# Discontinuous Data Assimilation

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**Abstract**

Data Assimilation is important in meteorology, oceanography and climatology because it is a way to improve the models with newly measured data, statically or dynamically. The problem is well know in control and system theory and a large number of methods applied to environmental sciences are issued from Kalman filters, optimal control etc. In this paper we give a short review of data assimilation by least squares and optimal control and then concentrate on the problem of finding a discontinuity known to be present in the data but of unknown position in space, such as a meteorological front. As standard control theory assumes differentiability, there are new mathematical difficulties here: if gradient methods are to be used computationally, one needs to establish that derivatives exists in the sense of $L^1$ instead of $L^2$. We show on simple examples the difficulties and give some numerical solutions for some flows with shocks.

**Keywords**: Inverse problems, data assimilation, meteorology, optimal control, discontinuities.

## Introduction

For obvious reasons, it is of prime importance to improve the numerical models for meteorology, oceanography and climatology. The fundamental equations of fluids are know and need no improvements. The numerical mesh for their discretisation are usually not adequate for lack of computing resource and turbulence modeling must be done. However even if the mesh could resolve all the scales in these flows, there would still be a problem of stability: however accurate the initial state, errors grow to an unacceptable level after some times. The numerical models need to be reinitialized or adjusted with new observations, a process which is called data assimilation.

For example, denote by $\Omega$ the domain occupied by the fluid (air or water), by $W(x,t)$ the vector field of the dynamic flow variables (density $\rho$, flux velocities $\rho u$, temperature $\theta$

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or pressure $p$, and possibly humidity, salinity) and let the set of equations for the fluid be the Euler equations

$$\partial_t W + \nabla \cdot F(W) = 0 \text{ for all } x \text{ in } \Omega, \text{ all } t \text{ in } (0,T) \tag{1}$$

with initial and boundary conditions

$$W(x,0) = V \text{ for all x in } \Omega \qquad (AW).n = v \text{ on the boundary } \Gamma = \partial\Omega \tag{2}$$

where the outer normal to $\Gamma$ is denoted by $n$. The matrix field $A(x,t)$ selects components of $W(x,t)$ which have to be given to ensure uniqueness.
Assume now that we have a new set of data $BW_d$ where $B(x,t)$ is a matrix field which selects the components of $W(x,t)$ which are measured at time $t$ and point $x$ ($B$ would contain Dirac masses if $W$ is measured at isolated points) . Then one would like to reset $V$ and/or $v$ so as to fit the new data. One way to do this is to solve

$$\min_{V,v} J_0(V,v) = \int_{\Omega\times(0,T)} |B(W - W_d)|^2 \quad \text{subject to (1)} \tag{3}$$

Since this is a least square procedure, Sasaki [7] proposed to adapt the norm to the probability measure of the state and observation variable because, after all, data assimilation is necessary because of random error on data. The so-called *4D-Var* method ([5]) proposes to replace $J_0$ by

$$J_1(V,v) = \int_{\Omega\times(0,T)} ((W - W_d)^T B^T \mathbf{R} B(W - W_d) + (W - W_1)^T \mathbf{S}(W - W_1)) \tag{4}$$

where $\mathbf{R}$ is the covariance probability matrix on the measurements and $\mathbf{S}$ is a covariance matrix on the predictive error to realize $W_1$.

# 1 Gradient Methods

Problem (1)-(4) is of the type

$$\min_{v\in\mathcal{V}} J(w,v) \ : \ Aw = f(v). \tag{5}$$

where $J$ is a real valued function, $A$ a linear operator from the *state space*$\mathcal{W}$ into its dual $\mathcal{W}'$. Let $q$ be a Lagrange multiplier associated to $Aw = f(v)$. By duality theory one may solve

$$\min_{v\in\mathcal{V}} \max_q L(w,q,v) = J(w,v) + < q, Aw - f(v) > . \tag{6}$$

where $<,>$ denotes the duality product in $\mathcal{W}$. When the hypotheses for the min-max theorem are met, a solution of (6) will be found by solving the *optimality conditions*

$$\partial_w L(w,q,v) = 0, \quad \partial_q L(w,q,v) = 0, \quad \partial_v L(w,q,v) = 0. \tag{7}$$

