Sensitivity and Error Propagation in Variational Data Assimilation

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Overview

- General Sensitivity Analysis
- Sensitivity and Data Assimilation
- Second Order Analysis
- An Application to a pollution problem

Introduction : Why second order methods ?

- A Data Assimilation problem, in a Variational Framework, is solution of an Optimality System
- The O.S. contains all the available information
- From this viewpoint the O.S. can be considered as a "Generalized Model"
- Therefore sensitivity with respect to parameters and/or observations must be carried out on the model

Sensitivity Analysis: Deterministic Approach

- Model: $\mathcal{F}$:

$$\mathcal{F}(\mathcal{X},\mathcal{U}) = 0 \tag{1}$$

- Scalar Response Function $\mathcal{G}$:

$$\mathcal{G}(\mathcal{X},\mathcal{U}) \tag{2}$$

- Sensitivity $\mathcal{S}$ is by definition the gradient of $\mathcal{G}$ with respect to $\mathcal{U}$:

$$\mathcal{S} = \nabla\mathcal{G}(\mathcal{X}(\mathcal{U}),\mathcal{U}) \tag{3}$$

Optimal Control Methods for D.A are efficient tools for deterministic sensitivity analysis

- An adjoint variable $\mathcal{P}$ is introduced as the solution of :

$$\left[\frac{\partial \mathcal{F}}{\partial \mathcal{X}}\right]^t . \mathcal{P} = \left[\frac{\partial \mathcal{G}}{\partial \mathcal{X}}\right] \tag{4}$$

- Then we get :

$$\mathcal{S} = \left[\frac{\partial \mathcal{G}}{\partial \mathcal{U}}\right] - \left[\frac{\partial \mathcal{F}}{\partial \mathcal{U}}\right]^t . \mathcal{P} \tag{5}$$

Data Assimilation for Pollution Modeling

- X is the state variable (velocity, surface elevation) governed by :

$$\begin{cases} \frac{dX}{dt} & = & F(X) \\ X(0) & = & U \end{cases} \tag{6}$$

- The concentration of pollutant C, produced by sources S verifies:

$$\begin{cases} \frac{dC}{dt} & = & G(X, C, S) \\ C(0) & = & V \end{cases} \tag{7}$$

- U and V are unknonw. The VDA problem is to evaluate them from observation X_{obs} and C_{obs}, in order to minimize the cost function J defined by:

$$J(U, V) = \frac{1}{2} \int_0^T \|EX - X_{obs}\|^2 dt + \frac{1}{2} \int_0^T \|DC - C_{obs}\|^2 dt \tag{8}$$

- For sake of simplicity regularization terms, of great practical importance, are not displayed

Data Assimilation for Pollution Modeling: Optimality System

- P and Q adjoint variables are introduced as the solution of the system :

$$\left\{ \begin{array}{rcl} \frac{dP}{dt} + \left[\frac{\partial F}{\partial X}\right]^t .P + \left[\frac{\partial G}{\partial X}\right]^t .Q & = & E^t(EX - X_{obs}) \\ P(T) & = & 0; \end{array} \right. \tag{9}$$

.;

$$\left\{ \begin{array}{rcl} \frac{dQ}{dt} + \left[\frac{\partial G}{\partial C}\right]^t .Q & = & D^t(DC - C_{obs}); \\ Q(T) & = & 0, \end{array} \right. \tag{10}$$

- Then the gradient of J with respect to U and V are given by :

$$\nabla J_U = -P(0) \tag{11}$$

$$\nabla J_V = -Q(0) \tag{12}$$

Sensitivity with respect to Sources

- If some response function $\mathcal{S}$ is introduced, how to evaluate the sensitivity with respect to observations? For instance how to evaluate the impact of an error of observation on a prediction?
- What should be the "model" $\mathcal{F}$ of the general sensitivity analysis?
- Because only the Optimality System contains the observation, the sensitivity analysis must be carried out on the O.S. considered as a Generalized Model
- Deriving the O.S. leads to carry out a **Second Order Analysis.**

Computing the sensitivity with respect to sources : second order adjoint.

