta T(0,Y); \tag{21}$$

$$\chi \frac{\partial \Delta \Psi}{\partial X}\Big|^{X=1} = 0; \tag{22}$$

And initial condition:

$$\Delta \Psi(t,x)\Big|^{t=t_f} = 0; \tag{23}$$

Because

$$\Psi(Q+\Delta Q)= \Psi(Q)+\Delta \Psi$$

and

$$\nabla \varepsilon_{Q+\Delta Q} = \nabla \varepsilon_Q + \nabla^2 \varepsilon \Delta Q$$

accounting

$$\nabla \varepsilon = -\Psi(t,1)$$

The Hessian action by the vector ΔQ equals

$$H\Delta Q = \nabla^2 \varepsilon \Delta Q = -\Delta \Psi(t,1) \tag{24}$$

Thus, in order to obtain the Hessian action by vector ΔQ, we sequentially solve the following four initial-boundary problems:

1. Forward problem, Eqs. (1-4) (where time is increasing)
2. First Order Adjoint problem, Eqs. (14-17) (where time is decreasing)
3. Tangent problem, Eqs. (9-11) (time is increasing)
4. Second Order Adjoint Problem, Eqs. (20-23) (time is decreasing)

In order to find the Hessian, the calculations for N orts should be performed, so the Hessian῀s computational cost equals $4N$.

Numerical Tests

The calculations of the Hessian are performed using the differentiation of First Order Adjoint problem as well as by using the solution of the Second Order Adjoint problem. The same finite-difference algorithm (first order accuracy in time and second order in space) is used for all problems under consideration. The test problem contains 28 time nodes for the heat flux interpolation, 20 cells in space, the specimen thickness being 0.003 m, the specific conductivity equals $\chi=4.18*10^{-4}$ $kW/(mK)$, and the specific volume heat is $\_\rho=2090$ $kJ/(m^3K)$. The heat flux is presented in Figure 1, and the temperature at the measurement point is provided in Figure 2. The comparison of the calculated Hessians shows that the direct differentiation causes a higher symmetry violation compared with the second order approach. The eigenvalues, computed via FOA (H_1) and SOA (H_2) (Eqs. (3) and (25), correspondingly) are presented in Table 1.

Table 1

j	1	2	3	4	5	6	7	8	9	10	11-17	18
H_1	5590	644	217	100	54.8	30.4	19.6	11.3	6.6	4.47	É	0
H_2	6060	640	212	97.2	51.7	30.1	18.2	11.3	7.6	5.07	É	0.145

The problem under the consideration has nonnegative eigenvalues due to the uniqueness of the Inverse Boundary Heat Conduction Problem [1]. Some eigenvalues should be close to zero due to the ill posedness of this problem. (See [3] for an in depth discussion on rank deficient and discrete ill-posed problems). Both methods yield a number of small negative eigenvalues, although the Second Order Adjoint problem yields a significantly smaller number of such eigenvalues. Nevertheless, from the viewpoint of uncertainty estimation, the largest eigenvalues are of interest and they practically coincide. The trace of the Hessian H_{ij} for FOA equals 7073, whereas for SOA it equals 6952. The rapid decrease of eigenvalues (Table 1) should be emphasized. Thereafter, we can use only maximum eigenvalue for uncertainty estimation $\varepsilon \approx 0.5\lambda_{max}\sigma^2$. The iterative calculation of the maximum eigenvalue λ_{max} may require a significantly smaller number of PDE solutions in comparison with the total Hessian calculation. The iterations for obtaining the maximum eigenvalue have the form

$X_{m+1}=AX_m;\ \lambda=max(X_{m+1})/max(X_m)$.

In the present case seven iterations yield a λ_{max} value of about 6423 (total spectrum for FOA provides λ_{max} =5590, for SOA λ_{max} =6060).

The estimation of the temperature uncertainty ε for normally distributed input data error of dispersion σ=0.01 via Hessian trace ($\varepsilon=0.5H_{ii}\sigma^2$, FOA and SOA), maximum eigenvalue ($0.5\lambda_{max}\sigma^2$), and averaging over the ensemble of 200 calculations are presented in the Table 2.

Table 2

	First order adjoint H_1	Second order adjoint H_2	λ_{max}	averaged
ε	0.354	0.345	0.32	0.326

Discussion

The total information regarding uncertainties in present problem (standard deviation of temperature at a certain point X) may be calculated (in the linear event) using sensitivities $<\delta T^2>=S_{ik}<dQ_k dQ_l>S_{il}$, $S_{ik}=\dfrac{\partial T(t_i,X)}{\partial Q(\tau_k)}$. The calculation of sensitivity implies the solution of a PDE system of higher order in comparison with the forward problem and requires storing multidimensional results. For small errors, the Fisher information matrix [1] (composed from sensitivities) approximate Hessian that provides correlation of sensitivity approach and the above-considered method.

$$H_{jk}=\frac{\partial^2\varepsilon}{\partial Q_j\partial Q_k}=\sum_i\frac{\partial T_i}{\partial Q_j}\frac{\partial T_i}{\partial Q_k}-2\sum_i\left(T_i^{exact}-T_i^{error}\right)\frac{\partial^2 T_i}{\partial Q_j\partial Q_k};$$

If we are interested in the time averaged temperature at a certain point (or another temperature functional), the adjoint approach may turn out to be more efficient from computer memory viewpoint. If the Hessian's eigenvalues decrease rapidly, fast uncertainty estimation via the maximum eigenvalue is feasible.

