

École Doctorale des Sciences de l'Environnement d'Île-de-France

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Modélisation Numérique
de l'Écoulement Atmosphérique
et Assimilation de Données

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Cours 7

21 Mai 2021

- Miscellaneous remarks and complements
- Weak constraint variational assimilation. Principle. The dual algorithm for variational assimilation. Examples.
- Impact of Stability and Instability on Assimilation. *Quasi-Static Variational Assimilation*

Bayesian Estimation (see course 2)

Data of the form

$$z = \Gamma x + \zeta, \quad \zeta \sim \mathcal{N}[0, S]$$

Known data vector z belongs to *data space* \mathcal{D} , $\dim \mathcal{D} = m$,

Unknown state vector x belongs to *state space* \mathcal{X} , $\dim \mathcal{X} = n$

Γ known ($m \times n$)-matrix, ζ unknown 'error'

Probability that $x = \xi$ given ? $x = \xi \Rightarrow \zeta = z - \Gamma \xi$

$$P(\zeta = z - \Gamma \xi) \propto \exp[-(z - \Gamma \xi)^T S^{-1} (z - \Gamma \xi)/2] \propto \exp[-(\xi - x^a)^T (P^a)^{-1} (\xi - x^a)/2]$$

where

$$x^a = (\Gamma^T S^{-1} \Gamma)^{-1} \Gamma^T S^{-1} z$$
$$P^a = (\Gamma^T S^{-1} \Gamma)^{-1}$$

Then conditional probability distribution is

$$P(x | z) = \mathcal{N}[x^a, P^a]$$

Bayesian Estimation (continuation 1)

$$z = \Gamma x + \xi, \quad \xi \sim \mathcal{N}[0, S]$$

Then

$$P(x | z) = \mathcal{N}[x^a, P^a]$$

with

$$x^a = (\Gamma^T S^{-1} \Gamma)^{-1} \Gamma^T S^{-1} z$$
$$P^a = (\Gamma^T S^{-1} \Gamma)^{-1}$$

Determinacy condition : $\text{rank} \Gamma = n$. Data contain information, directly or indirectly, on every component of state vector x . Requires $m \geq n$.

Variational form

$$P(x | z) \propto \exp[-(z - \Gamma\xi)^T S^{-1} (z - \Gamma\xi)/2] \propto \exp[-(\xi - x^a)^T (P^a)^{-1} (\xi - x^a)/2]$$

Conditional expectation x^a minimizes following scalar *objective function*, defined on state space \mathcal{X}

$$\xi \in \mathcal{X} \rightarrow \mathcal{J}(\xi) \equiv (1/2) [\Gamma\xi - z]^T S^{-1} [\Gamma\xi - z]$$

$$P^a = [\partial^2 \mathcal{J} / \partial \xi^2]^{-1}$$

$$\xi \in \mathcal{X} \rightarrow \mathcal{J}(\xi) \equiv (1/2) [\Gamma\xi - z]^T S^{-1} [\Gamma\xi - z]$$

$S = E(\zeta\zeta^T)$ is covariance matrix of data error ζ

Consider quantity $D = z_1^T S^{-1} z_2 = z_1^T [E(\zeta\zeta^T)]^{-1} z_2$

where z_1 and z_2 are any two vectors in data space

Change of coordinates $z \equiv Tw$

$$\zeta = T\chi \Rightarrow S = E(\zeta\zeta^T) = E[T\chi(T\chi)^T] = T E(\chi\chi^T)T^T$$

$$D = w_1^T T^T [T E(\chi\chi^T)T^T]^{-1} Tw_2$$

$$D = w_1^T [E(\chi\chi^T)]^{-1} w_2$$

Expression $D = z_1^T S^{-1} z_2$

defines proper scalar product, and associated norm, on data space

Mahalanobis norm



Prasanta Chandra Mahalanobis (1893 -1972)

From Course 5

If data still of the form

$$z = \Gamma x + \xi,$$

but ‘error’ ξ , which still has expectation 0 and covariance S , is not Gaussian, expressions

$$x^a = (\Gamma^T S^{-1} \Gamma)^{-1} \Gamma^T S^{-1} z$$

$$P^a = (\Gamma^T S^{-1} \Gamma)^{-1}$$

do not achieve Bayesian estimation, but define least-variance linear estimate of x from z (*Best Linear Unbiased Estimator, BLUE*), and associated estimation error covariance matrix. Significance of x^a and P^a is *different* from Gaussian (and Bayesian) case.

