Sensitivity Analysis in Pollution Models: Second and Third order Adjoint Methods

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Abstract

Understanding the consequences of emission changes from a source region onto a target region is a key factor for decision making. The source-target relationship is commonly studied by the sensitivity analysis of a response function with respect to the source. The basic approach determines the sensitivity by carrying out multiple simulations with variation of source parameters. The variability over the receptor is considered as the sensitivity. By definition, the sensitivity of a given response function with respect to the source is the gradient of that response function with respect to the source. A systematic approach uses the first order adjoint formulation. Both approaches assume that the transport velocity and the initial distribution of the pollutant are known. However, they are given by the solution of a Data Assimilation problem whose ingredients include, but are not limited to, the pollutant source, the mathematical model and physical measurements. As a consequence, the sensitivity analysis should be carried out on the optimality system of the Data Assimilation problem. It leads to a non standard problem on a second order adjoint system whose the solution requires the third order adjoint.

We present the mathematical derivation of the third order adjoint method for the sensitivity analysis, along with some numerical experiments and a comparison with the first order adjoint approach.

Introduction

The ability to know in advance and with accuracy the effect of the change of pollutant emission from a foreign region onto a target region would help decision makers to improve public health and protect the environment. Also, the knowledge of the exact location of an emission source that could impact a target region within a given time scale is an asset in choosing the right place for some events or the storage location for delicate products. Studies shown that the change in pollutant emission from a foreign region could have a significant impact on a target or response region, even at the intercontinental level. This is the case for the degradation of the air quality over remote continents [Wilkening 2000, Biscaye 2000, Holloway 2003, Akimoto 2003]. Some air pollution episodes in the US were reported to be associated with transpacific transport events [Jaffe 1999, Jaffe 2003]. During the last decades, ground based measurements and satellites remote sensing have provided evidence for foreign influence of pollutants [Allen 2004, Jaffe 2003, Seinfeld 2004]. The time scale for the influence of a remote source on a receptor region is highly dependent on weather conditions: [Jaffe1999] shows that under certain weather conditions, Asian emissions can be transported to North America within 5 to 8 days. As underlined by [Fiore 2003, Derwent 2003, Jonson 2005, Fiore 2009], attributing a given pollution to a specific source is complicated by the interplay of processes influencing the transport (export from the source region, the evolution in transit due to chemical and the depositional losses, dilution and mixing with local species over the receptor region). As it is difficult to diagnose source-receptor relationships from observation, such analysis rely on models: [Fiore 2009] uses a set of 21 numerical models to estimate the intercontinental source-receptor relationships for ozone pollution; [Wang 2009] made a similar study based on a high resolution model.

Sensitivity analysis: First order adjoint method

- Evolution of the pollutant:

$$\frac{dC}{dt} = G(X, C, S) \text{ in } \Omega \times [0, T]; \quad C(0) = V \tag{1}$$

C: concentration of the pollutant; S: production (source) of pollutant; G: evolution model (example: transport-diffusion); X: state of the geophysical system (velocity fields); Ω: physical domain of the system; $[0, T]$: interval of time of interest.

- Sensitivity problem: response function

$$\phi_A(C, S) = \int_0^T \int_{\Omega_A} \varphi(C, S) dx dt. \tag{2}$$

$\Omega_A \subset \Omega$: region of interest (response region); φ function giving the measure of the effect of interest (example, pollutant concentration).

- Sensitivity (gradient of ϕ_A with respect to S):

$$\nabla_S \phi_A = -\left[\frac{\partial G}{\partial S}\right]^t \Lambda + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A} \tag{3}$$

with Λ defined by (first order adjoint of the evolution model):

$$\frac{d\Lambda}{dt} + \left[\frac{\partial G}{\partial C}\right]^t \Lambda = \left[\frac{\partial \varphi}{\partial C}\right]^t 1_{\Omega_A}; \quad \Lambda(T) = 0, \tag{4}$$

Example 1: one dimensional transport-diffusion problem

We consider the problem of pollution by a single species that is produced by continuous sources defined on the physical space $\Omega = [-1, 1]$; The time interval of interest is $[0, 1]$. The concentration of the pollutant evolves according to the one dimensional transport-diffusion equation (5).

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \eta\frac{\partial^2 c}{\partial x^2} + s, x \in]-1, 1[, t \in [0, T]; c(x, 0) = c_0(x), \tag{5}$$

c, concentration of the pollutant; u, transport velocity; η, coefficient of diffusion; $s = s(x, t)$, source function. Response function:

$$\phi_A(c) = \frac{1}{T \times \|\Omega_A\|}\int_0^T \int_{-1}^1 1_{\Omega_A} c(x, t) dx dt, \tag{6}$$

$T = 1$, time scale of the study; $\varphi = c$.