- We need to introduce four second order adjoint variables Γ, Λ, Φ and Ψ as the solution of :

$$\left\{ \begin{array}{rcl} \frac{d\Gamma}{dt} + \left[\frac{\partial F}{\partial X}\right]^t \cdot \Gamma + \left[\frac{\partial F}{\partial X}\right]^t \cdot \Lambda + \left[\frac{\partial^2 F}{\partial X^2} P\right]^t \cdot \Phi & & \\ + \left[\frac{\partial^2 G}{\partial X^2} Q\right]^t \cdot \Phi + \left[\frac{\partial^2 G}{\partial C \partial X} Q\right]^t \cdot \Psi - E^t E \Phi & = & 0; \\ \Gamma(0) & = & 0; \\ \Gamma(T) & = & 0, \end{array} \right. \tag{13}$$

Computing the sensitivity with respect to sources 2

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$$\left\{\begin{array}{rcl} \dfrac{d\Lambda}{dt} + \left[\dfrac{\partial F}{\partial C}\right]^t \cdot \Lambda + \left[\dfrac{\partial^2 G}{\partial C \partial X} Q\right]^t \cdot \Phi & & \\ + \left[\dfrac{\partial^2 G}{\partial X^2} Q\right]^t \cdot \Psi - D^t D \Psi & = & \dfrac{\partial \varphi}{\partial C}; \\ \Lambda(0) & = & 0; \\ \Lambda(T) & = & 0, \end{array}\right. \tag{14}$$

$$\frac{d\Phi}{dt} + \left[\frac{\partial F}{\partial X}\right]^t \cdot \Phi = 0, \tag{15}$$

$$\frac{d\Psi}{dt} + \left[\frac{\partial G}{\partial C}\right]^t \cdot \Psi = 0, \tag{16}$$

- Then it comes :

$$\nabla \varphi = \left[\frac{\partial F}{\partial S}\right]^t \cdot \Lambda + \left[\frac{\partial^2 G}{\partial X^2} Q\right]^t \cdot \Phi + \left[\frac{\partial^2 G}{\partial C \partial S} Q\right]^t \cdot \Psi + \frac{\partial \varphi}{\partial S} \tag{17}$$

Remarks

- The sensitivity is obtained by solving the coupled system of four equations
- The System involves second order terms.
- We found a **non-standard problem : two equations have two conditions an initial condition and a final condition, the other two equations have no condition**

Solving the Non-Standard problem

- The Non-Standard problem can be symbolically written :

$$\begin{cases} \frac{dX}{dt} = K(X,Y), \ t \in [0,T]; \\ \frac{dY}{dt} = L(X,Y), \ t \in [0,T] \end{cases} \tag{18}$$

- with :

$$\begin{cases} X(0) = 0; \\ X(T) = 0 \end{cases} \tag{19}$$

and no condition on Y.
NSP is transformed into a problem of optimal control by introducing the control U and a cost-function $J_P(U)$ with :

$$\begin{cases} X(0) = 0; \\ Y(0) = U. \end{cases} \tag{20}$$

Solving the Non-Standard problem 2

A cost function $J_P(U)$ is defined by:

$$J_P(U) = \frac{1}{2}\|X(T,U)\|^2 + \frac{1}{2}\|U\|^2 \tag{21}$$

If Z and W are defined as the solution of:

$$\frac{dW}{dt} + \left[\frac{\partial K}{\partial X}\right]^t \cdot W + \left[\frac{\partial L}{\partial X}\right]^t \cdot Z = 0; \tag{22}$$

$$\frac{dZ}{dt} + \left[\frac{\partial K}{\partial Y}\right]^t \cdot W + \left[\frac{\partial L}{\partial Y}\right]^t \cdot Z = 0; \tag{23}$$

$$Z(T) = 0; W(T) = X(T), \tag{24}$$

then we get

$$\nabla J_P(U) = -Z(0) + U \tag{25}$$

Solving the Non-Standard problem 3

This problem involved third derivatives of the original model.
Recent developments on the NSP have been recently carried out by V. Shutyaev and F.-X. Le Dimet
The existence of a solution is demonstrated
Another method to solve NSP is proposed.

