An introduction to data assimilation

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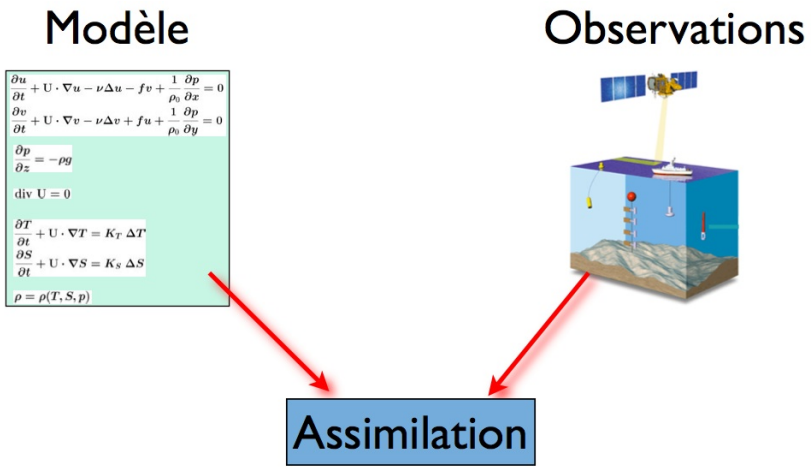
Data assimilation, the science of compromises

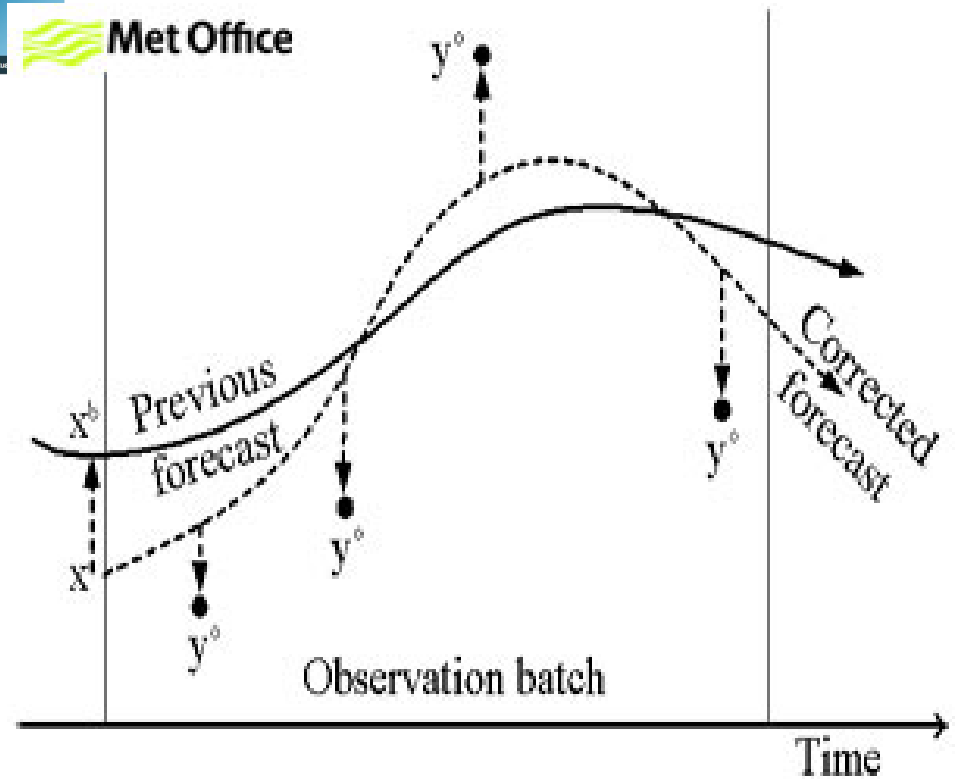
Context characterizing a (complex) system and/or forecasting its evolution, given several heterogeneous and uncertain sources of information



Widely used for geophysical fluids (meteorology, oceanography, atmospheric chemistry...), but also in other numerous domains (e.g. nuclear energy, medicine, agriculture planning...)

Closely linked to *inverse methods, control theory, estimation theory, filtering...*

A daily example: numerical weather forecast



Data assimilation, the science of compromises

Numerous possible aims:

- Forecast: estimation of the present state (initial condition)
- Model tuning: parameter estimation
- Inverse modeling: estimation of parameter fields
- Data analysis: re-analysis (model = interpolation operator)
- OSSE: optimization of observing systems
- ...

Objectives for this lecture

- introduce data assimilation from several points of view
- give an overview of the main families of methods
- point out the main difficulties and current corresponding answers

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Outline

1. Data assimilation for dummies: a simple model problem
2. Generalization: linear estimation theory, variational and sequential approaches
3. Main current challenges

Some references

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A simple but fundamental example

Model problem: least squares approach

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

Model problem: least squares approach

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

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

Model problem: least squares approach

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*
$y_1 = 66.2°\text{F}$ and $y_2 = 21°\text{C}$

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

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Drawback # 2: *if observation accuracies are inhomogeneous*

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

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

Model problem: statistical approach

Reformulation in a **probabilistic framework**:

- the goal is to estimate a scalar value x
- y_i is a realization of a random variable Y_i
- One is looking for an estimator (i.e. a r.v.) $\hat{X}$ that is
  - **linear**: $\hat{X} = \alpha_1 Y_1 + \alpha_2 Y_2$ (in order to be simple)
  - **unbiased**: $E(\hat{X}) = x$ (it seems reasonable)
  - **of minimal variance**: $\mathrm{Var}(\hat{X})$ minimum (optimal accuracy)

$\longrightarrow$ BLUE (Best Linear Unbiased Estimator)

Model problem: statistical approach

Let $Y_i = x + \varepsilon_i$ with

Hypotheses

- $E(\varepsilon_i) = 0 \qquad (i = 1, 2)$ — unbiased measurement devices
- $\mathrm{Var}(\varepsilon_i) = \sigma_i^2 \qquad (i = 1, 2)$ — known accuracies
- $\mathrm{Cov}(\varepsilon_1, \varepsilon_2) = 0$ — independent measurement errors

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Then, since $\hat{X} = \alpha_1 Y_1 + \alpha_2 Y_2 = (\alpha_1 + \alpha_2)x + \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$:

- $E(\hat{X}) = (\alpha_1 + \alpha_2)x + \alpha_1 E(\varepsilon_1) + \alpha_2 E(\varepsilon_2) \quad \Longrightarrow \alpha_1 + \alpha_2 = 1$

