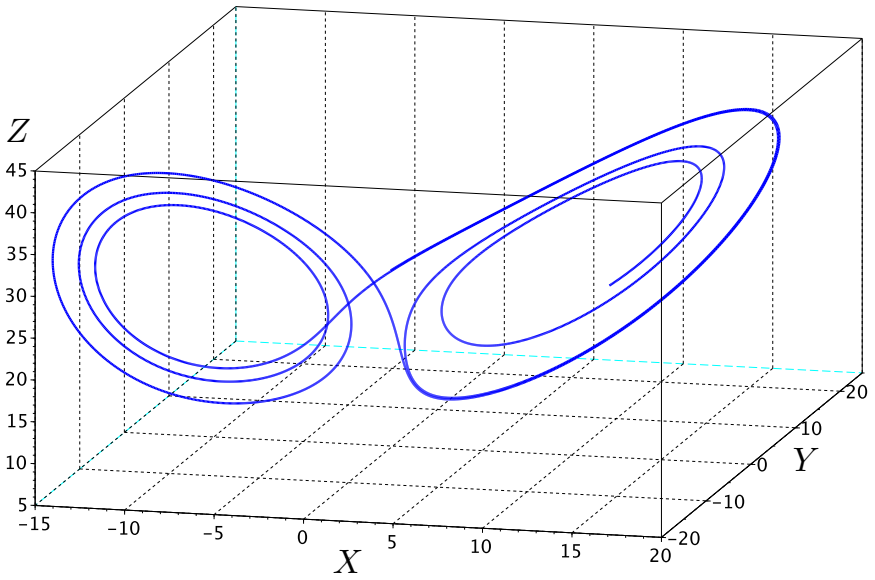
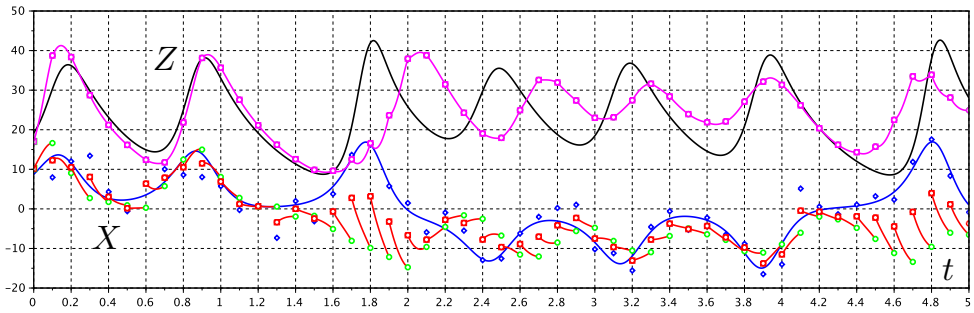
Olivier THUAL

Data assimilation for engineers





Toulouse INP - ENSEEIHT

"Fluid Mechanics, Energetics and Environment" Department

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Preamble

These notes are to be used in two M2 courses:

- "Mathematical methods for data exploitation" in the Teaching Unit "Big data and geosciences".
- "Data assimilation" in the Teaching Unit "Numerical methods for scientific computing in aerodynamics".

An online course can be found at the following reference:

[1] O. THUAL, Introduction to Data Assimilation for Scientists and Engineers, *Open Learn. Res. Ed. INP* **0202** (2013) 6h
`http://pedagotech.inp-toulouse.fr/130202`

The present notes provides improvement with respect to this resource.

See also the bibliography at the end of these notes.

Contents

Introduction

Data assimilation is at the meeting point of physical modelling, uncertainty analysis and mathematical algorithm (Figure 1). Given measurements with error and considering that modelling cannot be exact, the purpose of data assimilation is to mix these different sources of information with the proper weighting. Engineer applications based on modelling are making a growing use of data assimilation techniques with the increase of quantitative informations on the physical system and computer performances:

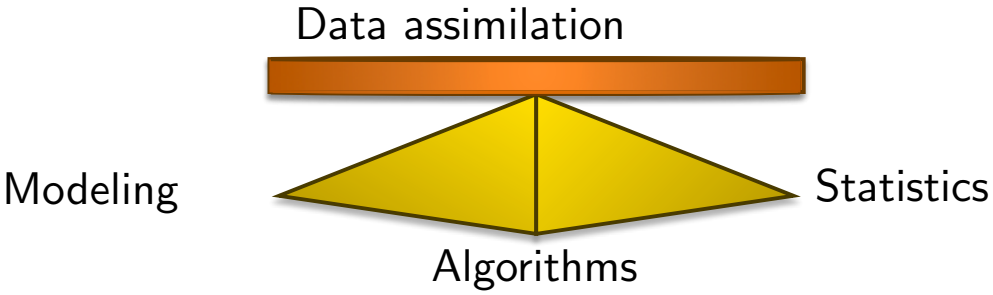

Figure 1: *Data assimilation is at the crossroad of several topics.*

In these notes, we will stress the following issues:

- Data assimilation combines the information issued from a model and observations;
- The information weight is proportional the inverses of square of their errors;
- Data assimilation is part of modeling for a wide variety of applications.

Chapter 1

From weather forecast to engineer applications

Contents

Introduction

With the drastic increase of data and computer perfomance, the modelling of physical systems is no longer reduced to a single numerical simulation of a system of equations. The engineer must take into account uncertainties, for instance through a large number of numerical simulations, and include informations coming from measurements of the physical system. The combination of data information and physical modelling, takin into account uncertainties, is called "data assimilation". Beyond weather forecast, which pioneered the field, numerous applications benefit from the progress of the data assimilation theory that mixes physical modelling, statistical analysis and algorithms. A series a example of increasing complexity is presented here to introduce this theory.

1 How is weather forecasted

The growing number of real time meteorological measurements, combined to the growing complexity of atmosphere numerical models, has necessitated sophisticated method to combine all the available information. Data assimilation enables to determine to best estimation of the present weather, which is then used as the initial condition to make forecasts.

1.1 An atmospheric model

A satellite picture of clouds provides a realistic feeling of weather (Figure 1.1). The principal meteorological fields are winds, pressure, temperature and humidity. Meteorology is among the most complex fluid mechanics flows.

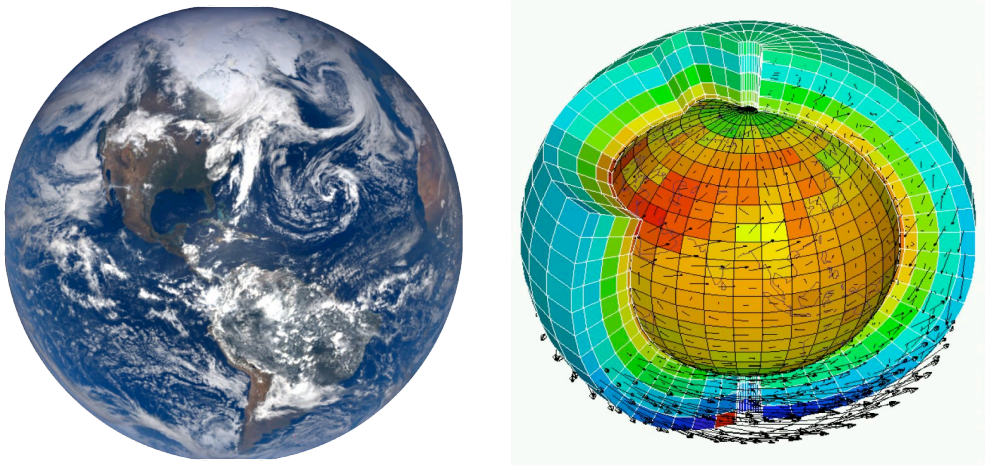

Figure 1.1: *Satelitte picture and numerical grid of an atmospheric model.*

Numerical simulations of the atmosphere dynamics are performed with models in which time and physical fields are discretized. The dynamics of the atmosphere is governed by fundamental laws such as mass, momentum or energy conservation. Subgrid processes are parametrized.

1.2 Measurements feeding a chain of forecast

Numerous observations of the atmosphere are constantly collected around the world. Satellite data have significantly increased the knowledge of atmosphere dynamics. In-situ data inequally covers the surface of the globe as well as vertical columns.

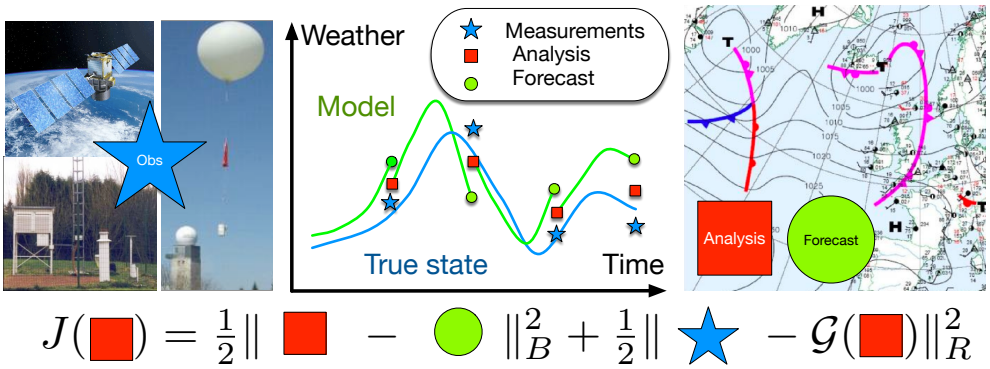

Figure 1.2: *Data assimilation chain in which the analysis minimizes the distances to both the measurements and the previous forecast.*

An analysis of the present weather combines information from both the model and observations, thanks to data assimilation. Weather forecast are performed by numerical simulation of the model, starting from this analysis. The analysis minimizes a combination J of distances (figure 1.2), where the "observation operator" $\mathcal{G}$ and the metrics B and R will be defined in the following.

The model provides a forecast from which the observation operator extracts quantities which are compared to actual data observation. The analysis is a field that combines these observations with the model forecast. It is then used as an initial condition for the next forecast. This adjustment is repeated at fixed time intervals.

1.3 Two century of data assimilation

Key features of the birth of data assimilation can be summarized as follow:

- End of the XVIII$^{\text{th}}$ century:
  - Planet orbit computations by Gauss
  - Least square method by Legendre
- Begining of the XX$^{\text{th}}$ century:
  - Concept of maximum likelyhood by Fisher
- Mid of the XX$^{\text{th}}$ century:
  - Kalman filter for the APOLLO program
  - Objective analysis of meteorological fields
- End of the XX$^{\text{th}}$ century:

– 3D-Var data assimilation method for weather forecast model
– Gain of 20% forecast quality at Météo-France going to 4D-Var (see Figure 1.3)

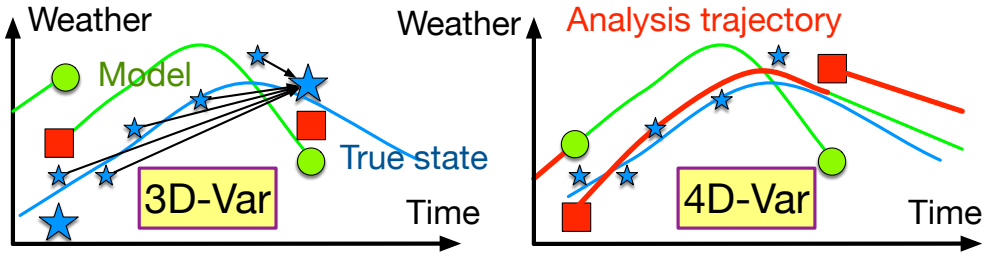

Figure 1.3: *3D-Var and 4D-Var.*

2 Other examples of data assimilation applications

2.1 The standard formalism of data assimilation

Most of the standard data assimilation methods can be presented with the following elements (Figure 1.4):

- A control space of column vectors $\underline{x} \in I\!R^N$;
- An observation space of column vectors $\underline{y} \in I\!R^M$;
- A control operator $\mathcal{G}$ linking the control space to the; observation space through the relation $\underline{y} = \mathcal{G}(\underline{x})$;
- A background $\underline{x}^b$ in the control space;
- Measurements $\underline{y}^o$ in the observation space.

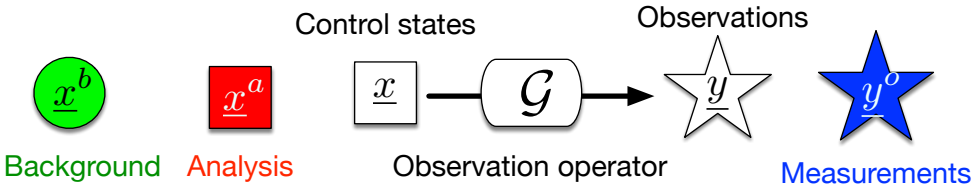

Figure 1.4: *The observation operator $\mathcal{G}$ links control and observation spaces.*

The analysis $\underline{x}^a$ is the state that minimizes the following cost function

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x} - \underline{x}^b\right)^T \underline{\underline{B}}^{-1}\left(\underline{x} - \underline{x}^b\right) + \frac{1}{2}\left[\underline{y}^o - \mathcal{G}(\underline{x})\right]^T \underline{\underline{R}}^{-1}\left[\underline{y}^o - \mathcal{G}(\underline{x})\right] \ , \quad (1.1)$$

where the metrics B and R are given by the following symmetric matrices:

- The $N \times N$ "background error covariance matrix" $\underline{\underline{B}}$;
- The $M \times M$ "observation error covariance matrix" $\underline{\underline{R}}$.

The cost function associates a real number to any vector $\underline{x}$ of the control space, given a background $\underline{x}^b$ state and a vector $\underline{y}^o$ of the observation space. The artificial observation $\underline{y} = \mathcal{G}(\underline{x})$ is "extracted" from the vector $\underline{x}$ through the observation operator $\mathcal{G}$.

The control space can contain the initial conditions of a time evolution model, parameter models or both, as presented in the following examples.

2.2 Examples of control spaces as initial conditions

When the observation operator $\mathcal{G}$ contains a time evolution model, the control space can be the initial condition of a model, in which case the background state $\underline{x}^b$ can be chosen as the previous forecast. One can wish to control the initial state $\underline{x}$ of the model leading to the artificial observation $\underline{y} = \mathcal{G}(\underline{x})$ to be compared with real observation $\underline{y}^o$.

This is the case of weather forecast presented in Section **1**, for which the control space, the observation operator and the observation space are described in Table **1**.1. Weather forecast is a significant example for data assimilation. Most of the time, the analysis is the initial condition of the meteorological model.

Control space	Observation operator	Observation space
• 3D fields: temperature, pressure, humidity, winds • Order ten millions of grid points	Evolution model of the primitive equations of the atmosphere	• Satellite data: surface temperatures, radiances, cloud cover... • Order one million of observations

Table **1**.1: Data assimilation for the atmospheric forecast.

Operational oceanography is more recent than operational meteorology. It shares common data assimilation methods. The forecast of the ocean dynamics, at temporal scales of order weeks rather than days for the atmosphere, shares similar features, as seen in Table **1**.2.

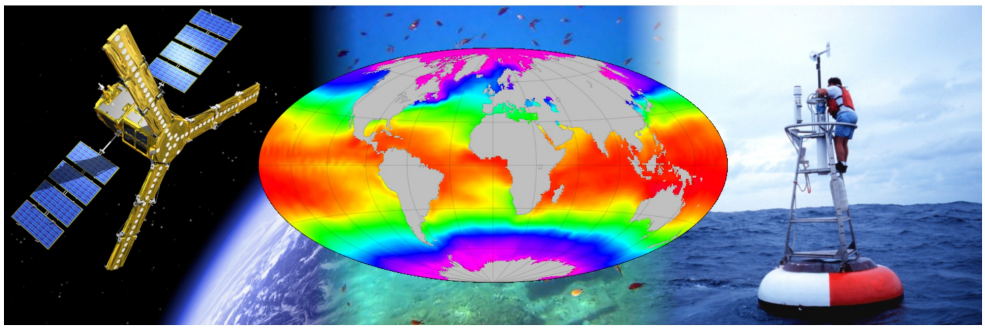

Figure **1**.5: *Data assimilation for oceanography with satellite and in-situ measurements.*

Control space	Observation operator	Observation space
• 3D fields: temperature, pressure, salinity, currents • 2D fields: sea surface level • Order ten millions of grid points	Evolution model of the primitive equations of the ocean	• Satelitte data: sea surface temperature, altimetry • In-situ data: temperature, salinity... • Order thousands of observations

Table 1.2: Data assimilation for the oceanic forecast.

2.3 Examples of control space as model parameters

Beyond geophysical applications, a large number of domains in which modelling plays an important role are concerned by the development of data assimilation. This is the case of the modelling of the core of nuclear plants (Figures 1.6), which characteristics are given in Table 1.3.

We want here to control the vector $\underline{x}$ of parameters of some model leading to the artificial observation $\underline{y} = \mathcal{G}(\underline{x})$ to be compared with real observation $\underline{y}^o$.

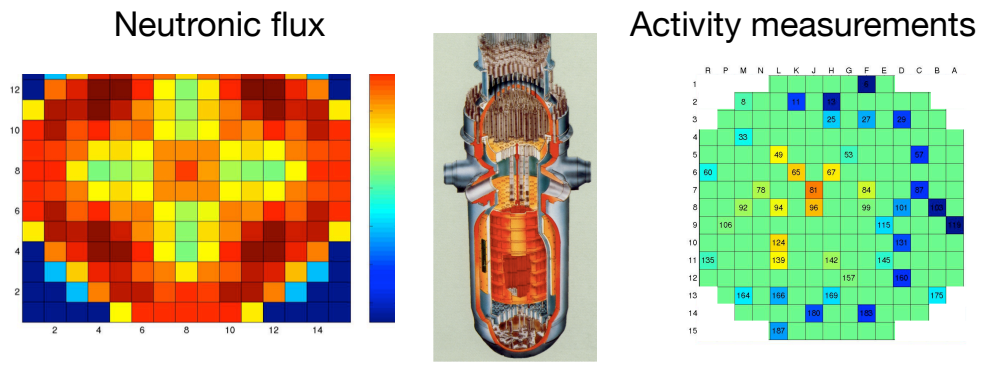

Figure 1.6: *Data assimilation for nuclear plants.*

Control space	Observation operator	Observation space
• 3D fields: neutronic flux, temperature, chemical concentration • Parameters: boundary reflections, diffusion coefficients • Order ten millions of grid points	Equilibrium model of the neutronic flux interacting with the heat transport fluid	• Neutronic and thermohydraulic sensors • Thousand of observations

Table 1.3: Data assimilation for nuclear plant core models.

3 What time is it?

Data assimilation deals with the mixing of measurements weighted by their certainty, i.e. the inverse of their error variance. The simple exemple developed in this section provides an illustration of the "Best Linear Unbiased Estimation" (BLUE) data assimilation method. The concept of correlation error matrix is illustrated with the simple example of clock time estimation. One considers time measurement as the realization of two independent or correlated gaussian random variables.

3.1 Errors as random variables

We consider that the error in the determination of a quantity, such a time for instance, is the result of a random draw of a gaussian random variable. If we denote by T_1 such random variable, we have to consider the probablity density

$$f_{T_1}(T) = \frac{1}{\sqrt{2\,\pi}\;\sigma_1}\;\exp\left[-\frac{(T-T_t)^2}{2\,\sigma_1^2}\right]\;, \tag{1.2}$$

from which we can compute the mean

$$T_t = \langle T_1 \rangle = \int_{I\!R} T\; f_{T_1}(T)\, dT \sim \frac{1}{R}\sum_{r=1}^{R} T_1^{(r)} \tag{1.3}$$

that can be estimated with a large number K of random draw $T_1^{(r)}$ and the variance $\sigma_1^2 = \left\langle T_1'^2 \right\rangle$ with $T_1' = T_1 - \langle T_1 \rangle$. The variance σ_1^2, square of the standard deviation σ_1, is a measure of the uncertainty of the random variable T_1.

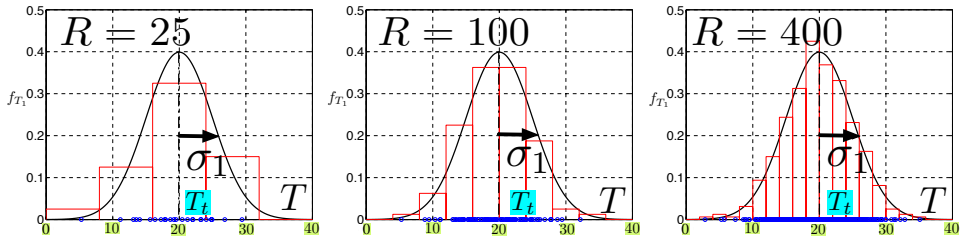

Figure 1.7: *Histogram of random variable converging towards it probability density function.*

We now consider two separate random variables T_1 et T_2 corresponding to two attempts to determine what time it is from two different clocks. We suppose that the two variables have the same mean T_t (there is no bias) and we denote by σ_1^2 and σ_2^2 their variances with $\sigma_1 \leq \sigma_2$. We then build the new random variable

$$T_a = (1-k)T_1 + kT_2\;, \tag{1.4}$$

where k is an ajustable constant.

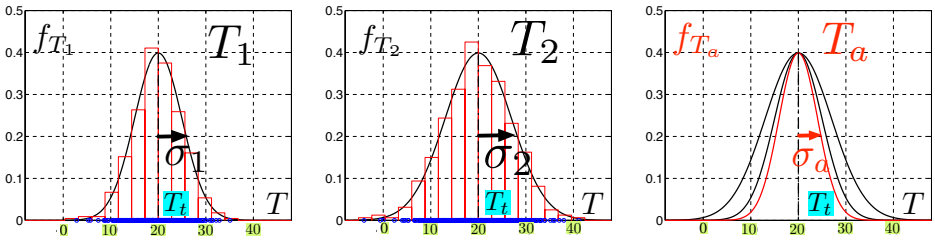

Figure 1.8: *Probability density function of T_1, T_2 and T_a.*

3.2 Uncorrelated random variables

We first suppose that T_1 and T_2 are independent, which means $\langle T_1' T_2' \rangle = 0$. If one clock is late, it does not systematically induces that other one is also late nor in advance. We can compute the variance σ_a^2 of T_a as $\sigma_a^2 = (1-k)^2 \sigma_1^2 + k^2 \sigma_2^2$. The minimum of σ_a^2, as a function of k (Figure 1.9), is obtained for $k_a = \sigma_2^{-2} / \left(\sigma_1^{-2} + \sigma_2^{-2}\right)$ and $\sigma_a^2 = \left(\sigma_1^{-2} + \sigma_2^{-2}\right)^{-1}$.

