Sensitivity of the optimal solution of variational data assimilation problems

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Statement of the problem

Consider the mathematical model of a physical process that is described by the evolution problem

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi), \quad t \in (0, T) \\ \varphi\big|_{t=0} = u, \end{cases} \tag{1}$$

where $\varphi = \varphi(t)$ is the unknown function belonging for any t to a Hilbert space X, $u \in X$, F is a nonlinear operator mapping Y into Y, $Y = L_2(0, T; X)$.

Let us introduce the functional

$$J(u) = \frac{1}{2}(V_1(u - u_0), u - u_0)_X + \frac{1}{2}(V_2(C\varphi - \varphi_{obs}), C\varphi - \varphi_{obs})_{Y_{obs}}, \tag{2}$$

where $u_0 \in X$ is a prior initial-value function (background state), $\varphi_{obs} \in Y_{obs}$ is a prescribed function (observational data), Y_{obs} is a Hilbert space (observation space), $C : Y \to Y_{obs}$ is a linear bounded operator, $V_1 : X \to X$ and $V_2 : Y_{obs} \to Y_{obs}$ are symmetric positive definite operators.

Data assimilation problem

Consider the following data assimilation problem with the aim to identify the initial condition: find $u \in X$ and $\varphi \in Y$ such that they satisfy (1), and on the set of solutions to (1), the functional $J(u)$ takes the minimum value, i.e.

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi), \quad t \in (0, T) \\ \varphi\Big|_{t=0} = u, \\ J(u) = \inf\limits_{v} J(v). \end{cases} \tag{3}$$

Optimality system

The necessary optimality condition reduces the problem (3) to the following optimality system:

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi), \quad t \in (0,T) \\ \varphi\big|_{t=0} = u, \end{cases} \tag{4}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\varphi))^* \varphi^* = -C^* V_2 (C\varphi - \varphi_{obs}), \quad t \in (0,T) \\ \varphi^*\big|_{t=T} = 0, \end{cases} \tag{5}$$

$$V_1(u - u_0) - \varphi^*\big|_{t=0} = 0 \tag{6}$$

with the unknowns φ, φ^*, u, where $(F'(\varphi))^*$ is the adjoint to the Frechet derivative of F with respect to φ, and C^* is the adjoint to C defined by $(C\varphi, \psi)_{Y_{obs}} = (\varphi, C^*\psi)_Y, \ \varphi \in Y, \psi \in Y_{obs}$.

Sensitivity of functionals after assimilation

Let us introduce a response function $G(\varphi, u)$, which is supposed to be a real-valued function and can be considered as a functional on $Y \times X$. We are interested in the sensitivity of G with respect to φ_{obs}, with φ and u obtained from the optimality system (4)–(6).

By definition, the sensitivity is defined by the gradient of G with respect to φ_{obs}:

$$\frac{dG}{d\varphi_{obs}} = \frac{\partial G}{\partial \varphi} \frac{\partial \varphi}{\partial \varphi_{obs}} + \frac{\partial G}{\partial u} \frac{\partial u}{\partial \varphi_{obs}}. \tag{7}$$

Optimality system for perturbations

If $\delta\varphi_{obs}$ is a perturbation on φ_{obs}, we get from the optimality system:

$$\begin{cases} \dfrac{\partial \delta\varphi}{\partial t} = F'(\varphi)\delta\varphi, \quad t \in (0,T) \\ \delta\varphi\big|_{t=0} = \delta u, \end{cases} \tag{8}$$

$$\begin{cases} -\dfrac{\partial \delta\varphi^*}{\partial t} - (F'(\varphi))^*\delta\varphi^* - (F''(\varphi)\delta\varphi)^*\varphi^* = -C^*V_2(C\delta\varphi - \delta\varphi_{obs}), \\ \delta\varphi^*\big|_{t=T} = 0, \end{cases} \tag{9}$$

