Sensitivity of the optimal solution of variational data assimilation problems

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Ocean thermodynamics model

$$
\begin{gathered}
T_t + (\bar{U}, \mathrm{Grad})T - \mathrm{Div}(\hat{a}_T \cdot \mathrm{Grad}\ T) = f_T \ \text{ in } \ D \times (t_0, t_1), \\
T = T_0 \text{ for } t = t_0 \text{ in } D, \\
-\nu_T \frac{\partial T}{\partial z} = Q \text{ on } \Gamma_S \times (t_0, t_1), \\
\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_{w,c} \times (t_0, t_1), \\
\bar{U}_n^{(-)} T + \frac{\partial T}{\partial N_T} = \bar{U}_n^{(-)} d_T + Q_T \text{ on } \Gamma_{w,op} \times (t_0, t_1), \\
\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_H \times (t_0, t_1).
\end{gathered}
\tag{1}
$$

Operator form of the problem

$$T_t + LT = \mathcal{F} + BQ, \quad t \in (t_0, t_1),$$
$$T = T_0, \qquad t = t_0, \tag{2}$$

where

$$(T_t, \widehat{T}) + (LT, \widehat{T}) = \mathcal{F}(\widehat{T}) + (BQ, \widehat{T}) \ \ \forall \widehat{T} \in W_2^1(D), \tag{3}$$

and L, $\mathcal{F}$, B are defined by:

$$(LT, \widehat{T}) \equiv -\int\limits_D T\mathrm{Div}(\bar{U}\widehat{T})dD + \int\limits_{\Gamma_{w,op}} \bar{U}_n^{(+)} T \widehat{T} d\Gamma + \int\limits_D \hat{a}_T \mathrm{Grad}(T) \cdot \mathrm{Grad}(\widehat{T}) dD,$$

$$\mathcal{F}(\widehat{T}) = \int\limits_{\Gamma_{w,op}} (Q_T + \bar{U}_n^{(-)} d_T) \widehat{T} dT + \int\limits_D f_T \widehat{T} dD,$$

$$(T_t, \widehat{T}) = \int\limits_D T_t \widehat{T} dD, \ \ (BQ, \widehat{T}) = \int\limits_\Omega Q \widehat{T}\big|_{z=0} d\Omega.$$

Data assimilation problem

Find T and Q such that

$$\begin{cases} T_t + LT &= \mathcal{F} + BQ, \quad \text{in} \quad D \times (t_0, t_1), \\ T &= T_0, \quad t = t_0 \\ J(Q) &= \inf\limits_{v} J(v), \end{cases} \tag{4}$$

where

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

and $Q^{(0)}$, $T_{\text{obs}} \in L_2(\Omega \times (t_0, t_1))$, $\alpha = const > 0$.

Optimality system

$$\begin{aligned} T_t + LT &= \mathcal{F} + BQ \quad \text{in} \;\; D \times (t_0, t_1), \\ T = T_0, &\qquad t = t_0, \end{aligned} \tag{5}$$

$$\begin{aligned} -(T^*)_t + L^* T^* &= Bm_0(T - T_{\mathrm{obs}}) \quad \text{in} \;\; D \times (t_0, t_1), \\ T^* = 0, &\qquad t = t_1, \end{aligned} \tag{6}$$

$$\alpha(Q - Q^{(0)}) + T^* = 0 \quad \text{on} \;\; \Omega \times (t_0, t_1). \tag{7}$$

Functionals of the sea surface temperature

$$G(T) = \int_{t_0}^{t_1} dt \int_{\Omega} F^*(x,y,t) T(x,y,0,t) d\Omega. \quad (8)$$

For example, if we are interested in the mean temperature of a specific region of the ocean ω for $z = 0$ in the interval $\bar{t} - \tau \le t \le \bar{t}$, then

$$F^*(x,y,t) = \begin{cases} 1\Big/(\tau \text{mes } \omega) & \text{if } (x,y) \in \omega, \bar{t} - \tau \le t \le \bar{t} \\ 0 & \text{else,} \end{cases} \quad (9)$$

and

$$G(T) = \frac{1}{\tau} \int_{\bar{t}-\tau}^{\bar{t}} dt \left(\frac{1}{\text{mes } \omega} \int_{\omega} T(x,y,0,t) d\Omega \right). \quad (10)$$

Sensitivity of functionals

The sensitivity is given by the gradient of G with respect to T_{obs}:

$$\frac{dG}{dT_{obs}} = \frac{\partial G}{\partial T}\frac{\partial T}{\partial T_{obs}}. \tag{11}$$

If δT_{obs} is a perturbation on T_{obs}, we get from the optimality system:

$$\begin{cases} \dfrac{\partial \delta T}{\partial t} + L\delta T = B\delta Q, \quad t \in (t_0, t_1) \\ \delta T\big|_{t=t_0} = 0, \end{cases} \tag{12}$$

$$\begin{cases} -\dfrac{\partial \delta T^*}{\partial t} + L^*\delta T^* = Bm_0(\delta T - \delta T_{obs}), \\ \delta T^*\big|_{t=T} = 0, \end{cases} \tag{13}$$

$$\alpha\delta Q + \delta T^*\big|_{z=0} = 0, \tag{14}$$

and

$$\left(\frac{dG}{dT_{obs}}, \delta T_{obs}\right) = \left(\frac{\partial G}{\partial T}, \delta T\right)_Y. \tag{15}$$

