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Study of the optimal solution sensitivity of variational data assimilation problem for a model of sea thermodynamics***V.P. Shutyaev, E.I. Parmuzin****

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Algorithms are proposed to study the sensitivity of the optimal solution to the errors of the observational data in the problem of variational assimilation of the sea surface temperature data with the aim of restoring heat fluxes for the nonstationary system of thermodynamic equations. Numerical experiments are presented in an application to the model of the thermodynamics of the Baltic Sea.

Keywords: mathematical modeling; variational data assimilation; optimal control; adjoint equations; sensitivity to errors

Introduction. In the mathematical modeling of climate change for various regions of the world, the sensitivity theory of selected functionals plays an important role in relation to the characteristics of continents, the World Ocean, initial data, external sources and internal parameters of the problem. The study of climate sensitivity makes it possible to evaluate the quality of models on the basis of real data and find new mechanisms responsible for climate formation.

At present, in connection with the research of global changes on the planet Earth, the problem of obtaining and rational use of measurement data for the purpose of retrospective analysis in various fields of knowledge is very important. The mathematical model of this problem can be formulated as a problem of assimilation and processing of multidimensional (including dependence on time and space variables) data, which is one of the problems of optimal control ([1]-[5]). Along with the development and justification of algorithms for numerical solution of problems of variational assimilation of observational data, the properties of the optimal solution play an important role ([6]-[9]). The question of the sensitivity of optimal solutions of variational assimilation problems to the errors of observational data and model parameters, which has not been studied until recently, is extremely important.

In this paper we consider the problem of studying the sensitivity of the optimal solution of the problem of variational assimilation of observational data on the sea surface temperature for the thermodynamic model in a formulation analogous to that introduced in [5]. On the basis of the relationships connecting the errors of the optimal solution of the problem of variational assimilation with the errors of the observational data through the Hessian of the cost functional, algorithms for calculating the sensitivity coefficients as the norms of the response operators arising in the equations for the errors are proposed.

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1. The problem of assimilation of observational data for the thermodynamics of the sea.

Let us consider the model of the thermodynamics of the sea in the form ([10], [11]):

$$\begin{aligned} T_t + (\bar{U}, \text{Grad})T - \text{Div}(\hat{a}_T \cdot \text{Grad} T) &= f_T \text{ in } D \times (t_0, t_1), \\ T &= T_0 \text{ at } t = t_0 \text{ in } D, \\ -v_T \frac{\partial T}{\partial z} &= Q \text{ on } \Gamma_S \times (t_0, t_1), \quad \frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_{w,c} \times (t_0, t_1), \\ \bar{U}_n^{(-)}T + \frac{\partial T}{\partial N_T} &= \bar{U}_n^{(-)}d_T + Q_T \text{ on } \Gamma_{w,op} \times (t_0, t_1), \\ \frac{\partial T}{\partial N_T} &= 0 \text{ on } \Gamma_H \times (t_0, t_1), \end{aligned} \quad (1.1)$$

where $T = T(x, y, z, t)$ – the unknown temperature function, $t \in (t_0, t_1)$, $(x, y, z) \in D = \Omega \times (0, H)$, $\Omega \subset R^2$, $H = H(x, y)$ – the bottom relief function, $Q = Q(x, y, t)$ – the heat flow through the upper boundary, $\bar{U} = (u, v, w)$, $a_T = \text{diag}((a_T)_{ii})$, $(a_T)_{11} = (a_T)_{22} = \mu_T$, $(a_T)_{33} = \nu_T$, $f_T = f_T(x, y, z, t)$ – given functions. The boundary of the region $\Gamma \equiv \partial D$ is represented as the union of four disjoint parts Γ_S , $\Gamma_{w,op}$, $\Gamma_{w,c}$, Γ_H , where $\Gamma_S = \Omega$ (unperturbed sea surface), $\Gamma_{w,op}$ – the liquid (open) part of the vertical lateral boundary, $\Gamma_{w,c}$ – the solid part of the vertical lateral boundary, Γ_H – the bottom of the sea. Other notations and a detailed description of the statement of the problem can be found in [5], [10].