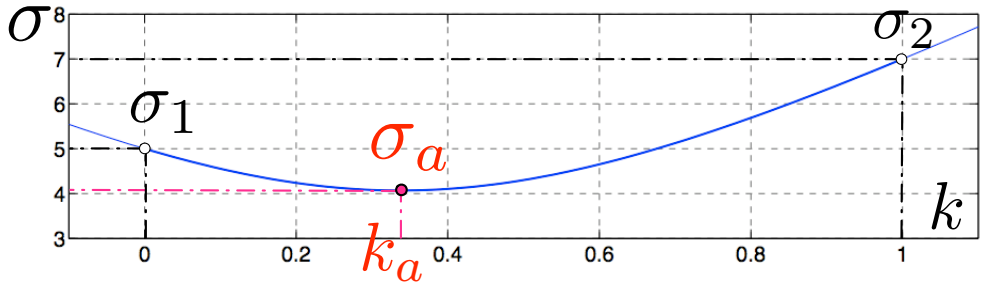

Figure 1.9: *Variance σ_a^2 as a function of k.*

For this optimal choice of k, on can write

$$T_a = \frac{C_1 T_1 + C_2 T_2}{C_1 + C_2} \text{ with } C_1 = \frac{1}{\sigma_1^2}\ ,\ C_2 = \frac{1}{\sigma_2^2} \text{ and } C_a = \frac{1}{\sigma_a^2} = C_1 + C_2\ . \quad (1.5)$$

We see that the weights are the "certainties" $C = 1/\sigma^2$ defined as the inverse of the error variances. One can show that any new independant measurement T_3 of certainty C_3, would increase the certainty of the analysis through $C_a = C_1 + C_2 + C_3$, provided that σ_1, σ_2, σ_3 are known, even approximatively.

One can notice that T_a minimize the cost function

$$J(T) = \frac{(T_1^o - T)^2}{2\,\sigma_1^2} + \frac{(T_2^o - T)^2}{2\,\sigma_2^2} = \frac{C_1}{2}\,(T_1^o - T)^2 + \frac{C_2}{2}\,(T_2^o - T)^2 \quad (1.6)$$

3.3 Correlated random variables

When T_1 and T_2 are no longer independent, their are correlated and we define the correlation coefficient by $\rho = \langle T_1' T_2' \rangle / (\sigma_1 \sigma_2)$. One can show that the choice of k that minimizes the variance of T_a is such that T^a minimizes the

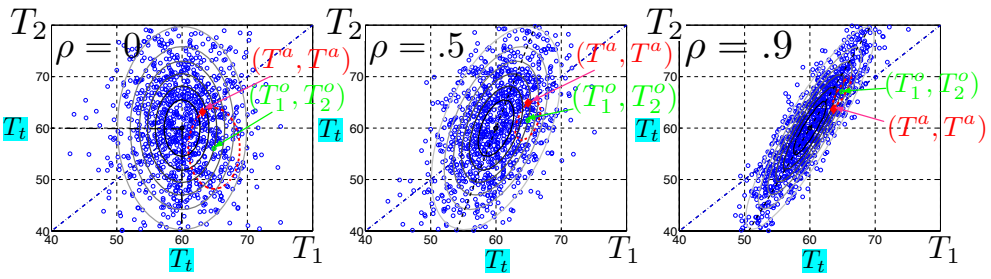

Figure 1.10: *The analysis T_a as the minimum of the cost function.*

new cost function

$$J(T) = \frac{1}{2}\,(T_1^o - T,\quad T_2^o - T)\begin{pmatrix}\sigma_1^2 & \rho\,\sigma_1\,\sigma_2\\ \rho\,\sigma_1\,\sigma_2 & \sigma_2^2\end{pmatrix}^{-1}\begin{pmatrix}T_1^o - T\\ T_2^o - T\end{pmatrix}\,, \qquad (1.7)$$

where the 2×2 matrix, can be seen as the "covariance observation error matrix" $\underline{\underline{R}}$. Indeed, the general formalism of this data assimilation problem is recovered by setting $\underline{x} = (T) \in I\!R$ as the control space, $\underline{y}^o = (T_1^o, T_2^o)^T \in I\!R^2$ as the observation space and $\mathcal{G}(\underline{x}) = (T, T)^T \in I\!R^2$.

EXERCICES

EXERCICE 1.1 Hands-on "What time is is?"

A demonstration program of the "What time is it?" example is available in several language (Octave, Scilab, Matlab) on the following page :

`http://pedagotech.inp-toulouse.fr/130202/co/2_goho_time.html`

1) Read the content of the program
2) Launch the program with the default parameters
3) Describe the program algorithm briefly
4) Change parameters and describe results

EXERCICE 1.2 BLUE and cost function for clocks

Best linear unbiased approximation

We consider two gaussian random variables T_1 and T_2 of respective root mean square σ_1 and σ_2 and sharing the same average $T_t =< T_1 >=< T_2 >$. We suppose that their correlation vanishes, that is $< T_1'\,T_2' >= 0$ with $T_1' = T_1 - T_t$ and $T_2' = T_2 - T_t$.

1) We consider the random variable $T_a = k\,T_1 + (1-k)\,T_2$ with $k \in [0,1]$. Compute the variance $\sigma_a^2(k)$ of T_a and draw its representative curve as a function of k.
2) Compute the value k_a for which $\sigma_a^2(k)$ is minimum. Show that the choice of this value for k leads to the expression $T_a = (C_1\,T_1 + C_2\,T_2)/(C_1 + C_2)$ where C_1 and C_2 are chosen such that $C_1 + C_2 = C_a$ with $C_a = 1/\sigma_a^2(k_a)$.

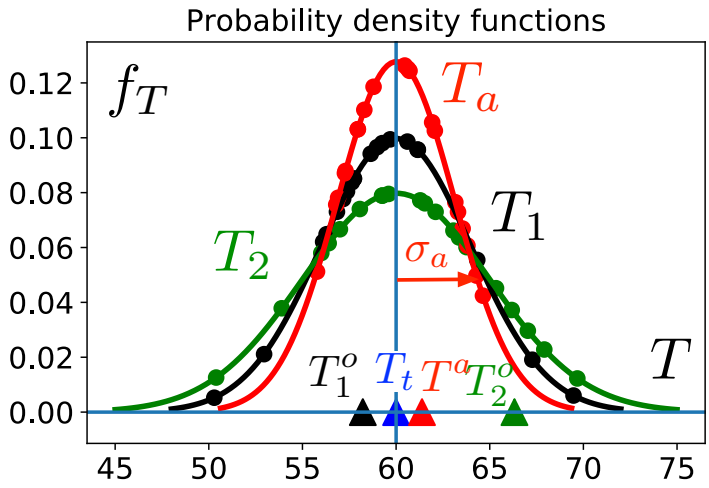

Figure 1.11: *Example of output of the demo program.*

3) What is the statistical meaning of C_1, C_2 and C_a. How can these quantities be named?

Minimum of a cost function

We consider the cost function $J(T) = (C_1/2)(T_1^o - T)^2 + (C_2/2)(T_2^o - T)^2$ where (C_1, C_2, T_1^o, T_2^o) are arbitrary constants.

4) Show that the value T^a that minimizes the cost function $J(x)$, is a the linear combination $T^a = k\,T_1^o + (1-k)\,T_2^o$ and compute the value of k. Compare it with k_a.

Bayesian approach

Given a value T, we consider a random vector $(T_1, T_2) \in I\!R^2$ with joint probability density function $f_T(T_1, T_2) = A\,g_1(T_1)\,g_2(T_1)$ where $g_i(T_i) = \exp[-(T_i - T)^2/(2\,\sigma_i^2)]$ for $i \in \{1, 2\}$ and the σ_i's are constants.

5) Compute the value of A such that $f_T(T_1, T_2)$ is a density probability function and deduce of it the value of $P(T) = f_T(T_1^o, T_2^o)$.
6) Compute the value $T = T_a$ such that $P(T)$ is maximum.

General formalism

We consider the cost function $J(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}^b)^T\,\underline{\underline{B}}^{-1}(\underline{x} - \underline{x}^b) + \frac{1}{2}[\underline{y}^o - \mathcal{G}(\underline{x})]^T\,\underline{\underline{R}}^{-1}[\underline{y}^o - \mathcal{G}(\underline{x})]$. We suppose that two independant unbiased clocks give the time T_1^o and T_2^o with the respective errors σ_1 and σ_2.

7) Describe $\underline{\underline{R}}$ and $\mathcal{G}$ when one considers that $\underline{y} = (T_1, T_2)^T$ is the observation vector and $\underline{x} = (T)$ is in the control space in the absence of background.
8) Describe $\underline{\underline{B}}$, $\underline{\underline{R}}$ and $\mathcal{G}$ when one considers that $\underline{y} = (T_2)$ is the observation vector and $\underline{x} = (T)$ is in the control space and (T_1^o) is considered as the background.
9) Give the link between the four parts of this problem.

EXERCICE 1.3 Convergence of estimators

We consider a random variable x with the gaussian probability density function of mean $x_t =< x >$ and variance $\sigma^2 = \left\langle x'^2 \right\rangle = \left\langle (x - x_t)^2 \right\rangle$. We consider an ensemble $x^{(r)}$ of draws of this random variable for $r = 1, ..., R$.

1) Show that $E_R = \frac{1}{R} \sum_{r=1}^{R} x^{(r)} \sim x^b$ is an unbiased estimator of x_t.
2) Show that $V_R = \frac{1}{R-1} \sum_{r=1}^{R} \left(x^{(r)} - E_R \right)^2$ is an unbiased estimator of σ.
3) Plot the scores $\log_{10}\left(|E_R - x^t| / |x_t| \right)$ and $\log_{10}\left(|V_R - \sigma| / \sigma \right)$ as functions of R for $R = 1, ..., 1000$.

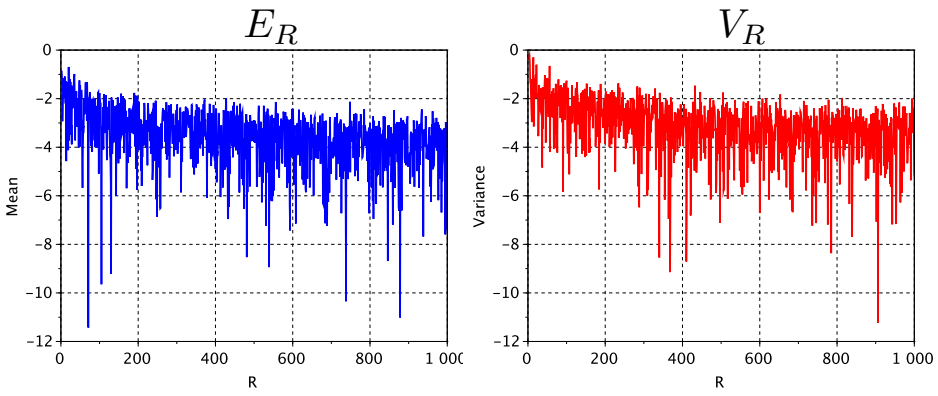

Figure 1.12: *Convergence of the estimators E_R and V_r of the the mean and the variance of a gaussian random variable.*

Chapter 2

Generic cost function

Contents

Introduction

The statistics for the uncertainities (erros) of physical quantities are often gaussian, due to the law of large numbers. This explains why most of the data assimilation methods used for engineer applications relies on a gaussian hypothesis for the error probablity density functions. Since gaussian processes are completly described by their mean (order one moment) and error covariances (order two moments), the minimization of the gaussian probability (best estimation) is equivalent to the minimization of a quadratic cost function involving the mean and the covariance error matrices. The minimization of such cost function is adressed in this chapter.

1 Looking for the minimum of a cost function

1.1 Generic cost function for data assimilation

Most of the usual data assimilation methods can be reduced to the minimisation of a cost function under the form:

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x}-\underline{x}^b\right)^T \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) + \frac{1}{2}\left[\underline{y}^o-\mathcal{G}(\underline{x})\right]^T \underline{\underline{R}}^{-1}\left[\underline{y}^o-\mathcal{G}(\underline{x})\right] \ , \quad (\mathbf{2}.1)$$

where $\underline{x} \in I\!R^N$ is a vector of the "control space", $\underline{x}^b$ is the "background" state, $\underline{y}^o \in I\!R^M$ a vector of measurements in the "observation space" and $\mathcal{G}$, the "observation operator" that links a vector $\underline{x} \in I\!R^N$ of the control space to a vector $\underline{y} = \mathcal{G}(\underline{x}) \in I\!R^M$ of the observation space (Figure **2**.1). The analysis $\underline{x}^a$ is the vector of the control state that minimizes the cost function $J(\underline{x})$, which can be written as $\underline{x}^a = \text{argmin}\,[J(\underline{x})]$. The $N \times N$ matrix $\underline{\underline{B}}$ and the $M \times M$ matrix $\underline{\underline{R}}$ are respectively called the "error covariance background matrix" and the "error covariance observation matrix".

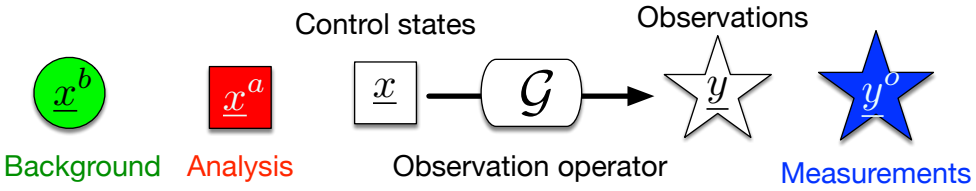

Figure **2**.1: *The analysis $\underline{x}^a$ is the vector $\underline{x} \in I\!R^N$ of the control space that is both close to the background $\underline{x}^b$ and such that $\underline{y} = \mathcal{G}(\underline{x}) \in I\!R^M$ in the observation state, obtained through the observation operator $\mathcal{G}$, is close to the measurements $\underline{y}^o$.*

We suppose that the background $\underline{x}^b$ is known with an error $\underline{\epsilon}^b \in I\!R^N$, modelled as a gaussian random field with zero mean (no bias). Similarily, $\underline{\epsilon}^o \in I\!R^N$ is a gaussian random field with zero mean (unbiased) that models the errors in the measurements $\underline{y}^o$. The symmetric matrices $\underline{\underline{B}}$ and $\underline{\underline{R}}$ are respectively defined by the relations

$$B_{ij} = \left\langle \epsilon_i^b \, \epsilon_j^b \right\rangle \quad \text{and} \quad R_{ij} = \left\langle \epsilon_i^o \, \epsilon_j^o \right\rangle \ , \quad (\mathbf{2}.2)$$

where the indices denote the components of the vectors or the matrices and $< \bullet >$ the statistical mean. We also suppose that the errors $\underline{\epsilon}^b$ and $\underline{\epsilon}^o$ are uncorrelated.

Since these matrices $\underline{\underline{B}}$ and $\underline{\underline{R}}$ are symmetric their eigenvalues are reals. These quantities represent the variances in the directions the eigenvectors. We suppose that they are all strictly positive, i.e. no information is completly certain. Thus, the respective inverses $\underline{\underline{B}}^{-1}$ and $\underline{\underline{R}}^{-1}$ of these matrices exist.

The bayesian approch of the present data assimilation formalism considers the probability density functions

$$f^b(\underline{x}) = K^b\, e^{-\,J_b(\underline{x})} \quad \text{with} \quad J_b(\underline{x}) = \frac{1}{2}\left(\underline{x}-\underline{x}^b\right)^T \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) \ , \tag{2.3}$$

$$f^o(\underline{y}) = K^o\, e^{-J_r(\underline{x})} \quad \text{with} \quad J_r(\underline{y}) = \frac{1}{2}\left(\underline{y}^o-\underline{y}\right)^T \underline{\underline{R}}^{-1}\left(\underline{y}^o-\underline{y}\right) \ , \tag{2.4}$$

$$f^{b/o}(\underline{x}) = f^b(\underline{x})\; f^o[\mathcal{G}(\underline{x})] = K^o\, K^b\, e^{-J(\underline{x})} \tag{2.5}$$

$$\text{with} \quad J(\underline{x}) = J_b(\underline{x}) + J_r\left[\mathcal{G}(\underline{x})\right] \ , \tag{2.6}$$

where K^o and K^b are normalization factors. Minimizing the probability density $f^{b/o}(\underline{x})$ of $\underline{x}^b$ "knowing" $\underline{y}^o$ is equivalent to minimizing its logarithm, that is minimizing the cost function J given by Equation (4.13).

1.2 Basic linear algebra

To find the minimum of a cost function such as J, we need some algebra involving vectors and matrices. In the following, $\underline{x} \in I\!R^N$ or $\underline{y} \in I\!R^M$ denote column vectors while their transposes $\underline{x}^T$ and $\underline{y}^T$ denote line vectors:

$$\underline{x} = \begin{pmatrix} x_1 \\ ... \\ x_j \\ ... \\ x_N \end{pmatrix} \ , \quad \underline{y} = \begin{pmatrix} y_1 \\ ... \\ y_i \\ ... \\ y_M \end{pmatrix} \ , \quad \begin{cases} \underline{x}^T = \left(x_1, ..., x_j, ..., x_N\right) \\ \\ \underline{y}^T = \left(y_1, ..., y_i, ..., y_M\right) \end{cases} . \tag{2.7}$$

Given a $M \times N$ matrix $\underline{\underline{H}}$, the product $\underline{y} = \underline{\underline{H}}\,\underline{x}$ can be explicited as follows:

$$\underline{y} = \underline{\underline{H}}\,\underline{x} \quad \Longleftrightarrow \quad \begin{pmatrix} y_1 \\ ... \\ y_i \\ ... \\ y_M \end{pmatrix} = \begin{pmatrix} H_{11} & ... & H_{1j} & ... & H_{1N} \\ ... & ... & ... & ... & ... \\ H_{i1} & ... & H_{ij} & ... & H_{iN} \\ ... & ... & ... & ... & ... \\ H_{M1} & ... & H_{Mj} & ... & H_{MN} \end{pmatrix} \begin{pmatrix} x_1 \\ ... \\ x_j \\ ... \\ x_N \end{pmatrix} . \tag{2.8}$$

If $\underline{x} \in I\!R^N$ is a $M \times 1$ (column) vector, $\underline{\underline{M}} \in I\!R^N \times I\!R^N$ is a $N \times N$ square matrix, $\underline{\underline{S}} \in I\!R^M \times I\!R^M$ a $M \times M$ square matrix, and $\underline{\underline{H}} \in I\!R^M \times I\!R^N$ a $M \times N$ rectangular matrix. Transposition rules read $\left(\underline{\underline{M}}\,\underline{x}\right)^T = \underline{x}^T\,\underline{\underline{M}}^T$ and $\left(\underline{\underline{S}}\,\underline{\underline{H}}\right)^T = \underline{\underline{H}}^T\,\underline{\underline{S}}^T$.

If a square matrix $\underline{\underline{M}}$ is inversible, i.e. if its determinant is not zero, we denote by $\underline{\underline{M}}^{-1}$ its inverse and $\underline{\underline{M}}^{-T} = \left[\underline{\underline{M}}^{-1}\right]^T$ its transpose. A square matrix $\underline{\underline{B}}$ is symmetric if $\underline{\underline{B}}^T = \underline{\underline{B}}$, that is $B_{ij} = B_{ji}$ for all indices.

1.3 Gradient of a scalar function

The gradient of a scalar I that associates to each vector $\underline{x} \in I\!R^N$ a real number $I(\underline{x}) \in I\!R$, is defined here as the column vector

$$\underline{\text{grad}}\, I(\underline{x}) = \left(\frac{\partial I}{\partial x_1}, \frac{\partial I}{\partial x_2}, \ldots \frac{\partial I}{\partial x_j}, \ldots . \frac{\partial I}{\partial x_N} \right)^T \tag{2.9}$$

made of the partial derivative with respect to the coordinates x_j.

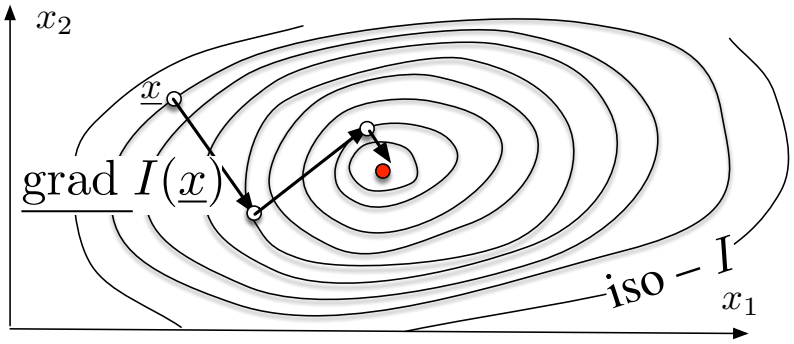

Figure 2.2: *Use of the gradient of the real function I for a descent methods looking for its minimum.*

Global or local minima of I are obtained when $\underline{\text{grad}}\ I = \underline{0}$. The gradient (column) vector is also useful to find these minima through "descent algorithms" such a the "steepest descent" method (Figures 2.2) or the "conjugate gradient" (more efficient) method.

The Hessian of a scalar function $I(\underline{x})$ with $\underline{x} \in I\!R^N$ is the $N \times N$ matrix $\underline{\underline{H}}(\underline{x}) = \underline{\underline{\text{Hess}}}\, I(\underline{x})$ whose components are $H_{ij} = \frac{\partial^2 I}{\partial x_i \partial x_j}$. This matrix is symmetric and its real eigenvalues represent the curvature of the function J for principal directions.

