Sensitivity of functionals in variational data assimilation for a sea thermodynamics model

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Abstract. The sensitivity of functionals of the optimal solution to a variational data assimilation problem for the sea thermodynamics model is studied. The variational data assimilation problem is formulated as an optimal control problem to find the initial state and the boundary condition. The sensitivity of the response functions as functionals of the optimal solution with respect to the observation data is determined by the gradient of the response function and reduces to the solution of a non-standard problem being a coupled system of direct and adjoint equations with mutually dependent initial and boundary values. The algorithm to compute the gradient of the response function is presented, based on the Hessian of the original cost functional. The sensitivity analysis of the response function with respect to errors of observation data is carried out. Numerical examples are presented for the Black Sea thermodynamics model.

1. Introduction

The methods of data assimilation are designed to combine mathematical models, observational data and a priori information. The data assimilation is aimed at constructing or refining the initial and/or boundary conditions (and other model parameters) to improve the accuracy of a prediction model. Mathematically, such problems may be formulated as optimal control problems [1–6]. Together with the development and justification of algorithms for the numerical solution to variational data assimilation problems [7], the key role belongs to the properties of the optimal solution and its sensitivity (see [8–15]).

As an extension of the approach in [14, 15], this paper considers the problem of sensitivity of functionals of the optimal solution of the variational data assimilation of the sea surface temperature for the sea thermodynamics model. The statement of the problem with the aim to restore the initial state and the boundary heat flux is given. The sensitivity of the response functions as functionals of the optimal solution with respect to the observation data is studied. The algorithm to compute the gradient of the response function, based on the Hessian of the original cost functional is presented. To illustrate the theory, numerical examples for the Black Sea thermodynamics model are presented.
2. Statement of the variational data assimilation problem

The sea thermodynamics problem is considered in the form [16], [17]:

\[ T_t + (\bar{U}, \text{Grad})T - \text{Div}(\bar{a}_T \cdot \text{Grad} T) = f_T \text{ in } D \times (t_0, t_1), \]

\[ T = T_0 \text{ for } t = t_0 \text{ in } D, \]

\[ -\nu_T \frac{\partial T}{\partial z} = Q \text{ on } \Gamma_S \times (t_0, t_1), \]

\[ \frac{\partial T}{\partial n} = 0 \text{ on } \Gamma_{w,c} \times (t_0, t_1), \]

\[ \bar{U}^{(-)}_n T + \frac{\partial T}{\partial n} = 0 \text{ on } \Gamma_{w,op} \times (t_0, t_1), \]

\[ \frac{\partial T}{\partial n} = 0 \text{ on } \Gamma_H \times (t_0, t_1), \]

where \( T = T(x, y, z, t) \) denotes temperature, \( t \in (t_0, t_1), (x, y, z) \in D = \Omega \times (0, H), \Omega \subset R^2, \)

\( H = H(x, y) \) is the bottom topography function, \( Q = Q(x, y, t) \) is the heat flux, \( \bar{U} = (u, v, w), \)

\( \bar{a}_T = \text{diag}(\alpha_{T,11}, \alpha_{T,22}, \alpha_{T,33}) = \nu_T = \bar{f}_T(x, y, z, t) \) are the given functions.

The boundary \( \Gamma \equiv \partial D \) of the domain \( D \) is supposed to consist of the disjoint parts \( \Gamma_S, \Gamma_{w,op}, \Gamma_{w,c}, \Gamma_H, \) where \( \Gamma_S = \Omega \) is the sea surface, \( \Gamma_{w,op} \) is the liquid (open) part of the vertical lateral boundary, \( \Gamma_{w,c} \) is the solid part of the vertical lateral boundary, \( \Gamma_H \) is the sea bottom,

\( \bar{U}^{(-)}_n = (|\bar{U}_n| - \bar{U}_n)/2, \) and \( \bar{U}_n \) is the normal component of \( \bar{U}. \)

We represent (1) in the form of an operator equation in \( (W_2^1(D))^*: \)

\[ T_t + LT = F + BQ, \quad t \in (t_0, t_1), \]

\[ T = T_0, \quad t = t_0, \]

being understood in the weak sense that

\[ (T_t, \hat{T}) + (LT, \hat{T}) = F(\hat{T}) + (BQ, \hat{T}) \forall \hat{T} \in W_2^1(D). \]