Computing the gradient

We introduce three adjoint variables $P_1 \in Y$, $P_2 \in Y$, P_3, such that

$$\left(\delta T, -\frac{\partial P_1}{\partial t} + L^* P_1 + B m_0 P_2\right)_Y + \left(\delta T\big|_{t=t_1}, P_1\big|_{t=t_1}\right)_X +$$
$$+\left(\delta\ T^*, \frac{\partial P_2}{\partial t} + LP_2 + BP_3\right)_Y + \left(\delta T^*\big|_{t=t_0}, P_2\big|_{t=t_0}\right)_X +$$
$$+\left(\delta Q, P_1\big|_{z=0} + \alpha P_3\right) - \left(\delta T_{obs}, m_0 P_2\big|_{z=0}\right) = 0, \quad X = L_2(D). \tag{16}$$

We put

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

$$P_1\big|_{z=0} + \alpha P_3 = 0, \ P_1\big|_{t=t_1} = 0, \ \frac{\partial P_2}{\partial t} + LP_2 + BP_3 = 0, \ P_2\big|_{t=t_0} = 0.$$

Hence, we can exclude P_3 and obtain the equation for P_2:

$$\frac{\partial P_2}{\partial t} + LP_2 - \frac{1}{\alpha} BP_1\big|_{z=0} = 0.$$

Non-standard problem

If P_1, P_2 are the solutions of the following system of equations

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} + L^* P_1 + B m_0 P_2 = \dfrac{\partial G}{\partial T}, & t \in (t_0, t_1) \\ P_1\big|_{t=t_1} = 0, \end{cases} \tag{17}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} + L P_2 = \dfrac{1}{\alpha} B P_1\big|_{z=0}, & t \in (t_0, t_1) \\ P_2\big|_{t=t_0} = 0, \end{cases} \tag{18}$$

then from (16) we get

$$\left(\frac{dG}{dT_{obs}}, \delta T_{obs}\right) = \left(\frac{\partial G}{\partial T}, \delta T\right)_Y = (m_0 P_2\big|_{z=0}, \delta T_{obs}),$$

and the gradient of G is given by

$$\frac{dG}{dT_{obs}} = m_0 P_2\big|_{z=0}. \tag{19}$$

Equivalent formulation

We write the non-standard problem (17)–(18) in the form:

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} + L^* P_1 + Bm_0 P_2 & = & \dfrac{\partial G}{\partial T}, \quad t \in (t_0, t_1) \\ P_1\Big|_{t=t_1} & = & 0, \end{cases} \tag{20}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} + LP_2 + Bv & = & 0, \quad t \in (t_0, t_1) \\ P_2\Big|_{t=t_0} & = & 0, \end{cases} \tag{21}$$

$$\alpha v + P_1\Big|_{z=0} = 0. \tag{22}$$

It is equivalent to the operator equation in $L_2(\Omega \times (t_0, t_1))$:

$$\mathcal{H} v = \Phi. \tag{23}$$

Hessian $\mathcal{H}$ and the right-hand side Φ

The operator $\mathcal{H}$ is defined on $w \in L_2(\Omega \times (t_0, t_1))$ by

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + L\phi + Bw = 0, & t \in (t_0, t_1) \\ \phi\Big|_{t=t_0} = 0, \end{cases} \tag{24}$$

$$\begin{cases} -\dfrac{\partial \phi^*}{\partial t} + L^*\phi^* = -Bm_0\phi, & t \in (t_0, t_1) \\ \phi^*\Big|_{t=t_1} = 0, \end{cases} \tag{25}$$

$$\mathcal{H}w = \alpha w + \phi^*\Big|_{z=0}. \tag{26}$$

The right-hand side Φ is given by $\Phi = \tilde{\phi}^*\Big|_{z=0}$, where $\tilde{\phi}^*$ is the solution to:

$$\begin{cases} -\dfrac{\partial \tilde{\phi}^*}{\partial t} + L^*\tilde{\phi}^* = -\dfrac{\partial G}{\partial T}, & t \in (t_0, t_1) \\ \tilde{\phi}^*\Big|_{t=t_1} = 0. \end{cases} \tag{27}$$

Solvability of the non-standard problem

For $\alpha > 0$ the operator $\mathcal{H}$ is positive definite, the equation $\mathcal{H}v = \Phi$ is correctly and everywhere solvable in $L_2(\Omega \times (t_0, t_1))$, i.e. for every Φ there exists a unique solution $v \in L_2(\Omega \times (t_0, t_1))$ and

$$\|v\| \leq c\|\Phi\|, \quad c = const > 0. \tag{28}$$

Therefore, the non-standard problem (17)–(18) has a unique solution $P_1, P_2 \in Y$.