From Course 4

Best Linear Unbiased Estimate

State vector \mathbf{x} , belonging to state space \mathcal{S} ($\dim \mathcal{S} = n$), to be estimated.

Available data in the form of

- A ‘background’ estimate (*e. g.* forecast from the past), belonging to state space, with dimension n

$$\mathbf{x}^b = \mathbf{x} + \boldsymbol{\zeta}^b$$

- An additional set of data (*e. g.* observations), belonging to observation space, with dimension p

$$\mathbf{y} = \mathbf{H}\mathbf{x} + \boldsymbol{\varepsilon}$$

\mathbf{H} is known linear observation operator.

Assume probability distribution is known for the couple $(\boldsymbol{\zeta}^b, \boldsymbol{\varepsilon})$.

Assume $E(\boldsymbol{\zeta}^b) = \mathbf{0}$, $E(\boldsymbol{\varepsilon}) = \mathbf{0}$, $E(\boldsymbol{\zeta}^b \boldsymbol{\varepsilon}^T) = \mathbf{0}$ (not restrictive)

Set $E(\boldsymbol{\zeta}^b \boldsymbol{\zeta}^{bT}) \equiv \mathbf{P}^b$ (also often denoted \mathbf{B}), $E(\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^T) \equiv \mathbf{R}$

$$\mathbf{x}^b = \mathbf{x} + \boldsymbol{\zeta}^b$$

$$\mathbf{y} = \mathbf{H}\mathbf{x} + \boldsymbol{\varepsilon}$$

$$E(\boldsymbol{\zeta}^b \boldsymbol{\varepsilon}^T) = 0 \text{ (not restrictive)}$$

If $E(\boldsymbol{\zeta}^b \boldsymbol{\varepsilon}^T) \neq 0$, one can estimate $\boldsymbol{\varepsilon}$ from $\boldsymbol{\zeta}^b$ through

$$\boldsymbol{\varepsilon}^a = E(\boldsymbol{\varepsilon} \boldsymbol{\zeta}^{bT}) [E(\boldsymbol{\zeta}^b \boldsymbol{\zeta}^{bT})]^{-1} \boldsymbol{\zeta}^b$$

Then $\boldsymbol{\varepsilon}' = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^a$ is uncorrelated with $\boldsymbol{\zeta}^b$, *i.e.* $E(\boldsymbol{\varepsilon}' \boldsymbol{\zeta}^{bT}) = 0$

Alternatively, if $E(\xi^b \varepsilon^T) = C \neq 0$, the gain matrix $C_{xy} [C_{yy}]^{-1}$ is modified,
 And the expressions for x^a and P^a become

$$x^a = x^b + [P^b H^T - C] [HP^b H^T + R - HC - C^T H^T]^{-1} (y - Hx^b)$$

$$P^a = P^b - [P^b H^T - C] [HP^b H^T + R - HC - C^T H^T]^{-1} [HP^b - C^T]$$

Structure of gain matrix

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{P}^b \mathbf{H}^T [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1} (\mathbf{y} - \mathbf{H} \mathbf{x}^b)$$

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{P}^a \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H} \mathbf{x}^b)$$

$$\mathbf{x}^a = (\mathbf{\Gamma}^T \mathbf{S}^{-1} \mathbf{\Gamma})^{-1} \mathbf{\Gamma}^T \mathbf{S}^{-1} \mathbf{z}$$

How to write the adjoint of a code ?

