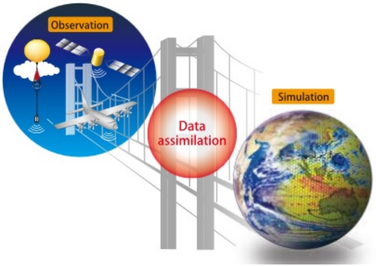
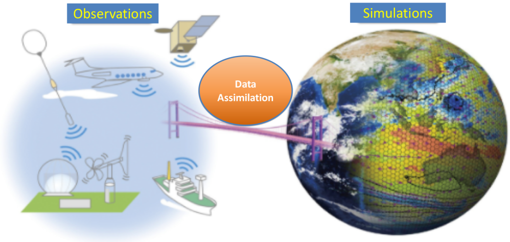
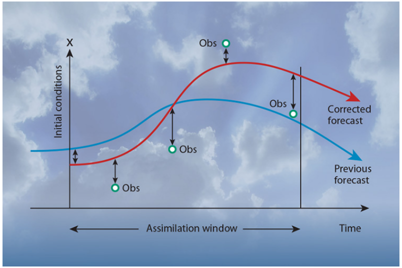
An introduction to data assimilation

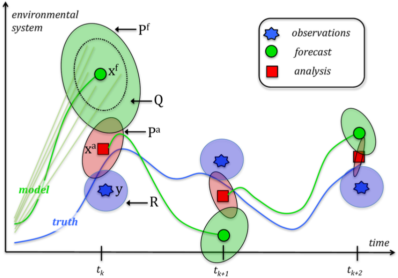
Eric Blayo
Univ. Grenoble Alpes and Inria

Data assimilation specialists can take advantage of these two hours to take a nap or visit the center of Paris.


Observation
Data
assimilation
Simulation

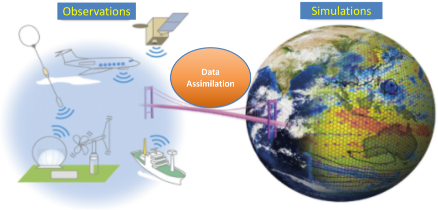

Observations
Simulations
Data
Assimilation


x
Initial conditions
Obs
Obs
Obs
Obs
Corrected
forecast
Previous
forecast
Assimilation window
Time


environmental
system
P^f
x^f
Q
P^a
x^a
y
R
model
truth
observations
forecast
analysis
time
t_k
t_{k+1}
t_{k+2}

Data assimilation, the science of compromise

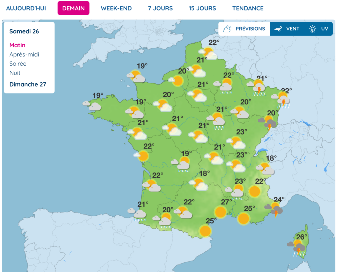
Context characterizing a (complex) system and/or forecasting its evolution, given several heterogeneous and uncertain sources of information

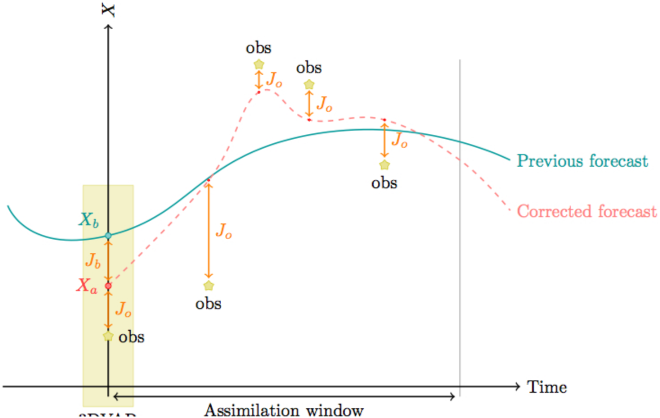


Widely used for geophysical fluids (meteorology, oceanography, river hydraulics. . .), but also in numerous other domains (e.g. nuclear energy, medicine, agriculture planning. . .)

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

A daily example: numerical weather forecast





A nightly example

Walking in a dark room

Data assimilation, the science of compromise

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
- ...

The "best estimate"

Several pieces of information:

- Model
- Prior (or background) value
- Observations
- Statistics
- ...

$\longrightarrow$ **Find the best possible estimate**

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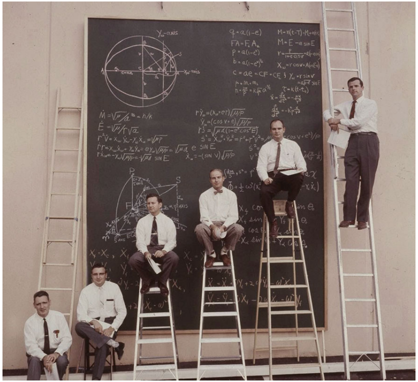
$\longrightarrow$ **Find the best possible estimate**

What does *the best possible estimate* means?

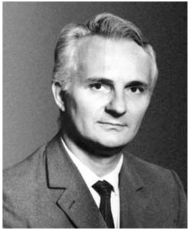
- **Estimate:** deterministic value? pdf? just a few moments of a pdf?
- **Best:** which criterion?

Historical perspective: from space rockets to weather forecasting...

Lev Pontryagin
(1908-1988)



NASA, 1961

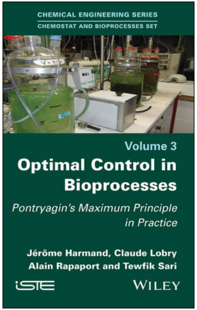


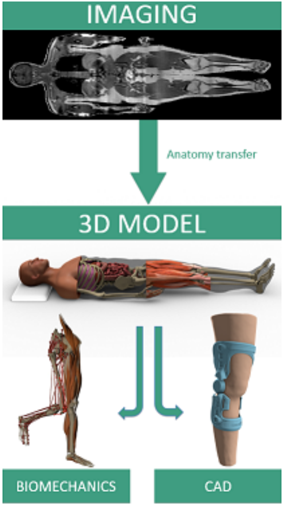
Jacques-Louis Lions
(1928-2001)

Rudolf Kalman
(1930-2016)

François-Xavier Le Dimet
(1945-2021)

… and many other applications





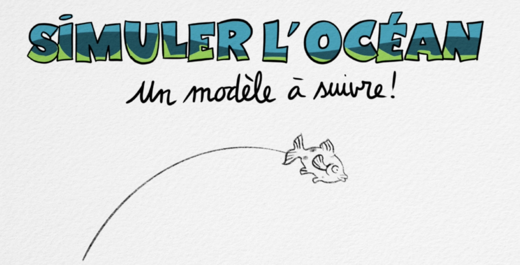
anatoscope.com

Objectives for this lecture

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

Data assimilation for dummies

Data assimilation for real dummies



on YouTube

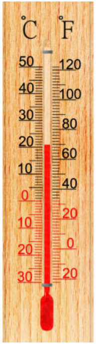
Data assimilation for average dummies

The simplest possible model problem Two pieces of information about the same quantity.
What is its true value?

Data assimilation for average dummies

The simplest possible model problem Two pieces of information about the same quantity. What is its true value?

Example a *prior* (or *background*) value $x^b = 19°\mathrm{C}$ and an *observation* $y = 21°\mathrm{C}$ of the (unknown) present temperature x^t



Model problem: least squares approach

A *prior* (or *background*) value $x^b = 19°\text{C}$ and an *observation* $y = 21°\text{C}$

- Let $J(x) = \frac{1}{2}\left[(x - x^b)^2 + (x - y)^2\right]$

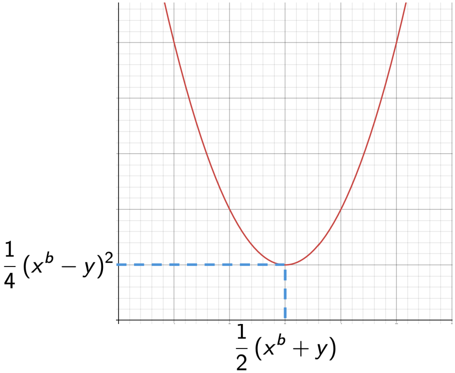
Model problem: least squares approach

A *prior* (or *background*) value $x^b = 19°\mathrm{C}$ and an *observation* $y = 21°\mathrm{C}$

- Let $J(x) = \dfrac{1}{2}\left[(x - x^b)^2 + (x - y)^2\right]$

$$= \left(x - \frac{x^b + y}{2}\right)^2 + \left(\frac{x^b - y}{2}\right)^2$$

- $\mathrm{Min}_x\, J(x) \quad \longrightarrow \quad x^a = \dfrac{x^b + y}{2} = 20°\mathrm{C}$



Model problem: least squares approach

Drawback # 1: if units are different

$x^b = 19°\mathrm{C}$ and $y = 69.8°\mathrm{F}$ $\longrightarrow$ need for a unit conversion

Let $H(x) = \dfrac{9}{5}x + 32$ **observation operator**

Then $J(x) = \dfrac{1}{2}\left[(x - x^b)^2 + (H(x) - y)^2\right]$

Model problem: least squares approach

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$\longrightarrow$ *adding apples and oranges !!*

Model problem: least squares approach

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Drawback # 2: if observation accuracies are different

If x^b is twice more accurate than y, one should obtain $x^a = \dfrac{2x^b + y}{3} = 19.67°\text{C}$

$\longrightarrow$ J should be $J(x) = \dfrac{1}{2}\left[\left(2(x - x^b)\right)^2 + (x - y)^2\right]$

Model problem: linear statistical approach

Reformulation in a **probabilistic framework**:

- the goal is to find an estimator X^a for the true unknown value x
- x^b and y are realizations of random variables X^b and Y

Model problem: linear statistical approach

Reformulation in a **probabilistic framework**:

- the goal is to find an estimator X^a for the true unknown value x
- x^b and y are realizations of random variables X^b and Y
- One is looking for an estimator (i.e. a random variable) X^a that is
  - **linear**: $X^a = \alpha_b X^b + \alpha_o Y$ (in order to be simple)
  - **unbiased**: $E(X^a) = x$ (it seems reasonable)
  - **of minimal variance**: $\mathrm{Var}(X^a)$ minimum (optimal accuracy)

$\longrightarrow$ **BLUE** (Best Linear Unbiased Estimator)

Model problem: linear statistical approach

Let $X^b = x + \varepsilon^b$ and $Y = x + \varepsilon^o$ with

Hypotheses

- $E(\varepsilon^b) = E(\varepsilon^o) = 0$ — unbiased background and measurement device
- $\mathrm{Var}(\varepsilon^b) = \sigma_b^2$ $\quad \mathrm{Var}(\varepsilon^o) = \sigma_o^2$ — known accuracies
- $\mathrm{Cov}(\varepsilon^b, \varepsilon^o) = 0$ — independent errors

Model problem: linear statistical approach

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- $\text{Cov}(\varepsilon^b, \varepsilon^o) = 0$ independent errors

Since $X^a = \alpha_b X^b + \alpha_o Y = (\alpha_b + \alpha_o)x + \alpha_b \varepsilon^b + \alpha_o \varepsilon^o$:

- $E(X^a) = (\alpha_b + \alpha_o)x + \alpha_b \underbrace{E(\varepsilon^b)}_{=0} + \alpha_o \underbrace{E(\varepsilon^o)}_{=0} \implies \alpha_b + \alpha_o = 1$

Model problem: linear statistical approach

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- $\mathrm{Var}(X^a) = E\left[(X^a - x)^2\right] = E\left[(\alpha_b \varepsilon^b + \alpha_o \varepsilon^o)^2\right] = \alpha_b^2 \sigma_b^2 + (1 - \alpha_b)^2 \sigma_o^2$

$$\frac{\partial}{\partial \alpha_b} = 0 \implies \alpha_b = \frac{\sigma_o^2}{\sigma_b^2 + \sigma_o^2}$$

Model problem: linear statistical approach

BLUE

$$X^a = \frac{\dfrac{1}{\sigma_b^2} X^b + \dfrac{1}{\sigma_o^2} Y}{\dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}}$$

Model problem: linear statistical approach

BLUE

$$X^a = \frac{\dfrac{1}{\sigma_b^2} X^b + \dfrac{1}{\sigma_o^2} Y}{\dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}} = X^b + \underbrace{\frac{\sigma_b^2}{\sigma_b^2 + \sigma_o^2}}_{\text{gain}} \underbrace{(Y - X^b)}_{\text{innovation}}$$

Model problem: linear statistical approach

BLUE

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Its accuracy: $\quad [\mathrm{Var}(X^a)]^{-1} = \dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}$ $\qquad$ accuracies are added

Model problem: linear statistical approach

BLUE

$$X^a = \frac{\dfrac{1}{\sigma_b^2} X^b + \dfrac{1}{\sigma_o^2} Y}{\dfrac{1}{\sigma_b^2} + \dfrac{1}{\sigma_o^2}} = X^b + \underbrace{\frac{\sigma_b^2}{\sigma_b^2 + \sigma_o^2}}_{\text{gain}} \underbrace{(Y - X^b)}_{\text{innovation}}$$

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- Hypotheses on the first two moments of $\varepsilon^b, \varepsilon^o$ lead to results on the first two moments of X^a

Model problem: linear statistical approach

Variational equivalence

This is equivalent to the problem:

$$\text{Minimize } J(x) = \frac{1}{2}\left[\frac{(x-x^b)^2}{\sigma_b^2} + \frac{(x-y)^2}{\sigma_o^2}\right]$$

Model problem: linear statistical approach

Variational equivalence

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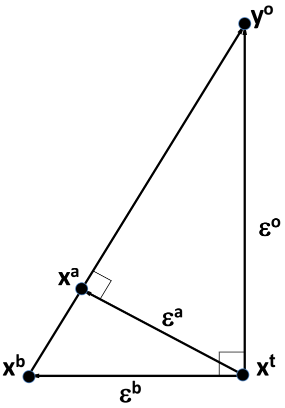
Remarks:

- 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
- $\underbrace{J''(x^a)}_{\text{convexity}} = \frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2} = \underbrace{[\mathrm{Var}(x^a)]^{-1}}_{\text{accuracy}}$

Model problem: linear statistical approach

Geometric interpretation

$$E(\varepsilon^o \varepsilon^b) = 0 \quad \Longrightarrow \quad E(\varepsilon^a (Y - X_b)) = 0$$



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

Model problem: linear statistical approach

Remark Most of these properties still hold if $\text{Cov}(\varepsilon^b, \varepsilon^o) = c \quad (\neq 0)$.