Algorithm to compute the gradient of $G(T)$

1) Solve the adjoint problem

$$\begin{cases} -\frac{\partial \tilde{\phi}^*}{\partial t} + L^* \tilde{\phi}^* & = & -\frac{\partial G}{\partial T}, \quad t \in (t_0, t_1) \\ \tilde{\phi}^*\big|_{t=t_1} & = & 0 \end{cases} \tag{29}$$

and put

$$\Phi = \tilde{\phi}^*\big|_{z=0}.$$

2) Find v by solving $\mathcal{H}v = \Phi$.

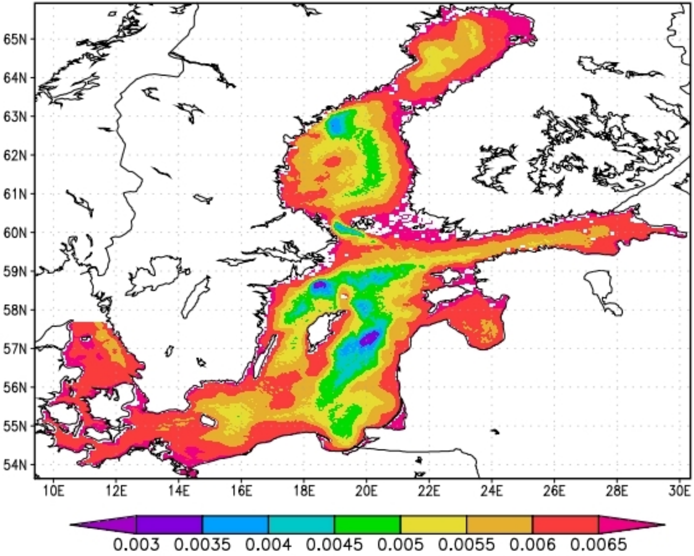
3) Solve the direct problem

$$\begin{cases} \frac{\partial P_2}{\partial t} + L_2 P_2 & = & -Bv, \quad t \in (t_0, t_1) \\ P_2\big|_{t=t_0} & = & 0. \end{cases} \tag{30}$$

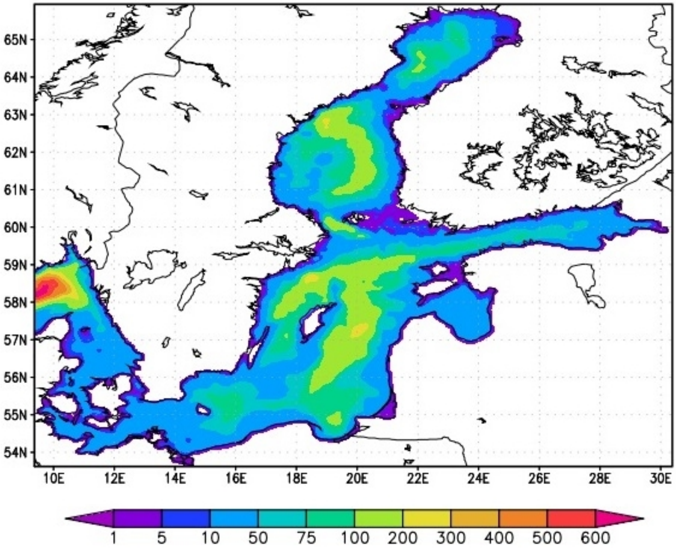
4) Compute the gradient of the response function as

$$\frac{dG}{dT_{obs}} = m_0 P_2\big|_{z=0}. \tag{31}$$

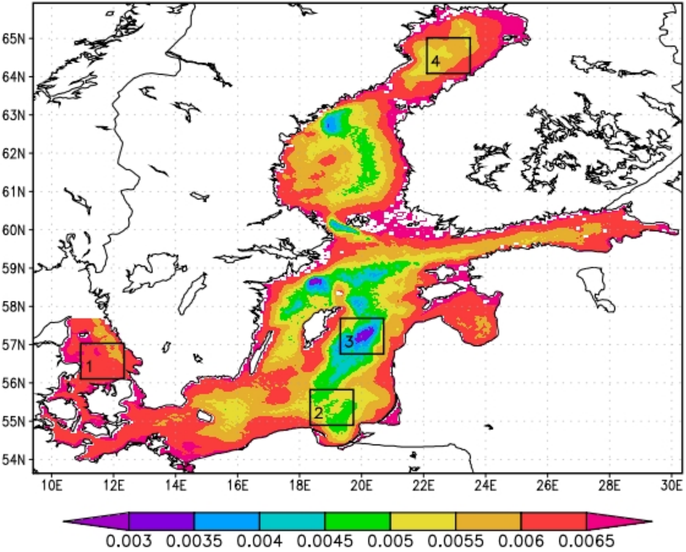
Gradient of the functional $G(T)$



Baltic Sea topography [m]



Regions in the Baltic Sea area



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