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- $E(\hat{X}) = (\alpha_1 + \alpha_2)x + \alpha_1 E(\varepsilon_1) + \alpha_2 E(\varepsilon_2) \quad \Longrightarrow \alpha_1 + \alpha_2 = 1$
- $\mathrm{Var}(\hat{X}) = E\left[(\hat{X} - x)^2\right] = E\left[(\alpha_1\varepsilon_1 + \alpha_2\varepsilon_2)^2\right] = \alpha_1^2\sigma_1^2 + (1-\alpha_1)^2\sigma_2^2$

$$\frac{\partial}{\partial \alpha_1} = 0 \Longrightarrow \alpha_1 = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2}$$

Model problem: statistical approach

In summary:

BLUE

$$\hat{X} = \frac{\frac{1}{\sigma_1^2} Y_1 + \frac{1}{\sigma_2^2} Y_2}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

Its accuracy: $\left[\mathrm{Var}(\hat{X})\right]^{-1} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}$ accuracies are added

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Remarks:

- The hypothesis $\mathrm{Cov}(\varepsilon_1, \varepsilon_2) = 0$ is not compulsory at all.
  $\mathrm{Cov}(\varepsilon_1, \varepsilon_2) = c \longrightarrow \alpha_i = \frac{\sigma_j^2 - c}{\sigma_1^2 + \sigma_2^2 - 2c}$
- Statistical hypotheses on the two first moments of $\varepsilon_1, \varepsilon_2$ lead to statistical results on the two first moments of $\hat{X}$.

Model problem: statistical approach

Variational equivalence

This is equivalent to the problem:

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

Model problem: statistical approach

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Remarks:

- This answers the previous problems of sensitivity to inhomogeneous units and insensitivity to inhomogeneous accuracies
- This gives a rationale for choosing the norm for defining J
- $$\underbrace{J''(\hat{x})}_{\text{convexity}} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} = \underbrace{[\mathrm{Var}(\hat{x})]^{-1}}_{\text{accuracy}}$$

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

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

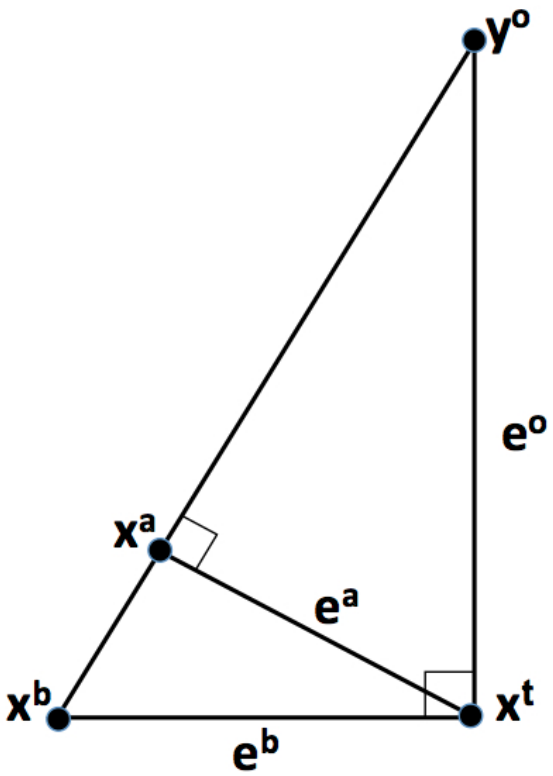
Model problem

Interpretation

If the background error and the observation error are uncorrelated: $E(e^o e^b) = 0$, then one can show that the estimation error and the innovation are uncorrelated:

$$E(e^a(Y - X_b)) = 0$$

$\rightarrow$ orthogonal projection for the scalar product $< Z_1, Z_2 >= E(Z_1 Z_2)$



Model problem: Bayesian approach

One can also consider x as a realization of a r.v. X, and be interested in the pdf $p(X|Y)$.

Several optimality criteria

- **minimum variance**: $\hat{X}_{MV}$ such that the spread around it is minimal
$$\longrightarrow \hat{X}_{MV} = E(X|Y)$$
- **maximum a posteriori**: most probable value of X given Y
$$\longrightarrow \hat{X}_{MAP} \text{ such that } \frac{\partial p(X|Y)}{\partial X} = 0$$
- **maximum likelihood**: $\hat{X}_{ML}$ that maximizes $p(Y|X)$

- Based on the Bayes rule:
$$P(X = x \mid Y = y) = \frac{P(Y = y \mid X = x)\, P(X = x)}{P(Y = y)}$$
- requires additional hypotheses on prior pdf for X and for $Y|X$
- In the Gaussian case, these estimations coincide with the BLUE

Model problem: Bayesian approach

Back to our example: observations y_1 and y_2 of an unknown value x.

The simplest approach: maximum likelihood (no prior on X)

Hypotheses:

- $Y_i \hookrightarrow \mathcal{N}(X, \sigma_i^2)$ — unbiased, known accuracies + known pdf
- $\mathrm{Cov}(Y_1, Y_2) = 0$ — independent measurement errors

Likelihood function: $\mathcal{L}(x) = dP(Y_1 = y_1 \text{ and } Y_2 = y_2 \,|\, X = x)$

One is looking for $\hat{x}_{ML} = \text{Argmax } \mathcal{L}(x)$ — maximum likelihood estimation

Model problem: Bayesian approach

$$\mathcal{L}(x) = \prod_{i=1}^{2} dP(Y_i = y_i \,|\, X = x) = \prod_{i=1}^{2} \frac{1}{\sqrt{2\pi}\,\sigma_i}\, e^{-\frac{(y_i - x)^2}{2\sigma_i^2}}$$

$$\begin{aligned}\text{Argmax } \mathcal{L}(x) &= \text{Argmin } \left(-\ln \mathcal{L}(x)\right) \\ &= \text{Argmin } \frac{1}{2}\left[\frac{(x-y_1)^2}{\sigma_1^2} + \frac{(x-y_2)^2}{\sigma_2^2}\right]\end{aligned}$$

Hence $\quad \hat{x}_{ML} = \dfrac{\dfrac{1}{\sigma_1^2}\, y_1 + \dfrac{1}{\sigma_2^2}\, y_2}{\dfrac{1}{\sigma_1^2} + \dfrac{1}{\sigma_2^2}}$

BLUE again

(because of Gaussian hypothesis)

Model problem: synthesis

Data assimilation methods are often split into two families: variational methods and statistical methods.

- Variational methods: minimization of a cost function (least squares approach)
- Statistical methods: algebraic computation of the BLUE (with hypotheses on the first two moments), or approximation of pdfs (with hypotheses on the pdfs) and computation of the MAP estimator
- There are strong links between those approaches, depending on the case (linear ? Gaussian ?)