$\mathbf{I}(\underline{\mathbf{x}})$	$\underline{\text{grad}}\ \mathbf{I}(\underline{\mathbf{x}})$	$\underline{\underline{\text{Hess}}}\, \mathrm{I}(\underline{\mathrm{x}})$
$\underline{u}^T\, \underline{x}$	$\underline{u}$	$\underline{\underline{0}}$
$\underline{u}^T\, \underline{\underline{M}}\, \underline{x}$	$\underline{\underline{M}}^T\, \underline{u}$	$\underline{\underline{0}}$
$\underline{x}^T\, \underline{\underline{M}}\, \underline{x}$	$(\underline{\underline{M}} + \underline{\underline{M}}^T)\, \underline{x}$	$\underline{\underline{M}} + \underline{\underline{M}}^T$
$\underline{x}^T\, \underline{\underline{H}}^T\, \underline{\underline{S}}\, \underline{\underline{H}}\, \underline{x}$	$\underline{\underline{H}}\, (\underline{\underline{S}} + \underline{\underline{S}}^T)\, \underline{\underline{H}}^T\, \underline{x}$	$\underline{\underline{H}}\, (\underline{\underline{S}} + \underline{\underline{S}}^T)\, \underline{\underline{H}}^T$

Table 2.1: *Gradient of usual fonctions J.*

Given a vector $\underline{u} \in I\!R^N$, a $N \times N$ matrix $\underline{\underline{M}}$, a $M \times M$ matrix $\underline{\underline{S}}$ and a $M \times N$ matric $\underline{\underline{H}}$, the expressions of the gradients and Hessians of several examples of real function $I(\underline{x})$ are given in Table 2.1. These formula will be useful, in the following, to compute the gradient of the cost function J.

2 Linearization methods

For some data assimilation applications, the observation operator $\mathcal{G}$ is linear. In this cas, the assimilation method that consists in the minimization of the

cost function J is called the "Best Linear Unbiased Estimation" (BLUE). When the observation operator $\mathcal{G}$ is nonlinear, it linearization around the background stage $\underline{x}^b$ is an approximation that defines the "incremental cost function", leading to an approximation of the analysis.

2.1 Best Linear Unbiased Estimation

When the observation operator $\mathcal{G}$ is linear, one can define the $M \times N$ matrix $\underline{\underline{G}}$ such that $\mathcal{G}(\underline{x}) = \underline{\underline{G}}\,\underline{x}$. In that case, the cost function reads

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x}-\underline{x}^b\right)^T \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) + \frac{1}{2}\left(\underline{y}^o-\underline{\underline{G}}\,\underline{x}\right)^T \underline{\underline{R}}^{-1}\left(\underline{y}^o-\underline{\underline{G}}\,\underline{x}\right) \ . \quad (\mathbf{2}.10)$$

Since $\underline{\underline{B}}$ and $\underline{\underline{R}}$ are symmetric matrices, the application of the formula of Table **2**.1 leads to the following expression of the gradient of the cost function:

$$\underline{\mathrm{grad}}\ J(\underline{x}) = \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) - \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\left[\underline{y}^o-\underline{\underline{G}}\,\underline{x}\right] \quad (\mathbf{2}.11)$$

$$= \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) - \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\left[\left(\underline{y}^o-\underline{\underline{G}}\,\underline{x}^b\right) - \underline{\underline{G}}\left(\underline{x}-\underline{x}^b\right)\right] \ . \quad (\mathbf{2}.12)$$

This gradient vanishes when $\underline{x}$ is equal to the analysis $\underline{x}^a$, such that

$$\underline{x}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d} \quad (\mathbf{2}.13)$$

$$\text{with} \quad \underline{\underline{K}} = \left(\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}\right)^{-1}\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1} \quad \text{and} \quad \underline{d} = \underline{y}^o - \underline{\underline{G}}\,\underline{x}^b \ , \quad (\mathbf{2}.14)$$

where $\underline{d}$ is called the "innovation vector" and $\underline{\underline{K}}$ the "gain matrix". Using cumbersome algebra, under the name of the "Sherman-Morrison-Woodbury" identity, the gain matrix can be expression with two equivalent formula:

$$\underline{\underline{K}} = \left(\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}\right)^{-1}\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1} = \underline{\underline{B}}\,\underline{\underline{G}}^T\left(\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}}\right)^{-1} \ . \quad (\mathbf{2}.15)$$

The choice of one formula rather the other one is dictated by the ratio between the dimension N of the control space and the dimension M of the observation space. If $N > M$, one should prefer to inverse the $M \times M$ matrix $\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}}$ rather the $N \times N$ matrix $\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}$, with the opposite choice if $N < M$.

The "covariance error analysis matrix" $\underline{\underline{A}}$ is the inverse of the Hessian of the cost function J, which reads

$$\underline{\underline{\mathrm{Hess}}}\,J(\underline{x}) = \underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}} \implies \underline{\underline{A}} = \left[\underline{\underline{\mathrm{Hess}}}\,J(\underline{x})\right]^{-1} = \left(\underline{\underline{I}} - \underline{\underline{K}}\,\underline{\underline{G}}\right)\underline{\underline{B}} \ , \quad (\mathbf{2}.16)$$

as can be prooved by cumbersome algebra. The matrix $\underline{\underline{A}}$ quantifies the uncertainy of the analysis $\underline{x}^a$ at the issue of the data analysis process. One can show that minimizing the cost fonction J is equivalent to minimizing the trace of $\underline{\underline{A}}$ if we look at $\underline{x}^a$ as a linear combination of both $\underline{x}^b$ and $\underline{y}^o$.

2.2 Incremental cost function

For the general case where the observation operator $\mathcal{G}$ in nonlinear, an usual approximation relies on its linearization around the background $\underline{x}^b$:

$$\mathcal{G}(\underline{x}^b + \underline{\delta x}) \ \approx \ \mathcal{G}(\underline{x}^b) + \underline{\underline{G}}\,\underline{\delta x} \ , \quad (\mathbf{2}.17)$$

where $\underline{\underline{G}}$, of components $G_{ij} = \frac{\partial \mathcal{G}_i}{\partial x_j}(\underline{x}^b)$ is the Jacobian matrix of $\mathcal{G}$ at $\underline{x}^b$. We then define the "incremental cost function"

$$J_{inc}(\underline{x}^b + \underline{\delta x}) = \frac{1}{2} \underline{\delta x}^T \ \underline{\underline{B}}^{-1} \ \underline{\delta x} + \frac{1}{2} \left(\underline{d} - \underline{\underline{G}} \, \underline{\delta x}\right)^T \ \underline{\underline{R}}^{-1} \ \left(\underline{d} - \underline{\underline{G}} \, \underline{\delta x}\right) \ , \qquad (\mathbf{2}.18)$$

where $\underline{d} = \underline{y}^o - \mathcal{G}(\underline{x}^b)$ is the innovation vector. Using algebra similar to the case of a linear observation operator, the analysis is given by $\underline{x}^a = \underline{x}^b + \underline{\underline{K}} \ \underline{d}$ with the gain matrix $\underline{\underline{K}} = \underline{\underline{B}} \, \underline{\underline{G}}^T \ \left(\underline{\underline{G}} \, \underline{\underline{B}} \, \underline{\underline{G}}^T + \underline{\underline{R}}\right)^{-1}$. The covariance analysis error matrix shares the same expression $\underline{\underline{A}} = (\underline{\underline{I}} - \underline{\underline{K}} \ \underline{\underline{G}}) \, \underline{\underline{B}}$ as for the linear case.

2.3 Finite difference linearization

The observation operator $\mathcal{G}$ links a vector $\underline{x}$ of the control space to the vector $\underline{y} = \mathcal{G}(\underline{x}) = [\mathcal{G}_1(\underline{x}), ...\mathcal{G}_i(\underline{x}), ...\mathcal{G}_M(\underline{x})]^T$ of the observation space. The Jacobian matrix $\underline{\underline{G}}$ of a nonlinear observation operator $\mathcal{G}$ around a state $\underline{x}^b$ is defined by

$$\mathcal{G}(\underline{x}^b + \underline{\delta x}) \ \approx \ \mathcal{G}(\underline{x}^b) + \underline{\underline{G}}(\underline{x}^b) \ \underline{\delta x} \quad \text{with} \quad \underline{\underline{G}} = (\underline{G}_1, ...\underline{G}_i ..., \underline{G}_M)^T \qquad (\mathbf{2}.19)$$

where the column vectors $\underline{G}_i$ are defined by

$$\underline{G}_i(\underline{x}^b) = \left[\frac{\partial \mathcal{G}_i}{\partial x_1}(\underline{x}^b)..., \frac{\partial \mathcal{G}_i}{\partial x_j}(\underline{x}^b)..., \frac{\partial \mathcal{G}_i}{\partial x_N}(\underline{x}^b)\right]^T \quad \text{for } i = 1, ...M \ . \qquad (\mathbf{2}.20)$$

When $\underline{\underline{G}}$ cannot be analytically computed, automatic differentiation can be thought if $\mathcal{G}$ is obtained through a computer program. If such differentiation cannot be developed, $\underline{\underline{G}}$ can be obtained through a finite difference method through the approximation

$$\frac{\partial \mathcal{G}_i}{\partial x_j}(\underline{x}^b) \sim \frac{\mathcal{G}_i(x_1^b..., x_j^b + \delta x_j, ...x_N^b) - \mathcal{G}_i(x_1^b..., x_j^b - \delta x_j, ...x_N^b)}{2 \, \delta x_j} \ , \qquad (\mathbf{2}.21)$$

where the δx_j's are "small" quantities. The "smallness" of these increments in all directions depends on the function $\mathcal{G}$ around $\underline{x}^b$ and must be tested by convergence computations.

When the computation cost of $\mathcal{G}$ is non negligible, this finite difference approximation is only viable when the dimension N is small enough.

3 How will the bore propagate?

We consider a simple example to illustrate the use of an incremental cost function an check the validity of the approximation.

3.1 Formulation of the cost function

We consider a uniform flow of height h_L and mean velocity U_L in an open channel (Figure **2**.3). For aerodynamic application, h_L can be seen as the density ρ_L of a compressible gaz in a tube.

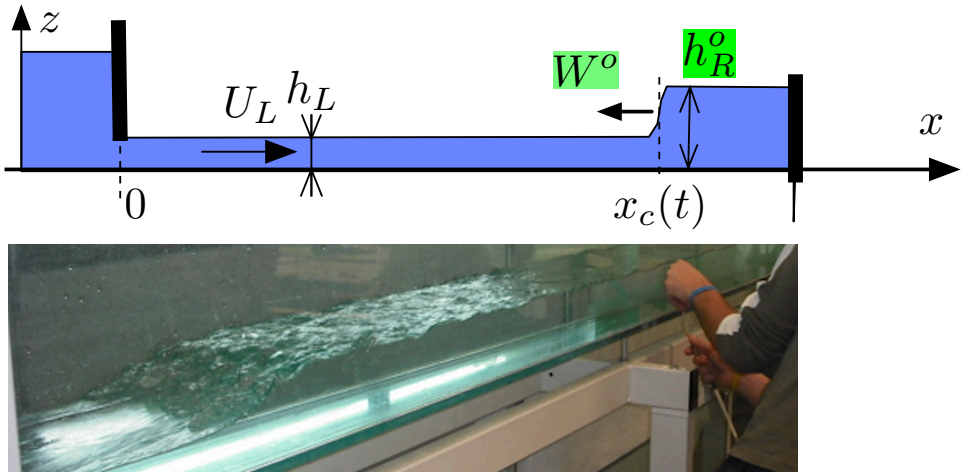

Figure **2**.3: *Moving hydraulic bore.*

We then suddenly close a gate at the end of the channel (hydraulics) or the tube (compressible gaz). This creates the upward propagation of a bore (hydraulics) or a shock (aerodynamics) of velocity $W < 0$. If h_R is the water height or the density (compressible gaz) at the right of the moving discontinuity, and U_R the associated mean velocity, mass conservation imposes the relation:

$$h_L(U_L - W) = h_R(U_R - W) \; . \tag{2.22}$$

If the gate is completly closed, the mean velocity between the shock and the gate is $U_R = 0$ and the shock velocity is given by

$$W = \frac{-h_L \, U_L}{h_R - h_L} \; . \tag{2.23}$$

We suppose that h_L and the lineic discharge flux $q = h_L \, U_L$ are know with infinite certainty while $h_R = h_R^b + \epsilon^b$ is known with an error ϵ^b of zero mean and standard deviation σ_r. We suppose that a measurement $W = W + \epsilon^o$ is made with an error ϵ^o of zero mean and standard deviation σ_r. We suppose that the errors ϵ^b and ϵ^o are uncorrelated.

We then arbitrarily decide that $x = h_R$ is in the control space of dimension $N = 1$ and $y = W$ is in the observation space of dimension $M = 1$. The opposite choice could have been made for this exemple. The observation operation is thus defined by

$$y = \mathcal{G}(x) = \frac{-q}{x - h_L} \; . \tag{2.24}$$

3.2 Minimum of the full cost function

Given the hypothesis of the data assimilation problem, we want to find the analysis $x^a = h_R^a$ that minimizes the cost function

$$J(x) = \frac{(x - x^b)^2}{2 \, \sigma_b^2} + \frac{[y^o - \mathcal{G}(x)]^2}{2 \, \sigma_r^2} = J_b(x) + J_r(x) \tag{2.25}$$

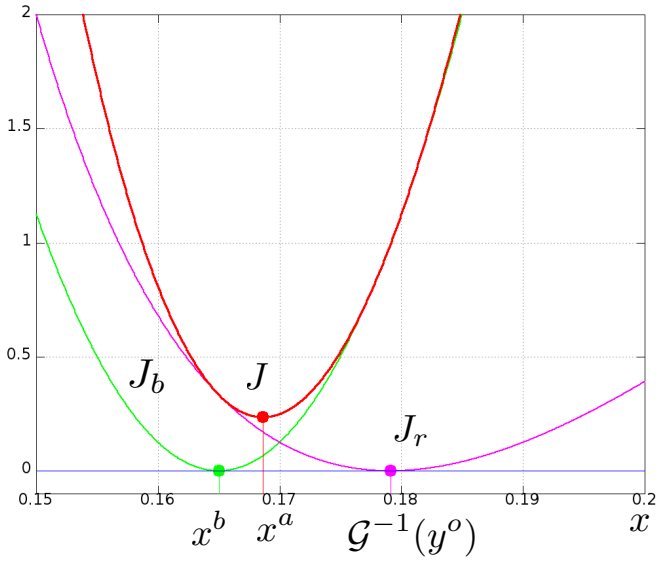

Figure **2**.4: *The analysis x^a is at the minimum of the cost function $J(x) = J_b(x) + J_r(x)$.*

with $J_b(x) = (x - x^b)^2/(2\,\sigma_b^2)$ and $J_r(x) = (y^o + \frac{q}{x-h_L})^2/(2\,\sigma_r^2)$.

The plot of the cost function $J(x)$ is shown in Figure **2**.4 with the plots of $J_b(x)$ and $J_r(x)$. The analysis x^a, which minimizes J is close to the measured height $x^b = h_R^b$ and the value $\mathcal{G}^{-1}(y^o) = \mathcal{G}^{-1}(W)$, which is the height that would induce the measured velocity W. The curvature (Hessian) of J_b and J_r indicate the uncertainty of the information respectively given by x^b and y^o.

3.3 Minimum of the incremental cost function

To approximate the minimization of the cost function

$$J(x) = \frac{(x - x^b)^2}{2\,\sigma_b^2} + \frac{[y^o - \mathcal{G}(x)]^2}{2\,\sigma_r^2} \qquad \text{with} \qquad \mathcal{G}(x) = \frac{-q}{x - h_L}\,, \tag{2.26}$$

we linearize $\mathcal{G}$ around x^b:

$$\mathcal{G}(x) = \mathcal{G}(x^b + \delta x) = \mathcal{G}(x^b) + G\,\delta x + O(\delta x^2)\,, \tag{2.27}$$

with $\delta x = x - x^b$ and $G = \mathcal{G}'(x^b) = q/(x^b - h_L)^2$. One can then write $J(x) = J_{inc}(x^b + \delta x) + O(\delta x^2)$, where the incremental cost function J_{inc} is defined by

$$J_{inc}(x^b + \delta x) = \frac{(\delta x)^2}{2\,\sigma_b^2} + \frac{(d - G\,\delta x)^2}{2\,\sigma_r^2} \tag{2.28}$$

where $d = y^o - \mathcal{G}(x^b)$ is the "innovation".

The gradient of the incremental function is simply the derivate of $J_{inc}(x)$, that reads

$$J'_{inc}(x^b + \delta x) = \frac{\delta x}{\sigma_b^2} + G\,\frac{G\,\delta x - d}{\sigma_r^2}. \tag{2.29}$$

It vanishes for $\widetilde{x}^a = \underline{x}^b + \widetilde{\delta x}^a$ with

$$\widetilde{\delta x}^a = K\,d \quad \text{with} \quad d = y^o - \mathcal{G}(x_b) \quad \text{and} \quad K = \left(\frac{1}{\sigma_b^2} + \frac{G^2}{\sigma_r^2}\right)^{-1} \frac{G}{\sigma_r^2} \tag{2.30}$$

We note that the gain K can also we written under the form

$$K = \sigma_b^2\, G\, \left(G^2\,\sigma_b^2 + \sigma_r^2\right)^{-1}\ , \tag{2.31}$$

which shows a simple form of the Sherman-Morrison-Woodbury identity.

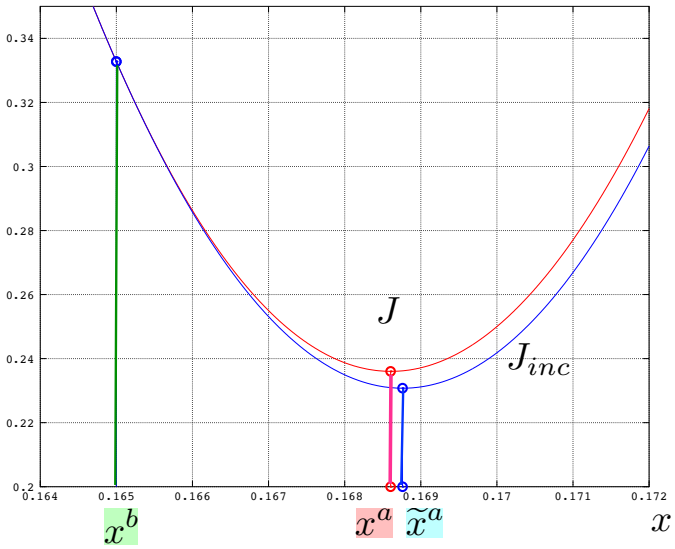

Figure 2.5: *Comparison of the minimun x^a of the cost function J with the mininum $\widetilde{x}^a$ of the incremental cost function J_{inc}.*

EXERCICES

EXERCICE 2.1 Hands-on "How will the bore propagate?"

A demonstration program of the "How will the bore propagate?" example is available in several language (Octave, Scilab, Matlab) on the following page :

`http://pedagotech.inp-toulouse.fr/130202/co/90-ho_jump.html`

1) Read the content of the program
2) Launch the program with the default parameters
3) Describe the program algorithm briefly
4) Change parameters and describe results
5) Replace $\mathcal{G}$ and $G = \mathcal{G}'(\underline{x}^b)$ by another function.

EXERCICE 2.2 Clocks

We suppose that $N = 1$ and $M = 2$ with the observation operator $\mathcal{G} : \mathbb{R} \to \mathbb{R}^2$ such that $x \mapsto \underline{y} = \underline{G}\,x$, where $\underline{G} = (1,1)^T$ can be seen as a $M \times N =$

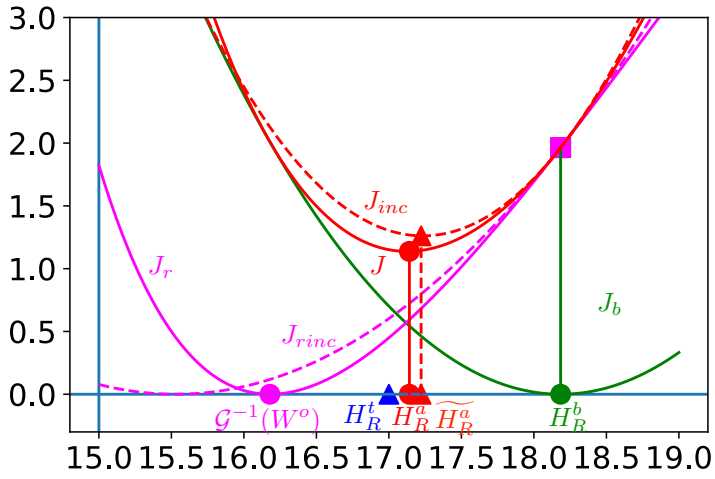

Figure **2**.6: *Example of output of the demo program.*

2×1 matrix or simply as column vector on $\mathbb{R}^2$. We consider the cost function $J(x) = \frac{1}{2}\,(\underline{y}^o - \underline{\underline{G}}\,x)^T\,\underline{\underline{R}}^{-1}\,(\underline{y}^o - \underline{\underline{G}}\,x)$ where $\underline{y} \in \mathbb{R}^2$ is a column vector and $\underline{\underline{R}}$ is a positively defined 2×2 symmetric matrix.

1) Show that $J'(x) = -\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,(\underline{y}^o - \underline{\underline{G}}\,x)$.
2) Express, as a function of $\underline{\underline{G}}$, $\underline{\underline{R}}$ and $\underline{y}^o$ the real number x^a that minimize $J(x)$.
3) Express x^a in the particular case where $\underline{\underline{R}} = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$.
4) We consider two gaussian random variables T_1 and T_2 of respective root mean square σ_1 and σ_2 and sharing the same average $T_t =< T_1 >=< T_2 >$. We suppose that their correlation vanishes, that is $< T_1'\,T_2' >= 0$ with $T_1' = T_1 - T_t$ and $T_2' = T_2 - T_t$. Let $\underline{y}^o = (y_1^o, y_2^o)^T = (T_1, T_2)^T$ be called the observation, where (T_1, T_2) is a random draw of the two variable. Show that the analysis x^a that minimize the previous cost function $J(x)$, is a the linear combination $x_a = T_a = k\,T_1 + (1-k)\,T_2$ such that $\sigma_a^2 =< T_a'^2 >$, with $T_a' =< T_a - T_t >$, is minimum when k varies in the set $k \in [0, 1]$.
5) We denote by $C_1 = 1/\sigma_1^2$ and $C_2 = 1/\sigma_2^2$ the inverses of the variances. Express T_a as a function of T_1, T_2, C_1 and C_2. How can you interpret the meaning of C_1 and C_2 in a statistical sense.

EXERCICE 2.3 Cost function and gain matrix

We consider column vectors $\underline{x} = (x_1, x_2, ..., x_N)^T \in \mathbb{R}^N$ and $\underline{y} = (y_1, y_2, ..., y_M)^T \in \mathbb{R}^M$. We denote by $\underline{x}^b \in \mathbb{R}^N$ and $\underline{y}^o \in \mathbb{R}^M$ two particular vectors. We denote by $\underline{\underline{B}}$ and $\underline{\underline{R}}$ two positively defined symmetric matrices of respective dimensions $N \times N$ and $M \times M$. We denote by $\underline{\underline{G}}$ a $M \times N$ matrix.
Give the expression of grad $J(x)$ for the following cost functions:

1) $J(\underline{x}) = \underline{b}^T\,\underline{x} = \underline{x}^T\,\underline{b}$ where $\underline{b}$ is a column vector of $\mathbb{R}^N$.
2) $J(\underline{x}) = \underline{u}^T\,\underline{\underline{M}}\,\underline{x}$ where $\underline{u}$ is a column vector of $\mathbb{R}^N$ and $\underline{\underline{M}}$ is a $N \times N$

matrix.