- $$X^a = \frac{\dfrac{1}{\sigma_b^2 - c} X^b + \dfrac{1}{\sigma_o^2 - c} Y}{\dfrac{1}{\sigma_b^2 - c} + \dfrac{1}{\sigma_o^2 - c}} = X^b + \underbrace{\frac{\sigma_b^2 - c}{\sigma_b^2 + \sigma_o^2 - 2c}}_{\text{gain}} \underbrace{(Y - X^b)}_{\text{innovation}}$$
- $\text{Var}(X^a) = \dfrac{\sigma_b^2 \sigma_o^2 - c^2}{\sigma_b^2 + \sigma_o^2 - 2c} \leq \min(\sigma_b^2\,,\,\sigma_o^2)$ (but accuracies are no longer added)
- $E(\varepsilon^a(Y - X_b)) = 0 \quad \longrightarrow$ the geometric interpretation still (more or less) holds
- The corresponding cost function is modified: $J(x) = \dfrac{1}{2}\left[\dfrac{(x - x^b)^2}{\sigma_b^2 - c} + \dfrac{(x - y)^2}{\sigma_o^2 - c}\right]$
- $$\underbrace{J''(x^a)}_{\text{convexity}} = \frac{1}{\sigma_b^2 - c} + \frac{1}{\sigma_o^2 - c} = \frac{\sigma_b^2 \sigma_o^2 - c^2}{(\sigma_b^2 - c)(\sigma_o^2 - c)} \underbrace{[\text{Var}(x^a)]^{-1}}_{\text{accuracy}}$$

Model problem: Bayesian approach

- x: a realization of a random variable X. What is the pdf $p(X|Y)$?
- Based on the Bayes rule:

$$P(X = x \,|\, Y = y) = \frac{\overbrace{P(Y = y \,|\, X = x)}^{\textit{likelihood}}\ \overbrace{P(X = x)}^{\textit{prior}}}{\underbrace{P(Y = y)}_{\textit{normalisation factor}}}$$

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- Back to our example:
  - Background $X^b \rightsquigarrow \mathcal{N}(19, \sigma_b^2)$
  - Observation $y = 21°$C, and $Y = X + \varepsilon^o$ with $\varepsilon^o \rightsquigarrow \mathcal{N}(0, \sigma_o^2)$

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$$P(X = x \mid Y = 21) = \frac{P(Y = 21 \mid X = x)\, P(X = x)}{P(Y = y)}$$

Model problem: Bayesian approach

- Background $X^b \rightsquigarrow \mathcal{N}(19, \sigma_b^2)$
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$$P(X = x \,|\, Y = 21) = \frac{P(Y = 21 \,|\, X = x)\, P(X = x)}{P(Y = y)}$$

- Prior: $P(X = x) = P(X^b = x) = \dfrac{1}{\sqrt{2\pi}\,\sigma_b} \exp\left(\dfrac{(x-19)^2}{2\sigma_b^2}\right)$

- Likelihood:

$$\begin{aligned} p(Y = 21 | \ X = x) &= p(\varepsilon^o = 21 - x | \ X = x) \\ &= p(\varepsilon^o = 21 - x) \qquad \varepsilon^o \text{ is assumed independent from } X \\ &= \frac{1}{\sqrt{2\pi}\,\sigma_o} \exp\left(-\frac{(21-x)^2}{2\,\sigma_o^2}\right) \end{aligned}$$

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- Hence

$$\begin{aligned}
p(X = x)\, p(Y = 21|\ X = x) &= \frac{1}{\sqrt{2\pi}\sigma_b} \exp\left(- \frac{(x-19)^2}{2\ \sigma_b^2} \right) \frac{1}{\sqrt{2\pi}\ \sigma_o} \exp\left(- \frac{(21-x)^2}{2\ \sigma_o^2} \right) \\
&= K\ \exp\left(- \frac{(x-m_a)^2}{2\sigma_a^2} \right)
\end{aligned}$$

$$\text{with } m_a = \frac{\frac{1}{\sigma_b^2}\, 19 + \frac{1}{\sigma_o^2}\, 21}{\frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}} \quad \text{and} \quad \sigma_a^2 = \left(\frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2} \right)^{-1}$$

Model problem: Bayesian approach

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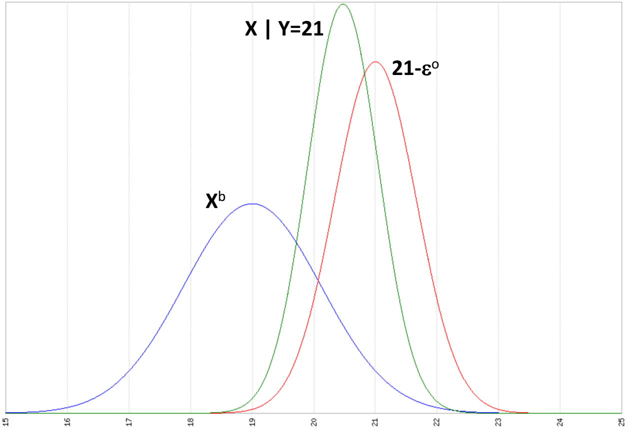
$$P(X = x \,|\, Y = 21) = \frac{P(Y = 21 \,|\, X = x)\, P(X = x)}{P(Y = y)}$$

- Hence

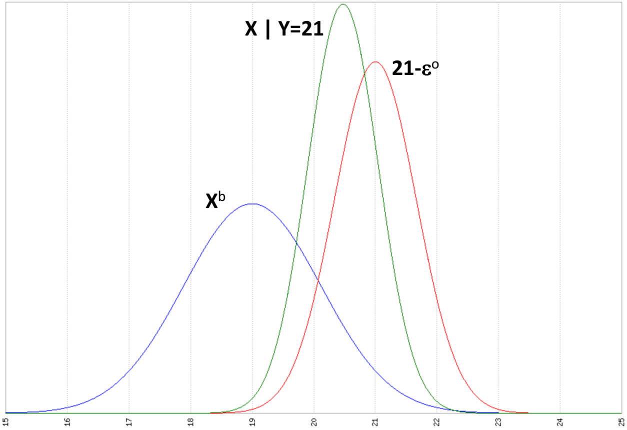
$$\begin{aligned}
p(X = x)\, p(Y = 21 |\, X = x) \quad &= \quad \frac{1}{\sqrt{2\pi}\sigma_b} \exp\left(-\frac{(x-19)^2}{2\,\sigma_b^2} \right) \frac{1}{\sqrt{2\pi}\,\sigma_o} \exp\left(-\frac{(21-x)^2}{2\,\sigma_o^2} \right) \\
&= \quad K\ \exp\left(-\frac{(x-m_a)^2}{2\sigma_a^2} \right) \\
&\quad\ \text{with } m_a = \frac{\frac{1}{\sigma_b^2}\,19 + \frac{1}{\sigma_o^2}\,21}{\frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}} \quad \text{and } \sigma_a^2 = \left(\frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2} \right)^{-1}
\end{aligned}$$

$$\longrightarrow X \,|\, Y = 21 \rightsquigarrow \mathcal{N}(m_a, \sigma_a^2)$$

Model problem: Bayesian approach



Model problem: Bayesian approach



Same as the BLUE, because of Gaussian hypothesis

Another example: source localization

Problem Find the position of the source of a signal, given a pointwise measurement

- **Signal intensity model**

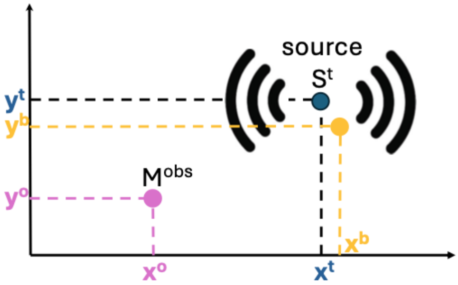
$$i(M) = i(x,y) = \frac{1}{\|S^t M\|^2 + \tau} = \frac{1}{(x - x^t)^2 + (y - y^t)^2 + \tau}$$

- **Observation**

$$i_{\text{obs}} = i(x^o, y^o) + \varepsilon^o = \frac{1}{\|S^t M^{\text{obs}}\|^2 + \tau} + \varepsilon^o = \frac{1}{(x^o - x^t)^2 + (y^o - y^t)^2 + \tau} + \varepsilon^o$$

ε^o: measurement error + model error $\rightsquigarrow \mathcal{N}(0, \sigma_o^2)$

- **First guess** $S^b = (x^b, y^b)$



Source localization: variational approach

$$
\begin{aligned}
J(x,y) &= J_b(x) + J_o(x) \\
&= \frac{1}{2\sigma_b^2}\underbrace{\Big((x-x^b)^2+(y-y^b)^2\Big)}_{\text{distance to the first guess location}} + \frac{1}{2\sigma_o^2}\underbrace{\left(i_{\text{obs}} - \frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2}_{\text{misfit between } i_{\text{obs}} \text{ and the theoretical intensity of the signal at point } M^{\text{obs}} \text{ if the source was located in } (x,y)}
\end{aligned}
$$

Source localization: variational approach

$$
\begin{aligned}
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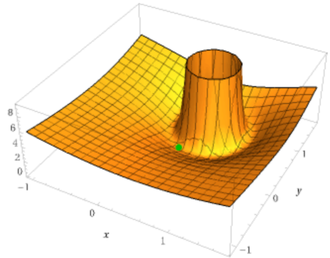
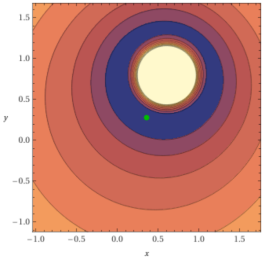
\end{aligned}
$$

3D and 2D views of $J(x,y)$

Green dot: location of the minimum





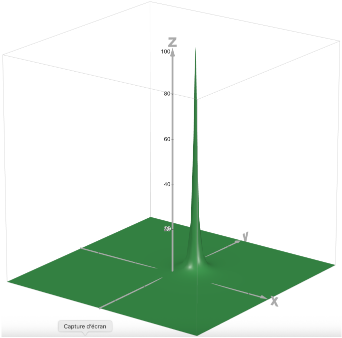
Source localization: statistical (BLUE) approach

The linear statistical approach makes several assumptions, including that of the linearity of the observation operator.

But $$H(x, y) = \frac{1}{(x^o - x)^2 + (y^o - y)^2 + \tau}$$

A linear approximation makes no sense.

$\longrightarrow$ this approach cannot be used



Source localization: Bayesian approach

Look for $P\Big((X^s, Y^s) = (x, y) \mid i(x^o, y^o) = i_{\mathrm{obs}}\Big)$ $\qquad X^s, Y^s$: random variables

Source localization: Bayesian approach

Look for $P\Big((X^s,Y^s)=(x,y) \mid i(x^o,y^o)=i_{\text{obs}}\Big)$ $\qquad X^s, Y^s$: random variables

Bayes theorem

$$P\Big((X^s,Y^s)=(x,y) \mid i(x^o,y^o)=i_{\text{obs}}\Big) = \frac{\overbrace{P\Big(i(x^o,y^o)=i_{\text{obs}} \mid (X^s,Y^s)=(x,y)\Big)}^{\textit{likelihood}}\ \overbrace{P\Big((X^s,Y^s)=(x,y)\Big)}^{\textit{prior}}}{P\Big(i(x^o,y^o)=i_{\text{obs}}\Big)}$$

Source localization: Bayesian approach

Look for $P\Big((X^s,Y^s)=(x,y)\mid i(x^o,y^o)=i_{\text{obs}}\Big)$ $\quad X^s, Y^s$: random variables

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Likelihood

$$\begin{aligned}
&P\Big(i(x^o,y^o)=i_{\text{obs}}\mid (X^s,Y^s)=(x,y)\Big)\\
&\quad=P\left(i_{\text{obs}}=\frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}+\varepsilon_o\right)\\
&\quad=P\left(\varepsilon_o=i_{\text{obs}}-\frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)\\
&\quad=\frac{1}{\sqrt{2\pi}\,\sigma_o}\exp\left(-\frac{\left(i_{\text{obs}}-\frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2}{2\sigma_o^2}\right)
\end{aligned}$$

Prior

$$\begin{aligned}
&P\Big((X^s,Y^s)=(x,y)\Big)\\
&\quad=\frac{1}{2\pi\sigma_b^2}\ \exp\left(-\frac{(x-x^b)^2+(y-y^b)^2}{2\sigma_b^2}\right)
\end{aligned}$$

Source localization: Bayesian approach

Hence $\quad P\Big((X^s, Y^s) = (x,y) \mid i(x^o,y^o) = i_{\text{obs}}\Big)$

$$\propto \exp\left(- \frac{\left(i_{\text{obs}} - \frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2}{2\sigma_o^2} \right) \exp\left(- \frac{(x-x^b)^2 + (y-y^b)^2}{2\sigma_b^2} \right)$$

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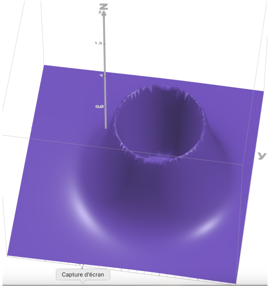
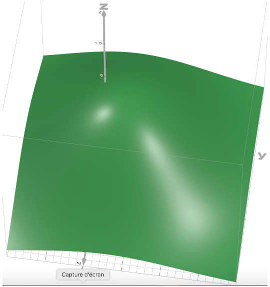
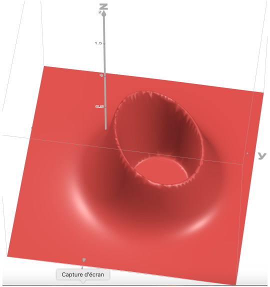


Likelihood



Prior



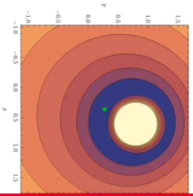
Posterior

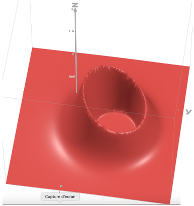
Source localization: Bayesian approach

Hence $$P\Big((X^s,Y^s)=(x,y)\mid i(x^o,y^o)=i_{\text{obs}}\Big)$$
$$\propto\ \exp\left(-\frac{\left(i_{\text{obs}}-\frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2}{2\sigma_o^2}\right)\ \exp\left(-\frac{(x-x^b)^2+(y-y^b)^2}{2\sigma_b^2}\right)$$

- The posterior is not Gaussian (at all!), even if ε^o and ε^b are Gaussian (due to the nonlinear observation operator)
- $P\Big((X^s,Y^s)=(x,y)\mid i(x^o,y^o)=i_{\text{obs}}\Big)\propto\exp\big(-J_o(x,y)-J_b(x,y)\big)$

$$\Longrightarrow\quad \text{Argmin } J(x,y)=\text{mode of the posterior}$$





Model problem: synthesis

Data assimilation methods are often split into 2-3 families:

- Variational methods: minimization of a cost function (least squares approach)
- Linear statistical approach: computation of the BLUE (with hypotheses on the first two moments)
- Bayesian approach: approximation of pdfs (with hypotheses on the pdfs)

- There are strong links between those approaches, depending on the case (linear operators, Gaussian errors...)

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Theorem

If you have understood this previous stuff, you have already understood a lot on data assimilation.