$$V_1\delta u - \delta\varphi^*\big|_{t=0} = 0, \tag{10}$$

and

$$\left(\frac{dG}{d\varphi_{obs}}, \delta\varphi_{obs}\right)_{Y_{obs}} = \left(\frac{\partial G}{\partial \varphi}, \delta\varphi\right)_Y + \left(\frac{\partial G}{\partial u}, \delta u\right)_X, \tag{11}$$

where $\delta\varphi$, $\delta\varphi^*$ and δu are the Gâteaux derivatives of φ, φ^* and u in the direction $\delta\varphi_{obs}$ (for example, $\delta\varphi = \frac{\partial\varphi}{\partial\varphi_{obs}}\delta\varphi_{obs}$).

Computing the gradient

To compute the gradient $\nabla_{\varphi_{obs}} G(\varphi, u)$, let us introduce three adjoint variables $P_1 \in Y$, $P_2 \in Y$ and $P_3 \in X$. By taking the inner product of (8) by P_1, (9) by P_2 and of (10) by P_3 and adding them, we obtain:

$$\left(\delta\varphi, -\frac{\partial P_1}{\partial t} - (F'(\varphi))^* P_1 - (F''(\varphi)P_2)^*\varphi^* + C^* V_2 C P_2\right)_Y + \left(\delta\varphi\big|_{t=T}, P_1\big|_{t=T}\right)_X$$
$$+\left(\delta\varphi^*, \frac{\partial P_2}{\partial t} - F'(\varphi)P_2\right)_Y + \left(\delta\varphi^*\big|_{t=0}, P_2\big|_{t=0} - P_3\right)_X +$$
$$+\left(\delta u, -P_1\big|_{t=0} + V_1 P_3\right)_X - \left(\delta\varphi_{obs}, V_2 C P_2\right)_{Y_{obs}} = 0. \qquad (12)$$

Here we put

$$-\frac{\partial P_1}{\partial t} - (F'(\varphi))^* P_1 - (F''(\varphi)P_2)^*\varphi^* + C^* V_2 C P_2 = \frac{\partial G}{\partial \varphi},$$

and

$$-P_1\big|_{t=0} + V_1 P_3 = \frac{\partial G}{\partial u},\ P_1\big|_{t=T} = 0,\ \frac{\partial P_2}{\partial t} - F'(\varphi)P_2 = 0,\ P_2\big|_{t=0} - P_3 = 0.$$

Thus, if P_1, P_2 are the solutions of the following system of equations

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} - (F'(\varphi))^* P_1 - (F''(\varphi)P_2)^*\varphi^* + C^* V_2 C P_2 &= \dfrac{\partial G}{\partial \varphi}, \quad t \in (0, T) \\ P_1\big|_{t=T} &= 0, \end{cases} \tag{13}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} - F'(\varphi)P_2 &= 0, \quad t \in (0, T) \\ V_1 P_2\big|_{t=0} &= \dfrac{\partial G}{\partial u} + P_1\big|_{t=0}, \end{cases} \tag{14}$$

then from (12) we get

$$\left(\frac{\partial G}{\partial \varphi}, \delta\varphi\right)_Y + \left(\frac{\partial G}{\partial u}, \delta u\right)_X = \left(\delta\varphi_{obs}, V_2 C P_2\right)_{Y_{obs}},$$

and due to (11) the gradient of G is given by

$$\frac{dG}{d\varphi_{obs}} = V_2 C P_2. \tag{15}$$

Equivalent formulation

Let us return to the former auxiliary variable $v = P_3 = P_2|_{t=0}$ and rewrite the non-standard problem (13)–(14) in an equivalent form:

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} - (F'(\varphi))^* P_1 - (F''(\varphi)P_2)^*\varphi^* + C^* V_2 C P_2 &= \dfrac{\partial G}{\partial \varphi}, \quad t \in (0, T) \\ P_1\Big|_{t=T} &= 0, \end{cases} \tag{16}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} - F'(\varphi)P_2 &= 0, \quad t \in (0, T) \\ P_2\Big|_{t=0} &= v, \end{cases} \tag{17}$$

$$V_1 v - P_1\Big|_{t=0} = \frac{\partial G}{\partial u}. \tag{18}$$

Here we have three unknowns: $v \in X,\ P_1, P_2 \in Y$. We will write (16)–(18) in the form of an operator equation for v.