Here

\[ (LT, \hat{T}) = \int_D (-T \text{Div}(\bar{U} \hat{T})) dD + \int_{\Gamma_{w,op}} \bar{U}^{(+)}_n \hat{T} d\Gamma + \int_D \bar{a}_T \text{Grad}(T) \cdot \text{Grad}(\hat{T}) dD, \]

\[ F(\hat{T}) = \int_{\Gamma_{w,op}} (Q_T + \bar{U}^{(-)}_n d_T) \hat{T} d\Gamma + \int_D \bar{f}_T \hat{T} dD, \]

\[ (T_t, \hat{T}) = \int_D T_t \hat{T} dD, \quad (BQ, \hat{T}) = \int_{\Omega} Q_{\hat{T}}^{1}_{z=0} d\Omega. \]

The functions \( \bar{a}_T, Q_T, f_T, Q \) are supposed to be regular enough such that equality (3) makes sense. The operator \( L \) was studied in [16].

Due to (3), equation (2) is considered in \( Y^* = L_2(t_0, t_1; (W_2^1(D))^*) \) because the operator \( B : L_2(\Omega \times (t_0, t_1)) \rightarrow Y^* \) maps the function \( Q \in L_2(\Omega \times (t_0, t_1)) \) to \( (BQ, \hat{T}) = \int_{\Omega} Q_{\hat{T}}^{1}_{z=0} d\Omega) \forall \hat{T} \in W_2^1(D) \) and, therefore, \( BQ \) is a linear bounded functional on \( Y = L_2(t_0, t_1; W_2^1(D)). \)
We consider the following data assimilation problem [18]: find \( T_0 \in L_2(D) \) and \( Q \in L_2(\Omega \times (t_0, t_1)) \) such that

\[
\begin{align*}
T_t + LT &= \mathcal{F} + BQ, \quad \text{in } D \times (t_0, t_1), \\
T &= T_0, \quad t = t_0, \\
J(T_0, Q) &= \inf_{v, w} J(v, w),
\end{align*}
\]

where

\[
J(T_0, Q) = \frac{\alpha}{2} \int_{t_0}^{t_1} \int_{\Omega} |Q - Q^{(0)}|^2 d\Omega dt + \frac{\beta}{2} \int_D |T_0 - T^{(0)}|^2 dD + \frac{1}{2} \int_{t_0}^{t_1} \int_{\Omega} m_0 |T|^2_{z=0} - T_{\text{obs}}|^2 d\Omega dt,
\]

and \( T^{(0)} = T^{(0)}(x, y, z) \in L_2(D), Q^{(0)} = Q^{(0)}(x, y, t), T_{\text{obs}} = T_{\text{obs}}(x, y, t) \in L_2(\Omega \times (t_0, t_1)) \) are the given functions, \( \alpha, \beta = \text{const} > 0 \). The function \( T_{\text{obs}}(x, y, t) \) is the sea surface temperature given from observations on some subset of \( \Omega \times (t_0, t_1) \) with the characteristic function \( m_0 \).

It is easy to see that for \( \alpha, \beta > 0 \), problem (4) has a unique solution. The solution \( T \) of (1) depends continuously on the initial condition \( T_0 \) and the flux \( Q \), and a priori estimates are valid in the corresponding functional spaces. The functional \( J \) is weakly lower semicontinuous, and the space of admissible controls \( L_2(D) \times L_2(\Omega \times (t_0, t_1)) \) is weakly compact, which gives the existence of the optimal solution to (4).

The necessary optimality condition \( \nabla J = 0 \) of the variational data assimilation problem under consideration is reduced to the optimality system of the form:

\[
\begin{align*}
T_t + LT &= \mathcal{F} + BQ, \quad \text{in } D \times (t_0, t_1), \\
T &= T_0, \quad t = t_0, \\
-(T^*)_t + L^*T^* &= Bm_0(B^*T - T_{\text{obs}}) \quad \text{in } D \times (t_0, t_1), \\
T^* &= 0, \quad t = t_1, \\
\beta(T_0 - T^{(0)}) + T^*|_{t=0} &= 0 \quad \text{in } D, \\
\alpha(Q - Q^{(0)}) + B^*T^* &= 0 \quad \text{on } \Omega \times (t_0, t_1),
\end{align*}
\]

where \( L^* \) and \( B^* \) are the operators adjoint to \( L \) and \( B \), respectively.