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Theorem

If you have understood this previous stuff, you have (almost) understood everything on data assimilation.

Generalization: variational approach

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

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

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

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

  Associated scalar product: $(\mathbf{u}, \mathbf{v})_{\mathbf{M}} = \mathbf{u}^T\mathbf{M}\,\mathbf{v} = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}\, u_i v_j$

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Remark

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

$$p \geq n$$

Formalism "background value + new observations"

$$\mathbf{z} = \begin{pmatrix} \mathbf{x}_b \\ \mathbf{y} \end{pmatrix} \begin{array}{l} \longleftarrow \text{background} \\ \longleftarrow \text{new observations} \end{array}$$

The cost function becomes:

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

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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.

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

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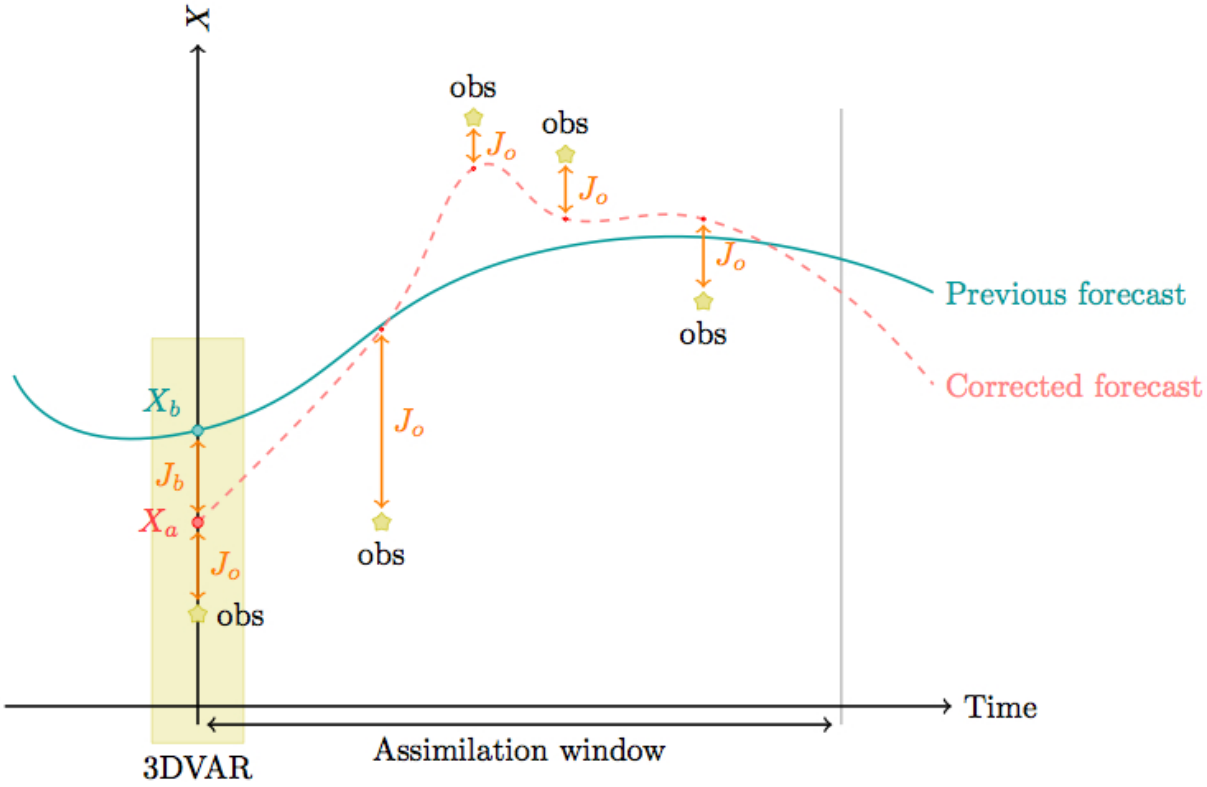

$$J(\mathbf{x}_0) = \underbrace{\frac{1}{2}\|\mathbf{x}_0 - \mathbf{x}_0^b\|_b^2}_{\text{background term } J_b} + \underbrace{\frac{1}{2}\sum_{i=0}^{N}\|H_i(\mathbf{x}(t_i)) - \mathbf{y}(t_i)\|_o^2}_{\text{observation term } J_o}$$

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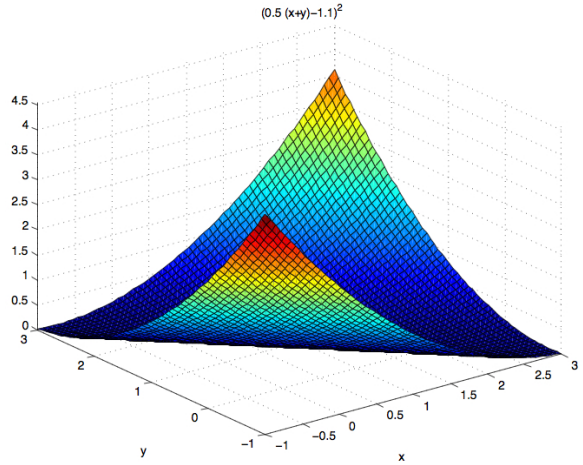
- If H and M are linear then J_o is quadratic.
- However J_o generally does not have a unique minimum, since the number of observations is generally less than the size of $\mathbf{x}_0$ (the problem is underdetermined: $p < n$).

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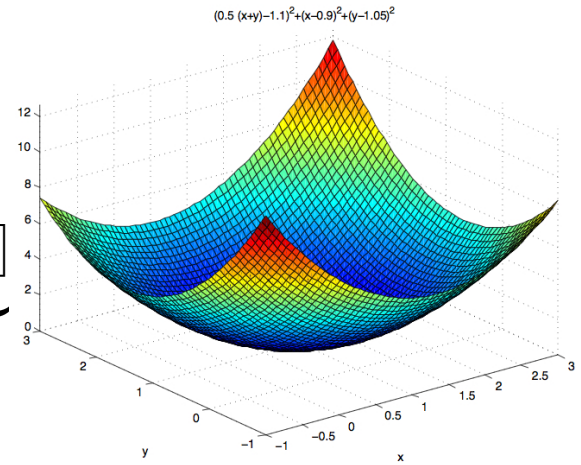
- If H and M are linear then J_o is quadratic.
- However it generally does not have a unique minimum, since the number of observations is generally less than the size of $\mathbf{x}_0$ (the problem is underdetermined).
- Adding J_b makes the problem of minimizing $J = J_o + J_b$ well posed.

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 $(x_1^b, x_2^b) = (0.9, 1.05)$

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

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



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/or M are nonlinear then J_o is no longer quadratic.