Hessian $\mathcal{H}$

We define the operator $\mathcal{H}$ by the successive solution of the following problems:

$$\begin{cases} \dfrac{\partial \phi}{\partial t} - F'(\varphi)\phi &= 0, \quad t \in (0,T) \\ \phi\big|_{t=0} &= w, \end{cases} \tag{19}$$

$$\begin{cases} -\dfrac{\partial \phi^*}{\partial t} - (F'(\varphi))^*\phi^* - (F''(\varphi)\phi)^*\varphi^* &= -C^* V_2 C\phi, \quad t \in (0,T) \\ \phi^*\big|_{t=T} &= 0, \end{cases} \tag{20}$$

$$\mathcal{H}w = V_1 w - \phi^*\big|_{t=0}. \tag{21}$$

Here φ and φ^* are the solutions of the optimality system (4)–(6).

Operator equation

The system (16)–(18) is equivalent to the following equation in X:

$$\mathcal{H}v = \mathcal{F} \tag{22}$$

with the right-hand side $\mathcal{F}$ defined by

$$\mathcal{F} = \frac{\partial G}{\partial u} + \tilde{\phi}^*\Big|_{t=0}, \tag{23}$$

where $\tilde{\phi}^*$ is the solution to the adjoint problem:

$$\begin{cases} -\dfrac{\partial \tilde{\phi}^*}{\partial t} - (F'(\varphi))^* \tilde{\phi}^* = \dfrac{\partial G}{\partial \varphi}, \quad t \in (0, T) \\ \tilde{\phi}^*\Big|_{t=T} = 0. \end{cases} \tag{24}$$

Solvability of the non-standard problem

It is easily seen that the operator $\mathcal{H}$ defined by (19)–(21) is the Hessian of the original functional J considered on the optimal solution u of the problem (4)–(6): $J''(u) = \mathcal{H}$. Under the assumption that $\mathcal{H}$ is positive definite, the operator equation (22) is correctly and everywhere solvable in X, i.e. for every $\mathcal{F}$ there exists a unique solution $v \in X$ and

$$\|v\|_X \leq c\|\mathcal{F}\|_X, \quad c = const > 0.$$

Therefore, under the assumption that $J''(u)$ is positive definite on the optimal solution, the non-standard problem (13)–(14) has a unique solution $P_1, P_2 \in Y$.

Algorithm to compute the gradient of the functional G

1) For $\dfrac{\partial G}{\partial u} \in X$, $\dfrac{\partial G}{\partial \varphi} \in Y$ solve the adjoint problem

$$\begin{cases} -\dfrac{\partial \tilde{\phi}^*}{\partial t} - (F'(\varphi))^* \tilde{\phi}^* &= \dfrac{\partial G}{\partial \varphi}, \quad t \in (0,T) \\ \tilde{\phi}^*\big|_{t=T} &= 0, \end{cases} \tag{25}$$

2) Find v by solving

$$\mathcal{H} v = \mathcal{F}, \;\; \mathcal{F} = \frac{\partial G}{\partial u} + \tilde{\phi}^*\big|_{t=0}.$$

3) Solve the direct problem

$$\begin{cases} \dfrac{\partial P_2}{\partial t} - F'(\varphi) P_2 &= 0, \quad t \in (0,T) \\ P_2\big|_{t=0} &= v. \end{cases} \tag{26}$$