3) $J_b(\underline{x}) = \frac{1}{2}\,(\underline{x}-\underline{x}^b)^T\,\underline{\underline{B}}^{-1}\,(\underline{x}-\underline{x}^b)$.

4) $J_r(\underline{x}) = \frac{1}{2}\,(\underline{y}^o-\underline{\underline{G}}\,\underline{x})^T\,\underline{\underline{R}}^{-1}\,(\underline{y}^o-\underline{\underline{G}}\,\underline{x})$.

5) $J(\underline{x}) = J_b(\underline{x}) + J_r(\underline{x})$

We denote by $\underline{d} = \underline{y}^o - \underline{\underline{G}}\,\underline{x}^b$ and $\underline{\delta x} = \underline{x} - \underline{x}^b$.

6) Show that minimum of $J(\underline{x})$ is obtained for $\underline{x}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d}$, where $\underline{\underline{K}}$ is are matrix that you will specify as a function of $\underline{\underline{B}}$, $\underline{\underline{R}}$ and $\underline{\underline{G}}$.

7) Add the ^{T} (transpose), $\underline{\ }$ (column vector) and $\underline{\underline{\ }}$ (matrix) notations so that the following relation be correct:

$$(G\,R^{-1}\,G + B^{-1})^{-1}\,G\,R^{-1} = B\,G\,(G\,B\,G + R)^{-1}\,. \qquad (\mathbf{2}.32)$$

8) Explain why this relation is useful in the context of data assimilation.

EXERCICE 2.4 Sherman-Morrison-Woodbury identity

1) The cost function of a standard assimilation problem reads :

$$J(\underline{x}) = \frac{1}{2}(\underline{x}-\underline{x}^b)^T\,\underline{\underline{B}}^{-1}\,(\underline{x}-\underline{x}^b) + \frac{1}{2}[\underline{y}^o-\mathcal{G}(\underline{x})]^T\,\underline{\underline{R}}^{-1}[\underline{y}^o-\mathcal{G}(\underline{x})]\,. \quad (\mathbf{2}.33)$$

We denote by N the dimension of the control space and by M the dimension of the observation space. Since $\underline{x}$ is considered as a column vector, one says that it is a matrix of size $N \times 1$. Give the names and matrix sizes of $\underline{x}^b$, $\underline{y}^o$, $\underline{\underline{B}}$ and $\underline{\underline{R}}$. Indicate the name of the operator $\mathcal{G}$ and the spaces that it links. Give the name and matrix size of the state $\underline{x}^a$ that minimizes J. Explain why $\underline{\underline{B}}$ and $\underline{\underline{R}}$ are symmetric.

2) We consider the approximation $\mathcal{G}(\underline{x}) = \mathcal{G}(\underline{x}^b) + \underline{\underline{G}}\,\underline{\delta x}$ with $\underline{\delta x} = \underline{x} - \underline{x}^b$. Show that the cost function is approximated by

$$J_{inc}(\underline{x}^b + \underline{\delta x}) = \frac{1}{2}\underline{\delta x}^T\,\underline{\underline{B}}^{-1}\,\underline{\delta x} + \frac{1}{2}(\underline{d}-\underline{\underline{G}}\,\underline{\delta x})^T\,\underline{\underline{R}}^{-1}(\underline{d}-\underline{\underline{G}}\,\underline{\delta x})\,, \quad (\mathbf{2}.34)$$

and give the expression of $\underline{d}$ as a function of $\underline{y}^o$, $\mathcal{G}$ and $\underline{x}^b$. Give the name and matrix size of $\underline{d}$. Give the name of the method that uses this approximation.

3) We admit without demonstration that

$$\underline{\text{grad}}\ (\underline{x}^T\,\underline{\underline{N}}\,\underline{x}) = (\underline{\underline{N}} + \underline{\underline{N}}^T)\,\underline{x} \qquad \text{and}$$
$$\underline{\text{grad}}\ \left[(\underline{\underline{H}}\,\underline{x}+\underline{u})^T\,\underline{\underline{N}}\,(\underline{\underline{H}}\,\underline{x}+\underline{u})\right] = \underline{\underline{H}}^T\,(\underline{\underline{N}} + \underline{\underline{N}}^T)\,(\underline{\underline{H}}\,\underline{x}+\underline{u})\,, \quad (\mathbf{2}.35)$$

where $\underline{\underline{N}}$ is a constant $N \times N$ matrix, $\underline{u}$ is a constant $N \times 1$ vector and the gradient of a scalar function $F(\underline{x})$ is defined by $\underline{\text{grad}}\ F(\underline{x}) = \left(\frac{\partial F}{\partial x_1}, ..., \frac{\partial F}{\partial x_N}\right)^T$. Show that the minimum of J_{inc} is obtained for

$$\underline{x}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d} \quad \text{with} \quad \underline{\underline{K}} = (\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}})^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,. \qquad (\mathbf{2}.36)$$

4) Give the matrix sizes of $\underline{\underline{C}}$ and $\underline{\underline{S}}$ defined by $\underline{\underline{C}} = \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}} + \underline{\underline{B}}^{-1}$ and $\underline{\underline{S}} = \underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}}$ and show that $\underline{\underline{K}} = \underline{\underline{C}}^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}$.

5) Show that $\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{S}} = \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{G}}^T = (\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}\,\underline{\underline{B}} + \underline{\underline{B}}^{-1}\,\underline{\underline{B}})\,\underline{\underline{G}}^T = \underline{\underline{C}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T$.

6) Show that the equality $\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{S}} = \underline{\underline{C}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T$ shown in the previous question implies (Sherman-Morrison-Woodbury identity):

$$\underline{\underline{K}} = \underline{\underline{B}}\,\underline{\underline{G}}^T\,(\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}})^{-1} = (\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}} + \underline{\underline{B}}^{-1})^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1} \qquad (\mathbf{2}.37)$$

7) If $\underline{\underline{B}}$, $\underline{\underline{B}}^{-1}$, $\underline{\underline{R}}$ and $\underline{\underline{R}}^{-1}$ are known, discuss the choice between the formula $\underline{\underline{K}} = \underline{\underline{B}}\,\underline{\underline{G}}^T\,\underline{\underline{S}}^{-1}$ and $\underline{\underline{K}} = \underline{\underline{C}}^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}$ depending on the relative sizes of N and M when computer resources is an issue.

8) In the particular cas $N = M = 1$, check the validity of the equality $\underline{\underline{B}}\,\underline{\underline{G}}^T\,\underline{\underline{S}}^{-1} = \underline{\underline{C}}^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}$ and give the expression of the $N \times M$ gain matrix $\underline{\underline{K}}$.

EXERCICE 2.5 Hydraulic jump

We consider a shallow water hydraulic channel with a stationnary lineic discharge flux $q = U_L\,h_L$ where U_L is the mean velocity and h_L the constant depth of the fluid. At $t = 0$, the flow is instantly blocked by a wall that induces a hydraulic jump of velocity W and a constant depth h_R at its right side with zero velocity $U_R = 0$ (see Figure **2**.7).

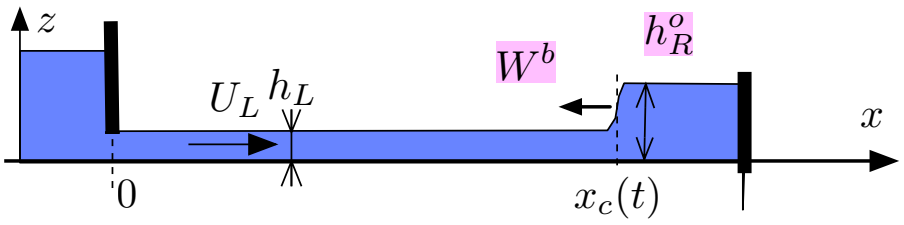

Figure **2**.7: Hydraulic jump experiment.

1) Starting with mass conservation $h_L\,(U_L - W) = h_R\,(U_R - W)$, show that $h_R = \mathcal{G}(W) = a + b/W$ and compute the constants a and b.

We suppose that an experiment gives W^b for the jump velocity with an error σ_b and h_R^o for the right depth with an error σ_r.

2) Considering $x^b = W^b$ as the background and $y^o = h_R^o$ as the observation, express the cost function $J(x)$ to minimize for a BLUE data assimilation method.

3) Draw exactly the curve of $J_b(x) = (x - x^b)^2/(2\,\sigma_b^2)$ and approximatively the curve of $J_r(x) = [y^o - \mathcal{G}(x)]^2/(2\,\sigma_r^2)$ as functions of x on the same graph. Draw the curve of $J(x)$ on the same graph.

4) Show that the incremental cost function is $J_{inc}(x^b + \delta x) = (\delta x)^2/(2\,\sigma_b^2) + (d - G\,\delta x)^2/(2\,\sigma_r^2)$ and give the expression of d and G.

5) Show that the analysis is $x^a = x^b + K\,d$ and give the expression of K.

6) Show that $1/J''_{inc}(x^a) = (I - K\,G)\,B$ with $I = 1$ and $B = \sigma_b^2$. What is the statistical meaning of $A = 1/J''_{inc}(x^a)$?

Chapter 3

Time dependent models

Contents

Introduction

Engineer applications are often involving time evolution processes, such as weather in meteorology, water dynamics in oceanography or hydrology of neutronic flux oscillation in nuclear plants. Data assimilation provides a way to find the best estimation of an initial state or model parameters. The analysis that results of the assimilation process provides an optimal estimation of the observed physical state and can enables forceast of the future states, if needed. In this chapter, we present two classes of data assimilation methods that adress evolution models: the 4D-Var "variationnal" methods and the Kalman filters. A simple example illustrates data assimilation for time dependent models.

1 The 4D-Var data assimilation

1.1 Temporal evolution

We suppose here that an observation vector $\underline{y} \in I\!R^M$ is made of several subvectors $\underline{y}_k$ of smaller dimensions, corresponding to several times t_k with $k = 1, ...K$. The observation operator $\mathcal{G}$ (Figure **3**.1) links a control vector $\underline{x} \in I\!R^N$ to an observation vector $\underline{y} = \mathcal{G}(\underline{x})$ such that

$$\underline{y} = (\underline{y}_1^T, ...\underline{y}_k^T, ...\underline{y}_K^T)^T \quad \text{with} \quad \underline{y}_k = \mathcal{G}_k(\underline{x}) \quad \text{for } k = 1, ...K \ . \tag{3.1}$$

The observation operateur can be written under the form $\mathcal{G} = \left(\mathcal{G}_1^T, ...\mathcal{G}_k^T, ...\mathcal{G}_K^T\right)^T$. The control space can be the initial conditions of a time evolution model, the parameters of such model or both.

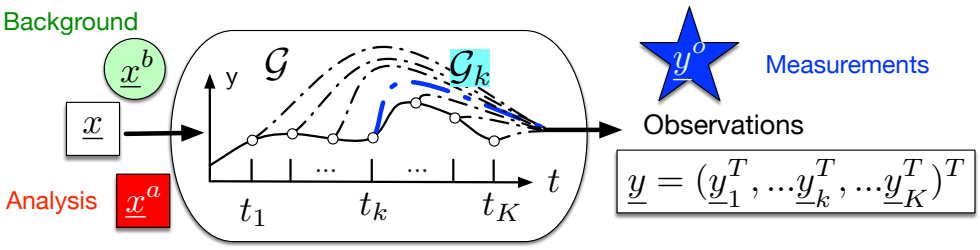

Figure **3**.1: *Observation operator $\mathcal{G}$ made of K observation sub-operators $\mathcal{G}_k$ at different times t_k for $k = 1, ..., K$.*

Assuming that the measurement errors at different times are uncorrelated, the covariance observation error matrix is bloc diagonal:

$$\underline{\underline{R}} = \text{diag} \ (\underline{\underline{R}}_1, ...\underline{\underline{R}}_k, ...\underline{\underline{R}}_K) \ , \tag{3.2}$$

where the $\underline{\underline{R}}_k$ covariance observation error submatrices have the respective square dimensions of the subvectors $\underline{y}_k$ at time t_k. Under this assumption, the

cost function read

$$J(\underline{x}) = J_b(\underline{x}) + \frac{1}{2}\left[\underline{y}^o - \mathcal{G}(\underline{x})\right]^T \underline{\underline{R}}^{-1} \left[\underline{y}^o - \mathcal{G}(\underline{x})\right] , \tag{3.3}$$

$$= J_b(\underline{x}) + \frac{1}{2}\sum_{k=1}^{K} \left[\underline{y}_k^o - \mathcal{G}_k(\underline{x})\right]^T \underline{\underline{R}}_k^{-1} \left[\underline{y}_k^o - \mathcal{G}_k(\underline{x})\right] , \tag{3.4}$$

$$\text{with} \qquad J_b(\underline{x}) = \frac{1}{2}\left(\underline{x} - \underline{x}^b\right)^T \underline{\underline{B}}^{-1} \left(\underline{x} - \underline{x}^b\right) . \tag{3.5}$$

1.2 Linear 4D-Var data assimilation

We now suppose that the time evolution of the considered physical problem is a linear Cauchy problem

$$\frac{d\underline{X}}{dt} = \underline{\underline{L}}(t)\,\underline{X} \quad \text{with} \quad \underline{X}(0) = \underline{x} , \tag{3.6}$$

where $\underline{X}(t)$ is the trajectory, $\underline{\underline{L}}(t)$ a linear matrix and $\underline{x}$ the initial condition at $t = 0$. The solution $\underline{X}(t_k)$ at time t_k of this dynamical system is deduced from the solution $\underline{X}(t_l)$ at time t_l through the relation

$$\underline{X}(t_k) = \underline{\underline{M}}_{l\to k}\,\underline{X}(t_l) \quad \text{with} \quad \underline{\underline{M}}_{l\to k} = \exp\left[\int_{t_l}^{t_k} \underline{\underline{L}}(t)\,dt\right] . \tag{3.7}$$

In particular, we have $\underline{X}(t_k) = \underline{\underline{M}}_{0\to k}\,\underline{x}$.

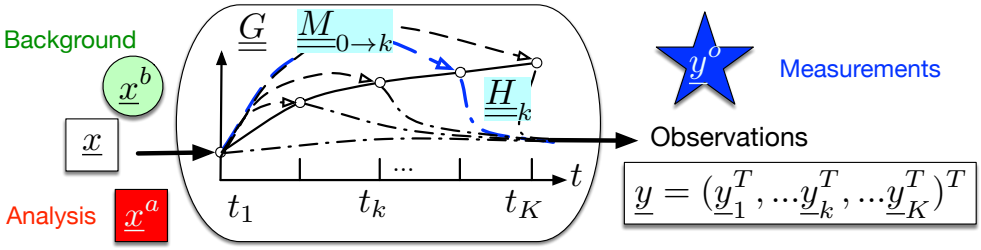

Figure 3.2: *Linear 4D-Var data assimilation method.*

We now suppose that measurements $\underline{y}_k^o$ are compared to the observation $\underline{y}_k = \underline{\underline{H}}_k\,\underline{\underline{M}}_{0\to k}\,\underline{x}$ for $k = 1, ..., K$, where the $\underline{\underline{H}}_k$'s are linear sub-observation operators. The observation operator $\underline{\underline{G}}$ is linear and can be written under the form of the $M \times M$ matrix

$$\underline{\underline{G}} = \text{diag}\left(\underline{\underline{H}}_1\,\underline{\underline{M}}_{0\to 1}, ...\underline{\underline{H}}_k\,\underline{\underline{M}}_{0\to k}, ...\underline{\underline{H}}_K\,\underline{\underline{M}}_{0\to K}\right) . \tag{3.8}$$

The cost function of this data assimilation problem now reads

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x} - \underline{x}^b\right)^T \underline{\underline{B}}^{-1} \left(\underline{x} - \underline{x}^b\right) + J_r(\underline{x}) \tag{3.9}$$

$$\text{with} \quad J_r(\underline{x}) = \frac{1}{2}\sum_{k=1}^{K} \left[\underline{y}_k^o - \underline{\underline{H}}_k\,\underline{\underline{M}}_{0\to k}\,\underline{x}\right]^T \underline{\underline{R}}_k^{-1} \left[\underline{y}_k^o - \underline{\underline{H}}_k\,\underline{\underline{M}}_{0\to k}\,\underline{x}\right] . \tag{3.10}$$

The analysis $\underline{x}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d}$ is given by the usual formula for the innovation vector $\underline{d}$ and the gain matrix $\underline{\underline{K}}$:

$$\underline{d} = \underline{y}^o - \underline{\underline{G}}\,\underline{x} \quad \text{and} \quad \underline{\underline{K}} = \left(\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}}\right)^{-1} \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1} , \tag{3.11}$$

where the Hessian $\underline{\underline{\text{Hess}}}\, J = \underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\, \underline{\underline{R}}^{-1}\, \underline{\underline{G}}$ now reads

$$\underline{\underline{\text{Hess}}}\, J = \underline{\underline{B}}^{-1} + \sum_{k=1}^{K} \underline{\underline{M}}_{0\to k}^T\, \underline{\underline{H}}_k^T\, \underline{\underline{R}}_k^{-1}\, \underline{\underline{H}}_k\, \underline{\underline{M}}_{0\to k} \,. \tag{3.12}$$

We now define the new Cauchy problem

$$\frac{\partial \underline{\widetilde{X}}}{\partial \tau} = \underline{\underline{L}}^T(t_K - \tau)\, \underline{\widetilde{X}} \quad \text{with} \quad \underline{\widetilde{X}}(0) = \underline{\widetilde{x}} \,. \tag{3.13}$$

Denoting $\tau_k = t_K - t_k$ for $k = 1, ...K$, we can write

$$\underline{\widetilde{X}}(\tau_l) = \underline{\underline{M}}^*_{k\to l}\, \underline{\widetilde{X}}(\tau_k) \quad \text{with} \quad \underline{\underline{M}}^*_{k\to l} = \exp\left[\int_{\tau_k}^{\tau_l} \underline{\underline{L}}^T(t_K - \tau)\, d\tau\right] \,. \tag{3.14}$$

Performing the change of variable $\tau = t_K - t$ in the integral, on can see that $\underline{\underline{M}}^*_{k\to l} = \underline{\underline{M}}^T_{l\to k}$, and thus $\underline{\underline{M}}^*_{k\to 0} = \underline{\underline{M}}^T_{0\to k}$. We also note that

$$\underline{\underline{M}}^*_{k\to 0} = \prod_{l=1}^{k} \underline{\underline{M}}^*_{l\to l-1} = \prod_{l=1}^{k} \underline{\underline{M}}^T_{l-1\to l} = \left(\prod_{l=k}^{1} \underline{\underline{M}}_{l-1\to l}\right)^T = \underline{\underline{M}}^T_{0\to k} \,. \tag{3.15}$$

The integration of the so called "adjoint equation" (3.13), lead to the adjoint model $\underline{\underline{M}}^*_{K\to k}$ which allow a direct expression of the Hessian of J or the gain matrix $\underline{\underline{K}}$ through the relations

$$\underline{\underline{M}}^T_{0\to k}\, \underline{\underline{H}}^T_k\, \underline{\underline{R}}^{-1}_k\, \underline{\underline{H}}_k\, \underline{\underline{M}}_{0\to k} = \underline{\underline{M}}^*_{k\to 0}\, \underline{\underline{H}}^T_k\, \underline{\underline{R}}^{-1}_k\, \underline{\underline{H}}_k\, \underline{\underline{M}}_{0\to k} \,. \tag{3.16}$$

1.3 The incremental 4D-Var cost function

We now suppose that the considered Cauchy problem is nonlinear:

$$\frac{d\underline{X}}{dt} = \mathcal{L}(t, \underline{X}) \quad \text{with} \quad \underline{X}(0) = \underline{x} \,, \tag{3.17}$$

where $\underline{X}(t)$ is the trajectory, $\mathcal{L}$ a nonlinear operator $\underline{x}$ the initial condition at $t = 0$. The solution $\underline{X}(t_k)$ at time t_k of this dynamical system is deduced from the solution $\underline{X}(t_l)$ at time t_l through the relation

$$\underline{X}(t_k) = \mathcal{M}_{l\to k}\, [\underline{X}(t_l)] \,, \tag{3.18}$$

where $\mathcal{M}_{l\to k}$ are nonlinear operators. We have $\underline{X}(t_k) = \mathcal{M}_{0\to k}(\underline{x})$.

We now suppose that measurements $\underline{y}^o_k$ are compared to the observation $\underline{y}_k = \mathcal{H}_k\, \mathcal{M}_{0\to k}(\underline{x})$ for $k = 1, ..., K$, where the $\mathcal{H}_k$ are nonlinear sub-operators applied to vectors $\mathcal{M}_{0\to k}(\underline{x})$. The observation operateur $\mathcal{G}$ is linear and can be written under the form of the

$$\mathcal{G} = \left(\mathcal{G}_1^T, ...\mathcal{G}_k^T, ...\mathcal{G}_K^T\right)^T \quad \text{with} \quad \mathcal{G}_k = \mathcal{H}_k\, \mathcal{M}_{0\to k} \,. \tag{3.19}$$

The cost function of this data assimilation problem now reads

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x} - \underline{x}^b\right)^T \underline{\underline{B}}^{-1} \left(\underline{x} - \underline{x}^b\right) + J_r(\underline{x}) \tag{3.20}$$

$$\text{with} \quad J_r(\underline{x}) = \frac{1}{2}\sum_{k=1}^{K} \left[\underline{y}^o_k - \mathcal{H}_k\, \mathcal{M}_{0\to k}(\underline{x})\right]^T \underline{\underline{R}}^{-1}_k \left[\underline{y}^o_k - \mathcal{H}_k\, \mathcal{M}_{0\to k}(\underline{x})\right] . \tag{3.21}$$

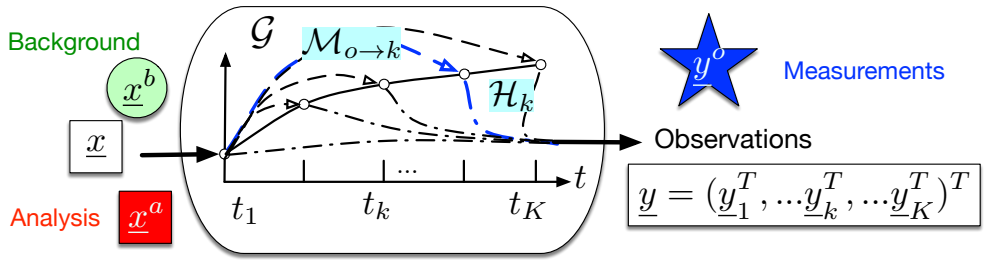

Figure **3**.3: *Nonlinear 4D-Var data assimilation methods.*

The incremental cost function J_{inc} is obtained by linearizing the observation operator around the background $\underline{x}^b$, which requires the linearizations

$$\mathcal{H}_k \, \mathcal{M}_{0\to k}(\underline{x}^b + \underline{\delta x}) \sim \mathcal{H}_k \, \mathcal{M}_{0\to k}(\underline{x}^b) + \underline{\underline{H}}_k \, \underline{\underline{M}}_{0\to k} \, \underline{\delta x} \; , \tag{3.22}$$

where $\underline{\underline{H}}_k$ is the linearized of $\mathcal{H}_k$ around $\mathcal{M}_{0\to k}(\underline{x}^b)$ and $\underline{\underline{M}}_{0\to k}$ is the "tangent model", linearized around the "background trajectory" $\underline{X}^b(t)$, solution of Equation (**3**.17) with the initial condition $\underline{X}^b(0) = \underline{x}^b$.