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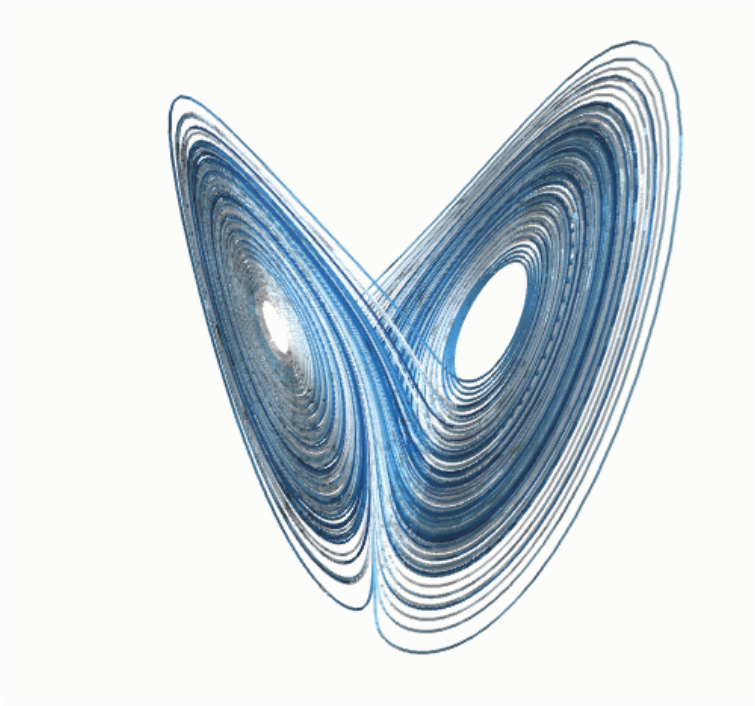

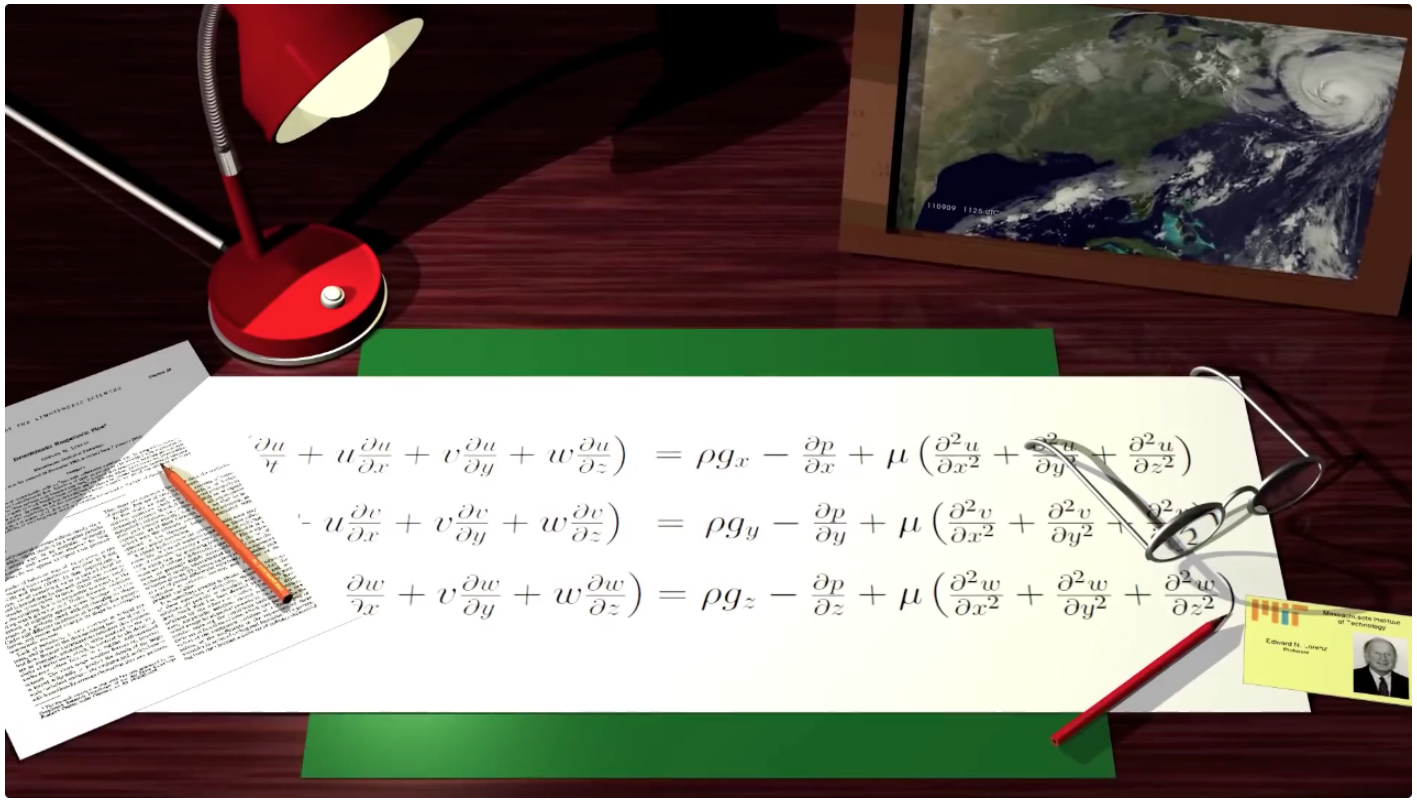

http://www.chaos-math.org

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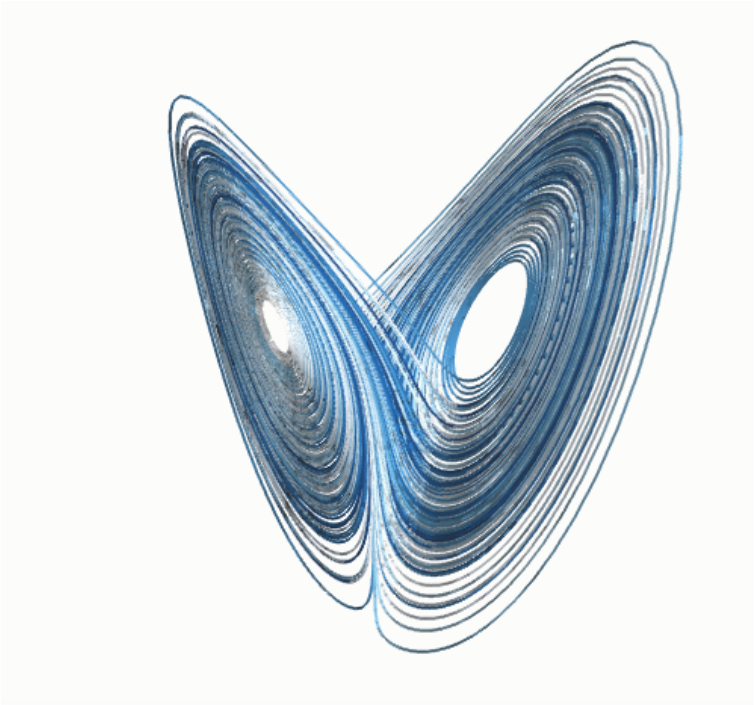

