Variational approach to data assimilation: optimization aspects and adjoint method

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Objectives

- introduce data assimilation as an optimization problem
- discuss the different forms of the objective functions
- discuss their properties w.r.t. optimization
- introduce the adjoint technique for the computation of the gradient

Link with statistical methods: cf lectures by E. Cosme

Variational data assimilation algorithms, tangent and adjoint codes: cf lectures by M. Nodet and A. Vidard

Outline

Model problem

Two different available measurements of a single quantity. Which estimation of its true value ? $\longrightarrow$ least squares approach

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Example 2 obs $y_1 = 19°\text{C}$ and $y_2 = 21°\text{C}$ of the (unknown) present temperature x.

- Let $J(x) = \frac{1}{2}\left[(x - y_1)^2 + (x - y_2)^2\right]$
- $\text{Min}_x \; J(x) \quad \longrightarrow \; \hat{x} = \dfrac{y_1 + y_2}{2} = 20°\text{C}$

Model problem

Observation operator If $\neq$ units: $y_1 = 66.2°\text{F}$ and $y_2 = 69.8°\text{F}$

- Let $H(x) = \dfrac{9}{5}x + 32$
- Let $J(x) = \dfrac{1}{2}\left[(H(x) - y_1)^2 + (H(x) - y_2)^2\right]$
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Drawback # 1: *if observation units are inhomogeneous*
$y_1 = 66.2°F$ and $y_2 = 21°C$

- $J(x) = \frac{1}{2}\left[(H(x) - y_1)^2 + (x - y_2)^2\right] \quad \longrightarrow \hat{x} = 19.47°C$!!

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Drawback # 2: *if observation accuracies are inhomogeneous*

If y_1 is twice more accurate than y_2, one should obtain $\hat{x} = \dfrac{2y_1 + y_2}{3} = 19.67°C$

$\longrightarrow$ J should be $J(x) = \frac{1}{2}\left[\left(\frac{x - y_1}{1/2}\right)^2 + \left(\frac{x - y_2}{1}\right)^2\right]$

Model problem

General form

$$\text{Minimize } J(x) = \frac{1}{2}\left[\frac{(H_1(x) - y_1)^2}{\sigma_1^2} + \frac{(H_2(x) - y_2)^2}{\sigma_2^2}\right]$$

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If $H_1 = H_2 = Id$: $$J(x) = \frac{1}{2}\,\frac{(x-y_1)^2}{\sigma_1^2} + \frac{1}{2}\,\frac{(x-y_2)^2}{\sigma_2^2}$$

which leads to $$\hat{x} = \frac{\dfrac{1}{\sigma_1^2}\,y_1 + \dfrac{1}{\sigma_2^2}\,y_2}{\dfrac{1}{\sigma_1^2} + \dfrac{1}{\sigma_2^2}}$$ *(weighted average)*

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Remark: $\underbrace{J''(\hat{x})}_{\text{convexity}} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} = \underbrace{[Var(\hat{x})]^{-1}}_{\text{accuracy}}$ *(cf BLUE)*

Model problem

Alternative formulation: background + observation If one considers that y_1 is a prior (or *background*) estimate x_b for x, and $y_2 = y$ is an independent observation, then:

$$J(x) = \underbrace{\frac{1}{2}\frac{(x - x_b)^2}{\sigma_b^2}}_{J_b} + \underbrace{\frac{1}{2}\frac{(x - y)^2}{\sigma_o^2}}_{J_o}$$

and

$$\hat{x} = \frac{\dfrac{1}{\sigma_b^2}x_b + \dfrac{1}{\sigma_o^2}y}{\dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}} = x_b + \underbrace{\frac{\sigma_b^2}{\sigma_b^2 + \sigma_o^2}}_{\text{gain}} \underbrace{(y - x_b)}_{\text{innovation}}$$

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Generalization: arbitrary number of unknowns and observations

To be estimated: $\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbf{R}^n$

Observations: $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_p \end{pmatrix} \in \mathbf{R}^p$

Observation operator: $\mathbf{y} \equiv H(\mathbf{x})$, with $H : \mathbf{R}^n \longrightarrow \mathbf{R}^p$

Generalization: arbitrary number of unknowns and observations

A simple example of observation operator

If $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$ and $\mathbf{y} = \begin{pmatrix} \text{an observation of } \frac{x_1+x_2}{2} \\ \text{an observation of } x_4 \end{pmatrix}$

then $H(\mathbf{x}) = \mathbf{H}\mathbf{x}$ with $\mathbf{H} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

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Cost function: $J(\mathbf{x}) = \frac{1}{2} \|H(\mathbf{x}) - \mathbf{y}\|^2$ with $\|.\|$ to be chosen.

Reminder: norms and scalar products

$$\mathbf{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \in \mathbf{R}^n$$

- Euclidian norm: $\|\mathbf{u}\|^2 = \mathbf{u}^T\mathbf{u} = \sum_{i=1}^{n} u_i^2$

  Associated scalar product: $(\mathbf{u},\mathbf{v}) = \mathbf{u}^T\mathbf{v} = \sum_{i=1}^{n} u_i v_i$

- Generalized norm: let $\mathbf{M}$ a symmetric positive definite matrix

  $\mathbf{M}$-norm: $\|\mathbf{u}\|_{\mathbf{M}}^2 = \mathbf{u}^T\mathbf{M}\ \mathbf{u} = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}\, u_i u_j$

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(Intuitive) necessary (but not sufficient) condition for the existence of a unique minimum:

$$p \geq n$$

Formalism "background value + new observations"

$$\mathbf{Y} = \begin{pmatrix} \mathbf{x}_b \\ \mathbf{y} \end{pmatrix} \begin{matrix} \longleftarrow \text{background} \\ \longleftarrow \text{new obs} \end{matrix}$$

The cost function becomes:

$$J(\mathbf{x}) \quad = \quad \underbrace{\frac{1}{2}\,\|\mathbf{x}-\mathbf{x}_b\|_b^2}_{J_b} \quad + \quad \underbrace{\frac{1}{2}\,\|H(\mathbf{x})-\mathbf{y}\|_o^2}_{J_o}$$

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$$= (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + (H(\mathbf{x}) - \mathbf{y})^T \mathbf{R}^{-1} (H(\mathbf{x}) - \mathbf{y})$$

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The necessary condition for the existence of a unique minimum ($p \geq n$) is automatically fulfilled.