The tangent model can be obtained by considering the linear Cauchy problem

$$\frac{\partial \underline{U}}{\partial t} = \underline{\underline{L}} \left[\underline{X}^b(t) \right] \underline{U} \quad \text{with} \quad \underline{U}(0) = \underline{\delta x} \; , \tag{3.23}$$

where $\underline{\underline{L}}$ is obtained through the linearization of $\mathcal{L}$ around the background trajectory: $\mathcal{L}[\underline{X}^b(t) + \underline{U}] \sim \mathcal{L}[\underline{X}^b(t)] + \underline{\underline{L}}[\underline{X}^b(t)] \, \underline{U}$. The tangent model $\underline{\underline{M}}_{l\to k}$ is thus defined by the relation

$$\underline{U}(t_k) = \underline{\underline{M}}_{l\to k} \, \underline{U}(t_l) \; . \tag{3.24}$$

The incremental cost function is then

$$J_{inc}(\underline{x}^b + \underline{\delta x}) = \frac{1}{2} \underline{\delta x}^T \underline{\underline{B}}^{-1} \underline{\delta x} + J_{r,inc}(\underline{x}^b + \underline{\delta x}) \qquad \text{with} \tag{3.25}$$

$$J_{r,inc}(\underline{x}^b + \underline{\delta x}) = \frac{1}{2} \sum_{k=1}^{K} \left[\underline{d}_k - \underline{\underline{H}}_k \, \underline{\underline{M}}_{0\to k} \, \underline{\delta x} \right]^T \underline{\underline{R}}_k^{-1} \left[\underline{d}_k - \underline{\underline{H}}_k \, \underline{\underline{M}}_{0\to k} \, \underline{\delta x} \right] , \tag{3.26}$$

where $\underline{d}_k = \underline{y}_k^o - \mathcal{H}_k \, \mathcal{M}_{0\to k}(\underline{x}^b)$ are the innovation subvectors. The incremental cost function is minimum for $\underline{\widetilde{x}}^a = \underline{x}^b + \underline{\underline{K}} \, \underline{d}$ where the innovation vector $\underline{d}$ and the gain matrix $\underline{\underline{K}}$ are given by the same equation (**3**.11). The adjoint model $\underline{\underline{M}}^*_{k\to 0}$ is obtained, as for the linear case, through a backtime integration of the transposed linear matrix $\underline{\underline{L}}^T \left[\underline{X}^b(t) \right]$.

Approximation of the 4D-Var can be obtained by replacing $\underline{\underline{M}}_{0\to k}$ and $\underline{\underline{M}}^*_{k\to 0}$ by the identity $\underline{\underline{I}}$ in the expression of the incremental cost function. This method is then called "First Guess at Appropriate Time" (FGAT).

A 4D-Var method can easily deduced from this presentation when $\underline{x}$ contains models parameters instead of the components of the initial conditions, or when its contains both the models parameters and the initial condition. An easy change of notations is necessary for these cases.

2 The Kalman filter data assimilation

2.1 Linear Kalman filter

We go back to the linear Cauchy problem (**3**.6). We note $\underline{\underline{M}}_k = \underline{\underline{M}}_{k-1\to k}$ for $k = 1, ...K$. We now suppose that the model is not perfect, such that

$$\underline{X}(t_k) = \underline{\underline{M}}_k \, \underline{X}(t_{k-1}) + \underline{\epsilon}^q_k \, , \tag{3.27}$$

where $\underline{\epsilon}^q_k$ are the model errors at time t_k, whose "covariance error model matrix" $\underline{\underline{Q}}_k$ is defined by its components $Q_{ij} = \left\langle \epsilon^q_i \, \epsilon^q_j \right\rangle$.

We suppose that we know the initial background $\underline{x}^b = \underline{X}(0)$ with an error $\underline{\epsilon}^b$ and measurements $\underline{y}^o_k$ at times t_k with errors $\underline{\epsilon}^o_k$. We denote by $\underline{\underline{B}}$ and $\underline{\underline{R}}_k$ the respective covariance errors matrices of these informations.

The Kalman filter is defined by the following iterations, for $k = 1, ...K$:

$$\begin{aligned}
\underline{x}_k &= \underline{\underline{M}}_k \, \underline{x}^a_{k-1} \quad \text{and} \quad \underline{\underline{B}}_k = \underline{\underline{M}}_k \, \underline{\underline{A}}_{k-1} \, \underline{\underline{M}}^T_k + \underline{\underline{Q}}_k \, , && (3.28)\\
\underline{x}^a_k &= \underline{x}_k + \underline{\underline{K}}_k \, \underline{d}_k \quad \text{with} && (3.29)\\
\underline{d}_k &= \underline{y}^o_k - \underline{\underline{H}}_k \, \underline{x}_k \quad \text{and} \quad \underline{\underline{K}}_k = \underline{\underline{B}}_k \, \underline{\underline{H}}^T_k \, (\underline{\underline{H}}_k \, \underline{\underline{B}}_k \, \underline{\underline{H}}_k + \underline{\underline{R}}_k)^{-1} \, , && (3.30)\\
\underline{\underline{A}}_k &= (\underline{\underline{I}} - \underline{\underline{K}}_k \, \underline{\underline{H}}_k) \, \underline{\underline{B}}_k \, , && (3.31)
\end{aligned}$$

where $\underline{y}^o_k$ are the measurements and $\underline{\underline{H}}_k$ are the observation operators at time t_k. The Kalman filter is initialized by $\underline{x}^a_0 = \underline{x}$ and $\underline{\underline{A}}_0 = \underline{\underline{B}}$.

This data assimilation method can be viewed as a chain of BLUE (Best Linear Unbiased Estimation) with $\underline{x}_k$ as the background $\underline{\underline{B}}_k$ as the covariance background error matrix and $\underline{\underline{R}}_k$ as the covariance observation error matrix. The covariance analysis error matrix $\underline{\underline{A}}_{k-1}$ is propagated through the linear model $\underline{\underline{M}}_k$ to give $\underline{\underline{B}}_k$, with the addition of the covariance model error matrix $\underline{\underline{Q}}_k$.

2.2 Extended Kalman filter

We now go back to the nonlinear Cauchy problem (**3**.17) and we denote $\mathcal{M}_k = \mathcal{M}_{k-1\to k}$ and $\underline{\underline{M}}_k = \underline{\underline{M}}_{k-1\to k}$ for $k = 1, ...K$ where $\mathcal{M}_{k\to l}$ is defined by Eauqtion (**3**.18) and $\underline{\underline{M}}_{l\to k}$ is defined by Equation (**3**.24).

The extend Kalman filter (Figure **3**.4) is the nonlinear version of the Kalman filter and reads, for $k = 1, ...K$:

$$\begin{aligned}
\underline{x}_k &= \mathcal{M}_k \left(\underline{x}^a_{k-1}\right) \quad \text{and} \quad \underline{\underline{B}}_k = \underline{\underline{M}}_k \, \underline{\underline{A}}_{k-1} \, \underline{\underline{M}}^T_k + \underline{\underline{Q}}_k && (3.32)\\
\underline{x}^a_k &= \underline{x}_k + \underline{\underline{K}}_k \, \underline{d}_k \quad \text{with} && (3.33)\\
\underline{d}_k &= \underline{y}^o_k - \mathcal{H}_k \left(\underline{x}_k\right) \quad \text{and} \quad \underline{\underline{K}}_k = \underline{\underline{B}}_k \, \underline{\underline{H}}^T_k \, (\underline{\underline{H}}_k \, \underline{\underline{B}}_k \, \underline{\underline{H}}_k + \underline{\underline{R}}_k)^{-1} \, , && (3.34)\\
\underline{\underline{A}}_k &= (\underline{\underline{I}} - \underline{\underline{K}}_k \, \underline{\underline{H}}_k) \, \underline{\underline{B}}_k \, , && (3.35)
\end{aligned}$$

where $\underline{y}^o_k$ are the measurements, $\mathcal{H}_k$ nonlinear observation sub-operators, $\underline{\underline{H}}_k$ their linearization around the states $\underline{x}_k$ at time t_k. The extended Kalman filter is initialized by $\underline{x}_0 = \underline{x}$ and $\underline{\underline{A}}_0 = \underline{\underline{B}}$.

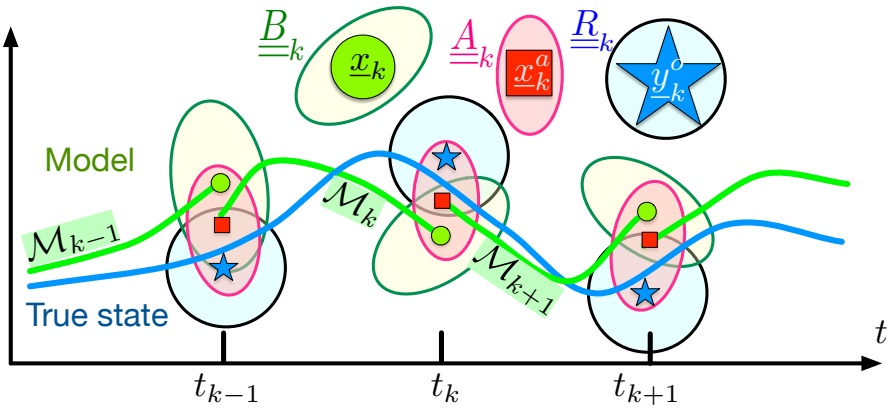

Figure **3**.4: *Extended Kalman filter.*

Approximation of this method can be obtained by replacing the expression of $\underline{\underline{B}}_k$ in Equation (**3**.32) by $\underline{\underline{B}}_k = \underline{\underline{B}}$ (chain of BLUE with constant $\underline{\underline{B}}$), $\underline{\underline{B}}_k = \underline{\underline{A}}_{k-1} + \underline{\underline{Q}}_k$ (chain of BLUE with $\underline{\underline{A}}$ propagate by identity) or ignoring $\underline{\underline{Q}}_k$ in one of these expressions.

2.3 Ensemble Kalman filters

Instead of considering one initial condition $\underline{x}^b$, the ensemble Kalman filters consider a number R of initial conditions $\underline{x}_0^{(r)}$ with $r = 1, ...R$, such that the covariance background error matrix $\underline{\underline{B}}$ and the background can be respectively approximated by

$$\underline{x}^b \sim \underline{x}_0 = \frac{1}{R}\sum_{r=1}^{R} \underline{x}_0^{(r)} \quad \text{and} \tag{3.36}$$

$$\underline{\underline{B}} \sim \frac{1}{R}\sum_{r=1}^{R} \left[\underline{x}_0^{(r)} - \underline{x}_0\right]\left[\underline{x}_0^{(r)} - \underline{x}_0\right]^T . \tag{3.37}$$

Such an ensemble can be obtained through a random function of probability density function $f^b(\underline{x}) = K^b \exp[-J_b(\underline{x})]$ with $J_b(\underline{x}) = \frac{1}{2}(\underline{x}-\underline{x}^b)^T\, \underline{\underline{B}}^{-1}\, (\underline{x}-\underline{x}^b)$.

When one can linearize the operator $\mathcal{H}_k$ around any state, i.e. compute $\underline{\underline{H}}_k$ for all $\underline{x}$, the algorithm of the ensemble Kalman filter reads, for $k = 1, ...K$:

$$\underline{x}_k^{(r)} = \mathcal{M}_k\left(\underline{x}_{k-1}^{a(r)}\right) \quad \text{for } r = 1, ...R \quad \text{and} \quad \underline{x}_k = \frac{1}{R}\sum_{r=1}^{R} \underline{x}_k^{(r)} , \tag{3.38}$$

$$\underline{\underline{B}}_k = \frac{1}{R-1}\sum_{r=1}^{R} \left(\underline{x}_k^{(r)} - \underline{x}_k\right)\left(\underline{x}_k^{(r)} - \underline{x}_k\right)^T + \underline{\underline{Q}}_k , \tag{3.39}$$

$$\underline{x}_k^{a(r)} = \underline{x}_k^{(r)} + \underline{\underline{K}}_k\, \underline{d}_k^{(r)} \quad \text{with} \quad \underline{d}_k^{(r)} = \underline{y}_k^o - \mathcal{H}_k\left(\underline{x}_k^{(r)}\right) \tag{3.40}$$

$$\text{and} \quad \underline{\underline{K}}_k = \underline{\underline{B}}_k\, \underline{\underline{H}}_k^T\, (\underline{\underline{H}}_k\, \underline{\underline{B}}_k\, \underline{\underline{H}}_k^T + \underline{\underline{R}}_k)^{-1}. \tag{3.41}$$

Instead of propagating the covariance analysis error matrix $\underline{\underline{A}}_{k-1}$ and using it as covariance background error matrix for a new analysis at time t_k, as in the

Extended Kalman filter, the spread of forcecast states are used as background states and the resulting spread of the analysis states provides an approximation of the covariance analysis error matrix (Figure **3**.5).

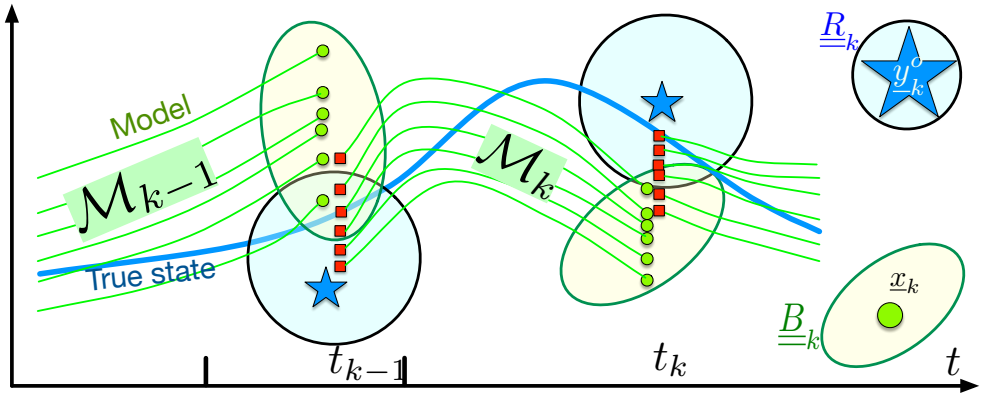

Figure **3**.5: *Ensemble Kalman filters.*

When the linearized operateur $\mathcal{H}_k$ is not available and assuming $\underline{\underline{Q}}_k = \underline{\underline{0}}$ (no model errors), the ensemble Kalman filter reads, for $k = 1, ...K$:

$$\underline{x}_k^{(r)} = \mathcal{M}_k\left(\underline{x}_{k-1}^{a(r)}\right) \quad \text{for } r = 1, ...R \quad \text{and} \quad \underline{x}_k = \frac{1}{R}\sum_{r=1}^{R} \underline{x}_k^{(r)} \ , \tag{3.42}$$

$$\underline{x}_k^{a(r)} = \underline{x}_k^{(r)} + \underline{\underline{K}}_k \, \underline{d}_k^{(r)} \quad \text{with} \quad \underline{d}_k^{(r)} = \underline{y}_k^{(r)} - \mathcal{H}_k\left(\underline{x}_k^{(r)}\right) \tag{3.43}$$

$$\text{and} \qquad \underline{\underline{K}}_k = \underline{\underline{\mathcal{A}}}_k^{BH^T} \left(\underline{\underline{\mathcal{A}}}_k^{HBH^T} + \underline{\underline{R}}_k\right)^{-1} , \tag{3.44}$$

where $\underline{\underline{\mathcal{A}}}_k^{BH^T}$ and $\underline{\underline{\mathcal{A}}}_k^{HBH^T}$ are respectively the approximation of $\underline{\underline{B}}_k \, \underline{\underline{H}}_k^T$ and $\underline{\underline{H}}_k \, \underline{\underline{B}}_k \, \underline{\underline{H}}_k^T$ with the expressions

$$\underline{\underline{\mathcal{A}}}_k^{BH^T} = \frac{1}{R-1}\sum_{r=1}^{R} \left(\underline{x}_k^{(r)} - \underline{x}_k\right) \left(\underline{y}_k^{(r)} - \underline{y}_k\right)^T , \tag{3.45}$$

$$\underline{\underline{\mathcal{A}}}_k^{HBH^T} = \frac{1}{R-1}\sum_{r=1}^{R} \left(\underline{y}_k^{(r)} - \underline{y}_k\right) \left(\underline{y}_k^{(r)} - \underline{y}_k\right)^T . \tag{3.46}$$

$$\text{with } \underline{y}_k^{(r)} = \mathcal{H}_k\left(\underline{x}_k^{(r)}\right) \quad \text{and} \quad \underline{y}_k = \frac{1}{R}\sum_{r=1}^{R} \mathcal{H}_k\left(\underline{x}_k^{(r)}\right) . \tag{3.47}$$

A variant of this ensemble data assimilation method is obtained by replacing the definion of $\underline{y}_k$ by $\underline{y}_k = \mathcal{H}_k\left(\underline{x}_k\right)$. With a little algebra, one recovers the previous method (with $\underline{\underline{Q}}_k = \underline{\underline{0}}$) with the approximation

$$\mathcal{H}_k(\underline{x}^{(r)}) - \mathcal{H}_k(\underline{x}) \sim \underline{\underline{H}}_k \left(\underline{x}^{(r)} - \underline{x}\right) . \tag{3.48}$$

This nonlinear method is thus a trick to approximate the linearization of $\mathcal{H}_k$.

As for the 4D-Var method, the control space of this last Ensemble Kalman filter can contain models parameters instead of the initial condition or both. New notation must be chosen in this case since the control parameter $\underline{x}$ no longer denotes an initial condition of the model $\mathcal{M}_k$.

3 Will the water overflow?

In this example, one estimates the water filling and discharge capacity of a tank with sequential measurements of its water height.

3.1 A reservoir model

We consider the reservoir model

$$\frac{dH(t)}{dt} = -\alpha\, H(t) + P \qquad \text{with} \qquad H(0) = H_0\ , \tag{3.49}$$

where $H(t)$ is the height of the reservoir, P a constant pouring flow into the reservoir and $Q(t) = \alpha\, H(t)$ the discharge flux, proportional to heigh. Such discharge flux are encounter for flow in porous media, let's say, for this example, water flowing through coffee powder (Figure **3**.6).

Equation (**3**.49) admits an exact solution $H(t) = (P/\alpha)\,[1 - \exp(-\alpha\, t)]$ that converges towards P/α when $t \to \infty$ (Figure **3**.6). Knowing P/α could be of significant importance if the upper limit of the reservoir is reached when $H(t)$ goes beyond some threshold.

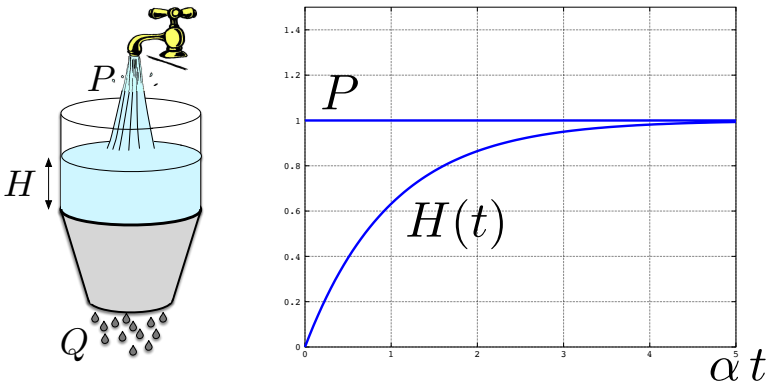

Figure **3**.6: *Solution $H(t)$ of the reservoir model starting with $H(0) = 0$.*

Given several measurements of the height $H(t_k)$ at several times t_k, one would like to determine the coefficients α and P that are only known with some uncertainties. Rather than doing the real experiment, a common procedure to test data assimilation methods consists in performing "twin experiments". We choose a set of parameters (α^t, P^t) and we decide that they are the "true parameters". We then compute (or analytically express) the "true trajectory" $H^t(t)$, obtained with these true parameters.

Artificial measurements at times t_k, for $k = 1, ...K$, are obtained by setting $y_k = H^t(t_k) + \epsilon^o$ where the artificial error ϵ^o is a gaussian random variable of zero mean and standard deviation σ_r. We then choose a background state made of $\alpha^b = \alpha^t + \epsilon_\alpha$ and $P^b = P^t + \epsilon_P$ where the errors ϵ_α and ϵ_P are gaussian random variable of zero mean, respective standard deviation σ_α and σ_P and correlation $\rho = \langle \alpha'\, P' \rangle \,/\sigma_\alpha\, \sigma_P$.

3.2 Assimilation of one control parameter

First, we consider that $\sigma_P = 0$, which meand that P is a fully certain parameter. We only have to determine on parameter $x = \alpha$ in a control space of dimension $N = 1$. The measurements $\underline{y}^o = (y_1^o, ...y_k^o, ...y_K^o)^T$ are in the observation space of dimension $M = K$. The observation operator $\mathcal{G} = (\mathcal{G}_1^T, ...\mathcal{G}_k^T, ...\mathcal{G}_K^T)^T$ is defined by $\mathcal{G}_k(\alpha) = (P/\alpha)[1 - \exp(-\alpha\, t_k)]$ (figure **3**.7).