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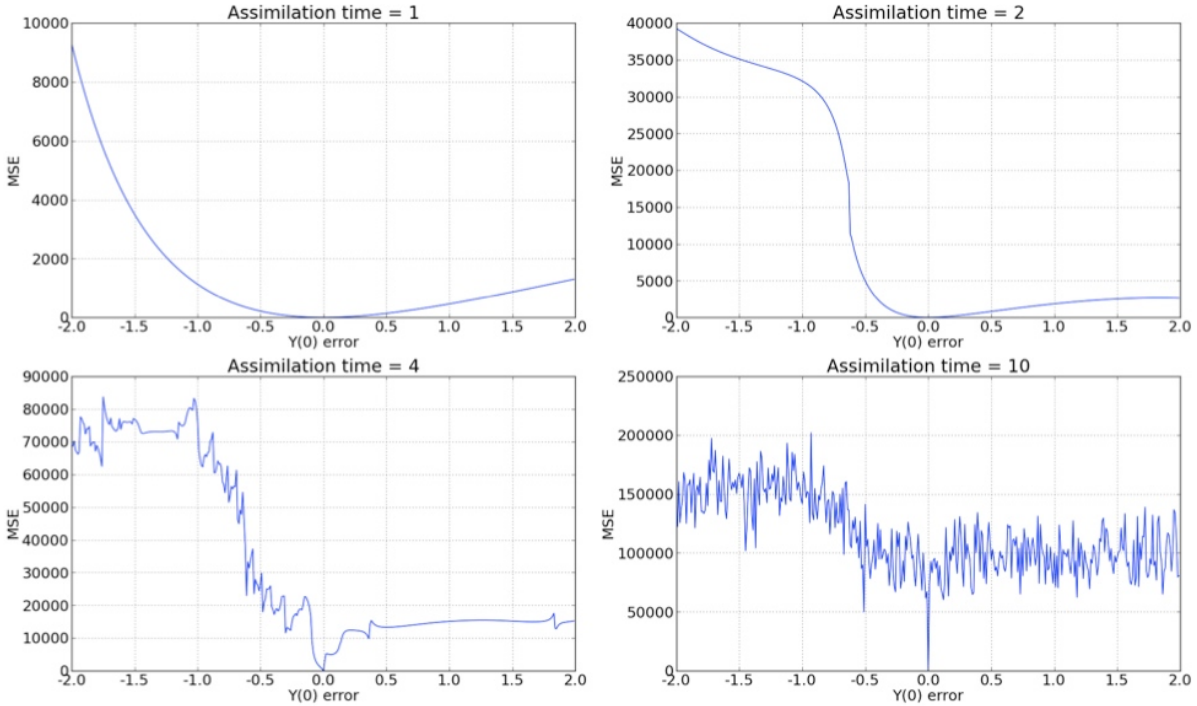

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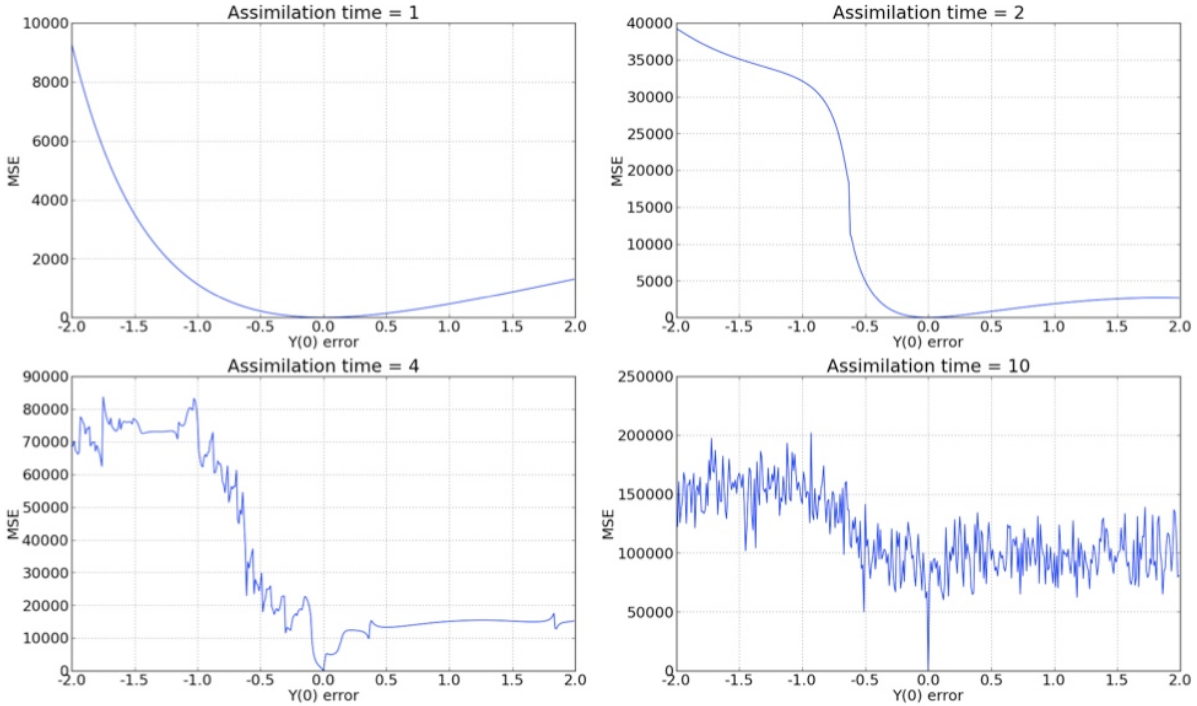

- Adding J_b makes it "more quadratic" (J_b is a regularization term), but $J = J_o + J_b$ may however have several local minima.

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.