When $A$ is invertible, one can look at (5) as a minimisation of $v \mapsto J(w(v), v)$ without constraint and apply calculus of variations:

$$\delta J := J(w(v+\delta v), v+\delta v) - J(w(v), v) = \partial_w J(w,v)\delta w + \partial_v J(w,v)\delta v + o(|\delta v|) \quad (8)$$

where $\delta w := w(v+\delta v) - w(v)$ satisfies the *linearized state equation*

$$A\delta w = \partial_v f(v)\delta v + o(|\delta v|) \quad (9)$$

Then, using the adjoint trick ([6])

$$< q, \partial_v f(v)\delta v >=< q, A\delta w >=< A^* q, \delta w >= \partial_w J(w,v)\delta w + o(|\delta v|) \quad (10)$$

provided $q$ is the solution of the *adjoint equation*

$$A^* q = \partial_w J(w,v). \quad (11)$$

So finally

$$\delta J =< q, \partial_v f(v)\delta v > + o(|\delta v|). \quad (12)$$

This calculus is helpful to set up a *gradient method* to solve the problem numerically because an iterative scheme of the type (where $w^m$ means $w(v^m)$)

$$v^{m+1} = v^m - \mu q^m \partial_v f(v^m) \qquad \text{with } \mu > 0 \text{ a small } \textit{step size} \text{ parameter} \quad (13)$$

generates a decreasing sequence of *cost function values* $\{J(w^m, v^m)\}$, independently of the *initial guess* $v^0$.

## 2 Discontinuous Data Assimilation

Gradient methods applied to the Euler system of equations can be difficult for several reasons:

1. The solution $W$ can be discontinuous (shocks).
2. The system is controllable but not the linearized one

Controllability is necessary because one is precisely looking for an inital state $V$ which drives the system to a desired state $W_1$. This problem has been studied by Coron et al [2]. However in the *4D-Var* approach, strictly speaking, exact controllability is not necessary since we search for a minimum of $J_1$, but there may be stability problems without it.

Shocks is a more serious difficulty as we shall show on the following example.

## 2.1 An Example with a Shock

Consider the *shock tube problem* with a constant state on each side of the shock denoted by $W^+$ on the right and $W^-$ on the left of the shock. The Euler equations for a perfect gas are given by (1) with, in dimension d,

$$W = (\rho, \rho u, \rho(\frac{|u|^2}{2} + \frac{\gamma}{\gamma - 1}\frac{p}{\rho}))$$
$$F_i(W) = (\rho u_i,\ \rho u_1 u_i + \delta_{1i}p, ..., \rho u_d u_i + \delta_{di}p,\ u_i(\frac{|u|^2}{2} + \frac{\gamma}{\gamma - 1}\frac{p}{\rho}))^T \quad (14)$$

Assume that $W^-$ is given and equal to $(A, B, C)$, that the geometry is a tube of length $L$, and that the Rankine-Hugoniot conditions are satisfied, so that the flow is at rest and

$$A = \rho^- u^- = \rho^+ u^+$$
$$B = \rho^- {u^-}^2 + p^- = \rho^+ {u^+}^2 + p^+$$
$$C = \rho^- u^- (\frac{|u^-|^2}{2} + \frac{\gamma}{\gamma - 1}\frac{p^-}{\rho^-}) = \rho^+ u^+ (\frac{|u^+|^2}{2} + \frac{\gamma}{\gamma - 1}\frac{p^+}{\rho^-}) \quad (15)$$

An equation for $\rho^\pm$ can be obtained:

$$2C(\gamma - 1)\rho^\pm - 2\gamma AB + A^3(\gamma + 1)\frac{1}{\rho^\pm} = 0 \quad (16)$$

With appropriate choice of $A, B, C$ there are two admissible solutions (the entropy inequality needs to be satisfied also), one corresponding to $\rho^-$ and the other to $\rho^+$. The position of the discontinuity is not fixed; this is because we are looking at the stationary problem. If this stationary state is a limit of a transient state then, invariants such as $I = \int_0^L \rho$, being independent of time, are fixed by the initial conditions. Therefore it is $I$ which fixes the position $x = a$ of the shock:

$$I = \int_0^L \rho = \rho^- a + \rho^+(L - a) \quad (17)$$

An analysis of the transient case in dimension one, done in the pioneering work of Godlewski et al [3], confirms the role of (17) to fix the shock.

## 2.2 Analysis

From (15) it is clear that knowing $\rho^-, u^-, p^+, I$, for instance, is enough to determine $a$, the number of equations being equal to the number of unknowns (but of course there may not be any physical solution). However any iterative algorithm will change $a$ as well, so the solution $\rho^\pm, u^\pm, p^\pm, a$ will be found as the limit of $\{{\rho^\pm}^m, {u^\pm}^m, {p^\pm}^m, a^m\}$. One then expects for instance $\rho^{m+1} - \rho^m \to 0$, but this cannot be true pointwise (but true in $L^1(0, L)$ only) because $\rho^{m+1}$ and $\rho^m$ are both discontinuous but not at the same point.
The same difficulty is found when Calculus of Variation is applied to (1)-(4); the meaning of the *little o* function in (8) and (10) is subtle and it is very easy to make a mistake.