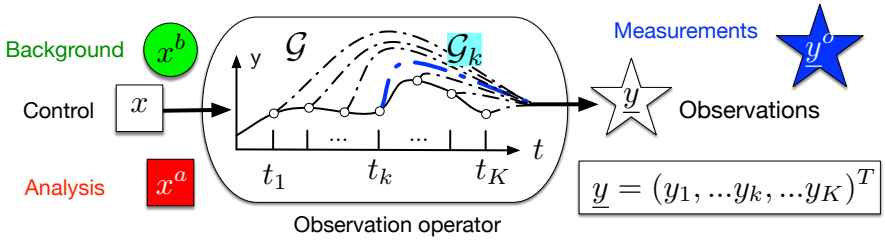

Figure **3**.7: *Assimilation of K data at times t_k to control one parameter x.*

The cost function to minimize reads

$$J(\alpha) = \frac{1}{2}\frac{(\alpha - \alpha^b)^2}{\sigma_b^2} + \sum_{k=1}^{K} \frac{\left[y_k^o - \mathcal{G}_k(\alpha)^2\right]}{2\,\sigma_r^2}\ , \qquad (\mathbf{3}.50)$$

were $\sigma_b = \sigma_\alpha$. The covariance observation error matrice reads $\underline{\underline{R}} = \sigma_r^2\, \underline{\underline{I}}$ where $\underline{\underline{I}}$ is the $M \times M$ identity matrix. The analysis x^a, which minizes J, give rise to an "analysis trajectory" $H^a(t)$ that can be compared to the "true trajectory" $H^t(t)$ and the "background trajectory", to see how the data assimilation of measurement improves the forecast of the asymptotic limit for $t \to \infty$ (Figure **3**.8).

3.3 Assimilation of two control parameters

We know suppose that both α and P are uncertain quantities and we consider the vectors $\underline{x} = (\alpha, P)^T \in I\!R^2$ in the control space of dimension $N = 2$. For this data assimilation problem, the observation operator components $\mathcal{G}_k(\alpha, P) = (P/\alpha)[1 - \exp(-\alpha\, t_k)]$ are now depending on two components. We still have $\underline{\underline{R}} = \sigma_r^2\, \underline{\underline{I}}$, a $M \times M$ matrix with $M = K$. The new cost function

$$J(\alpha, P) = \frac{1}{2}(\alpha - \alpha^b, P - P^b)\ \underline{\underline{B}}^{-1} \begin{pmatrix} \alpha - \alpha^b \\ P - P^b \end{pmatrix} + \sum_{k=1}^{K} \frac{\left[y_k^o - \mathcal{G}_k(\alpha, P)\right]^2}{2\,\sigma_r^2}\ , \qquad (\mathbf{3}.51)$$

where the covariance background error matrix reads

$$\underline{\underline{B}} = \begin{pmatrix} \sigma_\alpha^2 & \rho\,\sigma_\alpha\,\sigma_P \\ \rho\,\sigma_\alpha\,\sigma_P & \sigma_P^2 \end{pmatrix}\ . \qquad (\mathbf{3}.52)$$

Figure **3**.9 compares the background, the analysis and the true trajectory for several random draws of the measurements errors. We see that the assimilation of measurements improve the analysis, compared to the background.

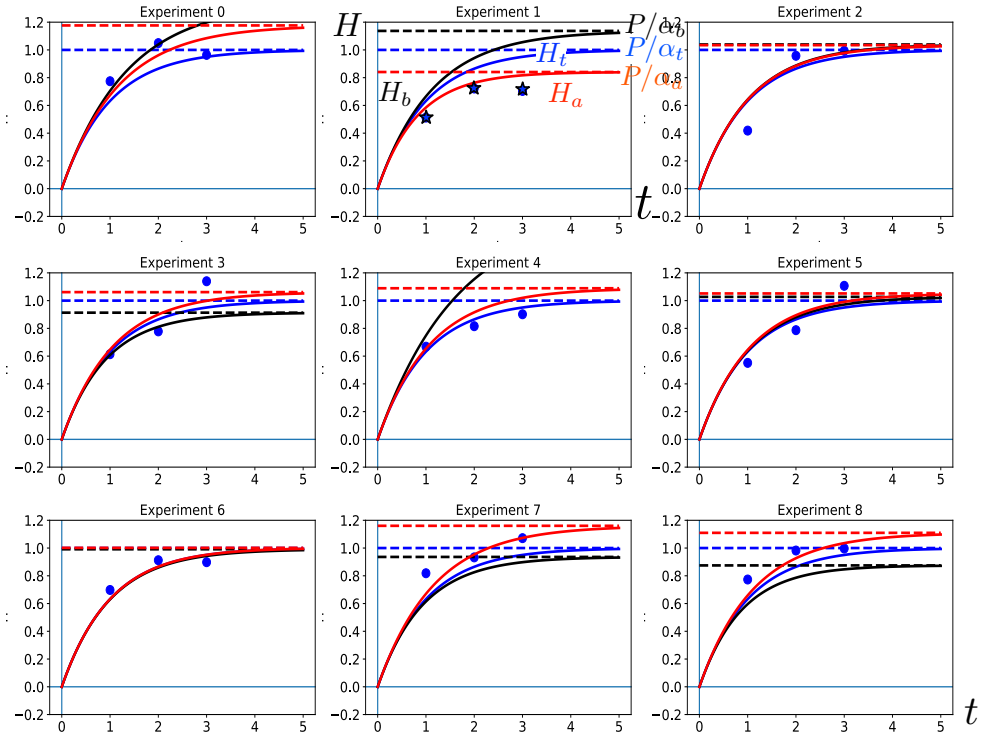

Figure **3**.8: *Control of a single model parameter $x = \alpha$. Comparison of the background trajectory (black) and the analysis trajectory (red) with the true trajectory (blue) $H^t(t)$, for random draws of the observations.*

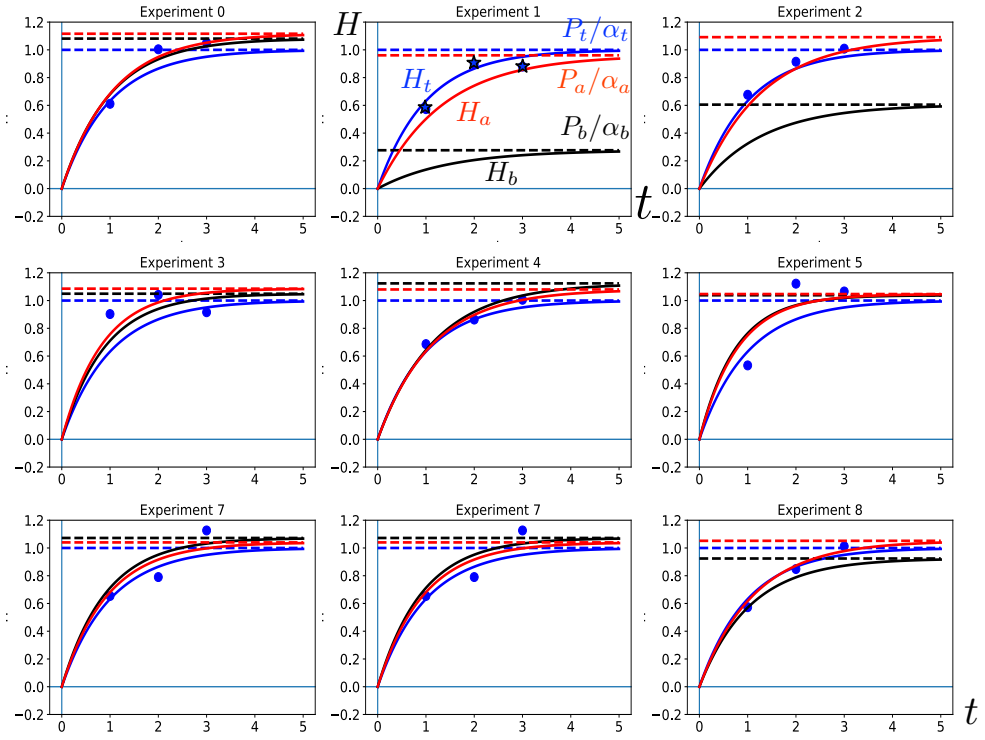

Figure **3**.9: *Control of a two model parameters $\underline{x} = (\alpha, P)^T$.*

EXERCICES

EXERCICE 3.1 Hands-on "Will the water overflow?"

A demonstration program of the "Will the water overflow?" example is available in several language (Octave, Scilab, Matlab) on the following page :

`http://pedagotech.inp-toulouse.fr/130202/co/90-ho_coffee.html`

1) Read the content of the program
2) Launch the program with the default parameters
3) Describe the program algorithm briefly
4) Change parameters and describe results
5) Enrich the program to compute scores

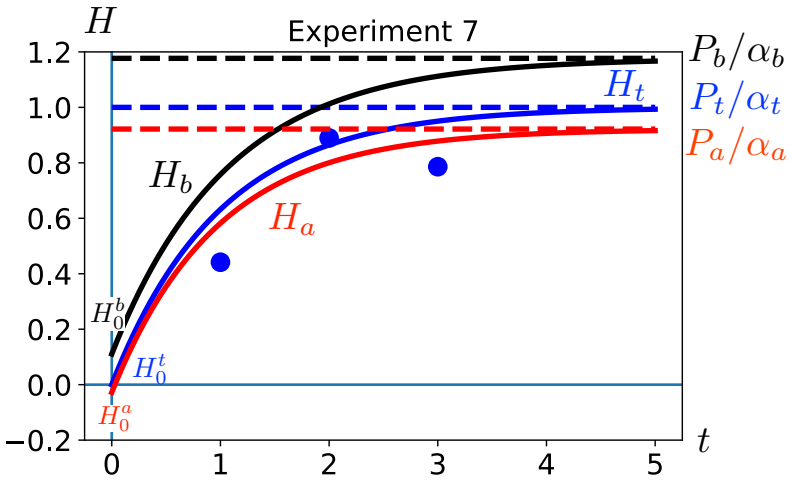

Figure 3.10: *Example of output of the demo program.*

EXERCICE 3.2 Reservoir

We consider the equation $\frac{dH}{dt} = 1 - H$ with $H(t) \in I\!R$ and the initial condition $H(0) = x$.

1) Give the analytical expression of the model $H(t) = \mathcal{M}_{0\to t}(x)$.
2) We consider the observation vector $\underline{y}^o = (y_1^o, y_2^o)^T$ where y_1^o and y_2^o are respective measurements of $H(t_1)$ and $H(t_2)$ with the independant errors of root mean square σ_r. If x is considered as the control space vector, express the observation operator $\underline{y} = \mathcal{G}(x)$ associated to this data assimilation problem.
3) We suppose that a guess x^b of the initial condition x is known with an error of root mean square σ_b. Show that the cost function of the 4D-Var data assimilation method can be written under the form $J(x+\delta x) = (\delta x)^2/(2\,B) + (d_1 - M_1\,\delta x)^2/(2\,R) + (d_2 - M_2\,\delta x)^2/(2\,R)$ where $\underline{d} = (d_1, d_2)^T$ and $\underline{\underline{G}} = (M_1, M_2)^T$ are 2×1 matrices. Express these vector as function of t_1, t_2, y_1^o, y_2^o and x^b and give their names and their meaning. Express

B and R.

4) We admit without demonstration that the gain function of a linear data assimilation based on $\underline{\underline{B}}$ and $\underline{\underline{R}}$ as covariance error matrices and $\underline{\underline{G}}$ as linear observation operator is given by the two equivalent expressions $\underline{\underline{K}} = \underline{\underline{B}}\,\underline{\underline{G}}^T\,(\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}})^{-1} = (\underline{\underline{B}}^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}})^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}$. Choose the most convenient expression to compute K_1 and K_2 in the expression of the analysis of the 4D-Var problem $x^a = x^b + K_1\,d_1 + K_2\,d_2$ where $d_i = y_i^o - 1 + \exp(-t_i)\,(1 - x^b)$ for $i \in \{1, 2\}$.

5) How varies K_2 when $t_2 \to \infty$? Deduce from this result that a too large data assimilation windows can jeopardize the convergence of a 4D-Var method.

EXERCICE 3.3 Chain of BLUE and the Lorenz model

We consider the Lorenz model $\frac{d}{dt}X = -\sigma\,X + \sigma\,Y$, $\frac{d}{dt}Y = \rho\,X - Y - X\,Z$ and $\frac{d}{dt}Z = X\,Y - \beta\,Z$, where $X(t)$, $Y(t)$ and $Z(t)$ evolve in time and $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$.

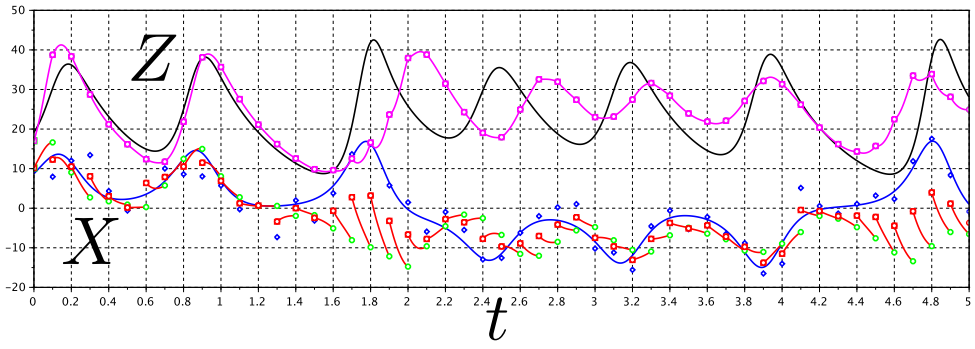

Figure **3**.11: Trajectories for a the chain of BLUE in a twin experiment.

We denote by $\underline{x}^a = \mathcal{F}_{blue}(\underline{x}^b, \underline{y}^o, \underline{\underline{B}}, \underline{\underline{R}}, \underline{\underline{G}})$ the minimum of the cost function

$$J(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}^b)^T\,\underline{\underline{B}}^{-1}\,(\underline{x} - \underline{x}^b) + \frac{1}{2}(\underline{y}^o - \underline{\underline{G}}\,\underline{x})^T\,\underline{\underline{R}}^{-1}(\underline{y}^o - \underline{\underline{G}}\,\underline{x})\,. \qquad (\mathbf{3}\cdot 53)$$

We assume that $\underline{\underline{B}} = \sigma_b^2\,\underline{\underline{I}}$, where $\underline{\underline{I}}$ is the 3×3 identity matrix, $\underline{\underline{R}} = \sigma_r^2$ and $\underline{\underline{G}} = (1, 0, 0)$. We consider the times $t_k = i\,\tau$ for $k = 1, ..., K$ where $K = 50$ and $\tau = 0,1$. We denote by $\underline{x}_{k+1} = \mathcal{M}_k(\underline{x}_k)$ the operator that computes the state $\underline{x}_{k+1}$ at time t_{k+1} obtained with the Lorenz model with the initial conditions $\underline{x}_k$ at time t_k.

We then define a chain of data assimilation methods by $\underline{x}_0^a = (X^b, Y^b, Z^b)^T$ and $\underline{x}_k^a = \mathcal{F}_{blue}\left[\mathcal{M}_k(\underline{x}_{k-1}^a), y_k^o, \underline{\underline{B}}, \underline{\underline{R}}, \underline{\underline{G}}\right]$ for $k = 1, ...K$.

1) Write a program, in the language of your choice, to integrate the Lorenz model on the interval $t \in [-10, 0]$ with initial conditions $X(-10) = 10$, $Y(-10) = 15$ and $Z(-10) = 20$.

2) Describe how to generate X^b, Y^b, Z^b and y_k^o in a twin experiment.

3) Express $\mathcal{F}_{blue}$ for any $\underline{x}^b = (X^b, Y^b, Z^b)^T$ and y^o using the notation $C_b = \sigma_b^{-2}$ and $C_r = \sigma_b^{-2}$.

4) Figure **3**.11 shows the result of the data assimilation methods for $\sigma_b = \sigma_r = 4$. Describe the various curves and points shown on the figure.
5) Describe the method in the cases $\sigma_b \gg \sigma_r$ and then $\sigma_r \gg \sigma_b$.
6) By comparison with the two independant clocks problem, show that $\underline{\underline{A}} = (\underline{\underline{I}} - \underline{\underline{K}}\,\underline{\underline{G}})\,\underline{\underline{B}}$ is the variance of the analysis error for the above twin experiment.
7) By denoting $\underline{\underline{M}}_k(\underline{x})$ the tangent linear operator of $\mathcal{M}_k$ with the initial condition $\underline{x}$, we now replace the analysis process by the extended Kalman filter $\underline{x}^a_k = \mathcal{F}_{blue}\left[\mathcal{M}_k(\underline{x}^a_{k-1}), \underline{y}^o_k, \underline{\underline{B}}_k, \underline{\underline{R}}, \underline{\underline{G}}\right]$, with $\underline{\underline{B}}_k = \underline{\underline{M}}_k(\underline{x}^a_{k-1})\,\underline{\underline{A}}_{k-1}\,\underline{\underline{M}}^T_k(\underline{x}^a_{k-1})$, $\underline{\underline{A}}_k = (\underline{\underline{I}} - \underline{\underline{K}}_k\,\underline{\underline{G}})\,\underline{\underline{B}}_k$, starting with $\underline{\underline{B}}_0 = \underline{\underline{B}}$, with gain matrices of the form $\underline{\underline{K}}_k = (\underline{\underline{B}}_k^{-1} + \underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}\,\underline{\underline{G}})^{-1}\,\underline{\underline{G}}^T\,\underline{\underline{R}}^{-1}$. Explain the choices underlying this data assimilation method, denoted by "Kalman filter with no model error".

EXERCICE 3.4 Data assimilation for a 1D field

In the interval $s \in [O, L]$, we consider a 1D field $h^t(s)$ considered as the "true state". We suppose that $h^b(s) = h^t(s) + \epsilon^b(s)$ is the "background state", where $\epsilon^b(s)$ is a gaussien random field such that

$$B(s, s') = \left\langle \epsilon^b(s)\,\epsilon^b(s') \right\rangle = \sigma_b^2\,\exp\left[\frac{-(s-s')^2}{2\,l_B^2}\right] . \qquad (\mathbf{3}.54)$$

We discretize the interval $[0, L]$ with N points s_j, for $j = 1, ...N$, and we consider the vector $\underline{x}^b \in I\!R^N$ of components $x^b_j = h^b(s_j)$ as the background state. We consider a measurement $y^0 = H^t(s_J) + \epsilon^o$ where s_J is one point in the interval and ϵ^o a gaussian variable of standard deviation σ_r (Figure **3**.12).

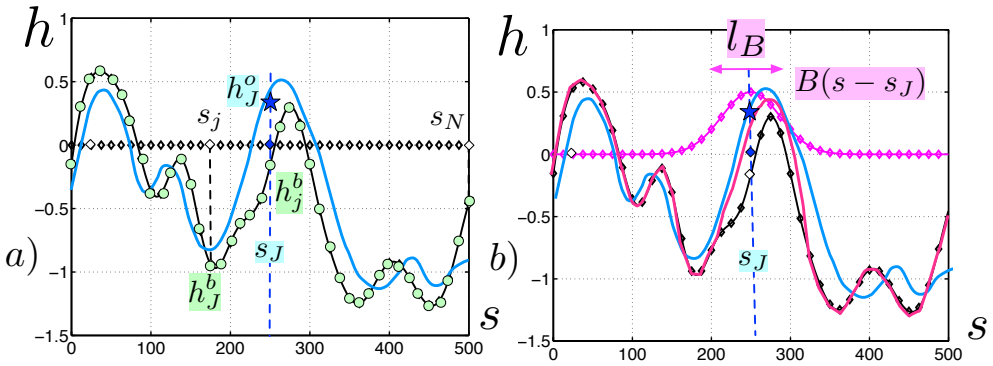

Figure **3**.12: *Data assimilation of one measurement in a 1D field. Background (plain black curve with green circles), True state (plain blue curve), measurement (blue star), analysis (plain red curve). Shape of B (plain magenta curve).*

We want to perform a BLUE analysis, with $\underline{x} \in I\!R^N$ as the control space, $y \in I\!R$ in the observation space and $\underline{G}(\underline{x}) = x_J$.

1) Show that the observation operator linear and describe the associated $1 \times N$ matrix $\underline{\underline{G}}$.
2) Describe the covariance observation error 1×1 matrix R.

3) Show that the covariance background error $N \times N$ matrix is such that

$$B_{jJ} = \mathcal{B}(x_j - x_J) = \sigma_b^2 \ \exp\left[-\frac{(x_j - x_J)^2}{2\, l_B^2}\right] \ . \qquad (\mathbf{3}.55)$$

4) Show that the components $x_j^a = h^a(x_j)$ of the analysis $\underline{x}^a$ are such that

$$h^a(x_j) = h^b(x_j) + \left[h_J^o - h^b(x_J)\right] \frac{\sigma_b^2}{\sigma_b^2 + \sigma_r^2} \ \exp\left[-\frac{(x_j - x_J)^2}{2\, l_B^2}\right] \ . \qquad (\mathbf{3}.56)$$

5) Comment Figure **3**.12b at the light of this result.

Chapter 4

Application projects

Contents

Introduction

This application project explores several data assimilation methods on the example of the Lorenz method: chain of BLUE with fixed or varing $\underline{\underline{B}}$ and Kalman filter without model error.

1 Data assimilation for the Lorenz model

1.1 The Lorenz model

We consider the Lorenz model :

$$\frac{dX}{dt} = -\sigma\, X + \sigma\, Y \;, \quad \frac{dY}{dt} = \rho\, X - Y - X\, Z \;, \quad \frac{dZ}{dt} = X\, Y - \beta\, Z \;, \quad (\mathbf{4}.1)$$

where $X(t)$, $Y(t)$ and $Z(t)$ evolve in time and $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$ are usual constant of this dynamical system.

Starting with the initial condition $(X_s, Y_s, Z_s) = (10, 15, 20)$ for $t = -10$, we integrate the model for $t \in [-10, 0]$ in order to reach the strange attractor through this transitory trajectory (Figure $\mathbf{4}.1$).