Generalization

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

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Example 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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If the problem is time dependent

- Observations are distributed in time: $\mathbf{y} = \mathbf{y}(t)$

- There is a model describing the evolution of $\mathbf{x}$: $\begin{cases} \dfrac{d\mathbf{x}}{dt} = M(\mathbf{x}) \\ \mathbf{x}(t=0) = \mathbf{x}_0 \end{cases}$

Generalization: variational approach

The cost function

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

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  (Intuitive) necessary (but not sufficient) condition
  for the existence of a unique minimum: $p \geq n$

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  (Intuitive) necessary (but not sufficient) condition
  for the existence of a unique minimum: $p \geq n$

- Augmented vector of information $\mathbf{z} = \begin{pmatrix} \mathbf{x}^b \\ \mathbf{y} \end{pmatrix}$ $\begin{array}{l} \longleftarrow \text{background} \\ \longleftarrow \text{new observations} \end{array}$

  The cost function becomes: $J(\mathbf{x}) = \underbrace{\dfrac{1}{2}\|\mathbf{x} - \mathbf{x}^b\|_b^2}_{J_b} + \underbrace{\dfrac{1}{2}\|H(\mathbf{x}) - \mathbf{y}\|_o^2}_{J_o}$

  The condition $p \geq n$ is automatically fulfilled.

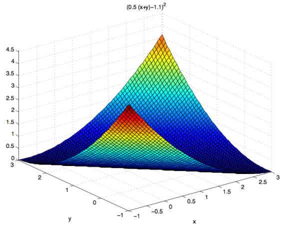
Uniqueness of the minimum

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

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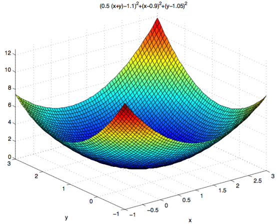
Adding J_b makes the problem of minimizing $J = J_o + J_b$ well posed.

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

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

$$\longrightarrow (x_1^a, x_2^a) = (0.94166\ldots, 1.09166\ldots)$$

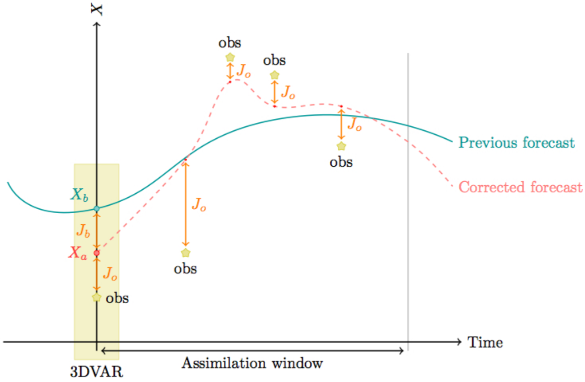


If the problem is time dependent

- $\mathbf{y} \longrightarrow \mathbf{y}(t) \quad \Longrightarrow \quad J_o(\mathbf{x}) = \dfrac{1}{2} \displaystyle\sum_{i=0}^{N} \| H_i(\mathbf{x}(t_i)) - \mathbf{y}(t_i) \|_o^2$
- $\left\{ \begin{aligned} \frac{d\mathbf{x}}{dt} &= M(\mathbf{x}) \\ \mathbf{x}(t=0) &= \mathbf{x}_0 \end{aligned} \right. \quad \Longrightarrow \quad J_o(\mathbf{x}) \longrightarrow J_o(\mathbf{x}_0)$

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

If the problem is time dependent



$$J(\mathbf{x}_0) = \underbrace{\frac{1}{2}\|\mathbf{x}_0 - \mathbf{x}_0^b\|_b^2}_{\text{background term } J_b}$$

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

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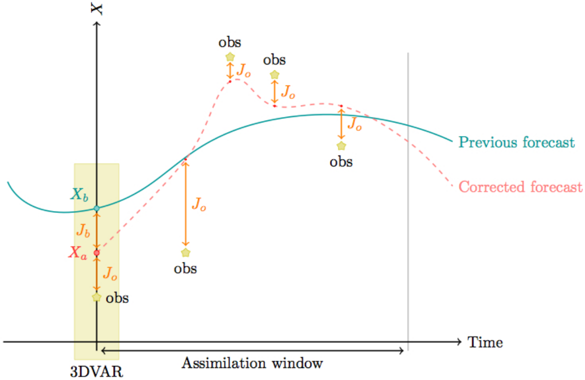

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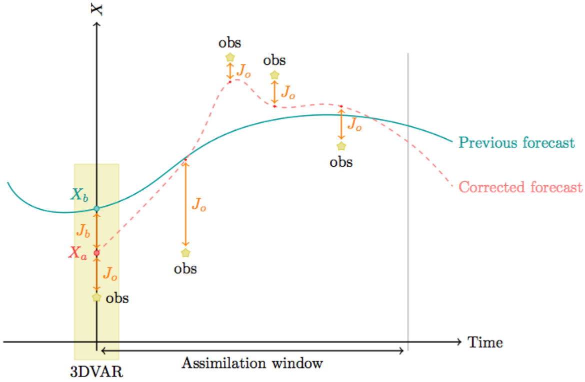
If H and M are linear then J_o is quadratic $\longrightarrow$ unique minimum

If the problem is time dependent



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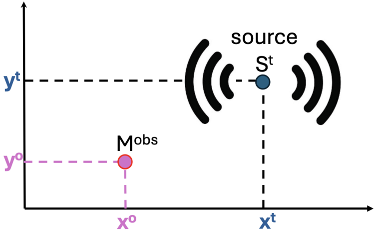
If H and/or M are nonlinear then J_o is no longer quadratic

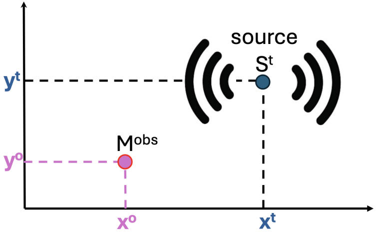
$\longrightarrow$ uniqueness of the minimum?

Uniqueness of the minimum: source localization



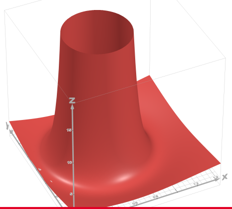
$$J_o(x,y) = \frac{1}{2\sigma_o^2}\left(i_{\text{obs}} - \frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2$$

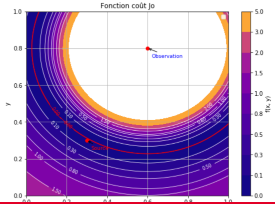
Uniqueness of the minimum: source localization



$$J_o(x,y) = \frac{1}{2\sigma_o^2}\left(i_{\text{obs}} - \frac{1}{(x^o-x)^2+(y^o-y)^2+\tau}\right)^2$$

$$\nabla J_o(x,y) = (0,0) \quad \Longleftrightarrow \quad \left\{ \begin{array}{ll} M(x,y) = M^{\text{obs}} & (\text{max of } J_o) \\ S \in \text{circle of center } M^{\text{obs}} \text{ and radius } \rho_o = \sqrt{\dfrac{1}{i_{\text{obs}}} - \tau} & (\text{min of } J_o\text{: } J_o(S)=0) \end{array} \right.$$



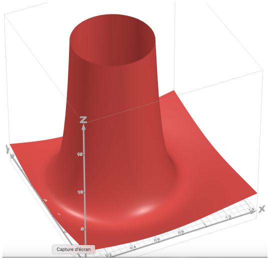


Infinite number of minima since the problem is underdetermined: 1 only observation and 2 values to estimate

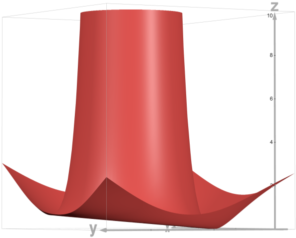
Uniqueness of the minimum: source localization

Effect of the background term

$$
\begin{aligned}
J(x,y) &= J_b(x) + J_o(x) \\
&= \frac{1}{2\sigma_b^2}\left((x-x_b)^2 + (y-y_b)^2 \right) + \frac{1}{2\sigma_o^2}\left(i_{\text{obs}} - \frac{1}{(x^o-x)^2+(y^o-y)^2+\tau} \right)^2
\end{aligned}
$$

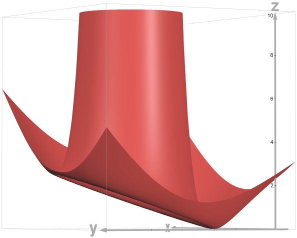


$J_o(x,y)$



$J_o(x,y) + J_b(x,y)$

$\sigma_b^2 = 1$



$J_o(x,y) + J_b(x,y)$

$\sigma_b^2 = 0.5$

Nonlinearity, chaos and all that sort of thing

Nous devons envisager l'état de l'Univers comme l'effet de son état antérieur et la cause de ce qui va suivre. Une intelligence qui pour un instant donné connaîtrait toutes les forces dont la nature est animée et la situation respective des êtres qui la composent, si d'ailleurs elle était assez vaste pour soumettre ces données à l'analyse, embrasserait dans la même formule le mouvement des plus grands corps de l'Univers et ceux du plus léger atome : rien ne serait incertain pour elle, l'avenir comme le passé serait présent à ses yeux.

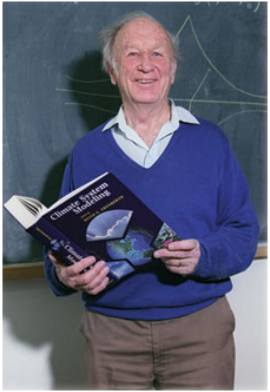
Pierre-Simon Laplace, *Essai philosophique sur les probabilités*, 1814

Pourquoi les météorologistes ont-ils tant de peine à prédire le temps avec quelque certitude ? [...] Nous voyons que les grandes perturbations se produisent généralement dans les régions où l'atmosphère est en équilibre instable. Les météorologistes voient bien que cet équilibre est instable, qu'un cyclone va naître quelque part ; mais où, ils sont hors d'état de le dire ; un dixième de degré en plus ou en moins en un point quelconque, le cyclone éclate ici et non pas là, et il étend ses ravages sur des contrées qu'il aurait épargnées. Si on avait connu ce dixième de degré, on aurait pu le savoir d'avance, mais les observations n'étaient ni assez serrées, ni assez précises, et c'est pour cela que tout semble dû à l'intervention du hasard. Ici encore nous retrouvons le même contraste entre une cause minime, inappréciable pour l'observateur, et des effets considérables, qui sont quelquefois d'épouvantables désastres.

Henri Poincaré, *Science et méthode*, 1908

Nonlinearity, chaos and all that sort of thing

A system is chaotic if a slight modification in the initial condition implies a large change in the solution.



Edward Lorenz
(1917-2008)

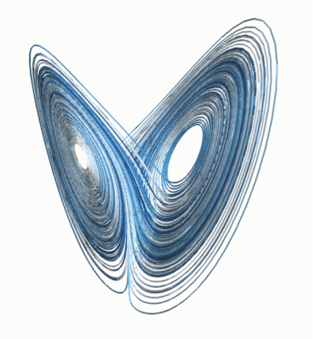
Nonlinearity, chaos and all that sort of thing

The historical Lorenz system (1963)

Edward Lorenz
(1917-2008)

Ellen Fetter
(1940 –)

$$\begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = \alpha(x_2 - x_1) \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = \beta x_1 - x_2 - x_1 x_3 \\ \dfrac{\mathrm{d}x_3}{\mathrm{d}t} = -\gamma x_3 + x_1 x_2 \end{cases}$$



Does the flap of a butterfly's wings in Brazil set off a tornado in Texas?

(139th meeting of the American Association for the Advancement of Science, 1972)

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
  $\longrightarrow$ uniqueness of the minimum?

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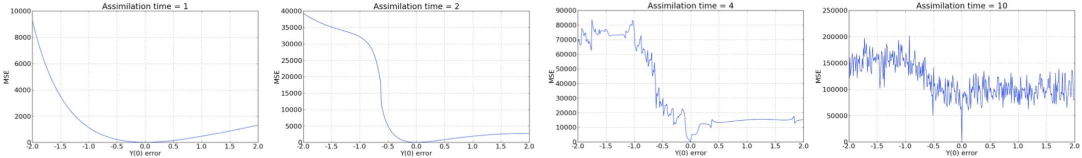
Lorenz system, observation of x_1, control of $x_2(t=0)$: $J_o(x_2(t=0)) = \dfrac{1}{2}\displaystyle\sum_{i=1}^{N}(x_1(t_i) - x_{1,\mathrm{obs}}(t_i))^2$



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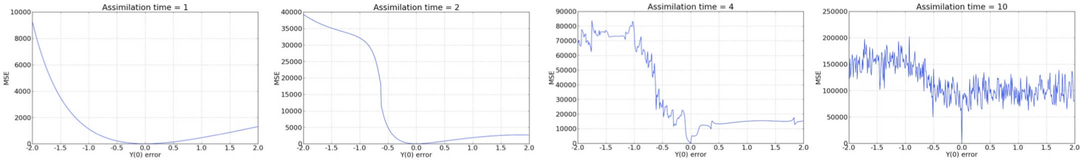
  $\longrightarrow$ uniqueness of the minimum?

Lorenz system, observation of x_1, control of $x_2(t=0)$: $J_o(x_2(t=0)) = \dfrac{1}{2}\displaystyle\sum_{i=1}^{N}\left(x_1(t_i) - x_{1,\mathrm{obs}}(t_i)\right)^2$

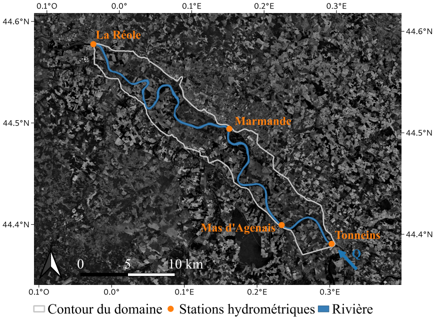


- Adding J_b makes it "more quadratic" (J_b is a regularization term), but $J = J_o + J_b$ may however have several local minima.