Sensitivity with respect to observations

- If some response function $\mathcal{S}$ is introduced, how to evaluate the sensitivity with respect to observations? For instance how to evaluate the impact of an error of observation on a prediction?
- What should be the "model" $\mathcal{F}$ of the general sensitivity analysis?
- Because only the Optimality System contains the observation, the sensitivity analysis must be carried out on the O.S. considered as a Generalized Model
- Deriving the O.S. leads to carry out a **Second Order Analysis.**

Optimality System: where are the observations?

- P and Q adjoint variables are introduced as the solution of the system :

$$\left\{ \begin{array}{rcl} \frac{dP}{dt} + \left[\frac{\partial F}{\partial X}\right]^t .P + \left[\frac{\partial G}{\partial X}\right]^t .Q & = & E^t(EX - X_{obs}) \\ P(T) & = & 0; \end{array} \right. \tag{26}$$

.;

$$\left\{ \begin{array}{rcl} \frac{dQ}{dt} + \left[\frac{\partial G}{\partial C}\right]^t .Q & = & D^t(DC - C_{obs}); \\ Q(T) & = & 0, \end{array} \right. \tag{27}$$

Sensitivity with respect to observations

- Therefore the sensitivity analysis has to be carried out on the O.S., the equations where observations are taken into account.
- We have to introduce some response function (e.g. the mean concentration in some area)
- The sensitivity is found as the solution of a non standard problem slightly different from the first one with initial/final conditions:
  $\Lambda(0) = \Phi(0)$;
  $\Lambda(T) = 0$,
- The method can be used to determine the optimal location of sensors

Mathematical formulation of the 2D water pollution problem

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (vh)}{\partial y} = 0, \qquad \text{in } \Omega, \tag{28}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial h}{\partial x} = -\frac{gu(u^2+v^2)^{1/2}}{K_x^2 h^{4/3}} - g\frac{\partial z_b}{\partial x}, \quad \text{in } \Omega, \tag{29}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial h}{\partial y} = -\frac{gv(u^2+v^2)^{1/2}}{K_y^2 h^{4/3}} - g\frac{\partial z_b}{\partial y}, \quad \text{in } \Omega, \tag{30}$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - \eta \Delta C = KC + S, \quad \text{in } \Omega, \tag{31}$$

Mathematical formulation of the 2D water pollution problem

$$\begin{cases} \dfrac{\partial X}{\partial t} + \dfrac{\partial \mathbf{A}(X)}{\partial x} + \dfrac{\partial \mathbf{B}(X)}{\partial y} & = & F(X), \quad \text{in } \Omega, \\ n_x u + n_y v & = & \bar{\mathbf{U}}_{in}, \quad \text{on } \Gamma_1, \\ n_x u + n_y v & = & 0, \quad \text{on } S_W, \\ h & = & \bar{h}(t), \quad \text{on } \Gamma_2, \\ X(0) & = & U, \end{cases} \tag{32}$$

$$\begin{cases} \dfrac{\partial C}{\partial t} + u\dfrac{\partial C}{\partial x} + v\dfrac{\partial C}{\partial y} - \eta \triangle C & = & KC + S, \quad \text{in } \Omega, \\ C & = & \bar{C}_{in}, \quad \text{on } \Gamma_1, \\ \frac{\partial C}{\partial \vec{n}} & = & 0, \quad \text{on } \Gamma_2 \bigcup S_W, \\ C(0) & = & V, \end{cases} \tag{33}$$

Mathematical formulation of the 2D water pollution problem

where:

$$\mathbf{A}(X) = \begin{pmatrix} uh \\ \frac{1}{2}u^2 + gh \\ uv \end{pmatrix}, \quad \mathbf{B}(X) = \begin{pmatrix} vh \\ uv \\ \frac{1}{2}v^2 + gh \end{pmatrix},$$

$$F(X) = \begin{pmatrix} 0 \\ \\ -gu\dfrac{\sqrt{u^2+v^2}}{K_x^2 h^{4/3}} + u\dfrac{\partial v}{\partial y} - g\dfrac{\partial z_b}{\partial x} \\ -gv\dfrac{\sqrt{u^2+v^2}}{K_y^2 h^{4/3}} + v\dfrac{\partial u}{\partial x} - g\dfrac{\partial z_b}{\partial y} \end{pmatrix}.$$