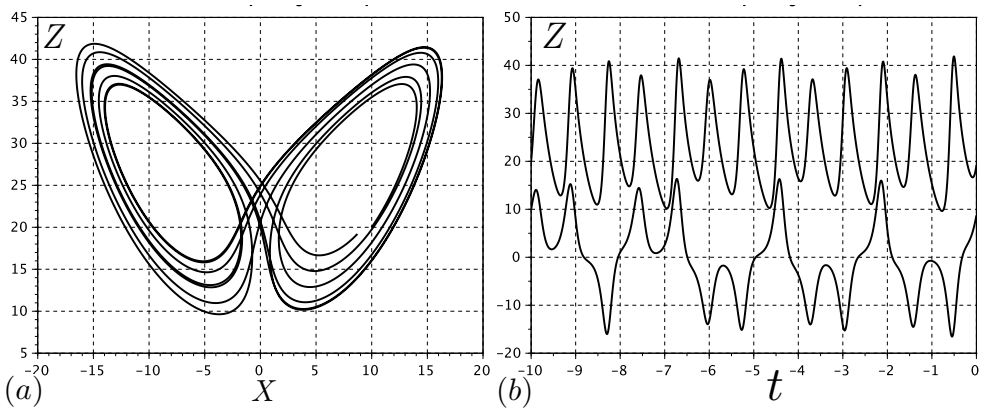

Figure $\mathbf{4}.1$: Transitory trajectory. a) $X(t)$ (low) and $Z(t)$ (high). b) Trajectory in the (X, Z) plane.

Starting with the initial condition $(X_0, Y_0, Z_0) = [X(0), Y(0), Z(0)]$ obtained at the end of the transitory trajectory for $t = 0$, we obtain a trajectory $[X^t(t), Y^t(t), Z^t(t)]$ for $t \in [0, t_f]$ that we call the "true state". We choose $t_f = K\,\tau$ with $K = 50$ and $\tau = 0.1$ (figure $\mathbf{4}.2$). We denote by $\mathcal{M}_k$ the nonlinear operator such that $(X, Y, Z)^T(t_k) = \mathcal{M}_k \left[(X, Y, Z)^T(t_{k-1})\right]$.

We then generate artificial measurements $y_k^o = X^t(t_k) + \epsilon^o$ for $k = 1, ..., 50$, where $t_k = k\,\tau$ and ϵ^o is a normal (gaussian) random function which standard deviation is equal to σ_r. We chose $\sigma_r = 2$ (figure $\mathbf{4}.2$).

We generate the initial guess (background) $(X^b, Y^b, Z^b) = (X_0, Y_0, Z_0) + (\epsilon_X, \epsilon_Y, \epsilon_Z)$ where ϵ_X, ϵ_Y and ϵ_Z are independant normal (gaussien) random functions which standard deviation are equal to σ_b. We chose $\sigma_b = 10$ (Figure $\mathbf{4}.2$). The challenge of this twin experiment is to estimate $[X^t(t_f), Y^t(t_f), Z^t(t_f)]$ the more accurately in a statistical sense.

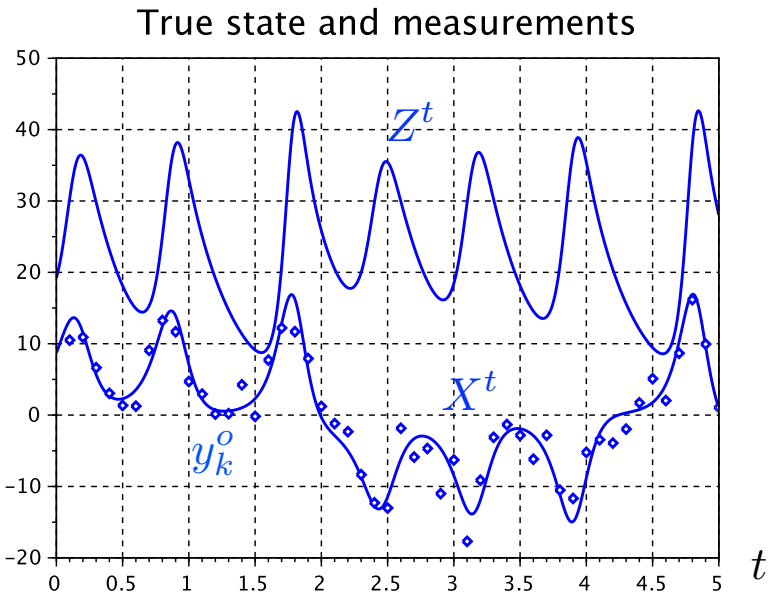

Figure **4.2**: True state $X^t(t)$ and $Z^t(t)$ (solid lines) and measurements $y^o(t_k)$ for $i = 1, ..., 50$ (diamonds).

1.2 Comparaison of three methods

Chain of BLUE (3D-Var) with constant $\underline{\underline{B}}$

The most simple data assimilation methods consists in fixing $\underline{\underline{B}} = \sigma_b^2 \, \underline{\underline{I}}$ as the covariance background error matrix in order to minimize the following cost function for each t_k with $k = 1, ..., K$:

$$J_k(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}_k^b)^T \, \underline{\underline{B}}^{-1} \, (\underline{x} - \underline{x}_k^b) + \frac{1}{2\,\sigma_r^2}(y_k^o - X)^2 \tag{4.2}$$

where $\underline{x} = (X, Y, Z)^T$ and $\underline{x}_k^b = \mathcal{M}_k(\underline{x}_{k-1}^b)$, starting with $\underline{x}_0^b = (X^b, Y^b, Z^b)^T$ and denoting $t_0 = 0$.

Since $\underline{\underline{R}} = R = \sigma_r^2$ is a scalar the gain matrix is

$$\underline{\underline{K}} = (\underline{\underline{B}}^{-1} + \underline{G}^T \, \underline{\underline{R}}^{-1} \, \underline{G})^{-1} \, \underline{G}^T \, \underline{\underline{R}}^{-1} = (\sigma_b^{-2} + \sigma_r^{-2})^{-1} \, \sigma_r^{-2} \, \underline{G}^T = \frac{\sigma_b^2}{\sigma_b^2 + \sigma_r^2} \, \underline{G}^T \, , \tag{4.3}$$

with $\underline{G} = (1, 0, 0)$. Thus, the analyzed state is

$$\underline{x}_k^a = \underline{x}_k^b + \underline{\underline{K}} \, d_k = \left[X_k^b + \frac{\sigma_b^2}{\sigma_b^2 + \sigma_r^2}(y_k^o - X_k^b), Y_k^b, Z_k^b \right]^T \tag{4.4}$$

where $d_k = y_k^o - \underline{G} \, \underline{x}_k^b = y_k^o - X_k^b$ is the innovation vector (here a scalar).

Therefore, the method consists in simulating the Lorenz model and adding $\frac{\sigma_b^2}{\sigma_b^2+\sigma_r^2}(y_k^o - X_k^b)$ to X at each observation time t_k. If $\sigma_b \gg \sigma_r$, the method consists in replacing X by y^o at each measurment time t_k for $k = 1, ..., K$.

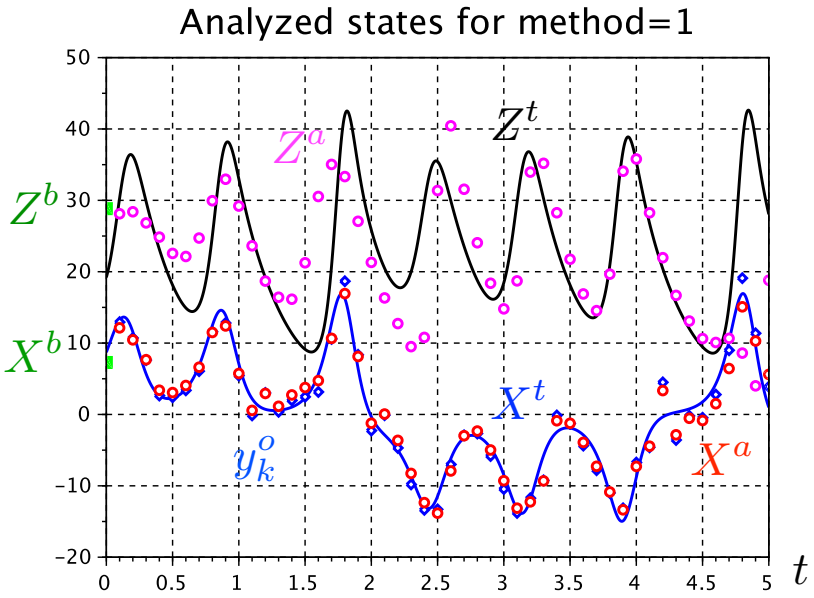

Figure 4.3: Chain of BLUE with a constant $\underline{\underline{B}}$: analyzed states X_k^a (low red circlesx) and Z_k^a (high pink circles) for the observation times t_k for $k = 1, ..., 50$. The initial guess X^b and Z^b are displayed in green for $t = 0$.

Chain of BLUE (3D-Var) with $\underline{\underline{B}}_k = \underline{\underline{A}}_{k-1}$

Since the analyzed covariance error matrix $\underline{\underline{A}} = (\underline{\underline{I}} - \underline{\underline{K}}\,\underline{\underline{G}})\,\underline{\underline{B}}$ can be computed, we can replace $\underline{\underline{B}}$ by $\underline{\underline{A}}$ at each observation time t_k. In this method, we minimize

$$J(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}_k^b)^T\,\underline{\underline{B}}_k^{-1}\,(\underline{x} - \underline{x}_k^b)^T + \frac{1}{2\,\sigma_r^2}(y_k^o - X)^2 \tag{4.5}$$

$$\underline{\underline{A}}_{k-1} = (\underline{\underline{I}} - \underline{\underline{K}}\,\underline{\underline{G}})\,\underline{\underline{B}}_{k-1} \qquad \text{and} \qquad \underline{\underline{B}}_k = \underline{\underline{A}}_{k-1} \tag{4.6}$$

for $k = 1, ..., K$ and $\underline{\underline{A}}_0 = \underline{\underline{B}}$.

Kalman filter with no error model

Instead of taking $\underline{\underline{A}}_{k-1}$ as the background covariance error matrix for the assimilation time t_k, we now choose $\underline{\underline{B}}_k = \underline{\underline{M}}_k\,\underline{\underline{A}}_{k-1}\,\underline{\underline{M}}_k^T$ where $\underline{\underline{M}}_k$ is the linear tangent model around the trajectory going from t_{k-1} to t_k. This Kalman filter method minimizes the cost function

$$J(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}_k^b)^T\,\underline{\underline{B}}_k^{-1}\,(\underline{x} - \underline{x}_k^b)^T + \frac{1}{2\,\sigma_r^2}(y_k^o - X)^2\,,$$
$$\underline{\underline{A}}_{k-1} = (\underline{\underline{I}} - \underline{\underline{K}}\,\underline{\underline{G}})\,\underline{\underline{B}}_{k-1} \qquad \text{and} \qquad \underline{\underline{B}}_k = \underline{\underline{M}}_k\,\underline{\underline{A}}_{k-1}\,\underline{\underline{M}}_k^T \tag{4.7}$$

for $k = 1, ..., K$ and $\underline{\underline{A}}_0 = \underline{\underline{B}}$.

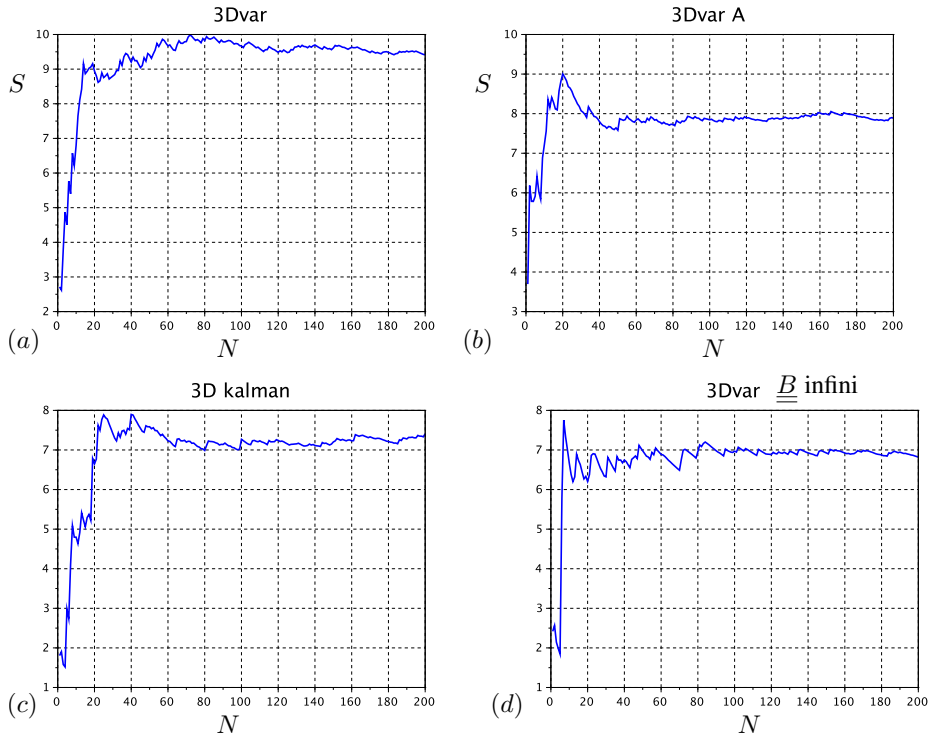

Figure **4**.4: Scores of the methods for the twin experiment. a) 3D-Var with fixed $\underline{\underline{B}}$. b) 3D-Var with $\underline{\underline{B}}$ replaced by $\underline{\underline{A}}$. c) Kalman filter. d) 3D-Var with infinite $\underline{\underline{B}}$ (not at $t = 0$).

The tangent model $\underline{\underline{M}}$ is obtained by simulating

$$\frac{d}{dt}(dX) = -\sigma\, dX + \sigma\, dY \tag{4.8}$$

$$\frac{d}{dt}(dY) = \rho\, dX - dY - dX\, Z^b(t) - X^b(t)\, dZ \tag{4.9}$$

$$\frac{d}{dt}(dZ) = dX\, Y^b(t) + X^b(t)\, dY - \beta\, dZ\ , \tag{4.10}$$

where $[X^b(t), Y^b(t), Z^b(t)]$ is the background trajectory from t_{k-1} to t_k.

The columns of $\underline{\underline{M}}_k$ are obtained by integrating the linear tangent model from t_{k-1} to t_k with the respective initial conditions $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ for (dX, dY, dZ).

1.3 Scores of the three methods

For each method we perform R experiments and we compare (X_f, Y_f, Z_f) to $[X^t, Y^t, Z^t](t_f)$. The score of the method is defined by

$$S(r) = \sqrt{\frac{1}{3\,R}\sum_{r=1}^{R}\left([D_X^{(r)}]^2 + [D_Y^{(r)}]^2 + [D_Z^{(r)}]^2\right)} \quad \text{with} \tag{4.11}$$

$$D_X^{(r)} = X_f^{(r)} - X^t(t_f),\ D_Y^{(r)} = Y_f^{(r)} - Y^t(t_f),\ D_Z^{(r)} = Z_f^{(r)} - Z^t(t_f)\ , \tag{4.12}$$

where $X^{(r)}$ is the value of X obtained at the random draw r. To see the statistical convergence of the score, we plot $S(R)$ as a function of R for $R \in [0, 1000]$.

The score of four method is presented in Figure **4**.4. The chain of BLUE with constant $\underline{\underline{B}}$ gives $S \sim 9.5$ for chosen values. If $\underline{\underline{B}}$ is replaced by $\underline{\underline{A}}$ in the method, the score is $S \sim 8$. The Kalman filter has a score of $S \sim 7$ close to the score of case where we simply replace X by y^0 at each assimilation time t_k.

2 Ensemble methods for two simple examples

2.1 Approximation of a gain matrix

Data assimilation applications are often governed by the generic cost function

$$J(\underline{x}) = \frac{1}{2}\left(\underline{x}-\underline{x}^b\right)^T \underline{\underline{B}}^{-1}\left(\underline{x}-\underline{x}^b\right) + \frac{1}{2}\left[\underline{y}^o-\mathcal{G}(\underline{x})\right]^T \underline{\underline{R}}^{-1}\left[\underline{y}^o-\mathcal{G}(\underline{x})\right] \ , \quad (\mathbf{4}.13)$$

with $\underline{x} \in I\!R^N$ in the control space, $\underline{x}^b \in I\!R^N$ as the the background state, $\underline{y}^o \in I\!R^M$ in the observation space and $\mathcal{G}$ such that $\underline{y} = \mathcal{G}(\underline{x})$. The $\underline{\underline{B}}$ and $\underline{\underline{R}}$ matrices are respectively the "error covariance background matrix" and the "error covariance observation matrix". An approximation $\widetilde{\underline{x}}^a$ of the analysis $\underline{x}^a$, that minimizes this cost function $J(\underline{x})$, is the given as the minimum of the incremental cost function J_{inc} defined by

$$J_{inc}(\underline{x}) = \frac{1}{2}\delta\underline{x}^T \underline{\underline{B}}^{-1} \delta\underline{x} + \frac{1}{2}\left(\underline{d}-\underline{\underline{G}}\,\delta\underline{x}\right)^T \underline{\underline{R}}^{-1}\left(\underline{d}-\underline{\underline{G}}\,\delta\underline{x}\right) \ , \quad (\mathbf{4}.14)$$

where $\delta\underline{x} = \underline{x}-\underline{x}^b$ is the increment, $\underline{d} = \underline{y}^o - \mathcal{G}(\underline{x}^b)$ is the innovation vector and $\underline{\underline{G}}$ is the Jacobian matrix of $\mathcal{G}$ around $\underline{x}^b$, such as $\mathcal{G}(\underline{x}^b+\delta\underline{x}) \approx \mathcal{G}(\underline{x}^b) + \underline{\underline{G}}\,\delta\underline{x}$. The approximate analysis $\widetilde{\underline{x}}^a$ of $\underline{x}^a$ is thus given by

$$\widetilde{\underline{x}}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d} \qquad \text{with} \qquad \underline{\underline{K}} = \underline{\underline{B}}\,\underline{\underline{G}}^T\left(\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T + \underline{\underline{R}}\right)^{-1} \ . \quad (\mathbf{4}.15)$$

Since the computation of the Jacobian matrix $\underline{\underline{G}}$ of $\mathcal{G}$ at $\underline{x}^b$ can be costly for high dimension control spaces, an approximation can be obtained through an ensemble method. We consider the ensemble $\underline{x}^{(r)}$ for $r = 1, ...R$ coming out of the sampling of a random gaussian vector of mean $\underline{x}^b$ and covariance variance $\underline{\underline{B}}$. We then compute $\underline{y}^{(r)} = \mathcal{G}\left(\underline{x}^{(r)}\right)$ for $r = 1, ...R$ and $\underline{y}^b = \mathcal{G}\left(\underline{x}^b\right)$ to approximate $\underline{\underline{B}}\,\underline{\underline{G}}^T$ and $\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T$, in the expression of the gain matrix $\underline{\underline{K}}$, by the following ensemble averages:

$$\begin{aligned}
\underline{\underline{B}}\,\underline{\underline{G}}^T \sim \underline{\underline{\mathcal{A}}}^{BG^T} &= \frac{1}{R}\sum_{r=1}^{R}\left(\underline{x}^{(r)}-\underline{x}^b\right)\left(\underline{y}^{(r)}-\underline{y}^b\right)^T \\
\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T \sim \underline{\underline{\mathcal{A}}}^{GBG^T} &= \frac{1}{R}\sum_{r=1}^{R}\left(\underline{y}^{(r)}-\underline{y}^b\right)\left(\underline{y}^{(r)}-\underline{y}^b\right)^T \ . \quad (\mathbf{4}.16)
\end{aligned}$$

The choice of this approximation is the be seen through the linear approximation $\underline{y}^{(r)} - \underline{y}^b = \mathcal{G}(\underline{x}^{(r)}) - \mathcal{G}(\underline{x}^b) \sim \underline{\underline{G}}(\underline{x}^{(r)} - \underline{x}^b)$, if the ensemble is not too much spread, and the statistical estimation $\underline{\underline{B}} \sim \frac{1}{R}\sum_{r=1}^{R}\left(\underline{x}^{(r)}-\underline{x}^b\right)\left(\underline{x}^{(r)}-\underline{x}^b\right)^T$.

To illustrate the validity of such an approximation, we consider the observation operator $\mathcal{G} = (\mathcal{G}_1^T, ...\mathcal{G}_M^T)^T$ such that $\mathcal{G}_i(\underline{x}) = [\underline{x} - 10 * \sin(i)\, \underline{e}_i]^2$ where $(\underline{e}_1, ..., \underline{e}_N)$ is the canonical basis. We define the true state as $\underline{x}^t = \sum_{j=1}^N \underline{e}_j$ and set the covariance matrices to $\underline{\underline{B}} = 0.1\ \underline{\underline{I}}$ and $\underline{\underline{R}} = \underline{\underline{I}}$. In figure **4**.5a, we plot $J_{inc}(\underline{x})$, $J_b(\underline{x}) = \frac{1}{2}\left(\underline{x} - \underline{x}^b\right)^T \underline{\underline{B}}^{-1} \left(\underline{x} - \underline{x}^b\right)$ and $J_{r,inc}(\underline{x}) = J_{inc}(\underline{x}) - J_b(\underline{x})$ as functions of z for $\underline{x} = \underline{x}^a + z\,(\underline{x}^a - \underline{x}^b)$. The scores $||\widetilde{\underline{x}}^a - \underline{x}^t||$ for the incremental method and its ensemble approximation are shown on figure **4**.5b.

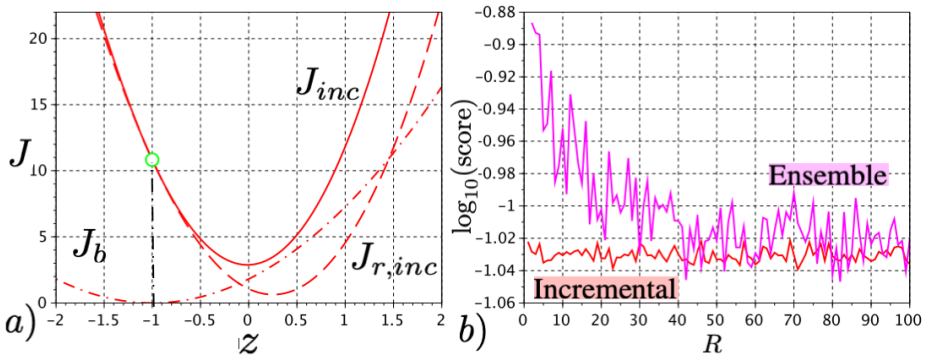

Figure **4**.5: a) Plot of J_{inc}, J_b and $J_{r,inc}$ as a function of z. b) Comparison of the scores of the incremental method and its ensemble approximation for the estimation of the true state.