Example: calibration of roughness coefficients for a flood model

Numerical simulation of a river flood

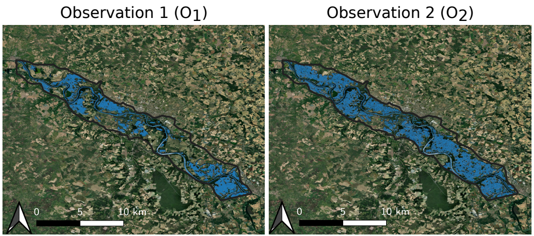
PhD thesis of Jean-Paul Travers, LNHE, 14 October 2025

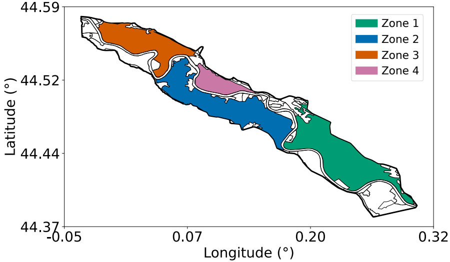


Example: calibration of roughness coefficients for a flood model

- Shallow water model (Telemac 2D)
- Assimilation of satellite images
- Control of roughness coefficients

$$\begin{cases} \dfrac{\partial h}{\partial t} + \dfrac{\partial (hu)}{\partial x} + \dfrac{\partial (hv)}{\partial y} = 0 \\ \dfrac{\partial (hu)}{\partial t} + \dfrac{\partial (hu^2)}{\partial x} + \dfrac{\partial (huv)}{\partial y} = -gh\dfrac{\partial \eta}{\partial x} - \dfrac{gQ^2}{{K_s}^2 h^{7/3}} + \dfrac{h}{\rho}F_x + \nabla\cdot(h\nu_e\nabla u) \\ \dfrac{\partial (hv)}{\partial t} + \dfrac{\partial (huv)}{\partial x} + \dfrac{\partial (hv^2)}{\partial y} = -gh\dfrac{\partial \eta}{\partial y} - \dfrac{gQ^2}{{K_s}^2 h^{7/3}} + \dfrac{h}{\rho}F_y + \nabla\cdot(h\nu_e\nabla v) \end{cases}$$





Example: calibration of roughness coefficients for a flood model

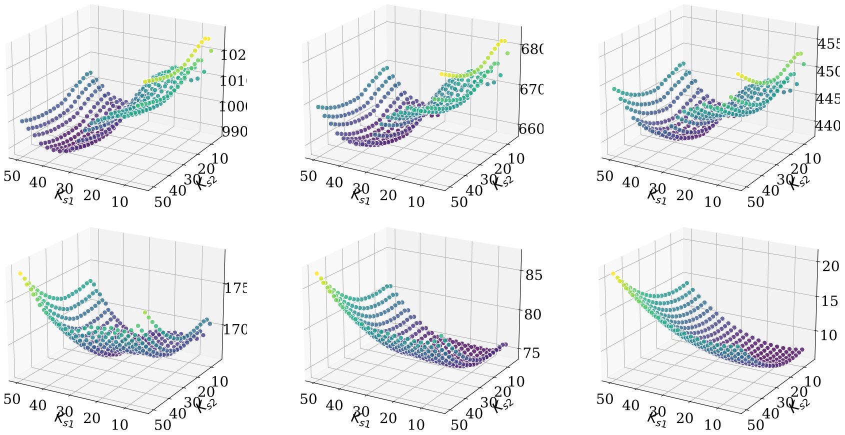
$J = J_b + \omega J_o$

—

Sections

$J(K_1, K_2, \bar{K}_3, \bar{K}_4)$

$\omega = 1520$ $\omega = 1010$ $\omega = 671$



$\omega = 253$ $\omega = 112$ $\omega = 10$

A fundamental remark

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 variational data assimilation lies in the definition of J.

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

Example: comparing two flood maps

- Many different possible distances...

List of Evaluated Geometric Performance Measures

Name	Method type	[Min, max, perfect value] description
Hausdorff distance (d_H)	Distance based	[0, ∞, 0] Maximum distance between points of two sets
Modified Hausdorff distance (d_{MH})	Distance based	[0, ∞, 0] Mean of the distances from each point in one set to the closest point in the other set
Procrustes analysis (P^2)	Shape alignment	[0, ∞, 0] Euclidean distance between shapes after rotation, scaling, and rotation
Sliced-Wasserstein distance (W_2)	Distribution based	[0, ∞, 0] Distance between probability distributions
Normalized Mutual Information (NMI)	Information theory	[1, 2, 2] Quantifies similarity using entropy
Flood Skill Score (FSS_n)	Neighborhood	[0, 1, 1] Quantifies overlap by comparing the flooded fraction over multiple neighborhood scales

Most Widely Used Performance Measures for Pixel-To-Pixel Comparison Based on the Confusion Matrix Adapted From Grimaldi et al. (2016)

Name	Evaluation	[Min, max, perfect value] description
False positive rate (FPR)/Precision (F)	$FP/(FP + TN)$	[0, 1, 0] Proportion of overprediction of flooded areas
True positive rate (TPR)/Recall (H)	$TP/(TP + FN)$	[0, 1, 1] Proportion correct of observed flooded areas
Positive predictive value (PPV)	$TP/(TP + FP)$	[0, 1, 1] Proportion of positive pixels that are true positive
Negative predictive value (NPV)	$TN/(FN + TN)$	[0, 1, 1] Proportion of negative pixels that are true negative
Peirce skill score (PSS)	H-F	[−1, 1, 1] Maximizing the difference between H and F
Accuracy (ACC)	$(TP + TN)/(TP + FP + TN + FN)$	[0, 1, 1] Proportion correct of total domain area
Fβ-score	$(1 + \beta^2)\cdot(H\cdot F)/(\beta^2\cdot F + H)$	[0, 1, 1] Combine precision and recall
Matthews correlation coefficient (MCC)	$\frac{TP\cdot TN - FP\cdot FN}{\sqrt{(TP+FP)\cdot(TP+FN)\cdot(TN+FP)\cdot(TN+FN)}}$	[−1, 1, 1] Balance of the four categories
Bias (B)	$(TP + FP)/(TP + FN)$	[0, ∞, 1] Ratio highlighting over/underprediction
Critical success index (CSI)	$TP/(TP + FP + FN)$	[0, 1, 1] Adaptation of ACC to focus on flooded areas
$F^{<3>}$	$(TP - FN)/(TP + FP + FN)$	[−1, 1, 1] Designed to penalize underprediction of flooded areas
$F^{<4>}$/Measure of fit	$(TP - FP)/(TP + FP + FN)$	[−1, 1, 1] Designed to penalize overprediction of flooded areas
Cohen's Kappa formula (κ)	$\frac{2\cdot(TP\cdot TN - FN\cdot FP)}{(TP+FP)\cdot(FP+TN)+(TP+FN)\cdot(FN+TN)}$	[−1, 1, 1] Balance of the four categories

Example: comparing two flood maps

- Many different possible distances...
- ... which do not quantify the same aspects...

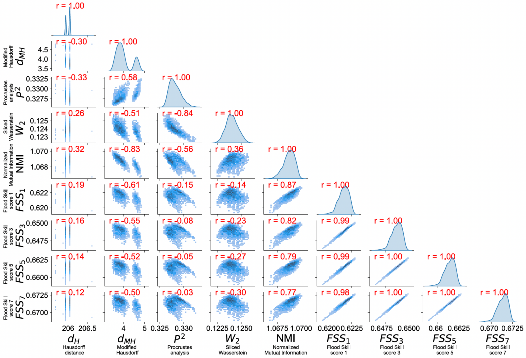


Figure 12. Scatter plots for geometric performance measures when evaluating the reference flood map with 4,000 simulated flood maps, with r being the Pearson correlation coefficient.

Example: comparing two flood maps

- Many different possible distances...
- ... which do not quantify the same aspects...
- ... and do not have the same properties.

Summary of the Metaverification Process for Pixel-To-Pixel and Geometric Comparisons

Pixel-to-pixel	FPR	TPR	PPV	NPV	PSS	ACC	$\beta = 1$	$\beta = 1.5$	$\beta = 2$	MCC	B	CSI	$\mathbf{F}^{<3>}$	$\mathbf{F}^{<4>}$	κ
Magnitude	×	×	×	×	✓	✓	∼	∼	∼	✓	✓	∼	∼	✓	✓
Translation	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Rotation	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	✓	✓	✓
Noise	×	✓	×	✓	✓	✓	✓	✓	✓	✓	×	✓	✓	✓	✓
Time	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

Geometric	$\mathbf{d_H}$	$\mathbf{d_{MH}}$	$\mathbf{P^2}$	$\mathbf{W_2}$	NMI	$\mathbf{FSS_1}$	$\mathbf{FSS_3}$	$\mathbf{FSS_5}$	$\mathbf{FSS_7}$
Magnitude	✓	✓	∼	✓	✓	∼	∼	∼	∼
Translation	×	✓	×	×	✓	✓	✓	✓	✓
Rotation	✓	✓	✓	✓	✓	✓	✓	✓	✓
Noise	×	✓	✓	✓	✓	✓	✓	✓	✓
Time	✓	✓	∼	✓	✓	×	×	×	×

Note. × = rejected by the criterion, ✓ = accepted by the criterion, and ∼ = in between.

Example: comparing two flood maps

- Many different possible distances...
- ... which do not quantify the same aspects...
- ... and do not have the same properties.

Water Resources Research®

RESEARCH ARTICLE

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Evaluation of Performance Measures for Comparing Flood Models With Satellite Observations

J.-P. Travert[1,2], S. Boyaval[2,3], C. Goeury[1,2], V. Bacchi[1], and F. Zaoui[1]

[1]EDF R&D, Laboratoire National d'Hydraulique et Environnement (LNHE), Chatou, France, [2]Laboratoire d'Hydraulique Saint-Venant (LHSV), ENPC, Institut Polytechnique de Paris, EDF R&D, Chatou, France, [3]Inria, Paris, France

Key Points:

- A methodology is reported to select a performance measure; for numerical comparison between flood models and satellite observation data

Minimizing J in the linear case

$$J(\mathbf{x}) = J_b(\mathbf{x}) + J_o(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})$$

Minimizing J in the linear case

$$J(\mathbf{x}) = J_b(\mathbf{x}) + J_o(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})$$

- Based on the Moore-Penrose inverse (least square problem)

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).

Proof of the Moore-Penrose inverse

$$J(\mathbf{x}) = \|\mathbf{Mx} - \mathbf{b}\|^2 = (\mathbf{Mx} - \mathbf{b})^T(\mathbf{Mx} - \mathbf{b}) \qquad \text{with } \mathbf{M}(p \times n) \text{ and } \mathbf{b} \in \mathbf{R}^p.$$

It uses two simple tools:

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

$$\frac{\partial J}{\partial \mathbf{d}}(\mathbf{x}) = \widehat{J}[\mathbf{x}](\mathbf{d}) = \lim_{\alpha \to 0} \frac{J(\mathbf{x} + \alpha \mathbf{d}) - J(\mathbf{x})}{\alpha}$$

- Gradient and directional derivative $\quad \dfrac{\partial J}{\partial \mathbf{d}}(\mathbf{x}) = \langle \nabla J(\mathbf{x}), \mathbf{d} \rangle$

Proof of the Moore-Penrose inverse

$$\begin{aligned} J(\mathbf{x}+\alpha\,\delta\mathbf{x}) &= (\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b})^T(\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b}) \\ &= (\mathbf{M}\mathbf{x}-\mathbf{b})^T(\mathbf{M}\mathbf{x}-\mathbf{b})+\alpha\left[(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{M}\mathbf{x}-\mathbf{b})+(\mathbf{M}\mathbf{x}-\mathbf{b})^T\mathbf{M}\delta\mathbf{x}\right]+\alpha^2\ (\ldots) \\ &= (\mathbf{M}\mathbf{x}-\mathbf{b})^T(\mathbf{M}\mathbf{x}-\mathbf{b})+2\alpha(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{M}\mathbf{x}-\mathbf{b})+\alpha^2\ (\ldots) \end{aligned}$$

Proof of the Moore-Penrose inverse

$$
\begin{aligned}
J(\mathbf{x}+\alpha\,\delta\mathbf{x}) &= (\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b})^T(\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b}) \\
&= (\mathbf{Mx}-\mathbf{b})^T(\mathbf{Mx}-\mathbf{b}) + \alpha\left[(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + (\mathbf{Mx}-\mathbf{b})^T\mathbf{M}\delta\mathbf{x}\right] + \alpha^2\ (\ldots) \\
&= (\mathbf{Mx}-\mathbf{b})^T(\mathbf{Mx}-\mathbf{b}) + 2\alpha(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + \alpha^2\ (\ldots)
\end{aligned}
$$

Hence $\dfrac{J(\mathbf{x}+\alpha\,\delta\mathbf{x})-J(\mathbf{x})}{\alpha} = 2\,(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + \alpha\ (\ldots) \quad\longrightarrow\quad 2\,(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b})$ as $\alpha\to 0$

i.e. $\dfrac{\partial J}{\partial\delta\mathbf{x}}(\mathbf{x}) = \langle\nabla J(\mathbf{x}),\delta\mathbf{x}\rangle = 2\,\delta\mathbf{x}^T\mathbf{M}^T(\mathbf{Mx}-\mathbf{b}) = \left\langle\delta\mathbf{x}, 2\,\mathbf{M}^T(\mathbf{Mx}-\mathbf{b})\right\rangle$

By identification: $\nabla J(\mathbf{x}) = 2\,\mathbf{M}^T(\mathbf{Mx}-\mathbf{b})$

Proof of the Moore-Penrose inverse

$$\begin{aligned} J(\mathbf{x}+\alpha\,\delta\mathbf{x}) &= (\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b})^T(\mathbf{M}(\mathbf{x}+\alpha\,\delta\mathbf{x})-\mathbf{b}) \\ &= (\mathbf{Mx}-\mathbf{b})^T(\mathbf{Mx}-\mathbf{b}) + \alpha\left[(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + (\mathbf{Mx}-\mathbf{b})^T\mathbf{M}\delta\mathbf{x}\right] + \alpha^2\ (\ldots) \\ &= (\mathbf{Mx}-\mathbf{b})^T(\mathbf{Mx}-\mathbf{b}) + 2\alpha(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + \alpha^2\ (\ldots) \end{aligned}$$

Hence $\quad \dfrac{J(\mathbf{x}+\alpha\,\delta\mathbf{x})-J(\mathbf{x})}{\alpha} = 2\,(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b}) + \alpha\ (\ldots) \quad\longrightarrow\quad 2\,(\mathbf{M}\,\delta\mathbf{x})^T(\mathbf{Mx}-\mathbf{b})$ as $\alpha\to 0$

i.e. $\quad \dfrac{\partial J}{\partial\delta\mathbf{x}}(\mathbf{x}) = \langle\nabla J(\mathbf{x}),\delta\mathbf{x}\rangle = 2\,\delta\mathbf{x}^T\mathbf{M}^T(\mathbf{Mx}-\mathbf{b}) = \left\langle\delta\mathbf{x}, 2\,\mathbf{M}^T(\mathbf{Mx}-\mathbf{b})\right\rangle$

By identification: $\quad \nabla J(\mathbf{x}) = 2\,\mathbf{M}^T(\mathbf{Mx}-\mathbf{b})$

$\nabla J(\mathbf{x}) = 0 \quad\Longleftrightarrow\quad \mathbf{M}^T\mathbf{Mx} = \mathbf{M}^T\mathbf{b}$, i.e. for $\hat{\mathbf{x}} = \mathbf{M}^+\mathbf{b}$ with $\mathbf{M}^+ = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$

Minimizing J in the linear case

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 $p \geq n$)*

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

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

(make $\mathbf{M} \longrightarrow \mathbf{N}^{1/2}\mathbf{M}$ and $\mathbf{b} \longrightarrow \mathbf{N}^{1/2}\mathbf{b}$ in the previous theorem)

Minimizing J in the linear case

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

For data assimilation: $J_o(\mathbf{x}) = \dfrac{1}{2}(\mathbf{Hx}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{Hx}-\mathbf{y}) \longrightarrow \hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\,\mathbf{y}$

Minimizing J in the linear case

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

For data assimilation: $J_o(\mathbf{x}) = \dfrac{1}{2}(\mathbf{Hx}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{Hx}-\mathbf{y}) \longrightarrow \hat{\mathbf{x}} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\,\mathbf{y}$

Similarly:

$$\begin{aligned} J(\mathbf{x}) &= \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}(\mathbf{Hx}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{Hx}-\mathbf{y}) \\ &= \frac{1}{2}(\mathbf{Mx}-\mathbf{b})^T\mathbf{N}\,(\mathbf{Mx}-\mathbf{b}) \end{aligned}$$