The problem (1.1) can be written in the form of an operator equation:

$$\begin{aligned} T_t + LT &= F + BQ, \quad t \in (t_0, t_1), \\ T &= T_0 \quad \text{at } t = t_0, \end{aligned} \quad (1.2)$$

where equality is understood in the weak sense, namely:

$$(T_t, T) + (LT, T) = F(T) + (BQ, T) \quad \forall T \in W_2^1(D), \quad (1.3)$$

in this case L , F , B are determined by the following relations:

$$\begin{aligned} (LT, T) &\equiv \int_D (-T \text{Div}(\bar{U}T)) dD + \int_{\Gamma_{w,op}} \bar{U}_n^{(+)} T T d\Gamma + \int_D a_T \text{Grad}(T) \cdot \text{Grad}(T) dD, \\ F(T) &= \int_{\Gamma_{w,op}} (Q_T + \bar{U}_n^{(-)} d_T) T d\Gamma + \int_D f_T T dD, \\ (T_t, T) &= \int_D T_t T dD, \quad (BQ, T) = \int_{\Omega} Q T|_{z=0} d\Omega, \end{aligned}$$

and the functions a_T , Q_T , f_T , Q are such that equality (1.3) makes sense. The properties of the operator L were investigated in [5].

We shall consider the problem of assimilating data on the temperature of the sea surface (see [5]). Suppose that the function $Q \in L_2(\Omega \times (t_0, t_1))$ is unknown in (1.1). Suppose that we have given a function of the observational data $T_{\text{obs}}(x, y, t)$ on $\bar{\Omega} \equiv \Omega \cup \partial\Omega$ at $t \in (t_0, t_1)$, which, in its physical meaning, is an approximation to the surface temperature function on Ω , i.e. to $T|_{z=0}$. We assume

that $T_{\text{obs}} \in L_2(\Omega \times (t_0, t_1))$, however, the function T_{obs} may not be more smooth, so it can not be used as the boundary condition on Γ_s . A case is possible when T_{obs} there is given only on a subset of $\Omega \times (t_0, t_1)$, whose characteristic function is denoted by m_0 . Outside this subset, for definiteness, T_{obs} is considered to be trivial.

Consider the following data assimilation problem: find T and Q such that

$$\begin{cases} T_t + LT = F + BQ, & \text{in } D \times (t_0, t_1), \\ T = T_0 & \text{at } t = t_0 \\ J(Q) = \inf_Q J(Q), \end{cases} \quad (1.4)$$

$$\text{where } J(Q) = \frac{\alpha}{2} \int_{t_0}^{t_1} \int_{\Omega} |Q - Q^{(0)}|^2 d\Omega dt + \frac{1}{2} \int_{t_0}^{t_1} \int_{\Omega} m_0 |T|_{z=0} - T_{\text{obs}}|^2 d\Omega dt, \quad (1.5)$$

$Q^{(0)} = Q^{(0)}(x, y, t)$ – specified function, $\alpha = \text{const} > 0$. The function J determines the root-mean-square deviation from the observed values.

With $\alpha > 0$ the problem of variational data assimilation has a unique solution. The existence of an optimal solution follows from the classical results of the theory of extremal problems, since it is not difficult to show that the solution of problem (1.2) depends continuously on the flow Q (a priori estimates hold in the corresponding function spaces). With $\alpha = 0$ the problem does not always have a solution, however, as shown in [5], there is a unique and dense solvability, which allows us to construct a sequence of regularized solutions that minimizes the functional.

The optimality system, which determines the solution of the problem of variational data assimilation (1.4)-(1.5) according to the necessary condition, has the form:

$$\begin{aligned} T_t + LT &= F + BQ & \text{in } D \times (t_0, t_1), \\ T &= T_0 & \text{at } t = t_0, \end{aligned} \quad (1.6)$$

$$\begin{aligned} -(T^*)_t + L^*T^* &= Bm_0(T - T_{\text{obs}}) & \text{in } D \times (t_0, t_1), \\ T^* &= 0 & \text{at } t = t_1, \end{aligned} \quad (1.7)$$

$$\alpha(Q - Q^{(0)}) + T^* = 0 \quad \text{on } \Omega \times (t_0, t_1), \quad (1.8)$$

where L^* – the operator adjoint to L .