If the problem is time dependent

- Observations are distributed in time: $\mathbf{y} = \mathbf{y}(t)$.
- The observation cost function becomes:

$$J_o(\mathbf{x}) = \frac{1}{2} \sum_{i=0}^{N} \| H_i(\mathbf{x}(t_i)) - \mathbf{y}(t_i) \|_o^2$$

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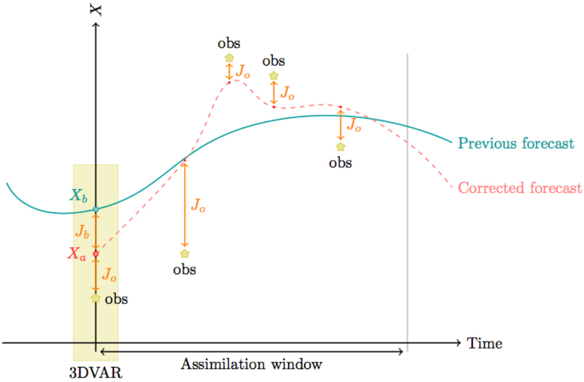
- There is a model describing the evolution of $\mathbf{x}$: $\dfrac{d\mathbf{x}}{dt} = M(\mathbf{x})$ with $\mathbf{x}(t=0) = \mathbf{x}_0$. Then J is often no longer minimized w.r.t. $\mathbf{x}$, but w.r.t. $\mathbf{x}_0$ only, or to some other parameters.

$$J_o(\mathbf{x}_0) = \frac{1}{2} \sum_{i=0}^{N} \| H_i(\mathbf{x}(t_i)) - \mathbf{y}(t_i) \|_o^2 = \frac{1}{2} \sum_{i=0}^{N} \| H_i(M_{0 \to t_i}(\mathbf{x}_0)) - \mathbf{y}(t_i) \|_o^2$$

If the problem is time dependent



$$J(\mathbf{x}_0) = \underbrace{\frac{1}{2}\|\mathbf{x}_0 - \mathbf{x}_0^b\|_b^2}_{\text{background term } J_b} + \underbrace{\frac{1}{2}\sum_{i=0}^{N}\|H_i(\mathbf{x}(t_i)) - \mathbf{y}(t_i)\|_o^2}_{\text{observation term } J_o}$$

Uniqueness of the minimum ?

$$J(\mathbf{x}_0) = J_b(\mathbf{x}_0) + J_o(\mathbf{x}_0) = \frac{1}{2}\,\|\mathbf{x}_0 - \mathbf{x}_b\|_b^2 + \frac{1}{2}\sum_{i=0}^{N}\|H_i(M_{0\to t_i}(\mathbf{x}_0)) - \mathbf{y}(t_i)\|_o^2$$

- If H and M are linear then J_o is quadratic.

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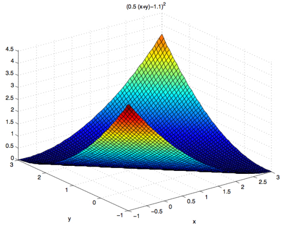
- If H and M are linear then J_o is quadratic.
- However it generally does not have a unique minimum, since the number of observations is generally less than the size of $\mathbf{x}_0$ (the problem is underdetermined: $p < n$).

Example: let $(x_1^t, x_2^t) = (1, 1)$ and $y = 1.1$ an observation of $\frac{1}{2}(x_1 + x_2)$.

$$J_o(x_1, x_2) = \frac{1}{2}\left(\frac{x_1 + x_2}{2} - 1.1\right)^2$$



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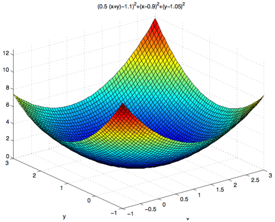
- If H and M are linear then J_o is quadratic.
- However it generally does not have a unique minimum, since the number of observations is generally less than the size of $\mathbf{x}_0$ (the problem is underdetermined).
- Adding J_b makes the problem of minimizing $J = J_o + J_b$ well posed.

Example: let $(x_1^t, x_2^t) = (1, 1)$ and $y = 1.1$ an observation of $\frac{1}{2}(x_1 + x_2)$. Let $(x_1^b, x_2^b) = (0.9, 1.05)$

$$J(x_1, x_2) = \underbrace{\frac{1}{2}\left(\frac{x_1 + x_2}{2} - 1.1\right)^2}_{J_o} + \underbrace{\frac{1}{2}\left[(x_1 - 0.9)^2 + (x_2 - 1.05)^2\right]}_{J_b}$$

$$\longrightarrow (x_1^*, x_2^*) = (0.94166..., 1.09166...)$$



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- If H and/or M are nonlinear then J_o is no longer quadratic.

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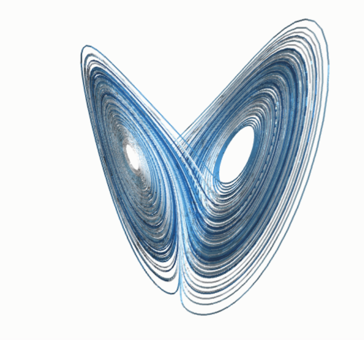
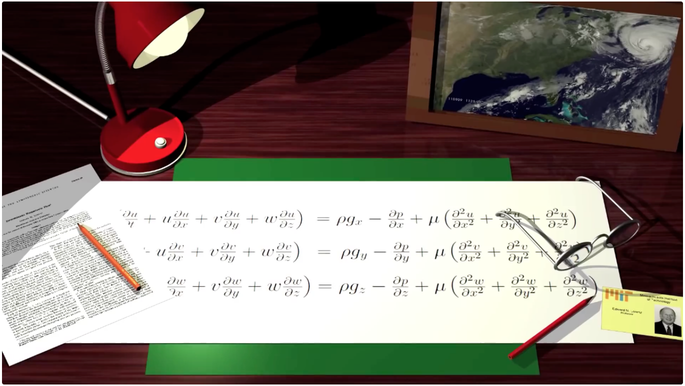
  Example: the Lorenz system (1963)

$$\begin{cases} \dfrac{dx}{dt} = \alpha(y - x) \\ \dfrac{dy}{dt} = \beta x - y - xz \\ \dfrac{dz}{dt} = -\gamma z + xy \end{cases}$$





http://www.chaos-math.org

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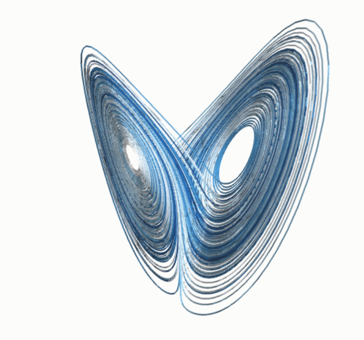