Operation $a = b \times c$

Input b, c Output a but also b, c

For clarity, we write

$$a = b \times c$$

$$b' = b$$

$$c' = c$$

$\partial J / \partial a$, $\partial J / \partial b'$, $\partial J / \partial c'$ available. We want to determine $\partial J / \partial b$, $\partial J / \partial c$

Chain rule

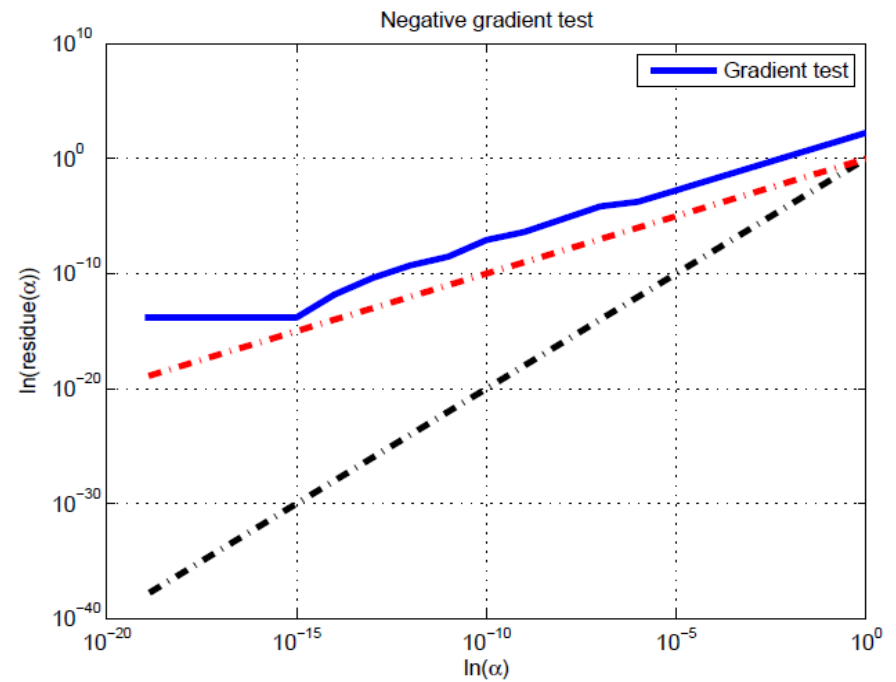
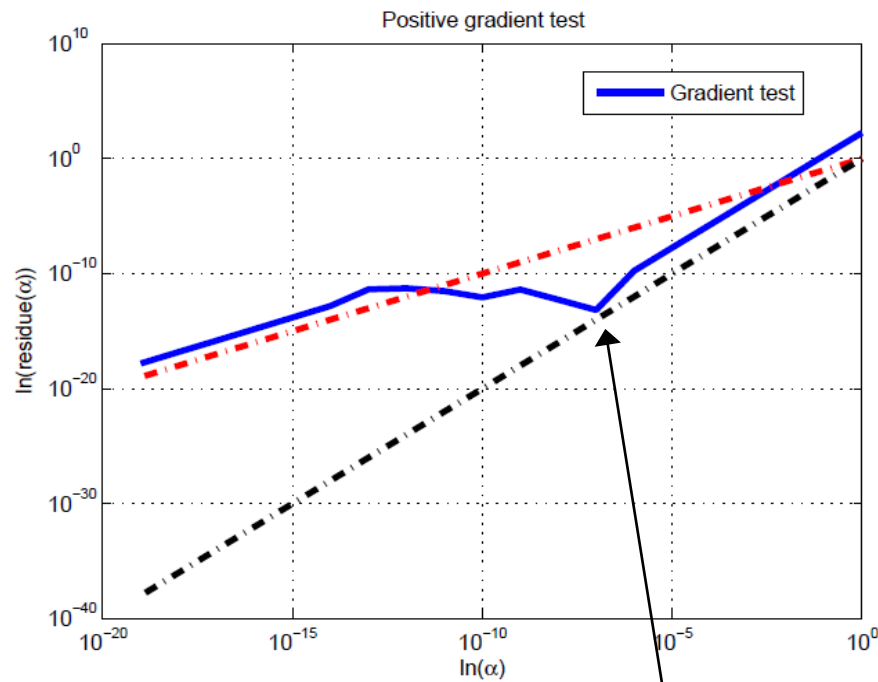
$$\partial J / \partial b = (\partial J / \partial a) \underset{c}{(\partial a / \partial b)} + (\partial J / \partial b') \underset{1}{(\partial b' / \partial b)} + (\partial J / \partial c') \underset{0}{(\partial c' / \partial b)}$$