Variational data assimilation problem

Define the cost function J by

$$J(U,V) = \frac{1}{2}\left(V_{1X}(U - X_0), (U - X_0)\right)_{X_X} + \frac{1}{2}\left(V_{1C}(V - C_0), (V - C_0)\right)_{X_C} \tag{34}$$

$$+\frac{1}{2}\left(V_{2X}(H_X X - X_{obs}), (H_X X - X_{obs})\right)_{Y_{Xobs}}$$

$$+\frac{1}{2}\left(V_{2C}(H_c C - C_{obs}), (H_c C - C_{obs})\right)_{Y_{Cobs}},$$

Variational data assimilation problem

$$
\left\{
\begin{array}{rcl}
\dfrac{\partial X}{\partial t} + \dfrac{\partial \mathbf{A}(X)}{\partial x} + \dfrac{\partial \mathbf{B}(X)}{\partial y} & = & F(X), \quad \text{in } \Omega, \\
\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - \eta \triangle C & = & KC + S, \quad \text{in } \Omega, \\
n_x u + n_y v & = & \bar{\mathbf{U}}_{in}, \quad \text{on } \Gamma_1, \\
n_x u + n_y v & = & 0, \quad \text{on } S_W, \\
h & = & \bar{h}(t), \quad \text{on } \Gamma_2, \\
C & = & \bar{C}_{in}, \quad \text{on } \Gamma_1 \\
\frac{\partial C}{\partial \vec{n}} & = & 0, \quad \text{on } \Gamma_2 \bigcup S_W, \\
C(0) & = & V \\
X(0) & = & U \\
J(U, V) & = & \inf\limits_{U^*, V^*} J(U^*, V^*).
\end{array}
\right.
\tag{35}
$$

Evaluation of sensitivities with respect to the source

$$G_A(X, C, S) = \int_0^T \int_{\Omega_A} C(x, y, t) dxdydt, \qquad (36)$$

where $\Omega_A \subset \Omega$ - the response region, C depends on S.

Simulation experiment on computing the response-function gradient for 2D water pollution model

The channel with L=3000m, W=800m, $z_b = 0$. Ω: 3000m$\times 800m$. Γ_1- the gate-into where $x = 0$, $y \in [0, 200]$, Γ_2 - the gate out of the channel : $x = 3000$, $y \in [600, 800]$. $C\mid_{\Gamma_1} = 24$ mg/l; $\mathbf{U}\vec{n}\mid_{\Gamma_1} = (un_x + vn_y)\mid_{\Gamma_1} = 0.35$ m/s. $\frac{\partial C}{\partial n}\mid_{S_W} = 0$ and $\mathbf{U}\vec{n}\mid_{S_W} = (un_x + vn_y)\mid_{S_W} = 0$. $\frac{\partial C}{\partial n}\mid_{\Gamma_2} = 0$ and $h\mid_{\Gamma_2} = 7$m. $u(x, y, 0) = 0, v(x, y, 0) = 0, h(x, y, 0) = 7$m and $C(x, y, 0) = 24$ mg/l.

K_x, K_y	Mesh type	η	K	Time step (s)
30.6	Triangular	$1.7e^{-6}$	$-4.05E^{-6}$	1

Table: Data of the channel

Simulation experiment on computing the response-function gradient for 2D water pollution model

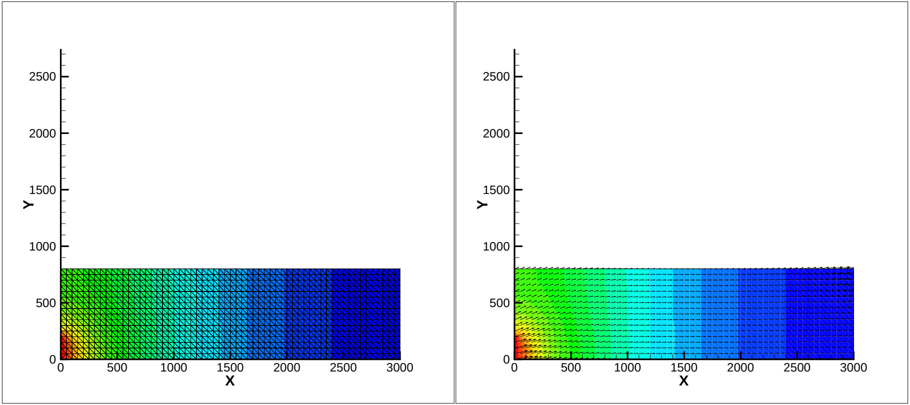

Figure: Unstructured net with triangular cells before putting the pollution source into the middle of the channel (Left); Velocity field before putting the pollution source into the middle of the channel (Right)