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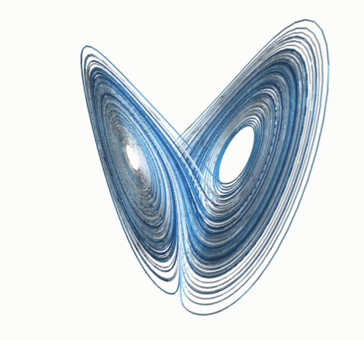

$$J_o(y_0) = \frac{1}{2}\sum_{i=0}^{N}\left(x(t_i) - x_{\mathrm{obs}}(t_i)\right)^2\ dt$$

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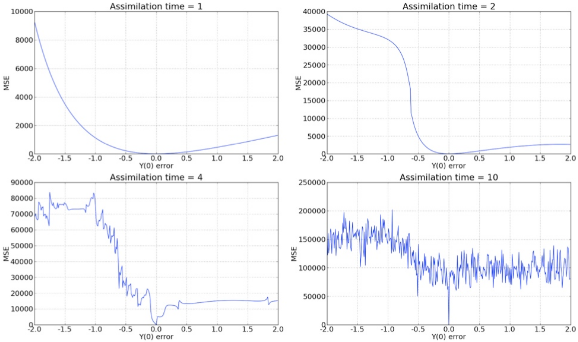

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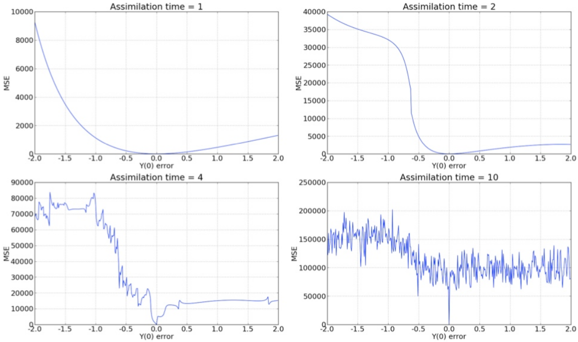

- Adding J_b makes it “more quadratic” (J_b is a regularization term), but $J = J_o + J_b$ may however have several (local) minima.

A fundamental remark before going into minimization aspects

Once J is defined (i.e. once all the ingredients are chosen: control variables, norms, observations. . .), the problem is entirely defined. Hence its solution.

The “physical” (i.e. the most important) part of data assimilation lies in the definition of J.

The rest of the job, i.e. minimizing J, is “only” technical work.

Outline

Reminder: norms and scalar products

$$\mathbf{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \in \mathbf{R}^n$$

- Euclidian norm: $\|\mathbf{u}\|^2 = \mathbf{u}^T\mathbf{u} = \sum_{i=1}^{n} u_i^2$

  Associated scalar product: $(\mathbf{u}, \mathbf{v}) = \mathbf{u}^T\mathbf{v} = \sum_{i=1}^{n} u_i v_i$

- Generalized norm: let $\mathbf{M}$ a symmetric positive definite matrix

  $\mathbf{M}$-norm: $\|\mathbf{u}\|_{\mathbf{M}}^2 = \mathbf{u}^T\mathbf{M}\,\mathbf{u} = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}\, u_i u_j$

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Reminder: norms and scalar products

$$u: \begin{array}{ccc} \Omega \subset \mathbf{R}^n & \longrightarrow & \mathbf{R} \\ \mathbf{x} & \longrightarrow & u(\mathbf{x}) \end{array} \qquad u \in L^2(\Omega)$$

- Euclidian (or L^2) norm: $\|u\|^2 = \int_\Omega u^2(\mathbf{x})\, d\mathbf{x}$

  Associated scalar product: $(u, v) = \int_\Omega u(\mathbf{x})\, v(\mathbf{x})\, d\mathbf{x}$

Reminder: derivatives and gradients

$f : E \longrightarrow \mathbf{R}$ (E being of finite or infinite dimension)

- Directional (or Gâteaux) derivative of f at point $x \in E$ in direction $d \in E$:

$$\frac{\partial f}{\partial d}(x) = \hat{f}[x](d) = \lim_{\alpha \to 0} \frac{f(x + \alpha d) - f(x)}{\alpha}$$

Example: partial derivatives $\dfrac{\partial f}{\partial x_i}$ are directional derivatives in the direction of the members of the canonical basis ($d = e_i$)

Reminder: derivatives and gradients

$f : E \longrightarrow \mathbf{R}$ (E being of finite or infinite dimension)

- Gradient (or Fréchet derivative): E being an Hilbert space, f is Fréchet differentiable at point $x \in E$ iff

$$\exists p \in E \text{ such that } f(x+h) = f(x) + (p,h) + o(\|h\|) \quad \forall h \in E$$

  p is the derivative or gradient of f at point x, denoted $f'(x)$ or $\nabla f(x)$.

- $h \rightarrow (p(x), h)$ is a linear function, called differential function or tangent linear function or Jacobian of f at point x

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- $h \to (p(x), h)$ is a linear function, called differential function or tangent linear function or Jacobian of f at point x

- Important (obvious) relationship: $\dfrac{\partial f}{\partial d}(x) = (\nabla f(x), d)$

Minimum of a quadratic function in finite dimension

Theorem: Generalized (or Moore-Penrose) inverse

Let $\mathbf{M}$ a $p \times n$ matrix, with rank n, and $\mathbf{b} \in \mathbf{R}^p$. *(hence $p \geq n$)*

Let $J(\mathbf{x}) = \|\mathbf{M}\mathbf{x} - \mathbf{b}\|^2 = (\mathbf{M}\mathbf{x} - \mathbf{b})^T(\mathbf{M}\mathbf{x} - \mathbf{b})$.