### 2.3 The Stationary Case

Going back to (1)-(4) but in the stationary case, assume that we wish to solve

$$\min_v\{ \quad J(v) = \int_\Omega |B(W - W_d)|^2$$
$$\text{subject to } \nabla \cdot F(W) = 0, \quad n^T AW = v, \quad \int_\Omega w_1 = I\} \tag{18}$$

by a gradient method. At some stage the derivative of $J$ with respect to a parameter $s$ of $v$ will be needed and it will require to differentiate the stationary Euler equation with respect to $s$.

### 2.4 Derivatives for Euler's equations

All primes denoting derivatives with respect to $s$, the equation of conservation of mass could be differentiated by the chain rule

$$\nabla \cdot (\rho u) = 0 \quad \Rightarrow \quad \nabla \cdot (\rho' u + \rho u') = 0 \tag{19}$$

Let us show that this makes no sense! This is because the position of the shock $\Sigma$ varies with $s$ too and so a discontinous function like $\rho$ is the sum of a smooth part $\tilde{\rho}$ and a jump $[\rho]$:

$$\rho(x) = \tilde{\rho}(x) + [\rho]\mathbf{I}_{\Sigma^-} \tag{20}$$

where $\mathbf{I}_{\Sigma^-}$ is the indicator function of the domain before the shock (this representation is not unique). So when (20) is differentiated with respect to $s$, the derivative of an indicator function being a Dirac function, we obtain:

$$\rho'(x) = \tilde{\rho}'(x) + [\rho]x'_\Sigma \cdot n_\Sigma \delta_\Sigma(x) \tag{21}$$

where $x = x_\Sigma$ is the equation of $\Sigma$ and $n_\Sigma$ its normal. Plugging (21) in (19) gives terms like $[\rho]\delta_\Sigma u$ which make no sense because $u$ is also discontinuous at $\Sigma$ (no way to choose between $[\rho]u^-$ and $[\rho]u^+$ when they appear in an integral).
The only way to differentiate (19) correctly is to introduce the conservative variable $\nu = \rho u$ and write

$$\nabla \cdot \nu = 0 \quad \Rightarrow \quad \nabla \cdot \nu' = 0 \tag{22}$$

Similarly, the momentum equation,

$$\nabla \cdot (\rho u \otimes u) + \nabla p = 0 \tag{23}$$

must be rewritten in terms of products of variables where only one of them jumps:

$$\nabla \cdot (\frac{1}{\rho}\nu \otimes \nu) + \nabla p = 0 \tag{24}$$

In this form it is correct to write

$$\nabla \cdot (\frac{1}{\rho}(\nu' \otimes \nu + \nu \otimes \nu')) + \nabla \cdot ((\frac{1}{\rho})'\nu \otimes \nu) + \nabla p' = 0 \tag{25}$$

One must be careful not to expand $(\rho^{-1})'$ because the result would be illicit. On the other hand one can write

$$\nabla\cdot(\frac{1}{\rho}(\nu'\otimes\nu+\nu\otimes\nu'))-\nabla\cdot(\frac{\tilde{\rho}'}{\rho^2}\nu\otimes\nu)+\nabla\tilde{p}'+\nabla\cdot((\nu\otimes\nu[\frac{1}{\rho}]+[p])\vec{x}'\cdot n_\Sigma\delta_\Sigma)=0 \quad (26)$$

Finally the energy equation is rewritten as

$$\nabla\cdot(\nu(\frac{1}{\rho^2}\frac{\nu^2}{2}+\frac{\gamma}{\gamma-1}\frac{p}{\rho}))=0 \quad (27)$$

and its s-derivative is

$$\nabla\cdot(\nu'(\frac{1}{\rho^2}\frac{\nu^2}{2}+\frac{\gamma}{\gamma-1}\frac{p}{\rho})+\nu(\frac{1}{\rho^2}\nu\cdot\nu'+\frac{\gamma}{\gamma-1}\frac{p}{\rho})+\nu((\frac{1}{\rho^2})'\frac{\nu^2}{2}+\frac{\gamma}{\gamma-1}(\frac{p}{\rho})'))=0 \quad (28)$$

with

$$(\frac{1}{\rho^2})'=-2\frac{\tilde{\rho}'}{\rho^3}+[\frac{1}{\rho^2}]\vec{x}'\cdot n_\Sigma\delta_\Sigma \qquad (\frac{p}{\rho})'=\frac{\tilde{p}'\rho-p\tilde{\rho}'}{\rho^2}+[\frac{p}{\rho}]\vec{x}'\cdot n_\Sigma\delta_\Sigma \quad (29)$$