$$\partial J / \partial b = (\partial J / \partial a) c + \partial J / \partial b'$$

Similarly

$$\partial J / \partial c = (\partial J / \partial a) b + \partial J / \partial c'$$

Gradient test



$\epsilon \cdot \tilde{\mathfrak{J}}$ (optimal control variable)

$\epsilon = 2^{-53}$ zero machine

$$\text{residue}(\alpha) = (\tilde{\mathfrak{J}}(x + \alpha dx) - \tilde{\mathfrak{J}}(x)) - \alpha \nabla \tilde{\mathfrak{J}}(x) dx$$

How to take model error into account in variational assimilation ?

Weak constraint variational assimilation

Allows for errors in the assimilating model

- Data

- Background estimate at time 0

$$x_0^b = x_0 + \xi_0^b \quad E(\xi_0^b \xi_0^{bT}) = P_0^b$$

- Observations at times $k = 0, \dots, K$

$$y_k = H_k x_k + \varepsilon_k \quad E(\varepsilon_k \varepsilon_k^T) = R_k \delta_{kk}$$

- Model

$$x_{k+1} = M_k x_k + \eta_k \quad E(\eta_k \eta_k^T) = Q_k \delta_{kk} \quad k = 0, \dots, K-1$$

Errors assumed to be unbiased and uncorrelated in time, H_k and M_k linear

Then objective function

$(\xi_0, \xi_1, \dots, \xi_K) \rightarrow$

$\mathcal{J}(\xi_0, \xi_1, \dots, \xi_K)$

$$\begin{aligned} &= (1/2) (x_0^b - \xi_0)^T [P_0^b]^{-1} (x_0^b - \xi_0) \\ &\quad + (1/2) \sum_{k=0, \dots, K} [y_k - H_k \xi_k]^T R_k^{-1} [y_k - H_k \xi_k] \\ &\quad + (1/2) \sum_{k=0, \dots, K-1} [\xi_{k+1} - M_k \xi_k]^T Q_k^{-1} [\xi_{k+1} - M_k \xi_k] \end{aligned}$$

Can include nonlinear M_k and/or H_k .

Implemented operationally at ECMWF for the assimilation in the stratosphere.

Becomes singular in the strong constraint limit $Q_k \rightarrow 0$

Dual Algorithm for Variational Assimilation (aka *Physical Space Analysis System, PSAS*, pronounced ‘pizzazz’; see in particular book and papers by Bennett)

$$x^a = x^b + P^b H^T [HP^b H^T + R]^{-1} (y - Hx^b)$$

$$x^a = x^b + P^b H^T \Lambda^{-1} d = x^b + P^b H^T m$$

where $\Lambda \equiv HP^b H^T + R$, $d \equiv y - Hx^b$ and $m \equiv \Lambda^{-1} d$ maximises

$$\mu \rightarrow \mathcal{K}(\mu) = -(1/2) \mu^T \Lambda \mu + d^T \mu$$

Maximisation is performed in (dual of) observation space.