We will study the sensitivity of the response functions as functionals of the optimal solution \( T_0, Q \) with respect to the observational data \( T_{\text{obs}} \).

3. The sensitivity of functionals of the optimal solution

The response functions as functionals of the optimal solution play an important role in applications. They are related to the outputs of the model after assimilation and it is often necessary to estimate their sensitivity with respect to observation errors.

Let us consider a response function \( G(T) \), which is supposed to be a real-valued function and can be considered as a functional on \( X = L_2(D \times (t_0, t_1)) \). We would like to study the sensitivity of the response function \( G \) with respect to the observation data \( T_{\text{obs}} \), with \( T, Q, T_0 \) obtained after the data assimilation from (6)–(9).

The sensitivity of \( G \) is determined by the gradient with respect to \( T_{\text{obs}} \) [1]:

\[
\frac{dG}{dT_{\text{obs}}} = \frac{\partial G}{\partial T} \frac{\partial T}{\partial T_{\text{obs}}},
\]

\(3\)
Let $\delta T_{\text{obs}}$ be a variation of $T_{\text{obs}}$, then from (6)–(9) we obtain:

$$
\begin{align*}
\left\{ \frac{\partial \delta T}{\partial t} + L \delta T, \delta T \right\}_{t=t_0} &= B \delta Q, \quad t \in (t_0, t_1) \\
\frac{-\partial \delta T^*}{\partial t} + L^* \delta T^* = B m_0 (B^* \delta T - \delta T_{\text{obs}}), \quad t \in (t_0, t_1)
\end{align*}
$$

(11)

Integrate by parts gives

$$
\beta \delta T_0 + \delta T^*|_{t=0} = 0 \quad \text{in} \quad D,
$$

(12)

$$
\alpha \delta Q + \delta T^*|_{z=0} = 0 \quad \text{on} \quad \Omega \times (t_0, t_1),
$$

(13)

and

$$
\left( \frac{dG}{dT_{\text{obs}}}, \delta T_{\text{obs}} \right) = \left( \frac{\partial G}{\partial T}, \delta T \right)_X,
$$

(14)

where $\delta T$, $\delta T^*$, $\delta T_0$, $\delta Q$ are the Gâteaux derivatives of $T$, $T^*$, $T_0$, $Q$, respectively, in the direction $\delta T_{\text{obs}}$.

We consider four adjoint variables $P_1 \in Y$, $P_2 \in Y$, $P_3 \in L_2(\Omega \times (t_0, t_1))$, $P_4 \in L_2(D)$ and take the inner product of (11) by $P_1$, (12) – by $P_2$, (14) – by $P_3$ and of (13) – by $P_4$. After summation, we come to:

$$
\begin{align*}
\left( \frac{\partial \delta T}{\partial t} + L \delta T, P_1 \right)_X - \left( B \delta Q, P_1 \right)_X + \left( -\frac{\partial \delta T^*}{\partial t} + L^* \delta T^*, P_2 \right)_X - \\
- \left( B m_0 (B^* \delta T - \delta T_{\text{obs}}), P_2 \right)_X + \left( \alpha \delta Q + \delta T^*|_{z=0}, P_3 \right)_{L_2(\Omega \times (t_0, t_1))} + \left( \beta \delta T_0 + \delta T^*|_{t=0}, P_4 \right)_{L_2(D)} = 0.
\end{align*}
$$