# 3 Justification in a Simple Case

Consider the case of a potential flow

$$u=\nabla\phi,\quad \nabla\cdot(\rho\nabla\phi)=0 \text{ in } \Omega \qquad \frac{\partial\phi}{\partial n}=g \text{ on } \Gamma:=\partial\Omega \quad (30)$$

Suppose that $\rho$ is known to be piecewise constant equal to $\rho^+$ or $\rho^-$ but the change from $\rho^-$ to $\rho^+$ happens across $\Sigma$ whose position is not known. We wish to identify $\Sigma$ from the knowledge of $\nabla\phi$ in a subdomain $D$ which does not intersect $\Sigma$. This will be done by solving

$$\min_\Sigma J(\rho)=\int_D|u_d-\nabla\phi|^2 \quad \text{subject to (30)} \quad (31)$$

In order to update $\Sigma$ so as to decrease $J$ by a gradient method we need to be able to compute the derivative of $J$ with respect to parameters $s$ defining $\Sigma$.
To do this we begin as usual:

$$J'=2\int_D(\nabla\phi-u_d)\nabla\phi' \quad (32)$$

Then we write (30) in mixed form with the conservation variable $V=\rho\nabla\phi$:

$$\nabla\cdot V=0,\quad \frac{1}{\rho}V-\nabla\phi=0 \quad (33)$$

and differentiate

$$\nabla\cdot V'=0,\quad \frac{1}{\rho}V'-\nabla\phi'+[\frac{1}{\rho}]V_n\vec{n}_\Sigma x'_\Sigma\cdot n_\Sigma\delta_\Sigma=0. \quad (34)$$

where $V_n$ means $V \cdot n$. Therefore, setting the adjoint state to be solution of

$$-\nabla \cdot (\rho \nabla q) = 2\mathbf{I}_D(\nabla \phi - u_d) \qquad \frac{\partial q}{\partial n}|_\Gamma = 0, \qquad Q = \rho \nabla q \tag{35}$$

we obtain

$$J' = 2\int_D (\nabla \phi - u_d)\nabla \phi' = \int_\Omega \rho \nabla q \nabla \phi' = \int_\Omega V' \nabla q + \int_\Sigma [\frac{1}{\rho}] V_n Q_n x'_\Sigma \cdot n_\Sigma$$
$$= \int_\Sigma [\frac{1}{\rho}](\rho u_n)(\rho q_n) x'_\Sigma \cdot n_\Sigma \tag{36}$$

This calculus has been justified mathematically in [1] for a similar problem on flow through porous media.

## 3.1 Numerical Simulation

The numerical implementation is done with `freefem++` [4]. To illustrate the theory we have solved the problem

$$-\nabla \cdot (\rho \nabla \phi) = 0 \text{ in } \Omega \qquad \phi|_\Gamma = xy \tag{37}$$

where $\Omega$ is the rectangle $(-5, 5) \times (-2.5, 2.5)$, $\rho$ is 6 inside an ellipse in the middle of the rectangle and 1 outside.

The discretisation is done with the finite element method on a mixed formulation of the problem by setting a system of equation for $\phi$ and $\Phi = \rho \nabla \phi$:

$$\int_\Omega (\frac{\Phi}{\rho} W + \phi \nabla \cdot W) = 0 \quad \forall W \in \mathcal{W} \qquad \int_\Omega w \nabla \cdot \Phi = 0 \quad \forall w \in L^2(\Omega) \tag{38}$$

where $\mathcal{W}$ is a subspace of the square integrable functions with square integrable divergence. These are approximated by piecewise linear discontinuous vector valued functions, continuous at the mid side nodes and piecewise constant functions respectively. Convergence of the numerical method on problems such as (35) is shown on the table below. The numerical solution with a mesh size $h = c\epsilon$ is compared with the $\epsilon$-divided difference of two numerical solutions of (33) on two geometries, the second one with $\Sigma$ moved by $|x'_\Sigma \cdot n_\Sigma| = \epsilon$

| $\epsilon$ | 0.1 | 0.05 | 0.025 | 0.0125 |
|---|---|---|---|---|
| $L^2$-error | 0.96 | 0.71 | 0.56 | 0.46 |

The data assimilation problem is (31) where $D$ is a disk on the right side of the domain and the discontinuity of $\rho$ occurs on the left side of the domain in a domain which is to be found. Such situation could occur when measurements are available on land and lacking in the ocean, such as shown on figure 3.1 with Scandinavia where a region of cold air in the ocean is to be identified.