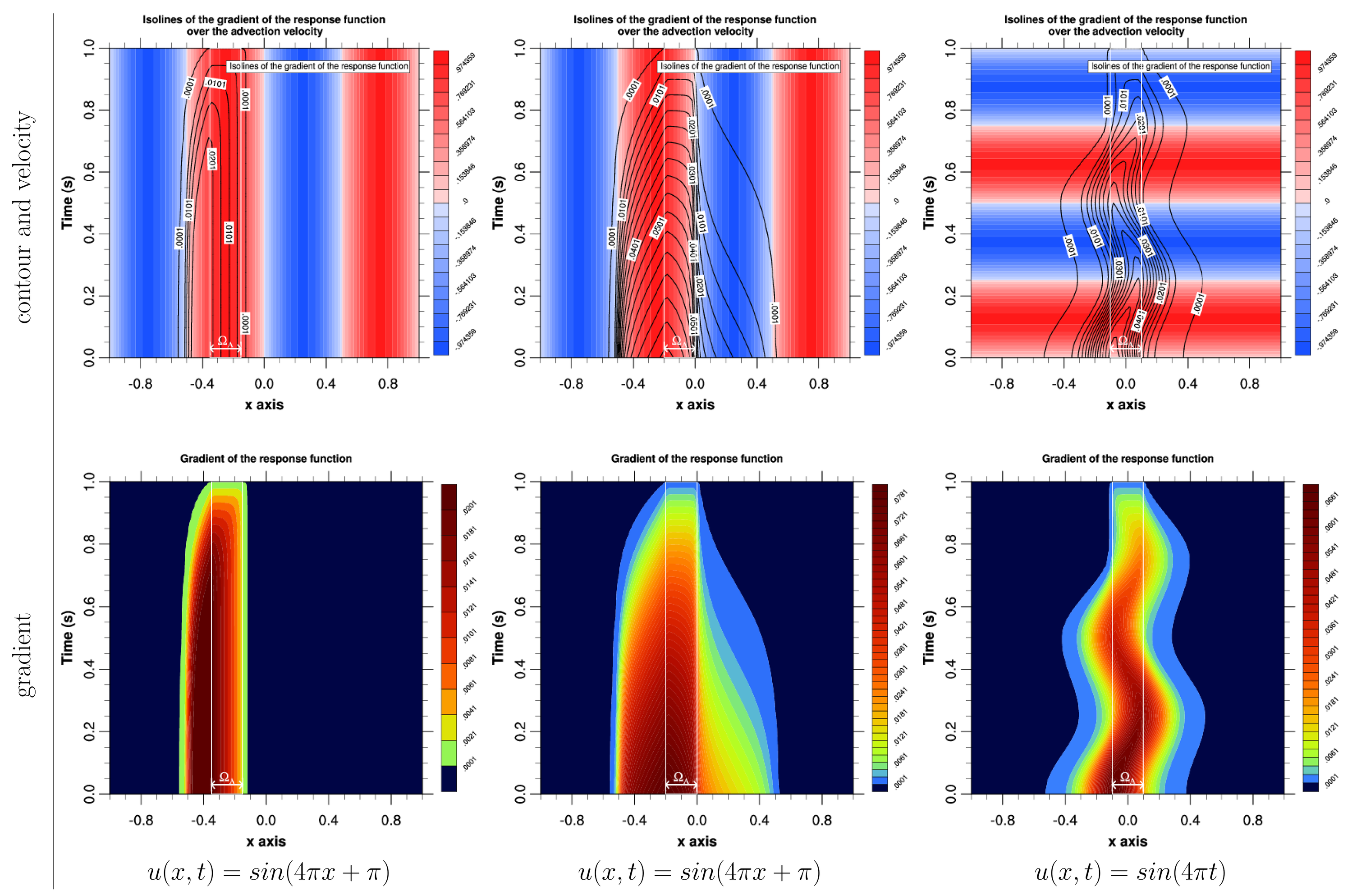
Gradient of the response function:

$$\nabla_s \Phi_A = -\Lambda \tag{7}$$

Λ is the solution of:

$$\frac{\partial \Lambda}{\partial t} - u\frac{\partial \Lambda}{\partial x} + \eta\frac{\partial^2 \Lambda}{\partial x^2} = 1_{\Omega_A}; \Lambda(t = T) = 0 \tag{8}$$