In what follows we assume that $\text{supp}(m_0) = \bar{\Omega} \times [t_0, t_1]$ and we will investigate the sensitivity of the optimal solution Q to the input data, namely, to the errors in the specification of the functions T_{obs} and $Q^{(0)}$.

As a result of solving the problem of variational assimilation of the data (1.6)-(1.8), we obtain the total flow function Q , which is the optimal solution in the sense of minimizing the functional (1.5). This solution depends on the function of the observational data T_{obs} on the sea surface. An important question is the sensitivity of the optimal solution to the changes in the function T_{obs} . This issue is of great importance from the point of view of the forecast, since the optimal solution found as a result of solving the variational assimilation problem is used to integrate the model in the next

time interval. In this section, algorithms for studying the sensitivity of the optimal solution to the errors of the observational data are considered.

Let the observation data be given with errors:

$$Q^{(0)} = \bar{Q} + \xi_1, T_{\text{obs}} = \bar{T}|_{z=0} + \xi_2, \quad (1.9)$$

where $\bar{T} \in L_2(\Omega \times (t_0, t_1))$, \bar{T} is the exact solution of the direct problem for: $Q = \bar{Q}$:

$$\begin{aligned} \bar{T}_t + L\bar{T} &= F + B\bar{Q} \quad \text{in } D \times (t_0, t_1), \\ \bar{T} &= T_0 \quad \text{at } t = t_0. \end{aligned} \quad (1.10)$$

The functions ξ_1, ξ_2 can be considered as errors in the input data $Q^{(0)}$ and T_{obs} accordingly. The influence of these errors on the optimal solution Q obtained from the optimality system (1.6)-(1.8) was investigated in [6, 12], where it was shown that the equation for the error of the optimal solution at $\alpha > 0$ has a unique solution

$$\delta Q = \alpha H^{-1} \xi_1 + H^{-1} R \xi_2, \quad (1.11)$$

where $H = H_0 + \alpha E$, E – the identity operator, H_0 is determined on $v \in L_2(\Omega \times (t_0, t_1))$ by sequential solution of the problems:

$$\begin{aligned} \psi_t + L\psi &= Bv \quad \text{in } D \times (t_0, t_1), \\ \psi &= 0 \quad \text{at } t = t_0, \end{aligned} \quad (1.12)$$

$$\begin{aligned} -(\psi^*)_t + L^*\psi^* &= Bm_0\psi \quad \text{in } D \times (t_0, t_1), \\ \psi^* &= 0 \quad \text{at } t = t_1, \end{aligned} \quad (1.13)$$

$$H_0 v = \psi^* \quad \text{on } \Omega \times (t_0, t_1), \quad (1.14)$$

and the operator R acts on functions $g \in L_2(\Omega \times (t_0, t_1))$ by the formula $Rg = \theta^*|_{z=0}$, where θ^* – is the solution of the adjoint problem

$$\begin{aligned} -(\theta^*)_t + L^*\theta^* &= Bm_0g \quad \text{in } D \times (t_0, t_1), \\ \theta^* &= 0 \quad \text{at } t = t_1. \end{aligned}$$

We note that the operator H is the Hessian of the functional J defined by (1.5).

Thus, the error of the optimal solution δQ is explicitly expressed in terms of the errors of the initial data ξ_1, ξ_2 . In [12] the properties of the operators of the problem are studied in detail and estimates for the sensitivity coefficients describing the sensitivity of the optimal solution of the problem of variational assimilation of observational data for the sea dynamics model are presented. As a characteristic of the sensitivity of the optimal solution to the errors of the observational data, we consider the value

$$r = \sqrt{\|H_0(H_0 + \alpha E)^{-2}\|}, \quad (1.15)$$

where H_0 is given by formulas (1.12)-(1.14). The coefficient r characterizes the magnitude of the norm of the response operator $H^{-1}R$ in equation (1.11). We note that the upper bound for the spectrum of the operator $H_0(H_0 + \alpha E)^{-2}$ can be considered as the norm in (1.15). For finite-dimensional approximation, the operator H_0 is a matrix and the coefficient r is calculated by the formula:

$$r = \sup_k \frac{\sqrt{\mu_k}}{\alpha + \mu_k}, \quad (1.16)$$

where μ_k – the eigenvalues of H_0 , and $\frac{\sqrt{\mu_k}}{\alpha + \mu_k}$ – the singular numbers of the operator $H^{-1}R$.