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

Remark: The gain matrix also reads $\mathbf{BH}^T(\mathbf{HBH}^T+\mathbf{R})^{-1}$ (Sherman-Morrison-Woodbury formula)

Minimizing J in the linear case

$$J(\mathbf{x}) = J_b(\mathbf{x}) + J_o(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})$$

- **Optimal estimation** $\mathbf{x}^a = \mathbf{x}^b + \underbrace{(\mathbf{B}^{-1}+\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}}_{\text{gain matrix}} \underbrace{(\mathbf{y}-\mathbf{H}\mathbf{x}^b)}_{\text{innovation vector}}$

Minimizing J in the linear case

$$J(\mathbf{x}) = J_b(\mathbf{x}) + J_o(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(\mathbf{H}\mathbf{x}-\mathbf{y})^T\mathbf{R}^{-1}(\mathbf{H}\mathbf{x}-\mathbf{y})$$

- **Optimal estimation** $\mathbf{x}^a = \mathbf{x}^b + \underbrace{(\mathbf{B}^{-1}+\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}}_{\text{gain matrix}} \quad \underbrace{(\mathbf{y}-\mathbf{H}\mathbf{x}^b)}_{\text{innovation vector}}$

- **Time dependent case**

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}_0-\mathbf{x}^b) + \frac{1}{2}\sum_{i=1}^{N}[\mathbf{y}_i-\mathbf{H}_i\mathbf{M}_{0,i}\mathbf{x}_0]^T\,\mathbf{R}_i^{-1}\,[\mathbf{y}_i-\mathbf{H}_i\mathbf{M}_{0,i}\mathbf{x}_0]$$

$$\mathbf{x}_0^a = \mathbf{x}^b + \left[\mathbf{B}^{-1}+\sum_{i=1}^{N}\mathbf{M}_{0,i}^T\mathbf{H}_i^T\mathbf{R}_i^{-1}\mathbf{H}_i\mathbf{M}_{0,i}\right]^{-1}\sum_{i=1}^{N}\mathbf{M}_{0,i}^T\mathbf{H}_i^T\mathbf{R}_i^{-1}(\mathbf{y}_i-\mathbf{H}_i\mathbf{M}_{0,i}\mathbf{x}^b)$$

Minimizing J

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 $\mathbf{x}^a$), the computation of $\mathbf{x}^a$ is performed using an optimization algorithm.

Implementation: *adjoint model, 3D-VAR, 3D-FGAT, 4D-VAR, incremental 4D-VAR...*

Generalization:
linear statistical approach

Generalization: linear statistical approach

To be estimated $\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbf{R}^n$ Observations $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_p \end{pmatrix} \in \mathbf{R}^p$

Linear observation operator $\mathbf{y} \equiv H(\mathbf{x}) = \mathbf{Hx}$

Statistical framework

- $\mathbf{y}$ is a realization of a random vector $\mathbf{Y}$, with covariance $\mathbf{R}$
- One is looking for the BLUE, i.e. a random variable $\mathbf{X}^a$ that is
  - **linear**: $\mathbf{X}^a = \mathbf{AY}$ with $\text{size}(\mathbf{A}) = (n, p)$
  - **unbiased**: $E(\mathbf{X}^a) = \mathbf{x}$
  - **of minimal variance**: $\text{Var}(\mathbf{X}^a) = \sum_{i=1}^{n} \text{Var}(X_i^a)$ minimum

Generalization: linear statistical approach

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  - **linear**: $\mathbf{X}^a = \mathbf{A}\mathbf{Y}$ with $\mathrm{size}(\mathbf{A}) = (n, p)$
  - **unbiased**: $E(\mathbf{X}^a) = \mathbf{x}$
  - **of minimal variance**: $\mathrm{Var}(\mathbf{X}^a) = \sum_{i=1}^{n} \mathrm{Var}(X_i^a)$ minimum

$$\mathbf{A} = (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}$$

(Gauss-Markov theorem)

Generalization: linear statistical approach

Background: $\mathbf{X}^b = \mathbf{x} + \varepsilon^b$ and new observations: $\mathbf{Y} = H(\mathbf{x}) + \varepsilon^o$

Hypotheses:

- $H(\mathbf{x}) = \mathbf{H}\mathbf{x}$ linear observation operator
- $E(\varepsilon^b) = 0$ and $E(\varepsilon^o) = 0$ unbiased background and observations
- $\mathrm{Cov}(\varepsilon^b, \varepsilon^o) = 0$ independent background and observation errors
- $\mathrm{Cov}(\varepsilon^b) = \mathbf{B}$ and $\mathrm{Cov}(\varepsilon^o) = \mathbf{R}$ known accuracies and covariances

BLUE

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

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

Link with the variational approach

Statistical approach: BLUE

$$\mathbf{X}^a = \mathbf{X}^b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{Y} - \mathbf{H}\mathbf{X}^b) \qquad \text{with } \mathrm{Cov}(\mathbf{X}^a) = (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}$$

Variational approach in the linear case

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

$$\min_{\mathbf{x}\in\mathbf{R}^n} J(\mathbf{x}) \quad \longrightarrow \quad \mathbf{x}^a = \mathbf{x}^b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^b\right)$$

Link with the variational approach

Statistical approach: BLUE

$$\mathbf{X}^a = \mathbf{X}^b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{Y} - \mathbf{H}\mathbf{X}^b) \qquad \text{with } \mathrm{Cov}(\mathbf{X}^a) = (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}$$

Variational approach in the linear case

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

$$\min_{\mathbf{x}\in\mathbf{R}^n} J(\mathbf{x}) \quad \longrightarrow \quad \mathbf{x}^a = \mathbf{x}^b + (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^b\right)$$

Same remarks as previously

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

If the problem is time dependent

Dynamical system $\mathbf{x}^t(t_{i+1}) = \mathbf{M}_{i,i+1}\mathbf{x}^t(t_i) + \varepsilon^m(t_i)$

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- Direct application of the BLUE on $[t_0, t_N]$ (hyp: $\varepsilon^m = 0$):

$$\mathbf{x}^a = \mathbf{x}^b + \left[\mathbf{B}^{-1} + \sum_{i=1}^{N} \mathbf{M}_{0,i}^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{M}_{0,i}\right]^{-1} \sum_{i=1}^{N} \mathbf{M}_{0,i}^T \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathbf{y}_i - \mathbf{H}_i \mathbf{M}_{0,i} \mathbf{x}^b)$$

$\longrightarrow$ equivalent to the 4D variational approach

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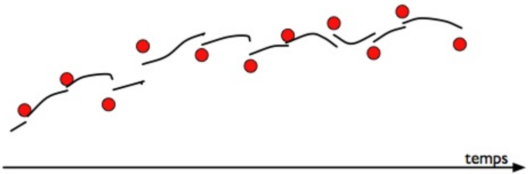
$\longrightarrow$ equivalent to the 4D variational approach

- Sequential application of the BLUE every observation time: $\longrightarrow$ Kalman filter



Rudolf Kalman
(1930-2016)

Kalman filter

Hypotheses

- $\varepsilon^m(t_i)$ is unbiased, with covariance matrix $\mathbf{Q}_i$. $\varepsilon^m(t_i)$ and $\varepsilon^m(t_j)$ are independent $(i \neq j)$.
- Unbiased observation $\mathbf{y}_i$, with error covariance matrix $\mathbf{R}_i$ (no Gaussian hypotheses
- $\varepsilon^m(t_i)$ and analysis error $\mathbf{x}^a(t_i) - \mathbf{x}^t(t_i)$ are independent on ε^o, ε^b, ε^m)

Evolution of the first two moments - Kalman filter

Initialization

$$\begin{aligned} \mathbf{x}^a(t_0) &= \mathbf{x}^b \\ \mathbf{P}^a(t_0) &= \mathbf{B} \end{aligned}$$

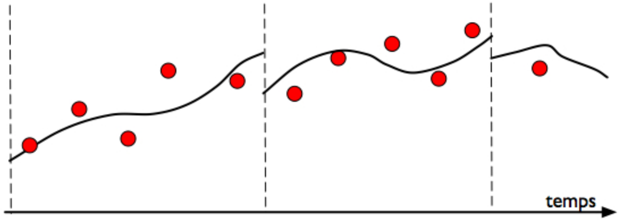
Step i *(prediction - correction, or forecast - analysis)*

$$\begin{aligned} \mathbf{x}^f(t_{i+1}) &= \mathbf{M}_{i,i+1}\,\mathbf{x}^a(t_i) & \text{Forecast} \\ \mathbf{P}^f(t_{i+1}) &= \mathbf{M}_{i,i+1}\,\mathbf{P}^a(t_i)\,\mathbf{M}^T_{i,i+1} + \mathbf{Q}_i \end{aligned}$$

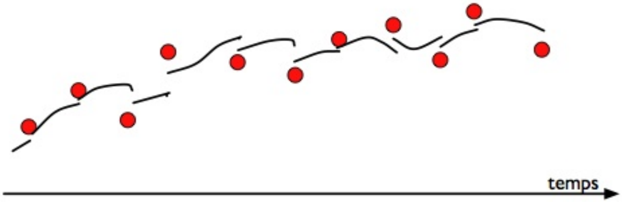
$$\begin{aligned} \mathbf{x}^a(t_{i+1}) &= \mathbf{x}^f(t_{i+1}) + \mathbf{K}_{i+1}\left[\mathbf{y}_{i+1} - \mathbf{H}_{i+1}\mathbf{x}^f(t_{i+1})\right] & \text{BLUE} \\ \mathbf{K}_{i+1} &= \mathbf{P}^f(t_{i+1})\mathbf{H}^T_{i+1}\left[\mathbf{H}_{i+1}\mathbf{P}^f(t_{i+1})\mathbf{H}^T_{i+1} + \mathbf{R}_{i+1}\right]^{-1}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

Kalman filter and 4D-Var

4D-Var



Kalman filter

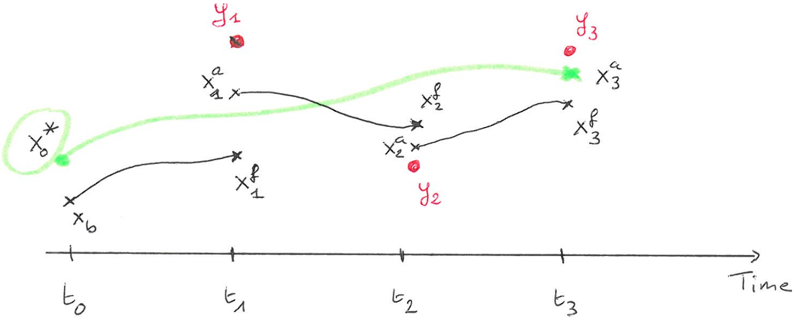


Kalman filter and 4D-Var

If $\mathbf{H}_i$ and $\mathbf{M}_{i,i+1}$ are linear, and if the model is perfect ($\varepsilon^m(t_i) = 0$), then the Kalman filter and the variational method minimizing

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathbf{H}_i\mathbf{M}_{0,i}\mathbf{x}_0 - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{M}_{0,i}\mathbf{x}_0 - \mathbf{y}_i)$$

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



Generalization:
Bayesian approach

Generalization: Bayesian approach

Several types of problem:

- Filtering $p(\mathbf{X}_N|\mathbf{Y}_{1:N} = \mathbf{y}_{1:N})$
- Forecast $p(\mathbf{X}_l|\mathbf{Y}_{1:N} = \mathbf{y}_{1:N}) \qquad (l > N)$
- Smoothing all other cases.
  - $p(\mathbf{X}_l|\mathbf{Y}_{1:N} = \mathbf{y}_{1:N}) \quad (l < N)$ fixed-point smoothing
  - $p(\mathbf{X}_{0:N}|\mathbf{Y}_{1:N} = \mathbf{y}_{1:N})$ fixed-interval smoothing
  - ...

Generalization: Bayesian approach

Two tools:

- Bayes theorem $$P(X=x\,|\,Y=y)=\frac{\overbrace{P(Y=y\,|\,X=x)}^{\textit{likelihood}}\;\overbrace{P(X=x)}^{\textit{prior}}}{\underbrace{P(Y=y)}_{\textit{normalisation factor}}}$$

- Marginalization rule $$p(\mathbf{X})=\int p(\mathbf{X}|\ \mathbf{Z})\,p(\mathbf{Z})\,d\mathbf{Z}$$

And some usual hypotheses:

- ε^o is independent from past and present states
- ε^m is dependent at most of the present state, but not from past states

Generalization: Bayesian approach

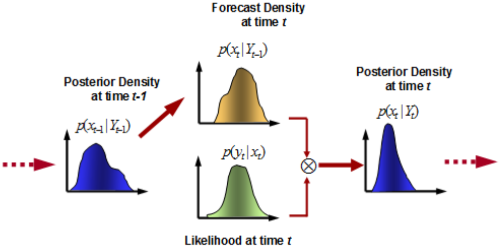
Filtering and forecast problems can be solved by a sequential algorithm alternating two phases:

- Analysis at time t_i :

$$p(\mathbf{X}_i = \mathbf{x}_i | \mathbf{Y}_{1:i} = \mathbf{y}_{1:i}) \propto p(\mathbf{Y}_i = \mathbf{y}_i | \mathbf{X}_i = \mathbf{x}_i)\, p(\mathbf{X}_i = \mathbf{x}_i | \mathbf{Y}_{1:i-1} = \mathbf{y}_{1:i-1})$$

- Forecast from t_i to t_{i+1} :

$$p(\mathbf{X}_{i+1} = \mathbf{x}_{i+1} | \mathbf{Y}_{1:i} = \mathbf{y}_{1:i}) = \int p(\mathbf{X}_{i+1} = \mathbf{x}_{i+1} | \mathbf{X}_i = \mathbf{x}_i)\, p(\mathbf{X}_i = \mathbf{x}_i | \mathbf{Y}_{1:i} = \mathbf{y}_{1:i})\, d\mathbf{x}_i$$



$$p(x_t | Y_t) = \frac{p(y_t | x_t)\, p(x_t | Y_{t-1})}{\int_{x_t} p(y_t | x_t)\, p(x_t | Y_{t-1})\, dx_t}$$

Generalization: Bayesian approach

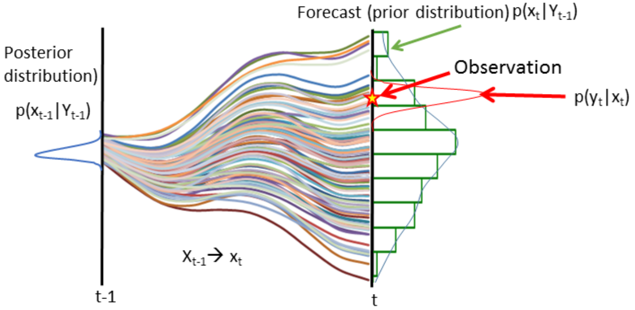
Links with previous methods

- The Kalman filter corresponds to the general Bayesian sequential algorithm in the case where errors are Gaussian, ε^m is independent from the present state, H and M are linear, and $\mathbf{X}_0 \rightsquigarrow \mathcal{N}(\mathbf{x}^b, \mathbf{B})$.