Minimizing J

$$
\begin{aligned}
J(\mathbf{x}) &= J_b(\mathbf{x}) + J_o(\mathbf{x}) \\
&= \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})
\end{aligned}
$$

Optimal estimation in the linear case

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

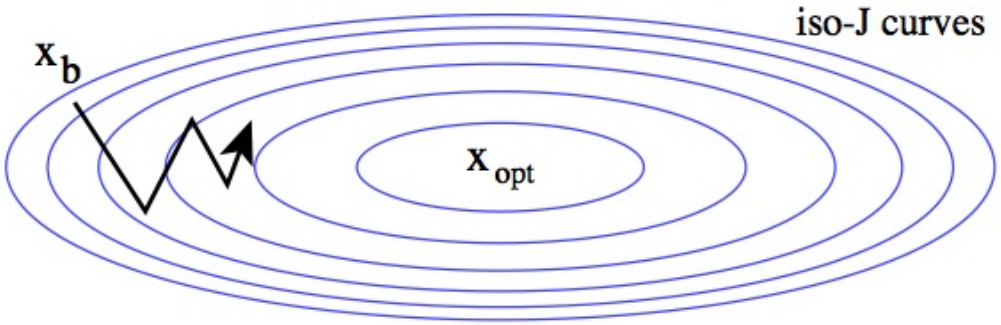
Given the size of n and p, it is generally impossible to handle explicitly $\mathbf{H}$, $\mathbf{B}$ and $\mathbf{R}$. So the direct computation of the gain matrix is impossible.

- 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.

Minimizing J: descent methods

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

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



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

Getting the gradient is not obvious

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

Example:

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

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

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

$\longrightarrow N + 1$ model runs

Getting the gradient is not obvious

In actual applications like meteorology / oceanography,
$N = [\mathbf{u}] = \mathcal{O}(10^6 - 10^9) \quad \longrightarrow$ this method cannot be used.

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

Example: an adjoint for the Burgers' equation

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

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

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Adjoint model

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

final condition !! $\rightarrow$ backward integration

Gradient of J

$$\nabla J = -p(.,0) \qquad \text{function of } x$$

Getting the gradient is not obvious

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

It requires writing a tangent linear code and an adjoint code (beyond the scope of this lecture):

- obeys systematic rules
- is not the most interesting task you can imagine
- there exists automatic differentiation softwares:
  $\longrightarrow$ cf http://www.autodiff.org

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

Generalization: statistical approach

Generalization: statistical approach

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 $H : \mathbf{R}^n \longrightarrow \mathbf{R}^p$

Statistical framework:

- $\mathbf{y}$ is a realization of a random vector $\mathbf{Y}$
- One is looking for the BLUE, i.e. a r.v. $\hat{\mathbf{X}}$ that is
  - **linear**: $\hat{\mathbf{X}} = \mathbf{AY}$ with $\text{size}(\mathbf{A}) = (n, p)$
  - **unbiased**: $E(\hat{\mathbf{X}}) = \mathbf{x}$
  - **of minimal variance**:

$$\text{Var}(\hat{\mathbf{X}}) = \sum_{i=1}^{n} \text{Var}(\hat{X}_i) = \text{Tr}(\text{Cov}(\hat{\mathbf{X}})) \text{ minimum}$$

Generalization: statistical approach

Hypotheses

- Linear observation operator: $H(\mathbf{x}) = \mathbf{H}\mathbf{x}$
- Let $\mathbf{Y} = \mathbf{H}\mathbf{x} + \varepsilon$ with ε random vector in $\mathbf{R}^p$
  - $E(\varepsilon) = 0$ unbiased measurement devices
  - $\mathrm{Cov}(\varepsilon) = E(\varepsilon\varepsilon^T) = \mathbf{R}$ known accuracies and covariances

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BLUE

$$\hat{\mathbf{X}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{Y} \quad \text{with } \mathrm{Cov}(\hat{\mathbf{X}}) = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}$$

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Reminder: variational approach in the linear case

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

$$\min_{\mathbf{x}\in\mathbf{R}^n} J_o(\mathbf{x}) \quad \longrightarrow \quad \hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\,\mathbf{y}$$

Formalism "background value + new observations"

Background: $\mathbf{X}_b = \mathbf{x} + \varepsilon_b$ and new observations: $\mathbf{Y} = \mathbf{H}\mathbf{x} + \varepsilon_o$

Hypotheses:

- $E(\varepsilon_b) = 0$ — unbiased background
- $E(\varepsilon_o) = 0$ — unbiased measurement devices
- $\mathrm{Cov}(\varepsilon_b, \varepsilon_o) = 0$ — independent background and observation errors
- $\mathrm{Cov}(\varepsilon_b) = \mathbf{B}$ et $\mathrm{Cov}(\varepsilon_o) = \mathbf{R}$ — known accuracies and covariances

BLUE

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

with $\left[\mathrm{Cov}(\hat{\mathbf{X}})\right]^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$ — accuracies are added

Link with the variational approach

Statistical approach: BLUE

$$\hat{\mathbf{X}} = \mathbf{X}_b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{Y} - \mathbf{H}\mathbf{X}_b)$$

with $\mathrm{Cov}(\hat{\mathbf{X}}) = (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}$

Variational approach in the linear case

$$\begin{aligned} J(\mathbf{x}) &= \frac{1}{2}\|\mathbf{x} - \mathbf{x}_b\|_b^2 + \frac{1}{2}\|H(\mathbf{x}) - \mathbf{y}\|_o^2 \\ &= \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \frac{1}{2}(\mathbf{H}\mathbf{x} - \mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x} - \mathbf{y}) \end{aligned}$$

$$\min_{\mathbf{x}\in\mathbf{R}^n} J(\mathbf{x}) \quad \longrightarrow \quad \hat{\mathbf{x}} = \mathbf{x}_b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\,(\mathbf{y} - \mathbf{H}\mathbf{x}_b)$$