2.2 Application to the bore example

The bore example is defined by $x \in I\!R$, $y = \in I\!R$ and $\mathcal{G}(x) = -q/(x - h_L)$ where q and h_L are known constants. The error covariance matrices are simply scalar variances such as $\underline{\underline{B}} = \sigma_b^2$ and $\underline{\underline{R}} = \sigma_r^2$. The gain matrix is

$$K = \sigma_b^2\, G\, \left(G^2\, \sigma_b^2 + \sigma_r^2\right)^{-1} \qquad \text{with} \qquad G = \mathcal{G}'(x^b) = \frac{q}{(x^b - h_L)^2}\ , \tag{4.17}$$

Pretending we do not know how to compute G, we build and ensemble $x^{(r)}$ for $r = 1, ...R$ out a gaussian random variable of mean x^b and variance σ_b^2. We then compute $y(r) = \mathcal{G}\left(x^{(r)}\right)$ and $y^b = \mathcal{G}\left(x^b\right)$ to build the approximations

$$\begin{aligned} \sigma_b^2\, G \sim \mathcal{A}^{\sigma_b^2\, G} &= \frac{1}{R} \sum_{r=1}^R \left(x^{(r)} - x^b\right) \left(y^{(r)} - y^b\right) \\ \sigma_b^2\, G^2 \sim \mathcal{A}^{\sigma_b^2\, G^2} &= \frac{1}{R} \sum_{r=1}^R \left(y^{(r)} - y^b\right) \left(y^{(r)} - y^b\right)\ . \end{aligned} \tag{4.18}$$

We see that this ensemble method approximates $G = \mathcal{G}'(x^b)$ since $\left(y^{(r)} - y^b\right) = \left[\mathcal{G}\left(x^{(r)}\right) - \mathcal{G}\left(x^b\right)\right] \sim G\ \left(x^{(r)} - x^b\right)$.

To assess the validity of such an approximation on an example, we choose $q = 7$, $h_L = 5$ $h_R = x^t = 17$, $x^b = 18$, $\sigma_b = 1$ and $\sigma_r = .03$. Figure **4**.6 shows the error $||\mathcal{A}^{\sigma_b^2\, G} - \sigma_b^2\, G||$ and $||\mathcal{A}^{\sigma_b^2\, G^2} - \sigma_b^2\, G||$ for various choices of R.

Figure **4**.7 compare the scores $||\widetilde{x}^a - x^t||$ of the incremental method and its ensemble approximation in the estimation of the true state.

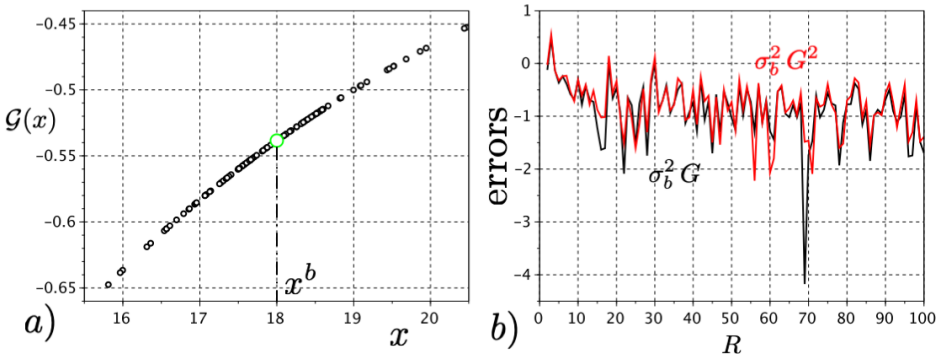

Figure 4.6: a) Dispersion of the ensemble in the estimation $\mathcal{G}(x)$. b) Errors in the approximation of $\sigma_b\, G$ and $\sigma_b\, G^2$ with the ensemble method.

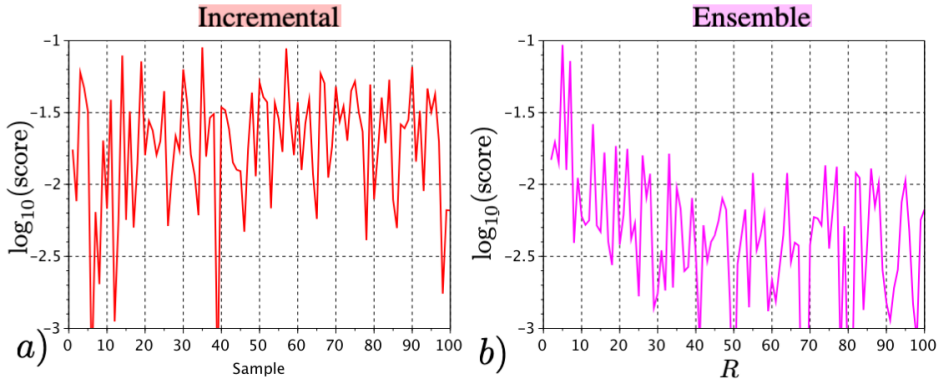

Figure 4.7: Scores of a)the incremental method and b) its ensemble approximation for the estimation of the true state.

2.3 Application to the reservoir example

The reservoir example is here defined by $\underline{x} = (\alpha, P, H_0) \in I\!R^3$ for the control space with a background state $\underline{x}^b = (\alpha^b, P^b, H_0^b)$, $\underline{y}^o = (y_1^o, ...y_k^o, ...y_K^o)^T \in I\!R^K$ for the measurements in the observation space and $\mathcal{G} = (\mathcal{G}_1^T, ...\mathcal{G}_k^T, ...\mathcal{G}_K^T)^T$ for the observation operator, with

$$\mathcal{G}_k(\alpha, P) = \frac{P}{\alpha}\left(1 - e^{-\alpha\, t_k}\right) + H_0\, e^{-\alpha\, t_k}\ . \tag{4.19}$$

We denote the background error covariance matrix by

$$\underline{\underline{B}} = \begin{pmatrix} \sigma_\alpha^2 & \rho\,\sigma_\alpha\,\sigma_P & 0 \\ \rho\,\sigma_\alpha\,\sigma_P & \sigma_P^2 & 0 \\ 0 & 0 & \sigma_{H_0}^2 \end{pmatrix}\ , \tag{4.20}$$

where ρ is a correlation coefficient. Assuming that the observation error covariance matrix in $I\!R^K$ is $\underline{\underline{R}} = \sigma_r^2\ \underline{\underline{I}}$ the cost function reads

$$J(\alpha, P) = \frac{1}{2}(\underline{x} - \underline{x}^b)^T\ \underline{\underline{B}}^{-1}\ (\underline{x} - \underline{x}^b) + \sum_{k=1}^{K} \frac{[y_k^o - \mathcal{G}_k(\alpha, P)]^2}{2\,\sigma_r^2}\ . \tag{4.21}$$

The ensemble methods consists in building an ensemble $\underline{x}^{(r)} = (\alpha^r, P^r, H_0^r)$ for $r = 1, ...R$ as gaussian draws of mean $\underline{x}^b$ and covariance matrix $\underline{\underline{B}}$, to obtain the approximations $\underline{\underline{B}}\,\underline{\underline{G}}^T \sim \underline{\underline{\mathcal{A}}}^{BG^T}$ and $\underline{\underline{G}}\,\underline{\underline{B}}\,\underline{\underline{G}}^T \sim \underline{\underline{\mathcal{A}}}^{GBG^T}$.

To illustrate the ensemble method, we choose $\underline{x}^t = (1, 1, 0)^T$, $(\sigma_\alpha, \sigma_P, \sigma_{H_0}) = (.2, .2, .1)$, $\rho = .3$, $\sigma_r = .1$ and $K = 4$. The background $\underline{x}^b$ and the measurments $\underline{y}^o$ are randomly chosen, according their probability laws. Figure **4**.8 shows two examples of draws leading to an ensemble of background trajectories and an analyzed trajectory, to be compared with the true trajectory.

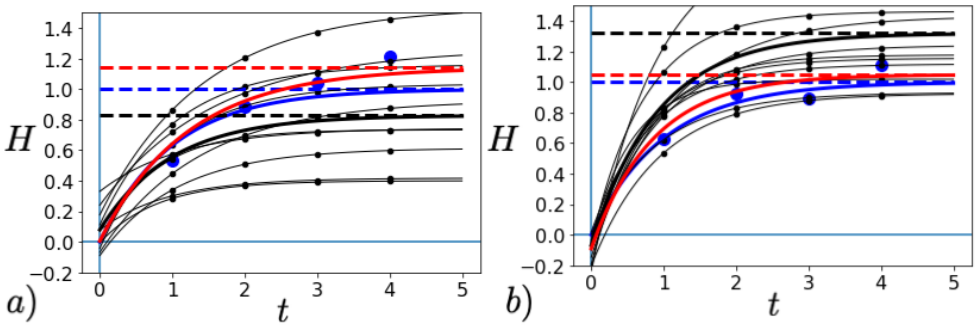

Figure **4**.8: Two samples of the ensemble method for the estimation of $\underline{x}^t$. Blue: true state trajectory. Black: background trajectory and its ensemble perturbations. Red: trajectory of the analysis.

3 Data assimilation for the advection-diffusion model

3.1 The advection-diffusion model

We consider the 1D advection-diffusion model

$$\frac{\partial h}{\partial t} + c\,\frac{\partial h}{\partial x} = \kappa\,\frac{\partial^2 h}{\partial x^2}\,, \tag{4.22}$$

where $h(x,t)$ is a real field, $c > 0$ advection velocity and κ a diffusion constant. This model can describe the propagation of heat in a fluid or the propogation of a small flood in a river. We consider the interval $x \in [0, L]$ with the open boundary conditions $\frac{\partial h}{\partial t}(L,t) + c\,\frac{\partial h}{\partial x}(L,t) = 0$ for $x = L$. For $x = 0$, we impose a Dirichlet condition $h(0,t) = q(t)$ where $q(t)$ is a gaussian random function with a gaussian whose autocorrelation fonction is

$$R_q(\tau) = \langle q(t)\,q(t+\tau)\rangle = q_m^2\,\exp\left(-\frac{\tau^2}{2\,\sigma_q^2}\right)\,. \tag{4.23}$$

Figure **4**.9 displays a sample of $q(t)$ for two different values of the standar deviation σ_q.

3.2 Twin experiments

An example of solution $h(x,t)$ is displayed in Figure **4**.10, with an intial condition $h_0(x) = h_m\,\exp\left(-\frac{x^2}{2l_0^2}\right)$ that gives a hint of the advection-diffusion process

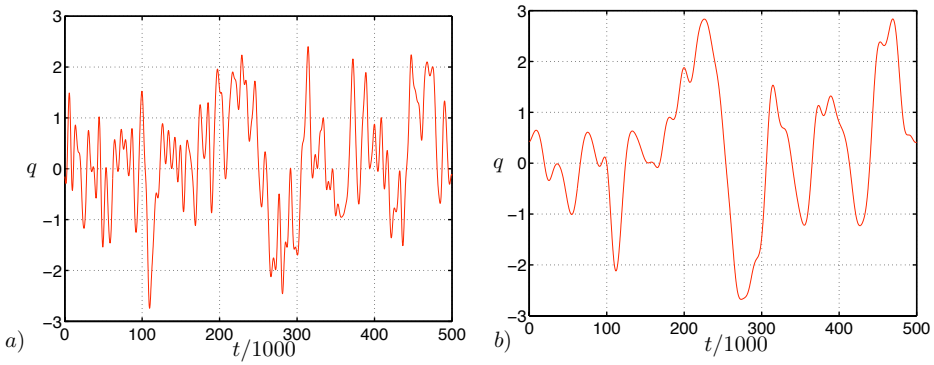

Figure 4.9: Condition aux limites amont aléatoire $q(t)$ pour $q_m = 1$. a) $\sigma_q = 3\ 10^3$. b) $\sigma_q = 9\ 10^3$.

for the chosen value, knowing the exact solution

$$h(x,t) = h_m \frac{l_0}{l(t)} \exp\left[-\frac{(x-ct)^2}{2l^2(t)}\right] \quad \text{with} \quad l^2(t) = l_0^2 + 2\,\kappa\, t\ . \tag{4.24}$$

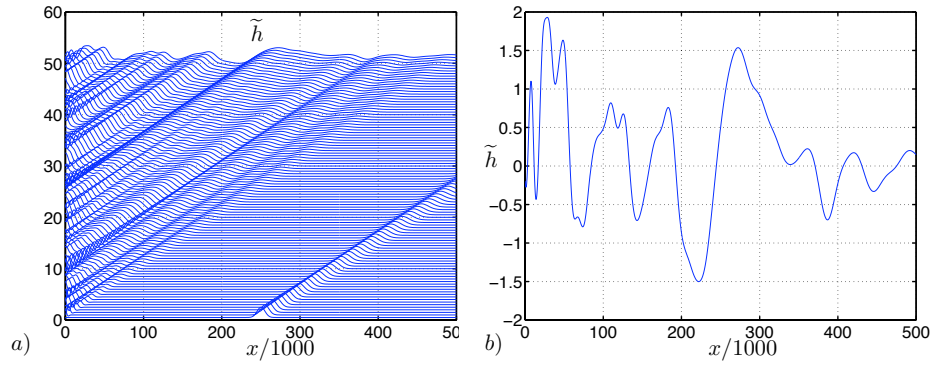

Figure 4.10: Solution $h(x,t)$ for $c = 1$ and $\kappa = 500$. a) Superposition of shifted $h(x,t)$ profile. b) Profile $h(x,T)$ for $T = 500$.

One can see, on Figure 4.10b that the correlation length of the profile $h(x,T)$ is small close to $x = 0$ than close to $x = L$. One can estimate that $l_0 = c\,\sigma_q$ for $x = 0$ and

$$l(x) = \sqrt{l_0^2 + 2\,\kappa\, x/c} \quad \text{for } x \in [0, L]\ , \tag{4.25}$$

based on an approximation in which the advection time is large compare to the diffusion time. Similarly, the correlation time $\sigma(x) = l(x)/c$ grows with x, as seen in Figure 4.11, which displays $h(L/10,t)$ and $h(L/2,t)$ as functions of time.

To perform twin experiments, we choose $c = c^t$ and $\kappa = \kappa^t$ with and input q^t generated by the parameters $(\sigma_q, q_m) = (\sigma_{qt}, q_{mt})$. We consider the corresponding solution $h^t(x,t)$ is the "true state". The model "without data assimilation" is characterized by the parameters $c = c_s$, $\kappa = \kappa_s$ and $q_s = q^t + \delta q$ where δq is a random function with of autocorrelation $R_{\delta q} = \delta q_m^2 \exp\left(-\frac{\tau^2}{2\,\sigma_q^2}\right)$.

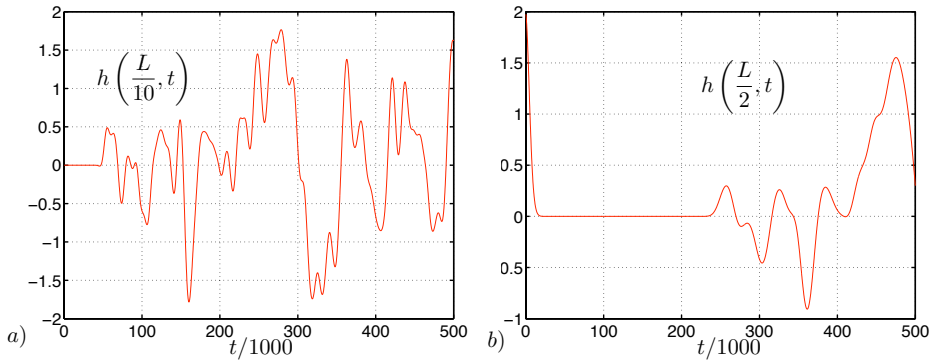

Figure **4**.11: Signal temporel $h(x,t)$ pour $c=1$ et $\kappa=500$ en a) $x=L/10$, b) $x=L/2$.

Figure **4**.12a compares $q^t(t)$ and $q_s(t)$ Figures **4**.12bcd compare $h^t(x,T)$ and $h_s(x,T)$ for $T = 500\,10^3$ and the choice of parameters $(c^t,c_s) = (1,.98)$, $(\kappa^t,\kappa_s)=(500,1000)$, $\sigma_{qt}=30\ 10^3$, $q_{mt}=1$ and $\delta q_m = .5$

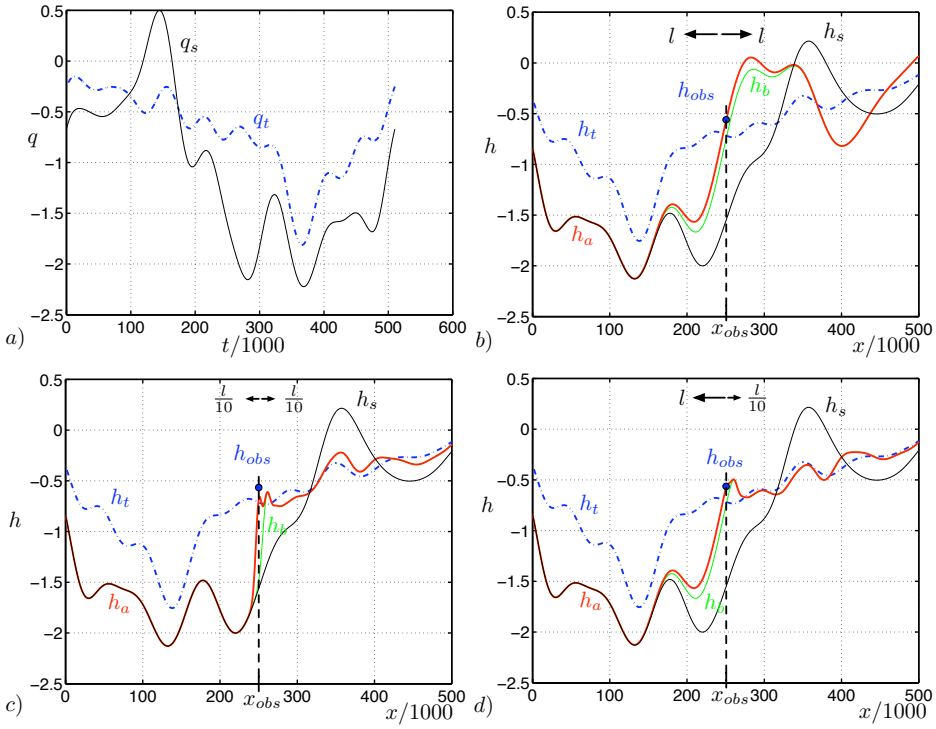

Figure **4**.12: Chain of BLUE. True state (dashed blue), model (plain black), background (plain green) and analysis (plain red). a) True forcing q^t and model q_s. bcd) Profiles for $t=T$: true profile h^t, background h_s, background h^b and analysis h^a, for the choices b) $l-l$, c) $l/10-l/10$ and d) $l-l/10$.

3.3 Chain of BLUE for one-point observations

We consider the observations $h^o(t_k) = h(x_{obs}, t) = h^t(x_{obs}, t) + \epsilon^o(t)$ where $\epsilon^o(t)$ is a gaussian white noise of standard deviation σ_r. We chose $x_{obs} = L/2$, $\sigma_r = 0.1$ and $t_{k+1} - t_k = \Delta t = 5\,10^3$. We choose to perform a BLUE data assimilation (3D-Var) for each new observation and use the analysis $h^a(x, t_k)$ as new initial condition $h^b(x, t_k)$ for the model (c_s, κ_s, q_s), that is carried by the model to become the new background $h^b(x, t_{j+1})$ for the next observation.

We have thus $\underline{\underline{R}} = \sigma_r^2$ and $\underline{H} = (0, ..., 0, 1, 0, ..., 0)^T$, the 1 being at the position n_{obs} where n_{obs} is the index x_{obs} in the spatial grid.

For the matrix $\underline{\underline{B}}$ we choose the discretized version of the correlation function

$$B(x, x') = \exp\left[-\frac{(x - x')^2}{2\, l_B^2(x, x')}\right] , \tag{4.26}$$

where $l_B(x, x')$ is a symmetric function with respect to the points (x, x').

For this data assimilation experiment with observations at x_{obs}, one only needs to know the function $B(x, x_{obs})$. The analysis reads $\underline{x}^a = \underline{x}^b + \underline{\underline{K}}\,\underline{d}$ where $\underline{d} = h^o(t_k) - h^b(x_{obs}, t_k)$ is the inovation, and $\underline{\underline{K}} = \underline{\underline{B}}\,\underline{\underline{H}}^T \left(\underline{\underline{H}}\,\underline{\underline{B}}\,\underline{\underline{H}}^T + \underline{\underline{R}}\right)^{-1}$ the gain matrix. For the present experiment, this leads to

$$h^a(x, t_k) = h^b(x, t_k) + \left[h^o(t_k) - h^b(x_{obs}, t_k)\right] \frac{\sigma_b^2}{\sigma_b^2 + \sigma_r^2} \exp\left[-\frac{(x - x_{obs})^2}{2\, l_B(x, x_{obs})^2}\right] . \tag{4.27}$$

In a first experiment, we choose $l_B(x, x_{obs}) = l(x_{obs})$ where $l(x)$ is given by Equation (4.25). Figure 4.12b shows the result of this data assimilation process for $t = T$ with $T = 500\ 10^3$. The analysis fail to match the true state with this choice.

In a second experiment, we choose $l_B(x, x_{obs}) = l(x_{obs})/10$, which lead to the results shown in Figure 4.12c. The analysis get close to the true state, but a one observes a too strong discontinuity in the profile.

At last, we choose, in Equation (4.26), the values $l_B(x, x_{obs}) = l(x_{obs})$ et pour $x < x_{obs}$ and $l_B(x, x_{obs}) = l(x_{obs})/10$ pour $x > x_{obs}$, which does not respect the symetry of $l_B(x, x_{obs})$. Figure 4.12d shows that this procedure enhance the quality of the data assimilation process.

A true extended Kalman filter, with a transport the matrix $\underline{\underline{A}}$ with the tangent model, would explain this asymmetry.

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