Numerical results



Example 2: shallow water pollution problem

We consider the problem of pollution by multiple species under the dynamics of a shallow water flow:

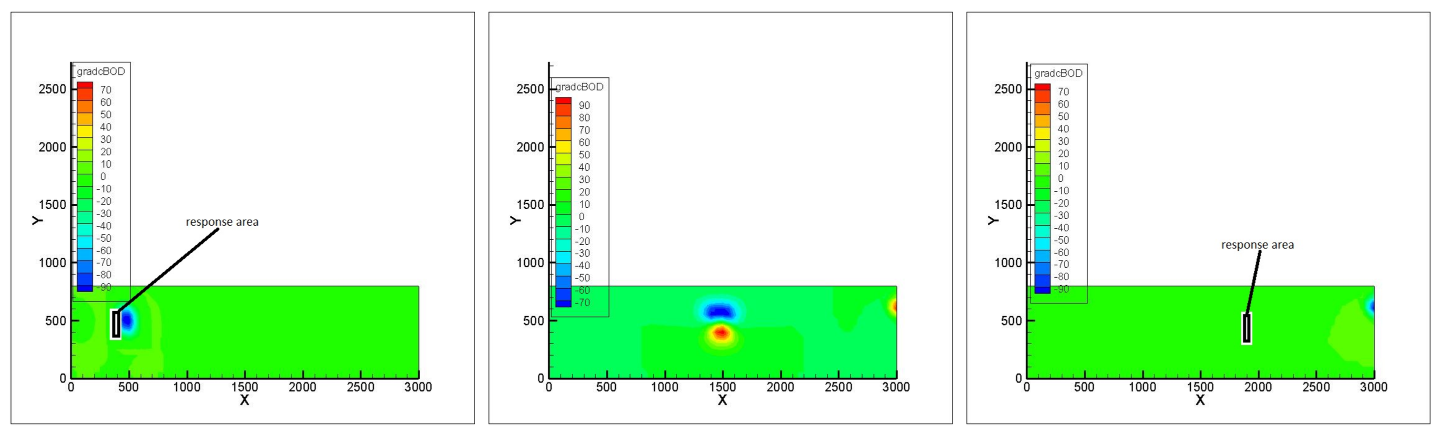
$$\begin{cases} \frac{\partial z}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (vh)}{\partial y} = 0, \\ \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial z}{\partial x} = -\frac{gu(u^2+v^2)^{1/2}}{K_x^2 h^{4/3}}, \\ \frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial z}{\partial y} = -\frac{gv(u^2+v^2)^{1/2}}{K_y^2 h^{4/3}}, \end{cases} \tag{9}$$

z, free surface elevation; h, water depth; (u, v), average horizontal velocity; g gravity acceleration; (K_x, K_y), Strickler coefficients

Pollution: transport and diffusion of m species of pollutants.

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} - \eta_i \Delta C_i = f_i(C) + S_i, \quad \text{in } \Omega, \ i = 1, \ldots, m. \tag{10}$$

Numerical results



Limitations

The first order adjoint supposed that the state of the geophysical system and the initial state of the pollution are known. However, this is not the case in real life problems. The state of the geophysical system and the initial state of the tracer are usually given by the solution of inverse problems using the Data Assimilation techniques. Those techniques use the sources and observations of the pollutant. The first order adjoint is thus insufficient for the sensitivity analysis.

Second order adjoint for the sensitivity analysis

Model: System and pollutant evolution

$$\frac{dX}{dt} = F(X); \quad X(0) = U. \tag{11}$$

$$\frac{dC}{dt} = G(X, C, S); \quad C(0) = V \tag{12}$$

Determination of the initial conditions

given the observation $X_{obs} \in \mathcal{X}_{obs}$ and $C_{obs} \in \mathcal{C}_{obs}$, we define the cost function:

$$J(U, V) = \frac{1}{2}\|U - U_b\|^2 + \frac{1}{2}\|V - V_b\|^2 + \frac{1}{2}\int_0^T \|H_1 X - X_{obs}\|^2 dt + \frac{1}{2}\int_0^T \|H_2 C - C_{obs}\|^2 dt \tag{13}$$

Minimization of the cost function using gradient based methods:

$$\nabla J_U = -P(0) + (U - U_b) \text{ and } \nabla J_V = -Q(0) + (V - V_b) \tag{14}$$