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Same remarks as previously

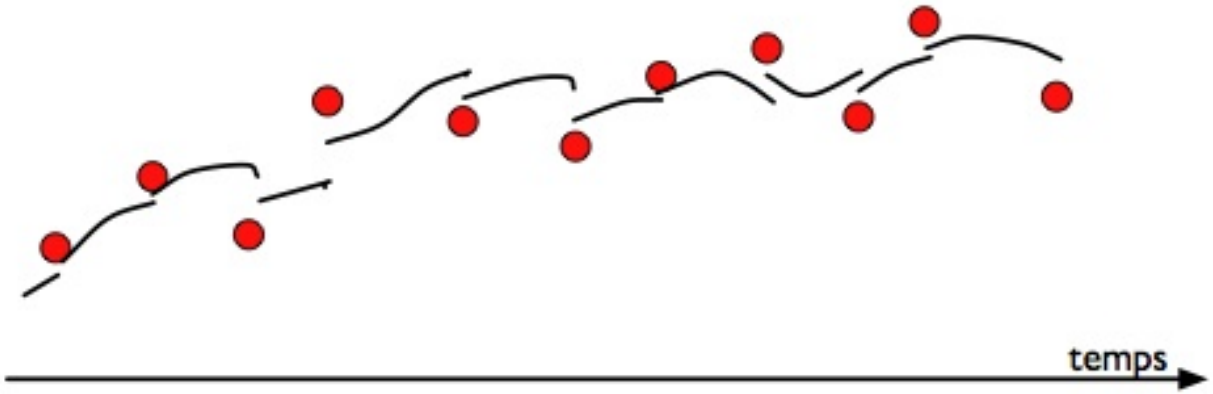
- The statistical approach rationalizes the choice of the norms for J_o and J_b in the variational approach.
- $\underbrace{\left[\mathrm{Cov}(\hat{\mathbf{X}})\right]^{-1}}_{\text{accuracy}} = \mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} = \underbrace{\mathrm{Hess}(J)}_{\text{convexity}}$

If the problem is time dependent

Dynamical system: $\mathbf{x}^t(t_{k+1}) = \mathbf{M}(t_k, t_{k+1})\mathbf{x}^t(t_k) + \mathbf{e}(t_k)$

- $\mathbf{x}^t(t_k)$ true state at time t_k
- $\mathbf{M}(t_k, t_{k+1})$ model assumed linear between t_k and t_{k+1}
- $\mathbf{e}(t_k)$ model error at time t_k

At every observation time t_k, we have an observation $\mathbf{y}_k$ and a model forecast $\mathbf{x}^f(t_k)$. The BLUE can be applied:



If the problem is time dependent

$$\mathbf{x}^t(t_{k+1}) = \mathbf{M}(t_k, t_{k+1})\,\mathbf{x}^t(t_k) + \mathbf{e}(t_k)$$

Hypotheses

- $\mathbf{e}(t_k)$ is unbiased, with covariance matrix $\mathbf{Q}_k$
- $\mathbf{e}(t_k)$ and $\mathbf{e}(t_l)$ are independent ($k \neq l$)
- Unbiased observation $\mathbf{y}_k$, with error covariance matrix $\mathbf{R}_k$
- $\mathbf{e}(t_k)$ and analysis error $\mathbf{x}^a(t_k) - \mathbf{x}^t(t_k)$ are independent

If the problem is time dependent

Kalman filter (Kalman and Bucy, 1961)

Initialization:

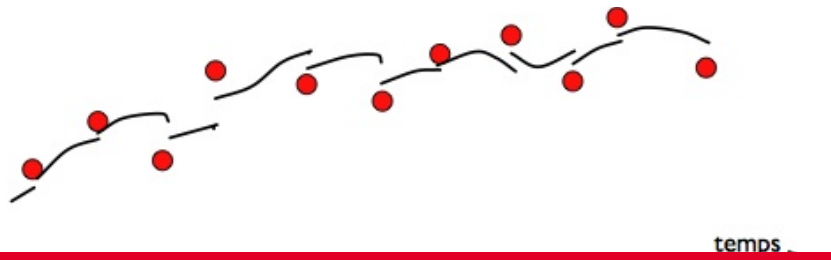
$$\begin{aligned} \mathbf{x}^a(t_0) &= \mathbf{x}_0 && \textit{approximate initial state} \\ \mathbf{P}^a(t_0) &= \mathbf{P}_0 && \textit{error covariance matrix} \end{aligned}$$

Step k: *(prediction - correction, or forecast - analysis)*

$$\begin{aligned} \mathbf{x}^f(t_{k+1}) &= \mathbf{M}(t_k, t_{k+1})\,\mathbf{x}^a(t_k) && \text{Forecast} \\ \mathbf{P}^f(t_{k+1}) &= \mathbf{M}(t_k, t_{k+1})\mathbf{P}^a(t_k)\mathbf{M}^T(t_k, t_{k+1}) + \mathbf{Q}_k \end{aligned}$$

$$\begin{aligned} \mathbf{x}^a(t_{k+1}) &= \mathbf{x}^f(t_{k+1}) + \mathbf{K}_{k+1}\left[\mathbf{y}_{k+1} - \mathbf{H}_{k+1}\mathbf{x}^f(t_{k+1})\right] && \text{BLUE} \\ \mathbf{K}_{k+1} &= \mathbf{P}^f(t_{k+1})\mathbf{H}_{k+1}^T\left[\mathbf{H}_{k+1}\mathbf{P}^f(t_{k+1})\mathbf{H}_{k+1}^T + \mathbf{R}_{k+1}\right]^{-1} \\ \mathbf{P}^a(t_{k+1}) &= \mathbf{P}^f(t_{k+1}) - \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{P}^f(t_{k+1}) \end{aligned}$$

where exponents ^{f} and ^{a} stand respectively for *forecast* and *analysis*.