J is minimum for $\hat{\mathbf{x}} = \mathbf{M}^+\mathbf{b}$, where $\mathbf{M}^+ = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$ (generalized, or Moore-Penrose, inverse).

Minimum of a quadratic function in finite dimension

Theorem: Generalized (or Moore-Penrose) inverse

Let $\mathbf{M}$ a $p \times n$ matrix, with rank n, and $\mathbf{b} \in \mathbf{R}^p$. *(hence $p \geq n$)*

Let $J(\mathbf{x}) = \|\mathbf{Mx} - \mathbf{b}\|^2 = (\mathbf{Mx} - \mathbf{b})^T(\mathbf{Mx} - \mathbf{b})$.

J is minimum for $\hat{\mathbf{x}} = \mathbf{M}^+\mathbf{b}$, where $\mathbf{M}^+ = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$
(generalized, or Moore-Penrose, inverse).

Corollary: with a generalized norm

Let $\mathbf{N}$ a $p \times p$ symmetric definite positive matrix.

Let $J_1(\mathbf{x}) = \|\mathbf{Mx} - \mathbf{b}\|_N^2 = (\mathbf{Mx} - \mathbf{b})^T\mathbf{N}\,(\mathbf{Mx} - \mathbf{b})$.

J_1 is minimum for $\hat{\mathbf{x}} = (\mathbf{M}^T\mathbf{N}\mathbf{M})^{-1}\mathbf{M}^T\mathbf{N}\,\mathbf{b}$.

Link with data assimilation

This gives the solution to the problem

$$\min_{\mathbf{x}\in\mathbf{R}^n} J_o(\mathbf{x}) = \frac{1}{2}\,\|\mathbf{H}\mathbf{x}-\mathbf{y}\|_o^2$$

in the case of a linear observation operator $\mathbf{H}$.

$$J_o(\mathbf{x}) = \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y}) \longrightarrow \hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\,\mathbf{y}$$

Link with data assimilation

Similarly:

$$
\begin{aligned}
J(\mathbf{x}) &= J_b(\mathbf{x}) + J_o(\mathbf{x}) \\
&= \frac{1}{2}\,\|\mathbf{x}-\mathbf{x}_b\|_b^2 \quad + \quad \frac{1}{2}\,\|H(\mathbf{x})-\mathbf{y}\|_o^2 \\
&= \frac{1}{2}\,(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}\,(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y}) \\
&= (\mathbf{M}\mathbf{x}-\mathbf{b})^T\mathbf{N}\,(\mathbf{M}\mathbf{x}-\mathbf{b}) = \|\mathbf{M}\mathbf{x}-\mathbf{b}\|_{\mathbf{N}}^2
\end{aligned}
$$

with $\mathbf{M} = \begin{pmatrix} \mathbf{I}_n \\ \mathbf{H} \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} \mathbf{x}_b \\ \mathbf{y} \end{pmatrix} \quad \mathbf{N} = \begin{pmatrix} \mathbf{B}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}^{-1} \end{pmatrix}$

Link with data assimilation

Similarly:

$$\begin{aligned} J(\mathbf{x}) &= J_b(\mathbf{x}) + J_o(\mathbf{x}) \\ &= \frac{1}{2}\,\|\mathbf{x}-\mathbf{x}_b\|_b^2 \quad + \quad \frac{1}{2}\,\|H(\mathbf{x})-\mathbf{y}\|_o^2 \\ &= \frac{1}{2}\,(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}\,(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y}) \\ &= (\mathbf{M}\mathbf{x}-\mathbf{b})^T\mathbf{N}\,(\mathbf{M}\mathbf{x}-\mathbf{b}) = \|\mathbf{M}\mathbf{x}-\mathbf{b}\|_{\mathbf{N}}^2 \end{aligned}$$

with $\mathbf{M} = \begin{pmatrix} \mathbf{I}_n \\ \mathbf{H} \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} \mathbf{x}_b \\ \mathbf{y} \end{pmatrix} \quad \mathbf{N} = \begin{pmatrix} \mathbf{B}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}^{-1} \end{pmatrix}$

which leads to

$$\hat{\mathbf{x}} = \mathbf{x}_b + \underbrace{(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}}_{\text{gain matrix}} \quad \underbrace{(\mathbf{y}-\mathbf{H}\mathbf{x}_b)}_{\text{innovation vector}}$$

Remark: The gain matrix also reads $\mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$

(Sherman-Morrison-Woodbury formula)

Link with data assimilation

Remark

$$\underbrace{\text{Hess}(J)}_{\text{convexity}} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} = \underbrace{[Cov(\hat{\mathbf{x}})]^{-1}}_{\text{accuracy}}$$

(cf BLUE)

Remark

Given the size of n and p, it is generally impossible to handle explicitly $\mathbf{H}$, $\mathbf{B}$ and $\mathbf{R}$. So the direct computation of the gain matrix is impossible.

► even in the linear case (for which we have an explicit expression for $\hat{\mathbf{x}}$), the computation of $\hat{\mathbf{x}}$ is performed using an optimization algorithm.

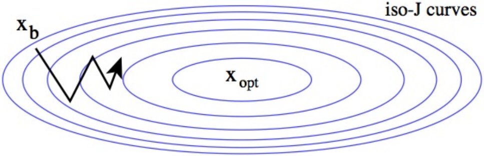
Outline

Outline

Descent methods

Descent methods for minimizing the cost function require the knowledge of (an estimate of) its gradient.

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \, \mathbf{d}_k$$



$$\text{with } \mathbf{d}_k = \begin{cases} -\nabla J(\mathbf{x}_k) & \text{gradient method} \\ -\left[\text{Hess}(J)(\mathbf{x}_k)\right]^{-1} \nabla J(\mathbf{x}_k) & \text{Newton method} \\ -\mathbf{B}_k \nabla J(\mathbf{x}_k) & \text{quasi-Newton methods (BFGS, \ldots)} \\ -\nabla J(\mathbf{x}_k) + \frac{\|\nabla J(\mathbf{x}_k)\|^2}{\|\nabla J(\mathbf{x}_{k-1})\|^2} d_{k-1} & \text{conjugate gradient} \\ \ldots & \ldots \end{cases}$$

The computation of $\nabla J(\mathbf{x}_k)$ may be difficult if the dependency of J with regard to the control variable $\mathbf{x}$ is not direct.