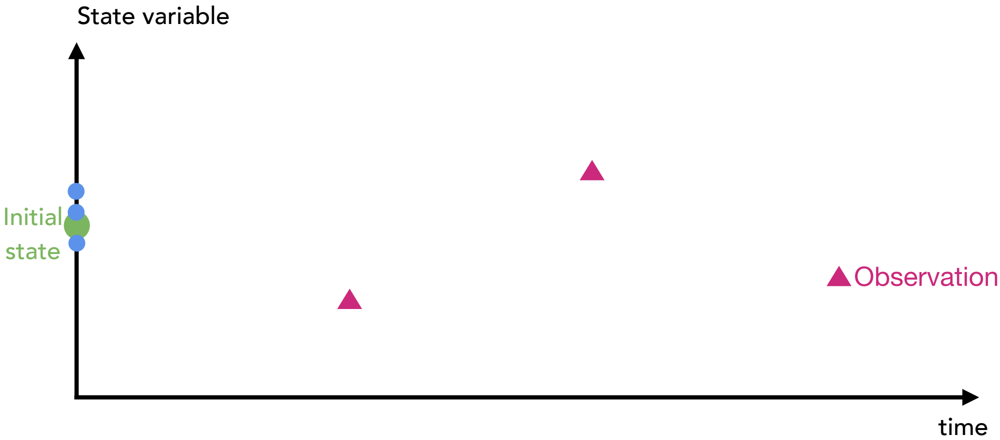
- Minimizing J in the variational approach is equivalent to looking for the mode of $p(\mathbf{X}_0 | \mathbf{Y}_{1:N} = \mathbf{y}_{1:N})$ if $\varepsilon^m = 0$, $\mathbf{X}_0 \rightsquigarrow \mathcal{N}(\mathbf{x}^b, \mathbf{B})$, and $\varepsilon_i^o \rightsquigarrow \mathcal{N}(\mathbf{0}, \mathbf{R}_i)$.

Implementation: ensemble methods (Monte Carlo approach)

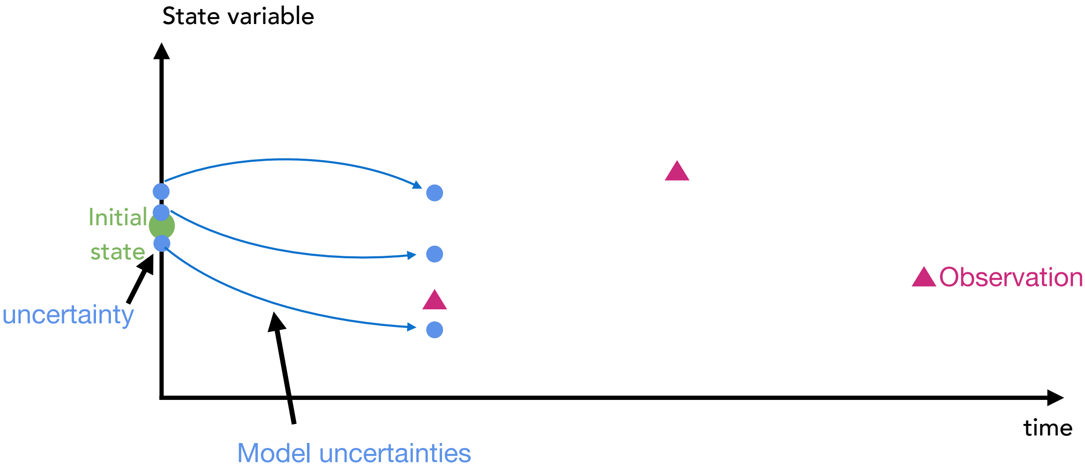
- Two main groups: *particle filters* and *Ensemble Kalman Filters*
- Differ mainly by their analysis step: *resampling methods* and *transformation methods*



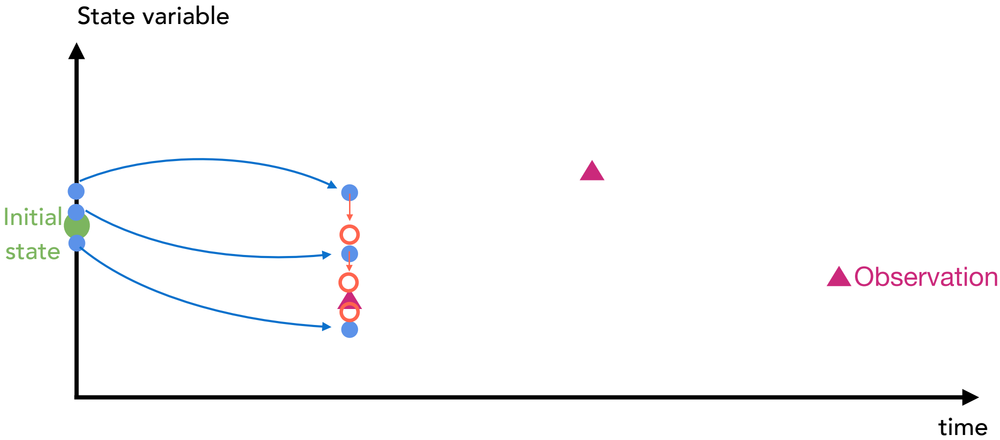
Implementation: ensemble methods (Monte Carlo approach)



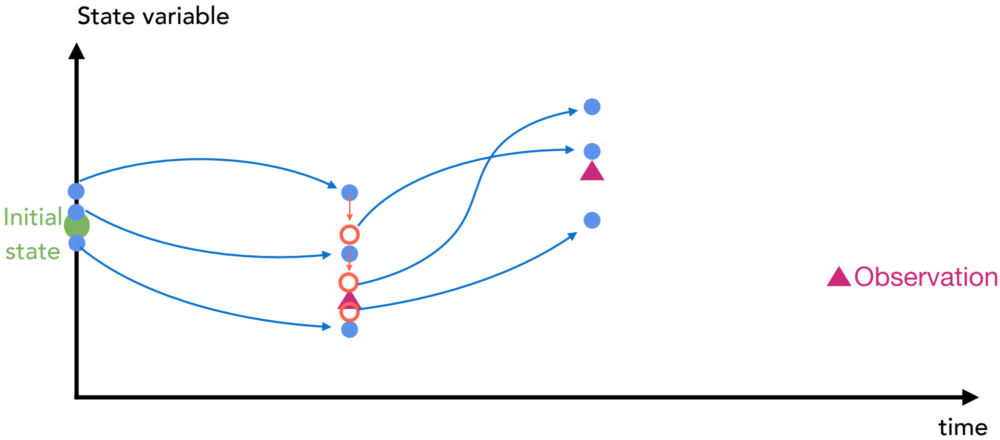
Implementation: ensemble methods (Monte Carlo approach)



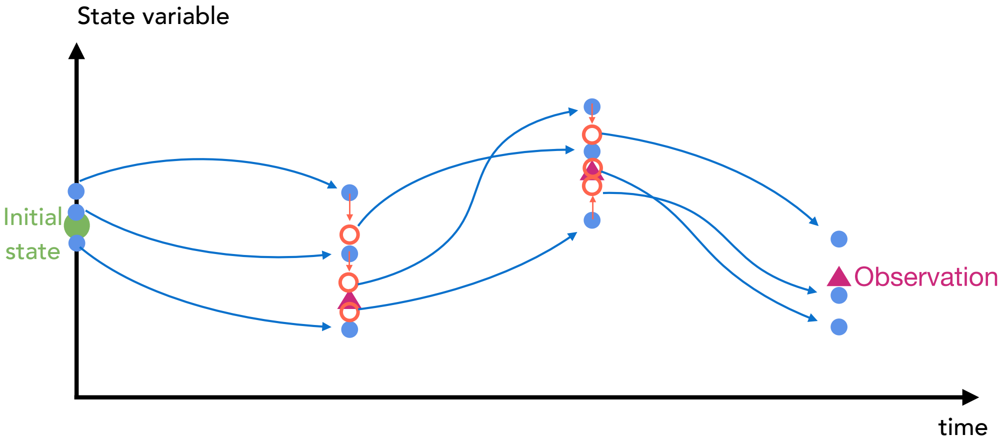
Implementation: ensemble methods (Monte Carlo approach)



Implementation: ensemble methods (Monte Carlo approach)

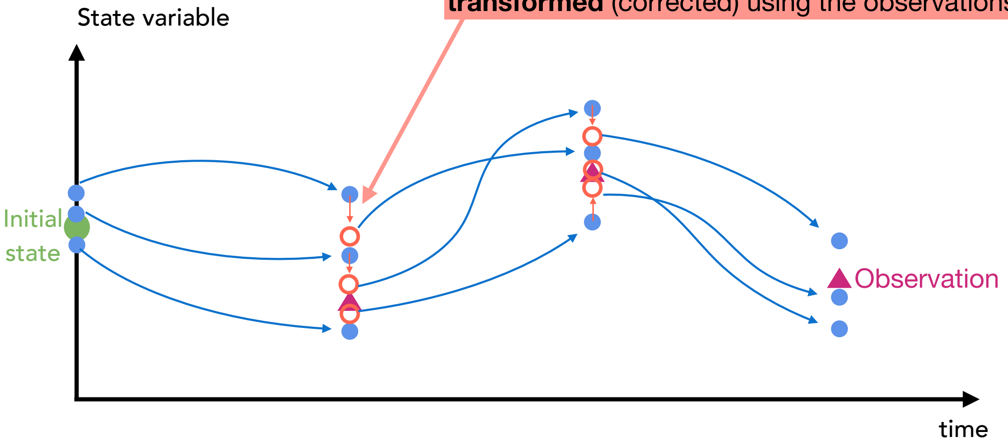


Implementation: ensemble methods (Monte Carlo approach)



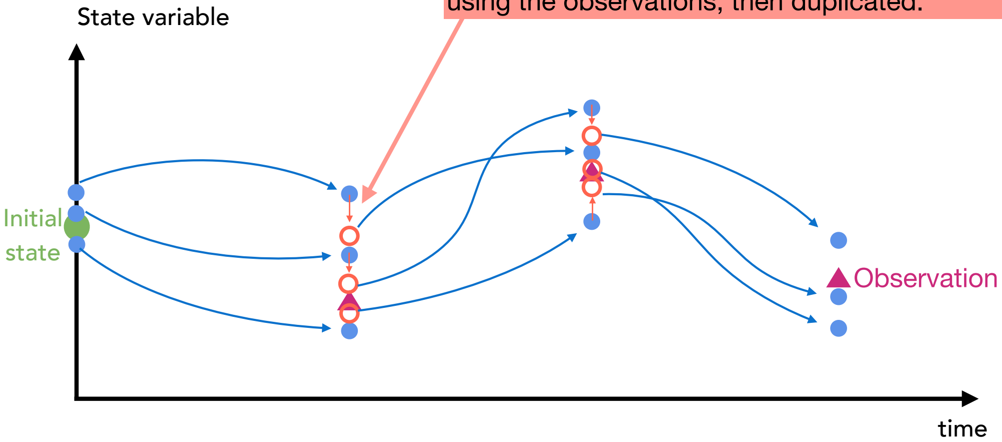
Implementation: ensemble methods (Monte Carlo approach)

In the **Ensemble Kalman** filter, the members are **transformed** (corrected) using the observations.



Implementation: ensemble methods (Monte Carlo approach)

In the **Particle** filter, the members are **selected** using the observations, then duplicated.



Minimization aspects

Minimizing J

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 $\mathbf{x}^a$), the computation of $\mathbf{x}^a$ is performed using an optimization algorithm.

Implementation: *adjoint model, 3D-VAR, 3D-FGAT, 4D-VAR, incremental 4D-VAR...*

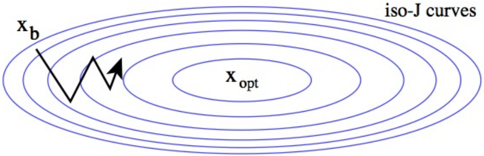
Minimizing J: descent methods

Minimizing J: descent methods

(thanks to Elise Arnaud)

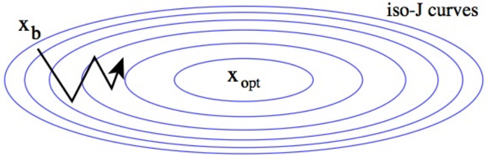
Minimizing J: descent methods

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



Minimizing J: descent methods

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



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

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

Getting the gradient is not obvious

- The simplest method: approximating the gradient by computing growth rates

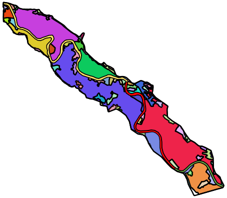
Example $\left\{ \begin{array}{l} \dfrac{d\mathbf{x}(t))}{dt} = M(\mathbf{x}(t)) \quad t \in [0, T] \\ \mathbf{x}(t=0) = \mathbf{u} \end{array} \right.$ with $\mathbf{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$

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

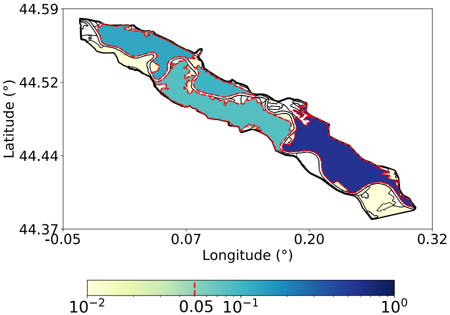
$$\nabla J(\mathbf{u}) = \begin{pmatrix} \dfrac{\partial J}{\partial u_1}(\mathbf{u}) \\ \vdots \\ \dfrac{\partial J}{\partial u_n}(\mathbf{u}) \end{pmatrix} \simeq \begin{pmatrix} [J(\mathbf{u} + \alpha\, \mathbf{e}_1) - J(\mathbf{u})] / \alpha \\ \vdots \\ [J(\mathbf{u} + \alpha\, \mathbf{e}_n) - J(\mathbf{u})] / \alpha \end{pmatrix} \qquad \longrightarrow n+1 \text{ model runs}$$

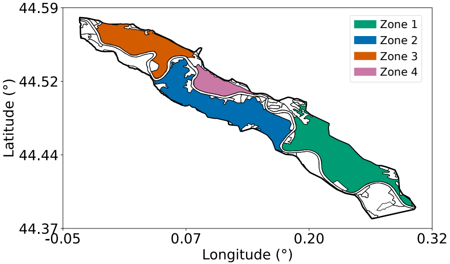
Example: calibration of roughness coefficients for a flood model

- Engineer's expertise: 92 subdomains with constant coefficient
- Evaluation of the gradient: 93 model runs (the adjoint of Telemac is not available) $\longrightarrow$ requires a reduction in the number of parameters $\longrightarrow$ sensitivity analysis



Total Sobol' index





Getting the gradient is not obvious

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

In such cases, the adjoint method provides an efficient way to compute ∇J.