Integration by parts gives

$$
\begin{align*}
\left( \delta T, \frac{-\partial P_1}{\partial t} + L^* P_1 - B m_0 B^* P_2 \right)_X + \left( \delta T|_{t=t_1}, P_1|_{t=t_1} \right)_{L_2(D)} - \left( \delta T_0, P_1|_{t=0} \right)_{L_2(D)} + \\
+ \left( \delta T^*, \frac{\partial P_2}{\partial t} + L P_2 + B P_3 \right)_X + \left( \delta T^*|_{t=t_0}, P_2|_{t=t_0} \right)_{L_2(D)} + \left( \delta Q, -P_1|_{z=0} + \alpha P_3 \right)_{L_2(\Omega \times (t_0, t_1))} + \\
+ \left( \delta T_{\text{obs}}, m_0 P_2|_{z=0} \right)_{L_2(\Omega \times (t_0, t_1))} + \left( \beta \delta T_0 + \delta T^*|_{t=0}, P_4 \right)_{L_2(D)} = 0.
\end{align*}
$$

(15)

(16)

Therefore,

$$
\begin{align*}
\left( \frac{-\partial P_1}{\partial t} + L^* P_1 - B m_0 B^* P_2, \delta T \right)_X + \left( -P_1|_{z=0} + \alpha P_3, \delta Q \right)_{L_2(\Omega \times (t_0, t_1))} + \left( \beta P_4 - P_1|_{t=0}, \delta T_0 \right)_{L_2(D)} + \\
\left( P_1|_{t=t_1}, \delta T|_{t=t_1} \right)_{L_2(D)} + \left( \frac{\partial P_2}{\partial t} + L P_2 + B P_3, \delta T^* \right)_X + \left( P_2|_{t=t_0} + P_4, \delta T^*|_{t=0} \right)_{L_2(D)} = \\
= - \left( m_0 P_2|_{z=0}, \delta T_{\text{obs}} \right)_{L_2(\Omega \times (t_0, t_1))}.
\end{align*}
$$

(17)

Assuming that

$$
\frac{\partial P_1}{\partial t} + L^* P_1 - B m_0 B^* P_2 = \frac{\partial G}{\partial T},
$$

we have

$$
\left\{ \frac{\partial \delta T}{\partial t} + L \delta T, \delta T \right\}_{t=t_0} = \delta T_0,
$$

(18)

and

$$
\frac{-\partial \delta T^*}{\partial t} + L^* \delta T^* = B m_0 (B^* \delta T - \delta T_{\text{obs}}), \quad t \in (t_0, t_1), \quad t \in (t_0, t_1).
$$

(19)
and

\[-P_1|_{z=0} + \alpha P_3 = 0, \beta P_4 - P_1|_{t=t_0}, P_1|_{t=t_1} = 0, \frac{\partial P_2}{\partial t} + LP_2 + BP_3 = 0, P_2|_{t=t_0} + P_4 = 0,\]

from (15), (17) we obtain

\[
\left( \frac{dG}{dT_{\text{obs}}}, \delta T_{\text{obs}} \right) = - \left( m_0 P_2|_{z=0}, \delta T_{\text{obs}} \right)_{L_2(\Omega \times (t_0, t_1))}.
\]

Therefore, the following statement is valid:

**Theorem 2.1.** Let \( P_1, P_2 \in Y, P_3 \in L_2(\Omega \times (t_0, t_1)), P_4 \in L_2(D) \) be the solutions of the following system of equations:

\[
\begin{cases}
\frac{\partial P_1}{\partial t} + L^* P_1 + Bm_0 B^* P_2 = \frac{\partial G}{\partial T}, & t \in (t_0, t_1) \\
P_1|_{t=t_1} = 0, \\
\frac{\partial P_2}{\partial t} + LP_2 = BP_3, & t \in (t_0, t_1) \\
-P_2|_{t=t_0} + P_4 = 0, \\
\beta P_4 - P_1|_{t=t_0} = 0, \alpha P_3 - P_1|_{z=0} = 0.
\end{cases}
\]

Then the gradient of \( G \) with respect to \( T_{\text{obs}} \) is given by

\[
\frac{dG}{dT_{\text{obs}}} = m_0 P_2|_{z=0}.
\]

The functions \( P_1, P_2 \in Y \) are the solutions of a non-standard problem, being a coupled system of two differential equations (18) and (19) of the first order with respect to time with the mutually dependent initial and boundary values.