Example:

- $u(x)$ solution of an ODE
- K a coefficient of this ODE
- $u^{\text{obs}}(x)$ an observation of $u(x)$
- $J(K) = \dfrac{1}{2} \left\| u(x) - u^{\text{obs}}(x) \right\|^2$

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- $u^{\text{obs}}(x)$ an observation of $u(x)$
- $J(K) = \frac{1}{2} \left\| u(x) - u^{\text{obs}}(x) \right\|^2$

$$\hat{J}[K](k) = (\nabla J(K), k) = < \hat{u}, u - u^{\text{obs}} >$$

$$\text{with } \hat{u} = \frac{\partial u}{\partial k}(K) = \lim_{\alpha \to 0} \frac{u_{K+\alpha k} - u_K}{\alpha}$$

It is often difficult (or even impossible) to obtain the gradient through the computation of growth rates.

Example:

$$\begin{cases} \dfrac{d\mathbf{x}(t))}{dt} = M(\mathbf{x}(t)) \quad t \in [0, T] \\ \mathbf{x}(t=0) = \mathbf{u} \end{cases} \qquad \text{with } \mathbf{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}$$

$$J(\mathbf{u}) = \frac{1}{2} \int_0^T \|\mathbf{x}(t) - \mathbf{x}^{obs}(t)\|^2 \qquad \longrightarrow \text{ requires one model run}$$

$$\nabla J(\mathbf{u}) = \begin{pmatrix} \dfrac{\partial J}{\partial u_1}(\mathbf{u}) \\ \vdots \\ \dfrac{\partial J}{\partial u_N}(\mathbf{u}) \end{pmatrix} \simeq \begin{pmatrix} \left[J(\mathbf{u} + \alpha\, \mathbf{e}_1) - J(\mathbf{u})\right]/\alpha \\ \vdots \\ \left[J(\mathbf{u} + \alpha\, \mathbf{e}_N) - J(\mathbf{u})\right]/\alpha \end{pmatrix}$$

$\longrightarrow N+1$ model runs

In most actual applications, $N = [\mathbf{u}]$ is large (or even very large: e.g. $N = \mathcal{O}(10^8 - 10^9)$ in meteorology) $\longrightarrow$ this method cannot be used.

Alternatively, the adjoint method provides a very efficient way to compute ∇J.

In most actual applications, $N = [\mathbf{u}]$ is large (or even very large: e.g. $N = \mathcal{O}(10^8 - 10^9)$ in meteorology) $\longrightarrow$ this method cannot be used.

Alternatively, the adjoint method provides a very efficient way to compute ∇J.

On the contrary, do not forget that, if the size of the control variable is very small ($< 10 - 20$), ∇J can be easily estimated by the computation of growth rates.

Reminder: adjoint operator

- General definition:
  Let $\mathcal{X}$ and $\mathcal{Y}$ two prehilbertian spaces (i.e. vector spaces with scalar products).
  Let $A : \mathcal{X} \longrightarrow \mathcal{Y}$ an operator.
  The adjoint operator $A^* : \mathcal{Y} \longrightarrow \mathcal{X}$ is defined by:

$$\forall x \in \mathcal{X}, \forall y \in \mathcal{Y}, \qquad < Ax, y >_{\mathcal{Y}} = < x, A^* y >_{\mathcal{X}}$$

  In the case where $\mathcal{X}$ and $\mathcal{Y}$ are Hilbert spaces and A is linear, then A^* always exists (and is unique).

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- Adjoint operator in finite dimension:
  $A : \mathbf{R}^n \longrightarrow \mathbf{R}^m$ a linear operator (i.e. a matrix). Then its adjoint operator A^* (w.r. to Euclidian norms) is A^T.

Outline

The continuous case

The assimilation problem

- $$\left\{ \begin{array}{ll} -u''(x) + c(x)\, u'(x) = f(x) & \quad x \in]0,1[\\ u(0) = u(1) = 0 \end{array} \right. \qquad f \in L^2(]0,1[)$$
- $c(x)$ is unknown
- $u^{\text{obs}}(x)$ an observation of $u(x)$
- Cost function: $J(c) = \dfrac{1}{2} \displaystyle\int_0^1 \left(u(x) - u^{\text{obs}}(x) \right)^2 \, dx$

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$\nabla J \rightarrow$ Gâteaux-derivative: $\hat{J}[c](\delta c) = < \nabla J(c), \delta c >$

$$\hat{J}[c](\delta c) = \int_0^1 \hat{u}(x)\left(u(x) - u^{\text{obs}}(x)\right)\, dx \quad \text{with } \hat{u} = \lim_{\alpha \to 0} \frac{u_{c+\alpha\delta c} - u_c}{\alpha}$$

What is the equation satisfied by $\hat{u}$?

$$\begin{cases} -\hat{u}''(x) + c(x)\,\hat{u}'(x) = -\delta c(x)\,u'(x) & x \in]0,1[\\ \hat{u}(0) = \hat{u}(1) = 0 & \end{cases}$$

tangent linear model

$$\left\{ \begin{array}{ll} -\hat{u}''(x) + c(x)\,\hat{u}'(x) = -\delta c(x)\,u'(x) & x \in]0,1[\\ \hat{u}(0) = \hat{u}(1) = 0 & \end{array} \right.$$ tangent linear model

Going back to $\hat{J}$: scalar product of the TLM with a variable p

$$-\int_0^1 \hat{u}''p + \int_0^1 c\,\hat{u}'p = -\int_0^1 \delta c\,u'p$$

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Integration by parts:

$$\int_0^1 \hat{u}\,(-p'' - (c\,p)') = \hat{u}'(1)p(1) - \hat{u}'(0)p(0) - \int_0^1 \delta c\,u'p$$

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adjoint model

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Then $\nabla J(c(x)) = -u'(x)\,p(x)$

Remark

Formally, we just made

$$(TLM(\hat{u}), p) = (\hat{u}, TLM^*(p))$$

We indeed computed the adjoint of the tangent linear model.