4) Compute the gradient of the response function as

$$\frac{dG}{d\varphi_{obs}} = V_2 C P_2. \tag{27}$$

Application: Ocean thermodynamics model

$$
\begin{aligned}
T_t + (\bar{U}, \mathrm{Grad})T - \mathrm{Div}(\hat{a}_T \cdot \mathrm{Grad}\ T) = f_T \ \text{ in } \ D \times (t_0, t_1), \\
T = T_0 \text{ for } t = t_0 \text{ in } D, \\
-\nu_T \frac{\partial T}{\partial z} = Q \text{ on } \Gamma_S \times (t_0, t_1), \\
\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_{w,c} \times (t_0, t_1), \\
\bar{U}_n^{(-)} T + \frac{\partial T}{\partial N_T} = \bar{U}_n^{(-)} d_T + Q_T \text{ on } \Gamma_{w,op} \times (t_0, t_1), \\
\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_H \times (t_0, t_1).
\end{aligned}
\tag{28}
$$

Operator form of the problem

$$T_t + LT = \mathcal{F} + BQ, \quad t \in (t_0, t_1),$$
$$T = T_0, \qquad t = t_0, \tag{29}$$

where

$$(T_t, \widehat{T}) + (LT, \widehat{T}) = \mathcal{F}(\widehat{T}) + (BQ, \widehat{T}) \;\; \forall \widehat{T} \in W_2^1(D), \tag{30}$$

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

$$\begin{cases} T_t + LT &= \mathcal{F} + BQ, \quad \text{in} \quad D \times (t_0, t_1), \\ T &= T_0, \qquad t = t_0 \\ J(Q) &= \inf\limits_{v} J(v), \end{cases} \tag{31}$$

where

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

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

Optimality system

$$
\begin{aligned}
T_t + LT &= \mathcal{F} + BQ \quad \text{in} \;\; D \times (t_0, t_1), \\
T = T_0, &\qquad t = t_0,
\end{aligned}
\tag{32}
$$

$$
\begin{aligned}
-(T^*)_t + L^* T^* &= Bm_0(T - T_{\mathrm{obs}}) \quad \text{in} \;\; D \times (t_0, t_1), \\
T^* = 0, &\qquad t = t_1,
\end{aligned}
\tag{33}
$$

$$
\alpha(Q - Q^{(0)}) + T^* = 0 \quad \text{on} \;\; \Omega \times (t_0, t_1). \tag{34}
$$

$$G(T) = \int_{t_0}^{t_1} dt \int_{\Omega} F^*(x, y, t) T(x, y, 0, t) d\Omega. \tag{35}$$

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

$$F^*(x, y, t) = \begin{cases} 1 \big/ (\tau \text{mes } \omega) & \text{if } (x, y) \in \omega, \bar{t} - \tau \le t \le \bar{t} \\ 0 & \text{else,} \end{cases} \tag{36}$$

and

$$G(T) = \frac{1}{\tau} \int_{\bar{t}-\tau}^{\bar{t}} dt \left(\frac{1}{\text{mes } \omega} \int_{\omega} T(x, y, 0, t) d\Omega \right). \tag{37}$$

Sensitivity of functionals

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

$$\frac{dG}{dT_{obs}} = \frac{\partial G}{\partial T}\frac{\partial T}{\partial T_{obs}}. \tag{38}$$

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

$$\left\{ \begin{array}{rcl} \frac{\partial \delta T}{\partial t} + L\delta T & = & B\delta Q, \quad t \in (t_0, t_1) \\ \delta T\Big|_{t=t_0} & = & 0, \end{array} \right. \tag{39}$$

$$\left\{ \begin{array}{rcl} -\frac{\partial \delta T^*}{\partial t} + L^*\delta T^* & = & Bm_0(\delta T - \delta T_{obs}), \\ \delta T^*\Big|_{t=T} & = & 0, \end{array} \right. \tag{40}$$

$$\alpha\delta Q + \delta T^*\Big|_{z=0} = 0, \tag{41}$$

and

$$\left(\frac{dG}{dT_{obs}}, \delta T_{obs}\right) = \left(\frac{\partial G}{\partial T}, \delta T\right)_Y. \tag{42}$$