It uses two simple tools:

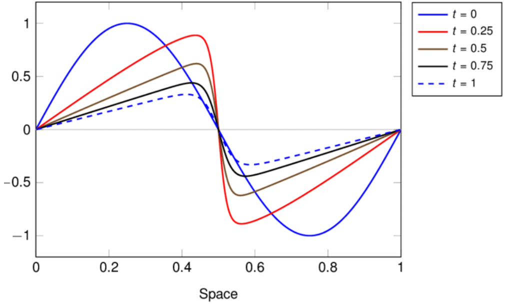
- Directional (or Gâteaux) derivative of f at point $\mathbf{x}$ in direction $\mathbf{d}$:

$$\frac{\partial J}{\partial \mathbf{d}}(\mathbf{x}) = \widehat{J}[\mathbf{x}](\mathbf{d}) = \lim_{\alpha \to 0} \frac{J(\mathbf{x} + \alpha \mathbf{d}) - J(\mathbf{x})}{\alpha}$$

- Gradient and directional derivative $\quad \dfrac{\partial J}{\partial \mathbf{d}}(\mathbf{x}) = (\nabla J(\mathbf{x}), \mathbf{d})$

Example: an adjoint for the viscous Burgers' equation

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



- $u^{obs}(x, t)$ an observation of $u(x, t)$
- Cost function:

$$J(u_0) = \frac{1}{2} \int_0^T \int_0^L \left(u(x, t) - u^{obs}(x, t)\right)^2 \, dx\, dt$$

Step 1: directional derivative of J

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

$$\begin{aligned} \frac{J(u_0+\alpha\,\delta u_0) - J(u_0)}{\alpha} &= \frac{1}{2\alpha}\int_0^T\!\!\int_0^L \left[(\tilde u - u^{\mathrm{obs}})^2 - (u-u^{\mathrm{obs}})^2\right] \\ &= \int_0^T\!\!\int_0^L \frac{\tilde u + u - 2u^{\mathrm{obs}}}{2}\,\frac{\tilde u - u}{\alpha} \end{aligned}$$

$$\alpha \to 0 \;:\; \frac{\partial J}{\partial \delta u_0}(u_0) = \langle \nabla J(u_0), \delta u_0\rangle = \int_0^T\!\!\int_0^L (u-u^{\mathrm{obs}})\;\widehat{u} \qquad \text{with } \widehat{u} = \lim_{\alpha\to 0}\frac{\tilde u - u}{\alpha} = \frac{\partial u}{\partial \delta u_0}$$

Step 1: directional derivative of J

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

$$\begin{aligned}\frac{J(u_0+\alpha\,\delta u_0)-J(u_0)}{\alpha} &= \frac{1}{2\alpha}\int_0^T\int_0^L\left[(\tilde u-u^{\text{obs}})^2-(u-u^{\text{obs}})^2\right]\\ &= \int_0^T\int_0^L \frac{\tilde u+u-2u^{\text{obs}}}{2}\;\frac{\tilde u-u}{\alpha}\end{aligned}$$

$$\alpha\to 0\ :\ \frac{\partial J}{\partial \delta u_0}(u_0)=\langle\nabla J(u_0),\delta u_0\rangle=\int_0^T\int_0^L (u-u^{\text{obs}})\ \widehat u \qquad \text{with } \widehat u=\lim_{\alpha\to 0}\frac{\tilde u-u}{\alpha}=\frac{\partial u}{\partial \delta u_0}$$

$\longrightarrow$ need information on $\widehat u$

Step 2: directional derivative of u - tangent linear model

$$\frac{(\tilde{S})-(S)}{\alpha}: \quad \left\{ \begin{array}{l} \dfrac{\partial\left(\frac{\tilde{u}-u}{\alpha}\right)}{\partial t} + \left(\dfrac{\tilde{u}-u}{\alpha}\right)\dfrac{\partial u}{\partial x} + \tilde{u}\,\dfrac{\partial\left(\frac{\tilde{u}-u}{\alpha}\right)}{\partial x} - \nu\,\dfrac{\partial^2\left(\frac{\tilde{u}-u}{\alpha}\right)}{\partial x^2} = 0 \quad x\in]0,L[,\, t\in[0,T] \\ \left(\dfrac{\tilde{u}-u}{\alpha}\right)(0,t) = \left(\dfrac{\tilde{u}-u}{\alpha}\right)(L,t) = 0 \quad t\in[0,T] \\ \left(\dfrac{\tilde{u}-u}{\alpha}\right)(x,0) = \delta u_0 \quad x\in[0,L] \end{array} \right.$$

$$\alpha \to 0: \quad (TLM) \left\{ \begin{array}{ll} \dfrac{\partial\widehat{u}}{\partial t} + \dfrac{\partial(u\widehat{u})}{\partial x} - \nu\,\dfrac{\partial^2\widehat{u}}{\partial x^2} = 0 & x\in]0,L[,\, t\in[0,T] \\ \widehat{u}(0,t) = \widehat{u}(L,t) = 0 & t\in[0,T] \\ \widehat{u}(x,0) = \delta u_0 & x\in[0,L] \end{array} \right.$$

tangent linear model

Step 2: directional derivative of u - tangent linear model

$$\frac{(\tilde S)-(S)}{\alpha}: \quad \begin{cases} \dfrac{\partial\left(\frac{\tilde u - u}{\alpha}\right)}{\partial t} + \left(\dfrac{\tilde u - u}{\alpha}\right)\dfrac{\partial u}{\partial x} + \tilde u \,\dfrac{\partial\left(\frac{\tilde u - u}{\alpha}\right)}{\partial x} - \nu\,\dfrac{\partial^2\left(\frac{\tilde u - u}{\alpha}\right)}{\partial x^2} = 0 & x \in]0,L[,\, t\in[0,T] \\ \left(\dfrac{\tilde u - u}{\alpha}\right)(0,t) = \left(\dfrac{\tilde u - u}{\alpha}\right)(L,t) = 0 & t \in [0,T] \\ \left(\dfrac{\tilde u - u}{\alpha}\right)(x,0) = \delta u_0 & x\in[0,L] \end{cases}$$

$$\alpha \to 0: \quad (TLM) \begin{cases} \dfrac{\partial \widehat u}{\partial t} + \dfrac{\partial(u\widehat u)}{\partial x} - \nu \dfrac{\partial^2 \widehat u}{\partial x^2} = 0 & x\in]0,L[,\, t\in[0,T] \\ \widehat u(0,t) = \widehat u(L,t) = 0 & t\in[0,T] \\ \widehat u(x,0) = \delta u_0 & x\in[0,L] \end{cases}$$

tangent linear model

TLM makes it possible to get $\displaystyle\int_0^T\int_0^L \left(u - u^{\text{obs}}\right)\,\widehat u \qquad \left(= \langle \nabla J(u_0), \delta u_0\rangle = \int_0^L \nabla J(u_0)(x)\,\delta u_0(x)\right)$

Step 3: adjoint model

$$\langle\,(TLM), p(x,t)\,\rangle : \qquad \int\int \frac{\partial \widehat{u}}{\partial t}\, p + \int\int \frac{\partial (u\widehat{u})}{\partial x}\, p - \nu \int\int \frac{\partial^2 \widehat{u}}{\partial x^2}\, p = 0$$

Integration by parts:

- $\displaystyle \int_0^T \frac{\partial \widehat{u}}{\partial t}\, p = \widehat{u}(.,T)\, p(.,T) - \underbrace{\widehat{u}(.,0)}_{\delta u_0}\, p(.,0) - \int_0^T \widehat{u}\, \frac{\partial p}{\partial t}$

- $\displaystyle \int_0^L \frac{\partial (u\widehat{u})}{\partial x}\, p = u(L,.)\,\underbrace{\widehat{u}(L,.)}_{=0}\, p(L,.) - u(0,.)\,\underbrace{\widehat{u}(0,.)}_{=0}\, p(0,.) - \int_0^L u\widehat{u}\, \frac{\partial p}{\partial x}$

- $\displaystyle \int_0^L \frac{\partial^2 \widehat{u}}{\partial x^2}\, p = \frac{\partial \widehat{u}}{\partial x}(L,.)\, p(L,.) - \frac{\partial \widehat{u}}{\partial x}(0,.)\, p(0,.) - \underbrace{\widehat{u}(L,.)}_{=0}\, \frac{\partial p}{\partial x}(L,.) + \underbrace{\widehat{u}(0,.)}_{=0}\, \frac{\partial p}{\partial x}(0,.) + \int_0^L \widehat{u}\, \frac{\partial^2 p}{\partial x^2}$

Hence

$$\int_0^T \int_0^L \widehat{u}\left(-\frac{\partial p}{\partial t} - u\frac{\partial p}{\partial x} - \nu\frac{\partial^2 p}{\partial x^2}\right) + \int_0^L \widehat{u}(.,T)\, p(.,T) + \int_0^T \frac{\partial \widehat{u}}{\partial x}(L,.)\, p(L,.) - \int_0^T \frac{\partial \widehat{u}}{\partial x}(0,.)\, p(0,.) = \int_0^L \delta u_0(.)\, p(.,0)$$

Step 3: adjoint model

In summary : $\displaystyle\int_0^T \int_0^L (u - u^{\text{obs}})\ \widehat{u} = \int_0^L \nabla J(u_0)(x)\, \delta u_0(x)$ and

$$\int_0^T \int_0^L \widehat{u} \left(-\frac{\partial p}{\partial t} - u\frac{\partial p}{\partial x} - \nu\,\frac{\partial^2 p}{\partial x^2}\right) + \int_0^L \widehat{u}(.,T)\, p(.,T) + \int_0^T \frac{\partial \widehat{u}}{\partial x}(L,.)\, p(L,.) - \int_0^T \frac{\partial \widehat{u}}{\partial x}(0,.)\, p(0,.) = \int_0^L \delta u_0(.)\, p(.,0)$$

Step 3: adjoint model

In summary : $\displaystyle\int_0^T\int_0^L (u-u^{\text{obs}})\;\widehat{u} = \int_0^L \nabla J(u_0)(x)\,\delta u_0(x)$ and

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Step 3: adjoint model

In summary : $\displaystyle\int_0^T\int_0^L (u-u^{\text{obs}})\ \hat{u} = \int_0^L \nabla J(u_0)(x)\,\delta u_0(x)$ and

$$\int_0^T\int_0^L \hat{u}\underbrace{\left(-\frac{\partial p}{\partial t} - u\frac{\partial p}{\partial x} - \nu\frac{\partial^2 p}{\partial x^2}\right)}_{u-u^{\text{obs}}} + \int_0^L \hat{u}(.,T)\ \underbrace{p(.,T)}_{=0} + \int_0^T \frac{\partial \hat{u}}{\partial x}(L,.)\ \underbrace{p(L,.)}_{=0} - \int_0^T \frac{\partial \hat{u}}{\partial x}(0,.)\ \underbrace{p(0,.)}_{=0} = \int_0^L \delta u_0(.)\,p(.,0)$$

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

adjoint model

Formally: $\langle\, TLM(\hat{u}), p\,\rangle = \langle\, \hat{u}, AD(p)\,\rangle$

Step 3: adjoint model

In summary : $\displaystyle\int_0^T\int_0^L (u-u^{\text{obs}})\;\widehat{u} = \int_0^L \nabla J(u_0)(x)\,\delta u_0(x)$ and

$$\int_0^T\int_0^L \widehat{u}\underbrace{\left(-\frac{\partial p}{\partial t} - u\frac{\partial p}{\partial x} - \nu\frac{\partial^2 p}{\partial x^2}\right)}_{u-u^{\text{obs}}} + \int_0^L \widehat{u}(.,T)\,\underbrace{p(.,T)}_{=0} + \int_0^T \frac{\partial \widehat{u}}{\partial x}(L,.)\,\underbrace{p(L,.)}_{=0} - \int_0^T \frac{\partial \widehat{u}}{\partial x}(0,.)\,\underbrace{p(0,.)}_{=0} = \int_0^L \delta u_0(.)\,p(.,0)$$

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

adjoint model

Formally: $\langle\, TLM(\widehat{u}), p\,\rangle = \langle\, \widehat{u}, AD(p)\,\rangle$

Conclusion: $\nabla J(u_0) = p(.,0)$

In summary

- Direct model

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

- Adjoint model

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

- Gradient $\quad \nabla J(u_0) = p(.,0)$

In summary

- Direct model

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

- Adjoint model

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

- Gradient $\quad \nabla J(u_0) = p(.,0)$

Discretized version: idem (integration by parts becomes change of index)

More generally

- **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** $J(U) = \dfrac{1}{2} \displaystyle\int_0^T \|H(X) - Y\|^2$

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.

More generally

Tangent linear model

$$\begin{cases} \dfrac{d\hat{X}(x,t)}{dt} = \mathbf{M}(\hat{X}) & (x,t) \in \Omega \times [0,T] \\ \hat{X}(x,0) = u(x) \end{cases}$$

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

Adjoint model

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

Gradient

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

The adjoint method

- The adjoint method provides an efficient way to compute ∇J.
- It 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.
- It requires writing a tangent linear code and an adjoint code:
  - obeys systematic rules
  - is not the most interesting task you can imagine
  - there exists automatic differentiation softwares $\longrightarrow$ cf http://www.autodiff.org
  - neural networks $\longrightarrow$ backward propagation
- Useful also for sensitivity analysis or stability analysis

To go a little bit further...

The main algorithms in short

Main methodological difficulties: non linearities, huge dimensions, poorly known error statistics, HPC issues...

- Variational methods
  - a series of approximations of the cost function, corresponding to a series of algorithms: 4DVar, incremental 4DVar, 3DFGAT, 3DVar
  - the more sophisticated ones (4DVar, incremental 4DVar) require the tangent linear and adjoint models (the development of which is a real investment). En4DVar algorithms try to avoid it.
- Statistical methods
  - Extended Kalman filter handles (weakly) non linear problems (requires the tangent linear model)
  - Reduced order Kalman filters address huge dimension problems
  - An efficient method, addressing both problems: ensemble Kalman filters (EnKF)
  - Particle filters: fully Bayesian approach - still limited to low dimension problems

Research directions

- Improved methods: more robust w.r.t. nonlinearities and/or non gaussianity, or without adjoint, or less expensive...
- Better management of errors (prior statistics, identification, a posteriori validation...)
- "Complex" observations (images, videos, Lagrangian data...)
- New application domains (often leading to new methodological questions)
- Definition of observing systems, sensitivity analysis...