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Actual calculations

- Solve for the direct model

$$\begin{cases} -u''(x) + c(x)\,u'(x) = f(x) & x \in]0,1[\\ u(0) = u(1) = 0 \end{cases}$$

- Then solve for the adjoint model

$$\begin{cases} -p''(x) - (c(x)\,p(x))' = u(x) - u^{\text{obs}}(x) & x \in]0,1[\\ p(0) = p(1) = 0 \end{cases}$$

- Hence the gradient: $\nabla J(c(x)) = -u'(x)\,p(x)$

The discrete case

Model

$$\begin{cases} -u''(x) + c(x)\, u'(x) = f(x) & x \in]0,1[\\ u(0) = u(1) = 0 \end{cases}$$

$$\longrightarrow \begin{cases} -\dfrac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + c_i \, \dfrac{u_{i+1} - u_i}{h} = f_i & i = 1 \ldots N \\ u_0 = u_{N+1} = 0 \end{cases}$$

Cost function

$$J(c) = \frac{1}{2} \int_0^1 \Big(u(x) - u^{\text{obs}}(x) \Big)^2 \, dx \qquad \longrightarrow \frac{1}{2} \sum_{i=1}^{N} \Big(u_i - u_i^{\text{obs}} \Big)^2$$

Gâteaux derivative:

$$\hat{J}[c](\delta c) = \int_0^1 \hat{u}(x) \Big(u(x) - u^{\text{obs}}(x) \Big) \, dx \qquad \longrightarrow \sum_{i=1}^{N} \hat{u}_i \, \Big(u_i - u_i^{\text{obs}} \Big)$$

Tangent linear model

$$\begin{cases} -\hat{u}''(x) + c(x)\,\hat{u}'(x) = -\delta c(x)\,u'(x) & x \in]0,1[\\ \hat{u}(0) = \hat{u}(1) = 0 \end{cases}$$

$$\begin{cases} -\dfrac{\hat{u}_{i+1} - 2\hat{u}_i + \hat{u}_{i-1}}{h^2} + c_i\,\dfrac{\hat{u}_{i+1} - \hat{u}_i}{h} = -\delta c_i\,\dfrac{u_{i+1} - u_i}{h} & i = 1 \dots N \\ \hat{u}_0 = \hat{u}_{N+1} = 0 \end{cases}$$

Adjoint model

$$\begin{cases} -p''(x) - (c(x)\,p(x))' = u(x) - u^{\text{obs}}(x) & x \in]0,1[\\ p(0) = p(1) = 0 \end{cases}$$

$$\begin{cases} -\dfrac{p_{i+1} - 2p_i + p_{i-1}}{h^2} - \dfrac{c_i\,p_i - c_{i-1}p_{i-1}}{h} = u_i - u_i^{\text{obs}} & i = 1 \dots N \\ p_0 = p_{N+1} = 0 \end{cases}$$

Gradient

$$\nabla J(c(x)) = -u'(x)\,p(x) \longrightarrow \begin{pmatrix} \vdots \\ -p_i\,\dfrac{u_{i+1} - u_i}{h} \\ \vdots \end{pmatrix}$$

Remark: with matrix notations

What we do when determining the adjoint model is simply transposing the matrix which defines the tangent linear model

$$(\mathbf{M}\hat{\mathbf{U}}, \mathbf{P}) = (\hat{\mathbf{U}}, \mathbf{M}^T \mathbf{P})$$

In the preceding example:

$$\mathbf{M}\hat{\mathbf{U}} = \mathbf{F} \quad \text{with } \mathbf{M} = \begin{bmatrix} 2\alpha - \beta_1 & -\alpha + \beta_1 & 0 & \cdots & 0 \\ -\alpha & 2\alpha - \beta_2 & -\alpha + \beta_2 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & -\alpha & 2\alpha - \beta_{N-1} & -\alpha + \beta_{N-1} \\ 0 & \cdots & 0 & -\alpha & 2\alpha - \beta_N \end{bmatrix}$$

$\alpha = 1/h^2$, $\beta_i = c_i/h$

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$\alpha = 1/h^2$, $\beta_i = c_i/h$

But **M** is generally not explicitly built in actual complex models...

Outline

Control of the coefficient of a 1-D diffusion equation

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial}{\partial x}\left(K(x)\dfrac{\partial u}{\partial x}\right) = f(x,t) \qquad x \in]0,L[,\, t \in]0,T[\\ u(0,t) = u(L,t) = 0 \quad t \in [0,T] \\ u(x,0) = u_0(x) \quad x \in [0,L] \end{cases}$$

- $K(x)$ is unknown
- $u^{\text{obs}}(x,t)$ an available observation of $u(x,t)$

$$\text{Minimize } J(K(x)) = \frac{1}{2}\int_0^T \int_0^L \left(u(x,t) - u^{\text{obs}}(x,t)\right)^2 \, dx\, dt$$

Gâteaux derivative

$$\hat{J}[K](k) = \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{\text{obs}}(x,t)\right)\, dx\, dt$$

Gâteaux derivative

$$\hat{J}[K](k) = \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{obs}(x,t)\right)\, dx\, dt$$

Tangent linear model

$$\left\{ \begin{array}{l} \dfrac{\partial \hat{u}}{\partial t} - \dfrac{\partial}{\partial x}\left(K(x)\dfrac{\partial \hat{u}}{\partial x}\right) = \dfrac{\partial}{\partial x}\left(k(x)\dfrac{\partial u}{\partial x}\right) \qquad x \in]0,L[,\ t \in]0,T[\\ \hat{u}(0,t) = \hat{u}(L,t) = 0 \qquad t \in [0,T] \\ \hat{u}(x,0) = 0 \qquad x \in [0,L] \end{array} \right.$$

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$$\hat{J}[K](k) = \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{\text{obs}}(x,t)\right)\, dx\, dt$$

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Adjoint model

$$\begin{cases} \dfrac{\partial p}{\partial t} + \dfrac{\partial}{\partial x}\left(K(x)\dfrac{\partial p}{\partial x}\right) = u - u^{\text{obs}} & x \in]0,L[,\ t \in]0,T[\\ p(0,t) = p(L,t) = 0 \qquad t \in [0,T] \\ p(x,T) = 0 \quad x \in [0,L] \quad \text{final condition !!} \rightarrow \text{backward integration} \end{cases}$$

Gâteaux derivative of J

$$\begin{aligned}\hat{J}[K](k) &= \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{\text{obs}}(x,t)\right)\, dx\, dt \\ &= \int_0^T \int_0^L k(x) \frac{\partial u}{\partial x} \frac{\partial p}{\partial x}\, dx\, dt\end{aligned}$$

Gradient of J

$$\nabla J = \int_0^T \frac{\partial u}{\partial x}(.,t) \frac{\partial p}{\partial x}(.,t)\, dt \qquad \text{function of } x$$

Discrete version:

same as for the preceding ODE, but with $\displaystyle\sum_{n=0}^{N}\sum_{i=1}^{I} u_i^n$

Matrix interpretation: $\mathbf{M}$ is much more complex than previously !!