Computing the gradient

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

$$\left(\delta T, -\frac{\partial P_1}{\partial t} + L^* P_1 + Bm_0 P_2\right)_Y + \left(\delta T\big|_{t=t_1}, P_1\big|_{t=t_1}\right)_X +$$

$$+\left(\delta\ T^*, \frac{\partial P_2}{\partial t} + LP_2 + BP_3\right)_Y + \left(\delta T^*\big|_{t=t_0}, P_2\big|_{t=t_0}\right)_X +$$

$$+\left(\delta Q, P_1\big|_{z=0} + \alpha P_3\right) - \left(\delta T_{obs}, m_0 P_2\big|_{z=0}\right) = 0, \ \ X = L_2(D). \quad (43)$$

We put

$$-\frac{\partial P_1}{\partial t} + L^* P_1 + Bm_0 P_2 = \frac{\partial G}{\partial T},$$

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

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

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} + L^* P_1 + B m_0 P_2 &= \dfrac{\partial G}{\partial T}, \quad t \in (t_0, t_1) \\ P_1\Big|_{t=t_1} &= 0, \end{cases} \tag{44}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} + L P_2 &= \dfrac{1}{\alpha} B P_1\Big|_{z=0}, \quad t \in (t_0, t_1) \\ P_2\Big|_{t=t_0} &= 0, \end{cases} \tag{45}$$

then from (43) 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

$$\frac{dG}{dT_{obs}} = m_0 P_2\big|_{z=0}. \tag{46}$$

Equivalent formulation

We write the non-standard problem (44)–(45) in the form:

$$\begin{cases} -\dfrac{\partial P_1}{\partial t} + L^* P_1 + Bm_0 P_2 = \dfrac{\partial G}{\partial T}, & t \in (t_0, t_1) \\ P_1\big|_{t=t_1} = 0, \end{cases} \tag{47}$$

$$\begin{cases} \dfrac{\partial P_2}{\partial t} + LP_2 + Bv = 0, & t \in (t_0, t_1) \\ P_2\big|_{t=t_0} = 0, \end{cases} \tag{48}$$

$$\alpha v + P_1\big|_{z=0} = 0. \tag{49}$$

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

$$\mathcal{H} v = \Phi. \tag{50}$$

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

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + L\phi + Bw & = & 0, \quad t \in (t_0, t_1) \\ \phi\big|_{t=t_0} & = & 0, \end{cases} \tag{51}$$

$$\begin{cases} -\dfrac{\partial \phi^*}{\partial t} + L^*\phi^* & = & -Bm_0\phi, \quad t \in (t_0, t_1) \\ \phi^*\big|_{t=t_1} & = & 0, \end{cases} \tag{52}$$

$$\mathcal{H}w = \alpha w + \phi^*\big|_{z=0}. \tag{53}$$

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

$$\begin{cases} -\dfrac{\partial \tilde{\phi}^*}{\partial t} + L^*\tilde{\phi}^* & = & -\dfrac{\partial G}{\partial T}, \quad t \in (t_0, t_1) \\ \tilde{\phi}^*\big|_{t=t_1} & = & 0. \end{cases} \tag{54}$$

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

$$\|v\| \leq c\|\Phi\|, \quad c = const > 0. \tag{55}$$

Therefore, the non-standard problem (44)–(45) has a unique solution $P_1, P_2 \in Y$.

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

1) Solve the adjoint problem

$$\begin{cases} -\dfrac{\partial \tilde{\phi}^*}{\partial t} + L^* \tilde{\phi}^* = -\dfrac{\partial G}{\partial T}, & t \in (t_0, t_1) \\ \tilde{\phi}^* \big|_{t=t_1} = 0 \end{cases} \tag{56}$$