In the non-standard problem (18)–(20) we have four unknowns: \( P_1, P_2 \in Y, P_3 \in L_2(\Omega \times (t_0, t_1)), P_4 \in L_2(D) \). Let us write down (18)–(20) in the form of an operator equation for \( U = (P_4, P_3)^T \). Consider the Hessian \( H \) of the original functional \( J \) from (5) defined on \( \Theta = (\xi, \eta)^T, \xi \in L_2(D), \eta \in L_2(\Omega \times (t_0, t_1)) \) by the equalities:

\[
\varphi_t + L \varphi = B \eta, \quad t \in (t_0, t_1),
\]

\[
\varphi = \xi \quad \text{for} \quad t = t_0,
\]

\[
-(\varphi^*)_t + L^* \varphi^* = Bm_0 B^* \varphi, \quad t \in (t_0, t_1),
\]

\[
\varphi^* = 0 \quad \text{for} \quad t = t_1,
\]

\[
H \Theta = (\beta \xi + \varphi^*|_{t=0}, \alpha \eta + B^* \varphi^*)^T.
\]

Then the non-standard problem (18)–(20) is equivalent to the operator equation:

\[
H U = \Phi
\]

with the right-hand side

\[
\Phi = (\phi^*|_{t=0}, \phi^*|_{z=0})^T.
\]
and $\phi^*$ being the solution of the adjoint problem:

$$
\begin{cases}
- \frac{\partial \phi^*}{\partial t} + L^* \phi^* = \frac{\partial G}{\partial T}, & t \in (t_0, t_1) \\
\phi^*|_{t=t_1} = 0
\end{cases}
$$

(27)

If $\alpha, \beta > 0$, then the operator $H$ is positive definite [18], equation (25) is correctly and everywhere solvable in $L^2(D) \times L^2(\Omega \times (t_0, t_1))$. Therefore, for every $\Phi \in L^2(D) \times L^2(\Omega \times (t_0, t_1))$ there exists a unique solution $U \in L^2(D) \times L^2(\Omega \times (t_0, t_1))$ and the non-standard problem (18)–(20) has a unique solution $P_1, P_2 \in Y, P_3 \in L^2(\Omega \times (t_0, t_1)), P_4 \in L^2(D)$.

From (18)–(27) we obtain the algorithm to find the gradient of the response function $G(T)$:

1) Find the solution of the adjoint problem

$$
\begin{cases}
- \frac{\partial \phi^*}{\partial t} + L^* \phi^* = \frac{\partial G}{\partial T}, & t \in (t_0, t_1) \\
\phi^*|_{t=t_1} = 0
\end{cases}
$$

(28)

and set $$(\phi^*|_{t=0}, \phi^*|_{z=0})^T.$$

2) Solve the Hessian equation $HU = \Phi$

and find $U = (U_1, U_2)^T$.

3) Find the solution of the problem

$$
\begin{cases}
\frac{\partial P_2}{\partial t} + LP_2 = BU_1, & t \in (t_0, t_1) \\
P_2|_{t=t_0} = U_2
\end{cases}
$$

(29)

4) Find the gradient of the response function by

$$
\frac{dG}{dT_{obs}} = m_0 P_2|_{z=0}.
$$

(30)

Using this algorithm, one can estimate the sensitivity of the response functions after the data assimilation with respect to observation errors.

4. Numerical experiments for the Black Sea dynamics model

The numerical experiments have been performed using the three-dimensional numerical model of the Black and the Azov seas hydrothermodynamics developed at the Marchuk Institute of Numerical Mathematics, the Russian Academy of Sciences. This model is based on the splitting method [19]. The data assimilation problem [18] was considered for the sea surface temperature $T_{obs}$ with the aim to find the initial state $T_0$ and the heat flux $Q$.

The parameters of the domain are the following: $\sigma$-grid is $306 \times 200 \times 27$ (in latitude, longitude, and depth, respectively). The first point of the "grid C" [20] has the coordinates $26.65^\circ$ E and $40.15^\circ$ N. The mesh sizes in $x$ and $y$ are equal to 0.05 and 0.036 degrees, respectively. The time step is $\Delta t = 2.5$ minutes.