Outline

General formal derivation

- **Model** $\begin{cases} \dfrac{dX(x,t)}{dt} = M(X(x,t)) \quad (x,t) \in \Omega \times [0,T] \\ X(x,0) = U(x) \end{cases}$
- **Observations** Y with observation operator H: $H(X) \equiv Y$
- **Cost function** $J(U) = \dfrac{1}{2} \displaystyle\int_0^T \|H(X) - Y\|^2$

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- **Observations** Y with observation operator H: $H(X) \equiv Y$
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Gâteaux derivative of J

$$\hat{J}[U](u) = \int_0^T < \hat{X}, \mathbf{H}^*(HX - Y) > \quad \text{with } \hat{X} = \lim_{\alpha \to 0} \frac{X_{U+\alpha u} - X_U}{\alpha}$$

where $\mathbf{H}^*$ is the adjoint of $\mathbf{H}$, the tangent linear operator of H.

Tangent linear model

$$\left\{ \begin{array}{l} \dfrac{d\hat{X}(x,t)}{dt} = \mathbf{M}(\hat{X}) \quad (x,t) \in \Omega \times [0,T] \\ \hat{X}(x,0) = u(x) \end{array} \right.$$

where $\mathbf{M}$ is the tangent linear operator of M.

Tangent linear model

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where **M** is the tangent linear operator of M.

Adjoint model

$$\begin{cases} \dfrac{dP(x,t)}{dt} + \mathbf{M}^*(P) = \mathbf{H}^*(HX - Y) \quad (x,t) \in \Omega \times [0,T] \\ P(x,T) = 0 \qquad \text{backward integration} \end{cases}$$

Tangent linear model

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where **M** is the tangent linear operator of M.

Adjoint model

$$\begin{cases} \dfrac{dP(x,t)}{dt} + \mathbf{M}^*(P) = \mathbf{H}^*(HX - Y) & (x,t) \in \Omega \times [0,T] \\ P(x,T) = 0 & \text{backward integration} \end{cases}$$

Gradient

$$\nabla J(U) = -P(.,0) \quad \text{function of } x$$

Example: the Burgers' equation

The assimilation problem

$$\left\{\begin{array}{ll} \dfrac{\partial u}{\partial t} + u\,\dfrac{\partial u}{\partial x} - \nu\,\dfrac{\partial^2 u}{\partial x^2} = f & x \in]0, L[,\ t \in [0, T] \\ u(0,t) = \psi_1(t) & t \in [0, T] \\ u(L,t) = \psi_2(t) & t \in [0, T] \\ u(x,0) = u_0(x) & x \in [0, L] \end{array}\right.$$

- $u_0(x)$ is unknown
- $u^{obs}(x,t)$ an observation of $u(x,t)$
- Cost function: $J(u_0) = \dfrac{1}{2}\displaystyle\int_0^T\int_0^L \left(u(x,t) - u^{obs}(x,t)\right)^2 \, dx\, dt$

Gâteaux derivative

$$\hat{J}[u_0](h_0) = \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{\text{obs}}(x,t)\right)\, dx\, dt$$

Gâteaux derivative

$$\hat{J}[u_0](h_0) = \int_0^T \int_0^L \hat{u}(x,t)\left(u(x,t) - u^{obs}(x,t)\right)\, dx\, dt$$

Tangent linear model

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} + \dfrac{\partial (u\hat{u})}{\partial x} - \nu \dfrac{\partial^2 \hat{u}}{\partial x^2} = 0 & x \in]0, L[, t \in [0, T] \\ \hat{u}(0,t) = 0 & t \in [0, T] \\ \hat{u}(L,t) = 0 & t \in [0, T] \\ \hat{u}(x,0) = h_0(x) & x \in [0, L] \end{cases}$$

Gâteaux derivative

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$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} + \dfrac{\partial (u\hat{u})}{\partial x} - \nu\,\dfrac{\partial^2 \hat{u}}{\partial x^2} = 0 & x \in]0,L[,\ t \in [0,T] \\ \hat{u}(0,t) = 0 & t \in [0,T] \\ \hat{u}(L,t) = 0 & t \in [0,T] \\ \hat{u}(x,0) = h_0(x) & x \in [0,L] \end{cases}$$

Adjoint model

$$\begin{cases} \dfrac{\partial p}{\partial t} + u\dfrac{\partial p}{\partial x} + \nu\,\dfrac{\partial^2 p}{\partial x^2} = \left(u - u^{obs}\right) & x \in]0,L[,\ t \in [0,T] \\ p(0,t) = 0 & t \in [0,T] \\ p(L,t) = 0 & t \in [0,T] \\ p(x,T) = 0 & x \in [0,L] \ \text{final condition !!} \to \text{backward integration} \end{cases}$$

Gâteaux derivative of J

$$\hat{J}[u_0](h_0) = \int_0^T \int_0^L \hat{u}(x,t) \left(u(x,t) - u^{obs}(x,t)\right) \, dx \, dt$$
$$= -\int_0^L h_0(x) p(x,0) \, dx$$

Gradient of J

$\nabla J = -p(.,0)$ function of x

Outline

Minimization with equality constraints

Optimization problem

- $J : \mathbf{R}^n \to \mathbf{R}$ differentiable
- $K = \{\mathbf{x} \in \mathbf{R}^n \text{ such that } h_1(\mathbf{x}) = \ldots = h_p(\mathbf{x}) = 0\}$, where the functions $h_i : \mathbf{R}^n \to \mathbf{R}$ are continuously differentiable.