and put

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

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

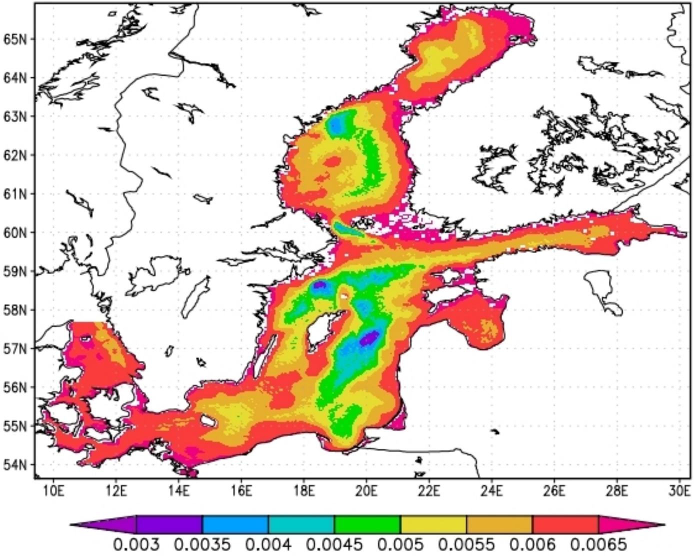
3) Solve the direct problem

$$\begin{cases} \dfrac{\partial P_2}{\partial t} + L_2 P_2 = -Bv, & t \in (t_0, t_1) \\ P_2 \big|_{t=t_0} = 0. \end{cases} \tag{57}$$

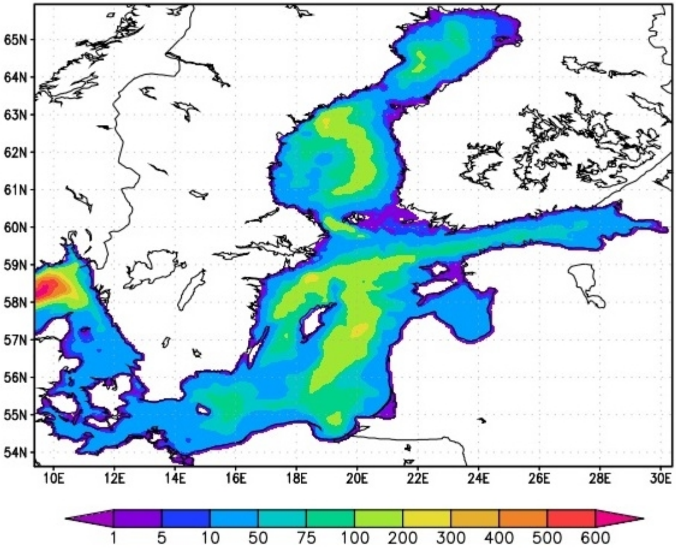
4) Compute the gradient of the response function as

$$\frac{dG}{dT_{obs}} = m_0 P_2 \big|_{z=0}. \tag{58}$$

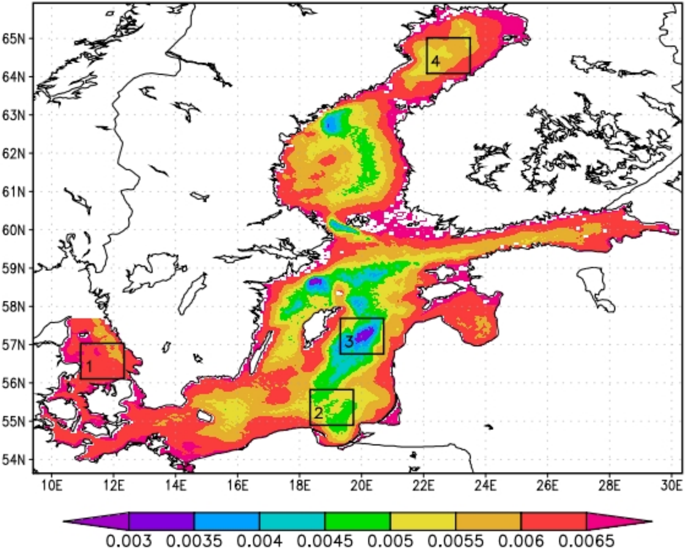
Gradient of the functional $G(T)$



Baltic Sea topography [m]



Regions in the Baltic Sea area



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Thank you!