The problem is simplified by taking only two parameters in the definition of the unknown shape:

$$x = -2 + (\sqrt{2} + r + s\cos t)\cos t, \quad y = (\sqrt{2} + r + s\cos t)\sin t \ \ t \in (0, 2\pi).$$

The gradient method is applied to $r$ and $s$ starting from $r = 0.8$ and $s = 0.4$. After 10 iterations

$$r^{10} = 0.120625 \ \ s^{10} = 0.01748 \ \ \frac{\partial J}{\partial r} = 0.00113 \ \ \frac{\partial J}{\partial s} = 0.00079 \ \ J = 0.0001516$$

while the exact solution is at $r = s = 0$.

Decreasing both $\epsilon$ and the mesh size gives convergence:

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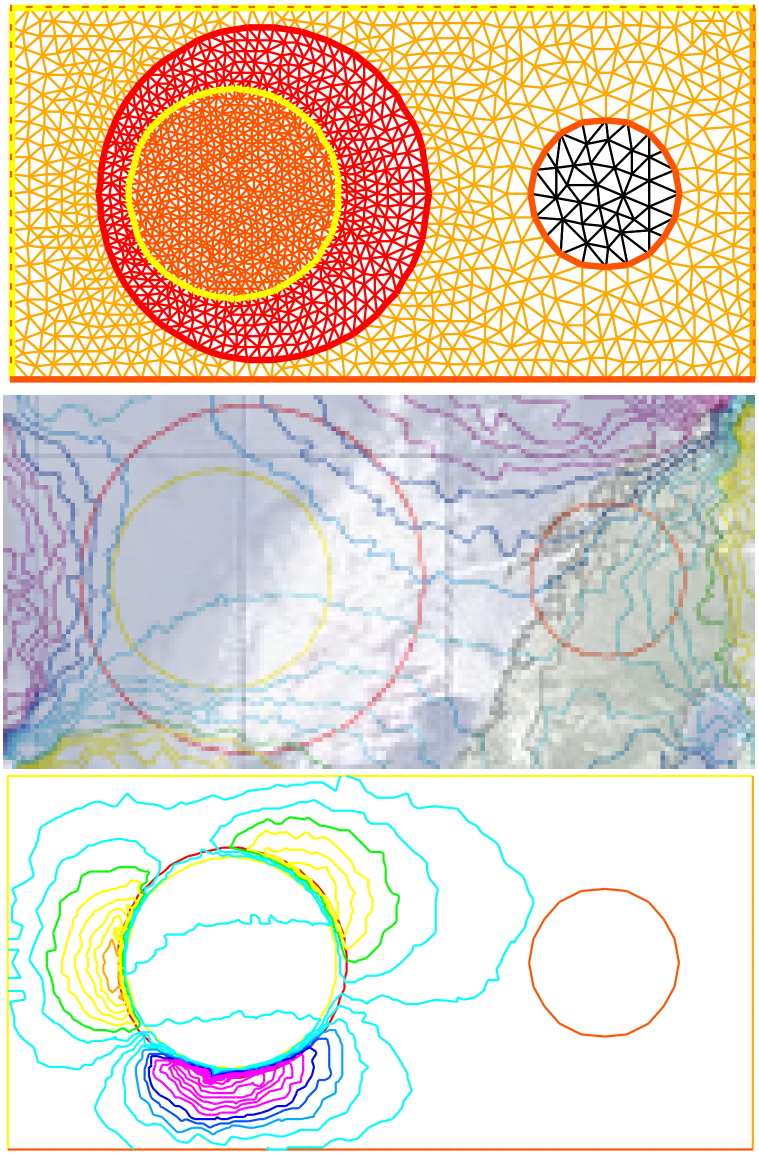

Figure 1: ***Top***: *The triangulation and the observation set (disk on the right), the initial guess (larger ellipse on the right) and the solution (smaller circle on the left).* ***Middle***: *Illustration of a possible meteorology application in the north sea west of Scandinavia where the density of air is found above the sea from data in the observation set (right) above the land. The figure shows also the level lines of the calculated velocity potential* $\phi$*.* ***Bottom***: *After 10 iterations the discontinuity curve has converged to a shape near to the analytical solution. The level line of the error are also shown (maximum error is about 10 per cent.)*