Find the solution of the constrained minimization problem $\min_{\mathbf{x} \in K} J(\mathbf{x})$

Theorem

If $\mathbf{x}^* \in K$ is a local minimum of J in K, and if the vectors $\nabla h_i(\mathbf{x}^*)$ $(i = 1, \ldots, p)$ are linearly independent,
then there exists $\lambda^* = (\lambda_1^*, \ldots, \lambda_p^*) \in \mathbf{R}^p$ such that

$$\nabla J(\mathbf{x}^*) + \sum_{i=1}^{p} \lambda_i^* \nabla h_i(\mathbf{x}^*) = 0$$

Let $\mathcal{L}(\mathbf{x};\lambda) = J(\mathbf{x}) + \sum_{i=1}^{p} \lambda_i h_i(\mathbf{x})$

- λ_i's: Lagrange multipliers associated to the constraints.
- $\mathcal{L}$: Lagrangian function associated to J.

Then minimizing J in K is equivalent to solving $\nabla\mathcal{L} = 0$ in $\mathbf{R}^n \times \mathbf{R}^p$,

since $$\begin{cases} \nabla_{\mathbf{x}}\mathcal{L} & = \nabla J + \sum_{i=1}^{p} \lambda_i \nabla h_i \\ \nabla_{\lambda_i}\mathcal{L} & = h_i \qquad i = 1,\ldots,p \end{cases}$$

This is a saddle point problem.

The adjoint method as a constrained minimization

The adjoint method can be interpreted as a minimization of $J(x)$ under the constraint that the model equations must be satisfied.

From this point of view, the adjoint variable corresponds to a Lagrange multiplier.

Example: control of the initial condition of the Burgers' equation

- Model:

$$\left\{\begin{array}{ll} \dfrac{\partial u}{\partial t} + u\,\dfrac{\partial u}{\partial x} - \nu\,\dfrac{\partial^2 u}{\partial x^2} = f & x \in]0, L[, t \in [0, T] \\ u(0,t) = \psi_1(t) & t \in [0, T] \\ u(L,t) = \psi_2(t) & t \in [0, T] \\ u(x,0) = u_0(x) & x \in [0, L] \end{array}\right.$$

- Full observation field $u^{obs}(x, t)$
- Cost function: $J(u_0) = \dfrac{1}{2}\displaystyle\int_0^T \int_0^L \left(u(x,t) - u^{obs}(x,t)\right)^2 \, dx\, dt$

Example: control of the initial condition of the Burgers' equation

- Model:

$$\begin{cases} \dfrac{\partial u}{\partial t} + u\,\dfrac{\partial u}{\partial x} - \nu\,\dfrac{\partial^2 u}{\partial x^2} = f & x \in]0, L[, t \in [0, T] \\ u(0, t) = \psi_1(t) & t \in [0, T] \\ u(L, t) = \psi_2(t) & t \in [0, T] \\ u(x, 0) = u_0(x) & x \in [0, L] \end{cases}$$

- Full observation field $u^{\text{obs}}(x, t)$
- Cost function: $J(u_0) = \dfrac{1}{2} \displaystyle\int_0^T \int_0^L \left(u(x, t) - u^{\text{obs}}(x, t)\right)^2 \, dx\, dt$

We will consider here that J is a function of u_0 and u, and will minimize $J(u_0, u)$ under the constraint of the model equations.

Lagrangian function

$$\mathcal{L}(u_0, u; p) = \underbrace{J(u_0, u)}_{\text{data ass cost function}} + \underbrace{\int_0^T \int_0^L \left(\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} - \nu\,\frac{\partial^2 u}{\partial x^2} - f \right) p}_{\text{model}}$$

Remark: no additional term (i.e. no Lagrange multipliers) for the initial condition nor for the boundary conditions: their values are fixed.

By integration by parts, $\mathcal{L}$ can also be written:

$$\begin{aligned}\mathcal{L}(u_0, u; p) = \quad & J(u_0, u) + \int_0^T \int_0^L \left(-u\frac{\partial p}{\partial t} - \frac{1}{2}u^2\,\frac{\partial p}{\partial x} - \nu u\frac{\partial^2 p}{\partial x^2} - fp \right) \\ & + \int_0^L [u(.,T)p(.,T) - u_0\,p(.,0)] + \int_0^T \left[\frac{1}{2}\psi_2^2\,p(L,.) - \frac{1}{2}\psi_1^2\,p(0,.)\right] \\ & -\nu\int_0^T \left[\frac{\partial u}{\partial x}(L,.)p(L,.) - \frac{\partial u}{\partial x}(0,.)p(0,.) + \psi_2\,\frac{\partial p}{\partial x}(L,.) - \psi_1\,\frac{\partial p}{\partial x}(0,.)\right]\end{aligned}$$

Saddle point:

- $$(\nabla_p \mathcal{L}, h_p) = \int_0^T \int_0^L \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} - f \right) h_p$$

- $$\begin{aligned}(\nabla_u \mathcal{L}, h_u) = & \int_0^T \int_0^L \left((u - u^{\text{obs}}) - \frac{\partial p}{\partial t} - u \frac{\partial p}{\partial x} - \nu \frac{\partial^2 p}{\partial x^2} \right) h_u \\ & + \int_0^L h_u(., T) p(., T) \\ & - \nu \int_0^T \left[\frac{\partial h_u}{\partial x}(L, .) p(L, .) - \frac{\partial h_u}{\partial x}(0, .) p(0, .) \right]\end{aligned}$$

- $$(\nabla_{u_0} \mathcal{L}, h_0) = - \int_0^L h_0(., 0) p(., 0)$$

$$\nabla \mathcal{L} = (\nabla_p \mathcal{L}, \nabla_u \mathcal{L}, \nabla_{u_0} \mathcal{L}) = 0$$

- $$\nabla_p \mathcal{L} = 0 \iff \frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} - \nu\,\frac{\partial^2 u}{\partial x^2} = f \qquad \forall x\, \forall t$$

- $$\nabla_u \mathcal{L} = 0 \iff \left\{ \begin{array}{l} \dfrac{\partial p}{\partial t} + u\,\dfrac{\partial p}{\partial x} + \nu\,\dfrac{\partial^2 p}{\partial x^2} = u - u^{obs} \\ p(x,T) = 0 \quad \forall x \\ p(0,t) = p(L,t) = 0 \quad \forall t \end{array} \right.$$

- $$\nabla_{u_0} \mathcal{L} = -p(.,0) = 0$$

Optimality system

This set of equations (direct model, adjoint model, Euler equation) is called the optimality system. It gathers all the information of the data assimilation problem.

Thank you !