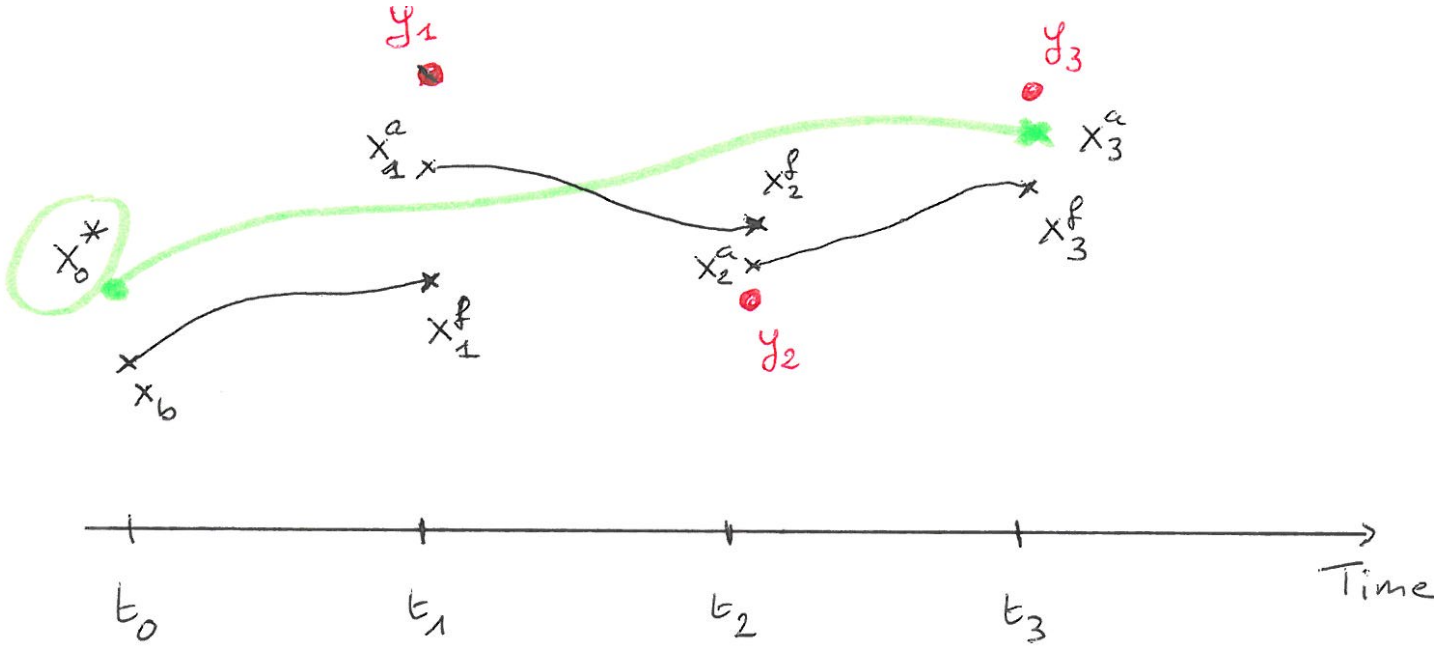
If the problem is time dependent

Equivalence with the variational approach

If $\mathbf{H}_k$ and $\mathbf{M}(t_k, t_{k+1})$ are linear, and if the model is perfect ($\mathbf{e}_k = 0$), then the Kalman filter and the variational method minimizing

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}_0)^T\mathbf{P}_0^{-1}(\mathbf{x}-\mathbf{x}_0) + \frac{1}{2}\sum_{k=0}^{N}(\mathbf{H_k}\mathbf{M}(t_0,t_k)\mathbf{x}-\mathbf{y}_k)^T\mathbf{R}_k^{-1}(\mathbf{H_k}\mathbf{M}(t_0,t_k)\mathbf{x}-\mathbf{y}_k)$$

lead to the same solution at $t = t_N$.



In summary

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variational approach least squares minimization (non dimensional terms)

- no particular hypothesis
- either for stationary or time dependent problems
- If M and H are linear, the cost function is quadratic: a unique solution if $p \geq n$
- Adding a background term ensures this property.
- If things are non linear, the approach is still valid. Possibly several minima

statistical approach

- hypotheses on the first two moments
- time independent + H linear + $p \geq n$: BLUE (first two moments)
- time dependent + M and H linear: Kalman filter (based on the BLUE)

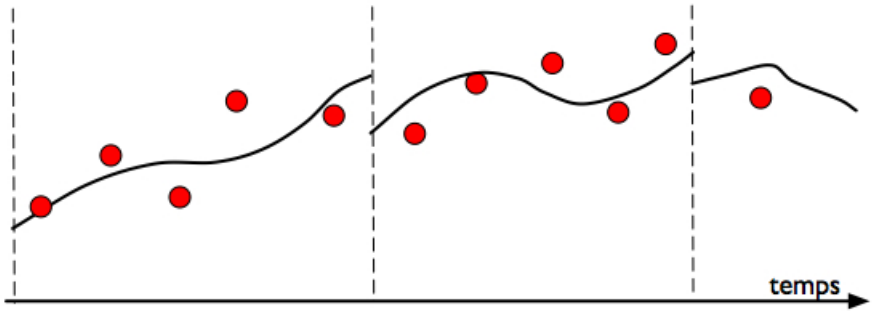
- hypotheses on the pdfs: Bayesian approach (pdf) + ML or MAP estimator

In summary

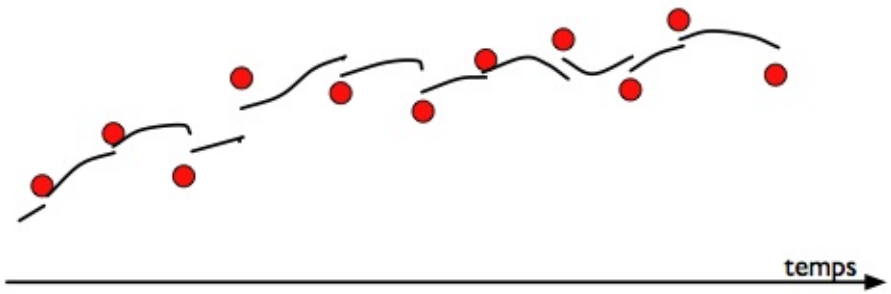
The statistical approach gives a rationale for the choice of the norms, and gives an estimation of the uncertainty.

time independent problems if H is linear, the variational and the statistical approaches lead to the same solution (provided $\|.\|_b$ is based on $\mathbf{B}^{-1}$ and $\|.\|_o$ is based on $\mathbf{R}^{-1}$)

time dependent problems if H and M are linear, if the model is perfect, both approaches lead to the same solution at final time.



4D-Var



Kalman filter

To go further...

Common main methodological difficulties

- Non linearities: J non quadratic / what about Kalman filter ?
- Huge dimensions $[\mathbf{x}] = \mathcal{O}(10^6 - 10^9)$: minimization of J / management of huge matrices
- Poorly known error statistics: choice of the norms / $\mathbf{B}, \mathbf{R}, \mathbf{Q}$
- Scientific computing issues (data management, code efficiency, parallelization...)

In short

- Variational methods:
  - a series of approximations of the cost function, corresponding to a series of methods: 4D-Var, incremental 4D-Var, 3D-FGAT, 3D-Var
  - the more sophisticated ones (4D-Var, incremental 4D-Var) require the tangent linear and adjoint models (the development of which is a real investment)
- Statistical methods:
  - extended Kalman filter handle (weakly) non linear problems (requires the tangent linear model)
  - reduced order Kalman filters address huge dimension problems
  - a quite efficient method, addressing both problems: ensemble Kalman filters (EnKF)
  - these are so called "Gaussian filters"
  - particle filters: currently being developed - fully Bayesian approach - still limited to low dimension problems

Some present research directions

- new methods: less expensive, more robust w.r.t. nonlinearities and/or non gaussianity (particle filters, En4DVar, BFN...)
- better management of errors (prior statistics, identification, a posteriori validation...)
- "complex" observations (images, Lagrangian data...)
- new application domains (often leading to new methodological questions)
- definition of observing systems, sensitivity analysis...

Two announcements

- CNA 2014: 5ème Colloque National d'Assimilation de données
  Toulouse, 1-3 décembre 2014
- Doctoral course "Introduction to data assimilation"
  Grenoble, January 5-9, 2015