The sea surface temperature (SST) observational data were provided by the "See the Sea" satellite service being a part of the CKP "IKI-Monitoring", which collects and processes various data on the state of the Earth’s surface and focuses on the satellite observations [21]. In this
experiment, the SST data for October 1, 2019 from the VIIRS spectrometer on the SNPP satellite were selected (at certain temporal points) as \( T_{\text{obs}} \), the data were recalculated on the model grid used for the numerical calculations. For \( Q^{(0)} \), we took the mean climatic flux obtained from the NCEP (National Centers for Environmental Prediction) reanalysis.

With the use of the model considered, calculations for the Black and the Azov area were carried out, with the sea surface assimilation algorithm working at certain time moments \( t_0 \), with \( t_1 = t_0 + \Delta t \). The sensitivity of functionals of the optimal solution \( Q \) with respect to observation errors over the interval \( (t_0, t_1) \) was numerically studied.

For \( G(T) \), the following functional was considered:

\[
G(T) = \int_{t_0}^{t_1} dt \int_{\Omega} F^*(x, y, t) T(x, y, 0, t) d\Omega,
\]

where \( F^*(x, y, t) \) is the weight function related to the temperature on the sea surface \( z = 0 \). If the mean temperature of a specific region \( \omega \) of the sea for \( z = 0 \) on the interval \( \bar{t} - \tau \leq t \leq \bar{t} \) is considered, then \( F^* \) is defined by

\[
F^*(x, y, t) = \begin{cases}
1/\left(\tau \text{mes } \omega\right) & \text{if } (x, y) \in \omega, \bar{t} - \tau \leq t \leq \bar{t} \\
0 & \text{else},
\end{cases}
\]

with \( \text{mes } \omega \) denoting the area of the region \( \omega \). In this case, (31) gives

\[
G(T) = \frac{1}{\tau} \int_{\bar{t} - \tau}^{\bar{t}} dt \left( \frac{1}{\text{mes } \omega} \int_{\omega} T(x, y, 0, t) d\Omega \right).
\]

Formula (31) may be represented in the form

\[
G(T) = \int_{t_0}^{t_1} (BF^*, T) dt = (BF^*, T)_X, \quad X = L_2(D \times (t_0, t_1)).
\]

Hence

\[
\left( \frac{\partial G}{\partial T}, \delta T \right)_X = (BF^*, \delta T)_X, \quad \frac{\partial G}{\partial T} = BF^*.
\]

The water area considered in the numerical experiments is shown in figure 1. Figure 2 presents the SST observation data used in the numerical experiment at a certain time moment.

The gradient of the response function \( G(T) \) defined by (33) with respect to the observation data \( T_{\text{obs}} \) on the sea surface is presented in figure 3, according to algorithm (28)–(30). Here \( \omega = \Omega, \tau = \Delta t, \ t = t_1, \alpha = \beta = 10^{-5} \). The sub-areas (in red) are revealed near the regions with a small depth, where the response function \( G(T) \) is most sensitive to errors in the observation data during variational assimilation. The direct computation of the response function \( G(T) \) by (33), with perturbations of the observation data \( T_{\text{obs}} \), has confirmed this result.

5. Conclusion
We have considered the problem of sensitivity of functionals of the optimal solution of the variational data assimilation of the sea surface temperature for the sea thermodynamics model. The variational data assimilation problem was formulated as an optimal control problem to find the initial state and the boundary heat flux. The sensitivity of the response functions as functionals of the optimal solution with respect to the observation data is defined by the
Figure 1. The Black Sea topography [m].

Figure 2. The SST observation data $T_{\text{obs}}$ at 23.40 on October 1, 2019, $^\circ$C.

Figure 3. The gradient of the functional $G(T)$.

gradient and is related to the solution of a non-standard problem being a coupled system of direct and adjoint equations with mutually dependent initial and boundary values. The algorithm to compute the gradient of the response function involves the Hessian of the original cost function. Numerical examples presented for the Black Sea dynamics model demonstrate the result of the gradient computation by the algorithm proposed for the response function related to the mean surface temperature. The experiments have revealed the sub-areas near the regions with a small depth, where the response function $G(T)$ is most sensitive to errors in the observation data during variational assimilation.

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