P and Q are defined as the solutions of the first order adjoint problems given by:

$$\frac{dP}{dt} + \left[\frac{\partial F}{\partial X}\right]^t \cdot P + \left[\frac{\partial G}{\partial X}\right]^t \cdot Q = H1^t(H_1 X - X_{obs}); \quad P(T) = 0 \tag{15}$$

$$\frac{dQ}{dt} + \left[\frac{\partial G}{\partial C}\right]^t \cdot Q = H_2^t \cdot (H_2 C - C_{obs}); \quad Q(T) = 0 \tag{16}$$

Evaluation of the sensitivities with respect to the sources

$$\text{Response function: } \Phi_A(C, S) = \int_0^T \int_{\Omega_A} \varphi(C, S) dx dt. \tag{17}$$

Sensitivity of Φ_A with respect S:

$$\nabla \Phi_A = -\left[\frac{\partial G}{\partial S}\right]^t \cdot \Lambda + \left[\frac{\partial^2 G}{\partial X^2} Q\right]^t \cdot \Phi + \left[\frac{\partial^2 G}{\partial C \partial S} Q\right]^t \cdot \Psi + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A} \tag{18}$$

Γ, Λ, Φ and Ψ are the solutions of the second order adjoint problem:

$$\begin{cases} \frac{d\Gamma}{dt} + \left[\frac{\partial F}{\partial X}\right]^t \cdot \Gamma + \left[\frac{\partial G}{\partial X}\right]^t \cdot \Lambda - \left[\frac{\partial^2 F}{\partial X^2} P\right] \cdot \Phi - \left[\frac{\partial^2 G}{\partial X^2} Q\right] \cdot \Phi - \left[\frac{\partial^2 G}{\partial C \partial X} Q\right] \cdot \Psi + E^t E \Phi = 0; \\ \frac{d\Lambda}{dt} + \left[\frac{\partial G}{\partial C}\right]^t \cdot \Lambda - \left[\frac{\partial^2 G}{\partial C \partial X} Q\right] \cdot \Phi - \left[\frac{\partial^2 G}{\partial X^2} Q\right] \cdot \Psi + D^t D \Psi = \left[\frac{\partial \varphi}{\partial C}\right]^t \cdot 1_{\Omega_A}; \\ \frac{d\Phi}{dt} - \left[\frac{\partial F}{\partial X}\right] \cdot \Phi = 0, \\ \frac{d\Psi}{dt} - \left[\frac{\partial G}{\partial C}\right] \cdot \Psi - \left[\frac{\partial G}{\partial X}\right] \cdot \Phi = 0, \\ \Gamma(0) + \Phi(0) = 0; \quad \Gamma(T) = 0 \\ \Lambda(0) + \Psi(0) = 0; \quad \Lambda(T) = 0 \end{cases} \tag{19}$$

This is a non standard system of 4 equations with simple final conditions on two equations and no simple conditions on two equations.

Solution of the non standard problem

For simplicity, let us consider the following system of two equations:

$$\begin{cases} \frac{dX}{dt} = K_1 X + K_2 Y + X_g, \ t \in [0, T]; \\ \frac{dY}{dt} = LY, \ t \in [0, T] \\ X(T) = 0; \quad X(0) + Y(0) = 0 \end{cases} \tag{20}$$

$$J_P(U) = \frac{1}{2}\|X(0, U) + U\|^2. \tag{21}$$

$$\nabla J_P(U) = -Z(0) + X(0) + U \tag{22}$$

$$\begin{cases} \frac{dW}{dt} + K_1^t W = 0; \\ \frac{dZ}{dt} + K_2^t W + L^t Z = 0; \\ W(0) = X(0) + U; \quad Z(T) = 0; \end{cases} \tag{23}$$

K_1, K_2 and L are linear operators; X_g is given. To turn it into a control problem, let us consider the problem with the initial condition $Y(0) = U$ on Y and the final condition $X(T) = 0$ on X. Assuming that under these conditions, (20) has a unique solution; let $X(0, U)$ be the value of X at time $t = 0$ for the value U of $Y(0)$, and define the cost function J_P: The problem becomes the determination of U^* minimizing J_P. We can expect that at the optimum, $X(T, U^*) = 0$ and the problem will be solved. Z and W are the third order adjoint variables. A theoretical question remains on the existence and the uniqueness of a solution. Development in this direction and numerical experiments are ongoing.

Design LaTeX , packages pgf et TikZ, PyNGL & PyNIO: Innocent Souopgui, oct. 2013