For estimation of uncertainty, the FOA differentiation is more advantageous compared with the SOA, because it is much simpler while providing similar accuracy for large eigenvalues. The SOA solution is preferable if we need an accurate calculation, for example, for the estimation of correctness subspace or for problem uniqueness.

Conclusion

The uncertainty of temperature from heat flux error may be estimated via First Order Adjoint equations, which are commonly used in Inverse Heat Transfer Problems, or via Second Order Adjoint equations. The adjoint codes developed for Inverse Heat Transfer may be directly used for the uncertainty estimation of the corresponding forward problems. The time computational cost is proportional to the input data dimension with the coefficient of about 2 or 4.

Numerical tests corroborate the feasibility of fast uncertainty estimation using Hessian maximum eigenvalue calculated in an iterative manner.

References

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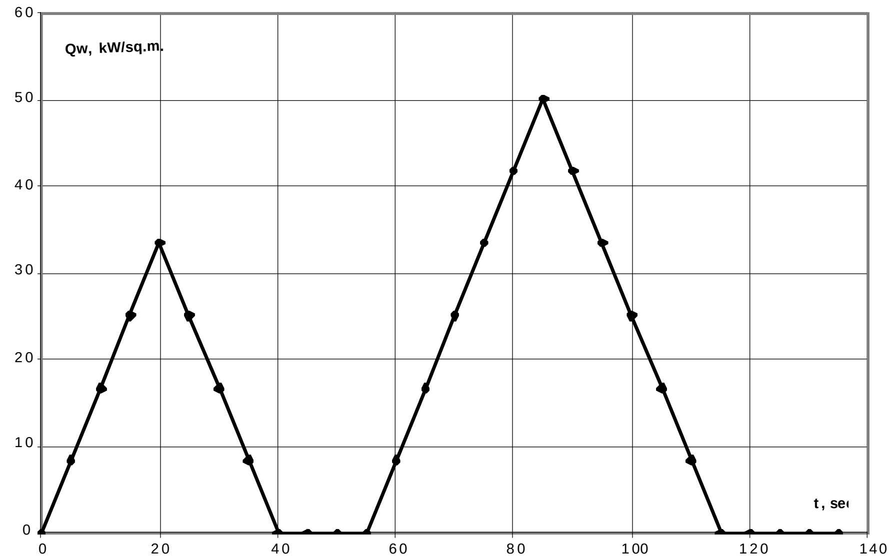
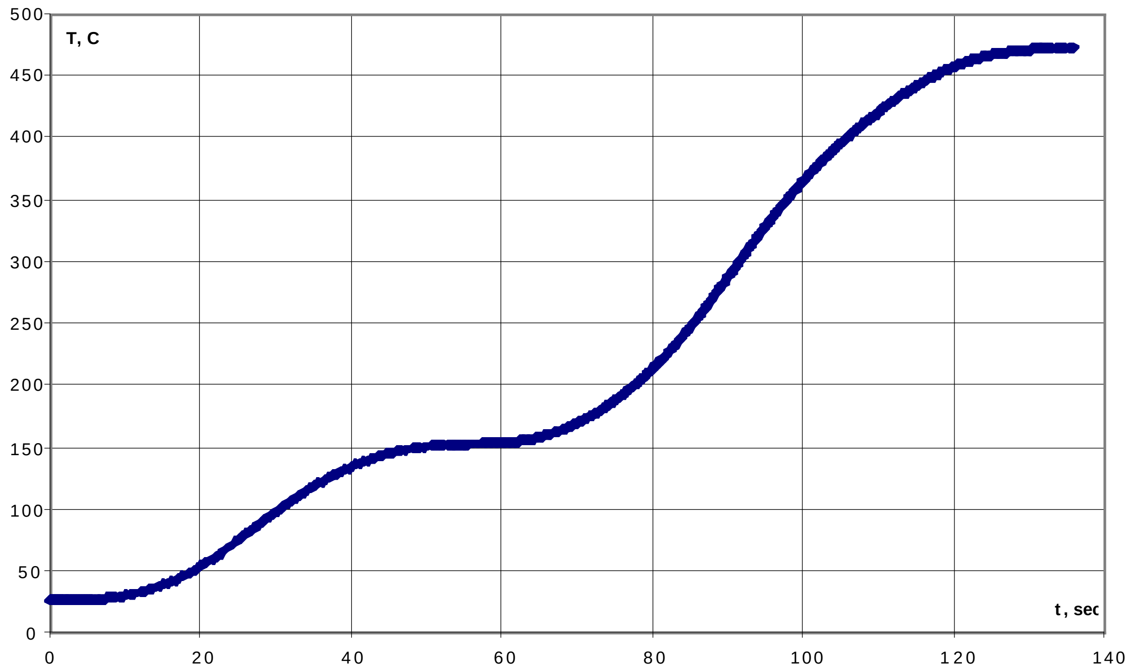
Figure Captions

Figure 1.
Heat flux on boundary in time dependence.

Figure 2.
The time variation of temperature at the point of uncertainty estimation.



Qw, kW/sq.m.
t, se
0
10
20
30
40
50
60
0
20
40
60
80
100
120
140


T, C
t , sec
0
50
100
150
200
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60
80
100
120
140