- IA-based / IA-using approaches

Announcement

Doctoral course "Introduction to data assimilation"

- Grenoble, January 5-9, 2026
- Elise Arnaud, Eric Blayo, Arthur Vidard
- https://adum.fr/script/catalogue.pl?mod=3697784&site=CDUDG
- Just contact us if you are interested

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var

4D-Var

4D-Var algorithm corresponds to the minimization of

$$J(\mathbf{x}_0) = \frac{1}{2}\,(\mathbf{x}_0 - \mathbf{x}_0^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{i=0}^{N}(H_i(\mathbf{x}_i) - \mathbf{y}_i)^T\mathbf{R}_i^{-1}(H_i(\mathbf{x}_i) - \mathbf{y}_i)$$

Preconditioned cost function

Defining $\mathbf{v} = \mathbf{B}^{-1/2}\,(\mathbf{x} - \mathbf{x}^b)$, J becomes

$$J(\mathbf{v}_0) = \frac{1}{2}\,\mathbf{v}_0^T\mathbf{v}_0 + \frac{1}{2}\sum_{i=0}^{N}(H_i(\mathbf{B}^{1/2}\mathbf{v}_i + \mathbf{x}_i^b) - \mathbf{y}_i)^T\mathbf{R}_i^{-1}(H_i(\mathbf{B}^{1/2}\mathbf{v}_i + \mathbf{x}_i^b) - \mathbf{y}_i)$$

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var

The problem is written in terms of $\delta\mathbf{x}_0 = \mathbf{x}_0 - \mathbf{x}_0^b$, and

$$J(\mathbf{x}_0) = \frac{1}{2}\,(\mathbf{x}_0 - \mathbf{x}_0^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{i=0}^{N}(H_i(\mathbf{x}_i) - \mathbf{y}_i)^T\mathbf{R}_i^{-1}(H_i(\mathbf{x}_i) - \mathbf{y}_i)$$

is approximated by a series of quadratic cost functions:

$$J^{(k+1)}(\delta\mathbf{x}_0) = \frac{1}{2}\,\delta\mathbf{x}_0^T\mathbf{B}^{-1}\delta\mathbf{x}_0 + \frac{1}{2}\sum_{i=0}^{N}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_i - \mathbf{d}_i)^T\mathbf{R}_i^{-1}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_i - \mathbf{d}_i)$$

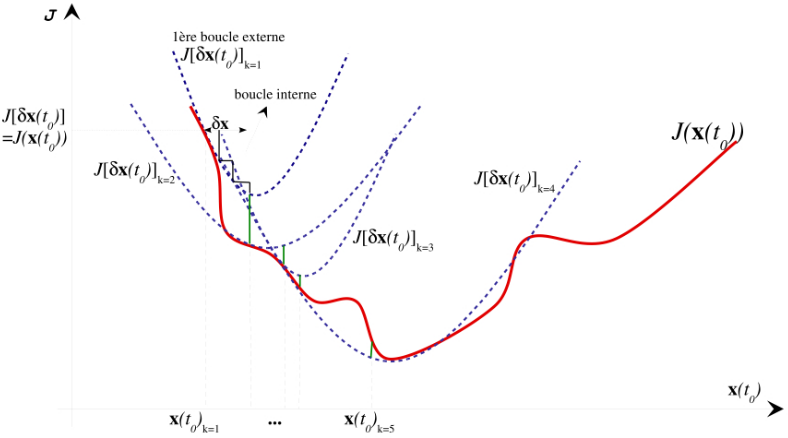
with $\delta\mathbf{x}_{i+1} = \mathbf{M}_{i,i+1}^{(k)}\delta\mathbf{x}_i$ and $\mathbf{d}_i = \mathbf{y}_i - H_i(\mathbf{x}_i^{(k)})$

- Kind of Gauss-Newton algorithm
- Tangent linear hypotheses must be satisfied:

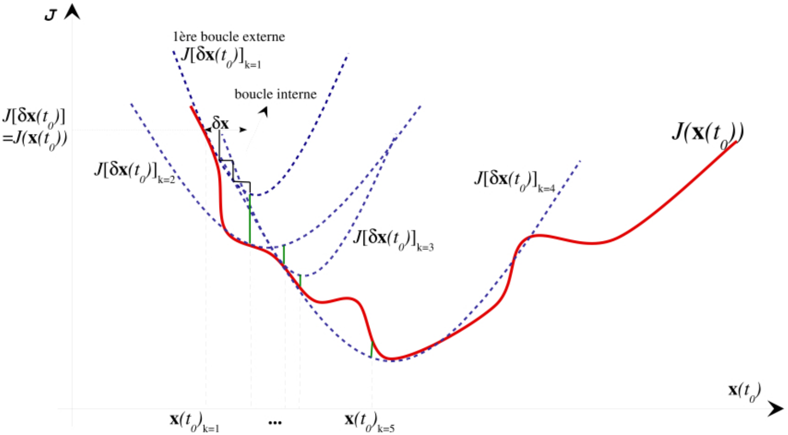
$$M(\mathbf{x}_0^{(k)} + \delta\mathbf{x}_0) \simeq M(\mathbf{x}_0^{(k)}) + \mathbf{M}^{(k)}\delta\mathbf{x}_0$$

$$H_i(\mathbf{x}_i^{(k)} + \delta\mathbf{x}_i) \simeq H_i(\mathbf{x}_i^{(k)}) + \mathbf{H}_i^{(k)}\delta\mathbf{x}_i$$

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var



4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var



Multi-incremental 4D-Var: inner loops can be made using some simplified physics and/or coarser resolution (Courtier et al. 1994, Courtier 1995, Veersé and Thépaut 1998, Trémolet 2005).

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var

The 3D-FGAT (First Guess at Appropriate Time) is an approximation of incremental 4D-Var where the tangent linear model is replaced by identity:

$$J^{(k+1)}(\delta \mathbf{x}_0) = \frac{1}{2}\, \delta \mathbf{x}_0^T \mathbf{B}^{-1} \delta \mathbf{x}_0 + \frac{1}{2} \sum_{i=0}^{N} (\mathbf{H}_i^{(k)} \delta \mathbf{x}_0 - \mathbf{d}_i)^T \mathbf{R}_i^{-1} (\mathbf{H}_i^{(k)} \delta \mathbf{x}_0 - \mathbf{d}_i)$$

$\longrightarrow$ something between 3D and 4D

Pros:

- much cheaper, does not require the adjoint model
- algorithm is close to incremental 4D-Var
- innovation is computed at the correct observation time

Cons: approximation!

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var

3D-Var: all observations are gathered as if they were all at time t_0.

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{i=0}^{N}(H_i(\mathbf{x}_0) - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(H_i(\mathbf{x}_0) - \mathbf{y}_i)$$

Pros: still cheaper
Cons: approximation!!

4D-Var / Incremental 4D-Var / 3D-FGAT / 3D-Var

3D-Var: all observations are gathered as if they were all at time t_0.

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{i=0}^{N}(H_i(\mathbf{x}_0) - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(H_i(\mathbf{x}_0) - \mathbf{y}_i)$$

Pros: still cheaper
Cons: approximation!!

Remark: 3D-Var = Optimal Interpolation = Krigging

Summary: simplifying $J \to$ a series of methods

4D-Var: $$J(\mathbf{x}_0) = \frac{1}{2}\,(\mathbf{x}_0 - \mathbf{x}_0^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\,\sum_{i=0}^{N}(H_i(\mathbf{x}_i) - \mathbf{y}_i)^T\mathbf{R}_i^{-1}(H_i(\mathbf{x}_i) - \mathbf{y}_i)$$

Incremental 4D-Var: $M(\mathbf{x}_0 + \delta\mathbf{x}_0) \simeq M(\mathbf{x}_0) + \mathbf{M}\delta\mathbf{x}_0$

$$J^{(k+1)}(\delta\mathbf{x}_0) = \frac{1}{2}\,\delta\mathbf{x}_0^T\mathbf{B}^{-1}\delta\mathbf{x}_0 + \frac{1}{2}\,\sum_{i=0}^{N}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_i - \mathbf{d}_i)^T\mathbf{R}_i^{-1}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_i - \mathbf{d}_i)$$

Multi-incremental 4D-Var: $M(\mathbf{x}_0 + \delta\mathbf{x}_0) \simeq M(\mathbf{x}_0) + \mathbf{S}^{-I}\mathbf{M}^L\delta\mathbf{x}_0^L$

$$J^{(k+1)}(\delta\mathbf{x}_0^L) = \frac{1}{2}\,(\delta\mathbf{x}_0^L)^T\mathbf{B}^{-1}\delta\mathbf{x}_0^L + \frac{1}{2}\,\sum_{i=0}^{N}(\mathbf{H}_i^{(k),L}\delta\mathbf{x}_i^L - \mathbf{d}_i)^T\mathbf{R}_i^{-1}(\mathbf{H}_i^{(k),L}\delta\mathbf{x}_i^L - \mathbf{d}_i)$$

3D-FGAT: $M(\mathbf{x}_0 + \delta\mathbf{x}_0) \simeq M(\mathbf{x}_0) + \delta\mathbf{x}_0$

$$J^{(k+1)}(\delta\mathbf{x}_0) = \frac{1}{2}\,\delta\mathbf{x}_0^T\mathbf{B}^{-1}\delta\mathbf{x}_0 + \frac{1}{2}\,\sum_{i=0}^{N}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_0 - \mathbf{d}_i)^T\mathbf{R}_i^{-1}(\mathbf{H}_i^{(k)}\delta\mathbf{x}_0 - \mathbf{d}_i)$$

3D-Var: $M(\mathbf{x}_0 + \delta\mathbf{x}_0) \simeq \mathbf{x}_0 + \delta\mathbf{x}_0$

$$J(\mathbf{x}_0) = \frac{1}{2}\,(\mathbf{x}_0 - \mathbf{x}_0^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\,\sum_{i=0}^{N}(H_i(\mathbf{x}_0) - \mathbf{y}_i)^T\mathbf{R}_i^{-1}(H_i(\mathbf{x}_0) - \mathbf{y}_i)$$

Non linearities: extended Kalman filter

The Kalman filter assumes that M and H are linear. If not: linearization

$$\mathbf{x}^f_{k+1} = M_{k,k+1}(\mathbf{x}^a_k) \simeq M_{k,k+1}(\mathbf{x}^t_k) + \mathbf{M}_{k,k+1} \underbrace{(\mathbf{x}^a_k - \mathbf{x}^t_k)}_{\mathbf{e}^a_k}$$

$$\Longrightarrow \quad \mathbf{x}^f_{k+1} - \mathbf{x}^t_{k+1} = \mathbf{e}^f_{k+1} = \underbrace{M_{k,k+1}(\mathbf{x}^t_k) - \mathbf{x}^t_{k+1}}_{\mathbf{e}_k} + \mathbf{M}_{k,k+1}\mathbf{e}^a_k$$

$$\Longrightarrow \quad \mathbf{P}^f_{k+1} = \mathrm{Cov}(\mathbf{e}^f_{k+1}) = \mathbf{M}_{k,k+1}\mathbf{P}^a_k\mathbf{M}^T_{k,k+1} + \mathbf{Q}_k$$

and similarly for the other equations of the filter

Non linearities: extended Kalman filter

Extended Kalman filter

Initialization:

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

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

$$\begin{array}{rcll} \mathbf{x}^f_{k+1} & = & M_{k,k+1}(\mathbf{x}^a_k) & \text{Forecast} \\ \mathbf{P}^f_{k+1} & = & \mathbf{M}_{k,k+1}\mathbf{P}^a_k\mathbf{M}^T_{k,k+1} + \mathbf{Q}_k & \end{array}$$

$$\begin{array}{rcll} \mathbf{x}^a_{k+1} & = & \mathbf{x}^f_{k+1} + \mathbf{K}_{k+1}\left[\mathbf{y}_{k+1} - H_{k+1}(\mathbf{x}^f_{k+1})\right] & \text{BLUE analysis} \\ \mathbf{K}_{k+1} & = & \mathbf{P}^f_{k+1}\mathbf{H}^T_{k+1}\left[\mathbf{H}_{k+1}\mathbf{P}^f_{k+1}\mathbf{H}^T_{k+1} + \mathbf{R}_{k+1}\right]^{-1} & \\ \mathbf{P}^a_{k+1} & = & \mathbf{P}^f_{k+1} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{P}^f_{k+1} & \end{array}$$

Non linearities: extended Kalman filter

Extended Kalman filter

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)*

$$\begin{aligned} \mathbf{x}^f_{k+1} &= M_{k,k+1}(\mathbf{x}^a_k) && \text{Forecast} \\ \mathbf{P}^f_{k+1} &= \mathbf{M}_{k,k+1}\mathbf{P}^a_k\mathbf{M}^T_{k,k+1} + \mathbf{Q}_k \end{aligned}$$

$$\begin{aligned} \mathbf{x}^a_{k+1} &= \mathbf{x}^f_{k+1} + \mathbf{K}_{k+1}\left[\mathbf{y}_{k+1} - H_{k+1}(\mathbf{x}^f_{k+1})\right] && \text{BLUE analysis} \\ \mathbf{K}_{k+1} &= \mathbf{P}^f_{k+1}\mathbf{H}^T_{k+1}\left[\mathbf{H}_{k+1}\mathbf{P}^f_{k+1}\mathbf{H}^T_{k+1} + \mathbf{R}_{k+1}\right]^{-1} \\ \mathbf{P}^a_{k+1} &= \mathbf{P}^f_{k+1} - \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{P}^f_{k+1} \end{aligned}$$

- OK if nonlinearities are not too strong
- Requires the availability of $\mathbf{M}_{k,k+1}$ and $\mathbf{H}_k$
- More sophisticated approaches have been developed $\longrightarrow$ unscented Kalman filter (exact up to second order, requires no tangent linear model nor Hessian matrix)

Huge dimension: reduced order filters

As soon as $[\mathbf{x}]$ becomes huge, it's no longer possible to handle the covariance matrices.

Idea: a large part of the system variability can be represented (or is assumed to) in a reduced dimension space.

$\longrightarrow$ RRSQRT filter, SEEK filter, SEIK filter...

Huge dimension: reduced order filters

Example: Reduced Rank SQuare Root filter

- $\mathbf{P}_0^f \simeq \mathbf{S}_0^f \left(\mathbf{S}_0^f\right)^T$ with $\text{size}(\mathbf{S}_0^f) = (n, r)$ (r leading modes, $r \ll n$)
- This is injected in the filter equations. This leads for instance to $\mathbf{P}_k^a = \mathbf{S}_k^a \left(\mathbf{S}_k^a\right)^T$, with

$$\mathbf{S}_k^a = \underbrace{\mathbf{S}_k^f}_{(n,r)} \left(\underbrace{\mathbf{I}_r - \mathbf{\Psi}_k^T [\mathbf{\Psi}_k \mathbf{\Psi}_k^T + \mathbf{R}_k]^{-1} \mathbf{\Psi}_k}_{(r,r)} \right)^{1/2} \qquad \text{where } \mathbf{\Psi}_k = \underbrace{\mathbf{H}_k \mathbf{S}_k^f}_{(p,r)}$$

Pros: most computations in low dimension
Cons: choice and time evolution of the modes

The Ensemble Kalman filter

- addresses both problems of non linearities and huge dimension
- rather simple and intuitive

Idea: generation of an ensemble of N trajectories, by N perturbations of the set of observations (consistently with $\mathbf{R}$). Standard extended Kalman filter, with covariance matrices computed using the ensemble:

$$\mathbf{P}_k^f = \frac{1}{N-1}\sum_{j=1}^{N}(\mathbf{x}_{j,k}^f - \bar{x}_k^f)(\mathbf{x}_{j,k}^f - \bar{x}_k^f)^T \text{ with } \bar{x}_k^f = \frac{1}{N}\sum_{j=1}^{N}\mathbf{x}_{j,k}^f$$

$$\mathbf{P}_k^a = \frac{1}{N-1}\sum_{j=1}^{N}(\mathbf{x}_{j,k}^a - \bar{x}_k^a)(\mathbf{x}_{j,k}^f - \bar{x}_k^f)^T \text{ with } \bar{x}_k^a = \frac{1}{N}\sum_{j=1}^{N}\mathbf{x}_{j,k}^a$$