Simulation experiment on computing the response-function gradient for 2D water pollution model

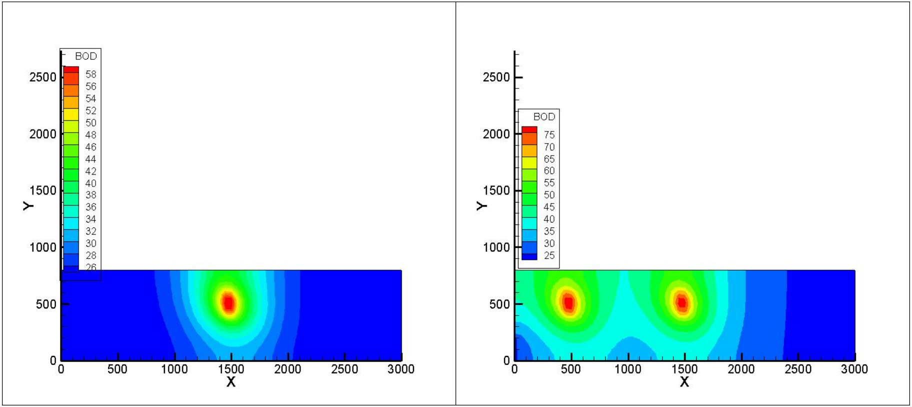

Figure: Concentration picture after putting 1 pollution source into the channel (Left); Concentration picture after putting 2 pollution sources into the channel (Right)

Simulation experiment on computing the response-function gradient for 2D water pollution model

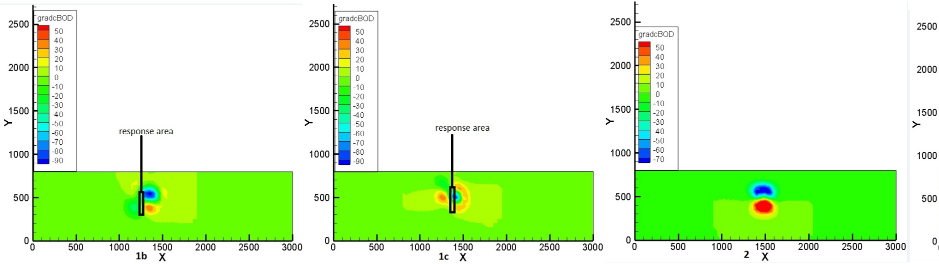

Figure: One source in the channel - Relative gradients of the response function in 6 cases of response region places (from left to right) : Response region in the left-hand place of the source region; Response region in the left-hand place of the source region; Response region in the left-hand place of the source region; Response region in the place of the source region; Response regions in the right-hand and far right-hand places of the source region

Simulation experiment on computing the response-function gradient for 2D water pollution model

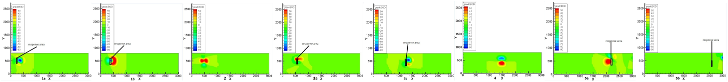

Figure: Two sources in the channel - Relative gradients of the response function in 9 cases of the response region places (from left to right) : Response region in the left-hand place of the source regions; Response region in the place of the first source region; Response region in the right-hand place nearby the first source region; Response region in the right-hand place nearby the first source region; Response region in the middle between 2 sources; Response region in the left-hand place nearby the second source region; Response region in the place of the second source region; Response region in the right-hand place of source region; Response region in the right-hand place of the source region

Conclusion

More numerical results in Le Dimet, Tran Thu Ha, Shutyaev (2014)

- Observations and analysis are linked only in the Optimality System
- A sensitivity Analysis with respect to the observation must be carried out on the O.S.
- Second Order Adjoint can be used for uncertainties propagation and evaluation of a posteriori covariance analysis (Gejadze, Shutyaev, Le Dimet, 2013, QJRMS)
- Singular Evolutive Interpolated Kalman filter has been applied and is under development (Ha Tran Thu et al. 2013, CRAS)