On the basis of the above, we can formulate the following algorithm for calculating the sensitivity coefficient of the optimal solution to the errors of the observational data:

- 1) calculate the Hessian H_0 , determined by the formulas (1.12)-(1.14);
- 2) find the eigenvalues of the Hessian H_0 ;
- 3) calculate the sensitivity coefficient r by formula (1.16).

Here it should be emphasized that for finite-dimensional approximation H_0 turns out to be a poorly conditioned matrix, for which the smallest eigenvalue μ_{\min} is close to zero. In this case, when

$\alpha = 0$ the coefficient $r = \frac{1}{\sqrt{\mu_{\min}}}$ can be sufficiently large, i.e. the optimal solution can be very

sensitive to observation errors. This means that in this case it is necessary to introduce a regularizer with a parameter $\alpha > 0$, which will make the task of determining the optimal solution stable with respect to errors of observations.

2.Results of numerical experiments. For numerical experiments, we used the three-dimensional numerical model of the hydrothermodynamics of the Baltic Sea, developed in the INM of the Russian Academy of Sciences on the basis of the splitting method [13] and supplemented with the assimilation procedure [5] of the surface temperature with the aim of restoring heat fluxes. We present some results of numerical experiments on the sensitivity of the optimal solution.

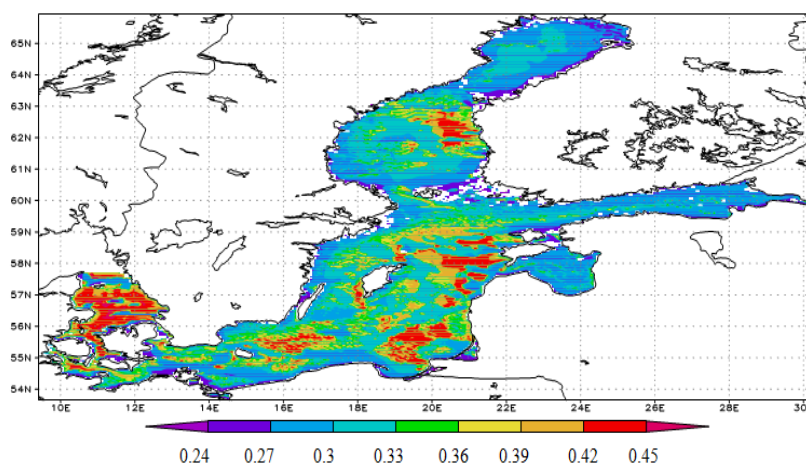


Fig. 1. Singular numbers of the operator after 1000 calculation steps

Fig. 1 shows the singular numbers of the operator $H^{-1}R$, which determine the sensitivity coefficient r . The largest singular numbers correspond to points lying near the regions with a small depth, especially in places on the slopes of the depressions. Thus, the optimal solution proves to be

sensitive to the errors of observations at the points of the surface near these regions, and the stability of the problem of restoring heat fluxes on the surface can degrade at these points.

Conclusion. In this paper, numerical algorithms for studying the sensitivity of the solution of the problem of variational assimilation of data on the temperature of the sea surface with the aim of restoring heat fluxes on the surface are considered. The equation for the error of the optimal solution through errors in the observational data is related to the Hessian of the original observation functional. This equation leads to the determination of the sensitivity coefficients as norms of response operators that characterize the degree of influence of errors in the observational data on the optimal solution of the problem of variational assimilation. The proposed methodology makes it possible to determine the subregions in which the optimal solution is most sensitive to observation errors in the variational assimilation of data, image processing, in the case where the values of the errors are not known in advance.

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Исследование чувствительности оптимального решения задачи вариационного усвоения данных для модели термодинамики моря *

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Предложены алгоритмы исследования чувствительности оптимального решения к погрешностям данных наблюдений в задаче вариационного усвоения данных о температуре поверхности моря с целью восстановления потоков тепла для нестационарной системы уравнений термодинамики. Представлены численные эксперименты в приложении к модели термодинамики Балтийского моря.

Ключевые слова: математическое моделирование; вариационное усвоение данных; оптимальное управление; сопряженные уравнения; чувствительность к погрешностям

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