Dual Algorithm for Variational Assimilation (continuation 2)

Extends to time dimension, and to weak-constraint case, by defining state vector as

$$x \equiv (x_0^T, x_1^T, \dots, x_K^T)^T$$

or, equivalently, but more conveniently, as

$$x \equiv (x_0^T, \eta_0^T, \dots, \eta_{K-1}^T)^T$$

where, as before

$$\eta_k = x_{k+1} - M_k x_k \quad , \quad k = 0, \dots, K-1$$

The background for x_0 is x_0^b , the background for η_k is 0 . Complete background is

$$x^b = (x_0^{bT}, 0^T, \dots, 0^T)^T$$

It is associated with error covariance matrix

$$P^b = \text{diag}(P_0^b, Q_0, \dots, Q_{K-1})$$

Dual Algorithm for Variational Assimilation (continuation 3)

Define global observation vector as

$$y \equiv (y_0^T, y_1^T, \dots, y_K^T)^T$$

and global innovation vector as

$$d \equiv (d_0^T, d_1^T, \dots, d_K^T)^T$$

where

$$d_k \equiv y_k - H_k x_k^b, \text{ with } x_{k+1}^b \equiv M_k x_k^b, \quad k = 0, \dots, K-1$$

Dual Algorithm for Variational Assimilation (continuation 4)

For any state vector $\xi = (\xi_0^T, v_0^T, \dots, v_{K-1}^T)^T$, the observation operator H

$$\xi \rightarrow H\xi = (u_0^T, \dots, u_K^T)^T$$

is defined by the sequence of operations

$$u_0 = H_0 \xi_0$$

then for $k = 0, \dots, K-1$

$$\begin{aligned}\xi_{k+1} &= M_k \xi_k + v_k \\ u_{k+1} &= H_{k+1} \xi_{k+1}\end{aligned}$$

The observation error covariance matrix is equal to

$$R = \text{diag}(R_0, \dots, R_K)$$

Dual Algorithm for Variational Assimilation (continuation 5)

Maximization of dual objective function

$$\mu \rightarrow \mathcal{K}(\mu) = -(1/2) \mu^T \Lambda \mu + d^T \mu$$

requires explicit repeated computations of its gradient

$$\nabla_{\mu} \mathcal{K} = - \Lambda \mu + d = - (HP^b H^T + R) \mu + d$$

Starting from $\mu = (\mu_0^T, \dots, \mu_K^T)^T$ belonging to (dual) of observation space, this requires 5 successive steps

- Step 1. Multiplication by H^T . This is done by applying the transpose of the process defined above, viz.,

Set $\chi_K = 0$

Then, for $k = K-1, \dots, 0$

$$\begin{aligned} \mathbf{v}_k &= \chi_{k+1} + H_{k+1}^T \mu_{k+1} \\ \chi_k &= M_k^T \mathbf{v}_k \end{aligned}$$

Finally

$$\lambda_0 = \chi_0 + H_0^T \mu_0$$

The output of this step, which includes a backward integration of the adjoint model, is the vector

$$(\lambda_0^T, \mathbf{v}_0^T, \dots, \mathbf{v}_{K-1}^T)^T$$

Dual Algorithm for Variational Assimilation (continuation 6)

- Step 2. Multiplication by P^b . This reduces to

$$\begin{aligned}\xi_0 &= P_0^b \lambda_0 \\ \mathbf{v}_k &= Q_k \mathbf{v}_k, \quad k = 0, \dots, K-1\end{aligned}$$

- Step 3. Multiplication by H . Apply the process defined above on the vector $(\xi_0^T, \mathbf{v}_0^T, \dots, \mathbf{v}_{K-1}^T)^T$, thereby producing vector $(u_0^T, \dots, u_K^T)^T$.

- Step 4. Add vector $R\mu$, *i. e.* compute

$$\begin{aligned}\varphi_0 &= \xi_0 + R_0 \mu_0 \\ \varphi_k &= \mathbf{v}_{k-1} + R_k \mu_k, \quad k = 1, \dots, K,\end{aligned}$$

- Step 5. Change sign of vector $\varphi = (\varphi_0^T, \dots, \varphi_K^T)^T$, and add vector $d = y - Hx^b$,

Dual Algorithm for Variational Assimilation (continuation 7)

Temporal correlations can be introduced.

Dual algorithm remains regular in the limit of vanishing model error. Can be used for both strong- and weak-constraint assimilation.

No significant increase of computing cost in comparison with standard strong constraint variational assimilation (Courtier, Louvel)

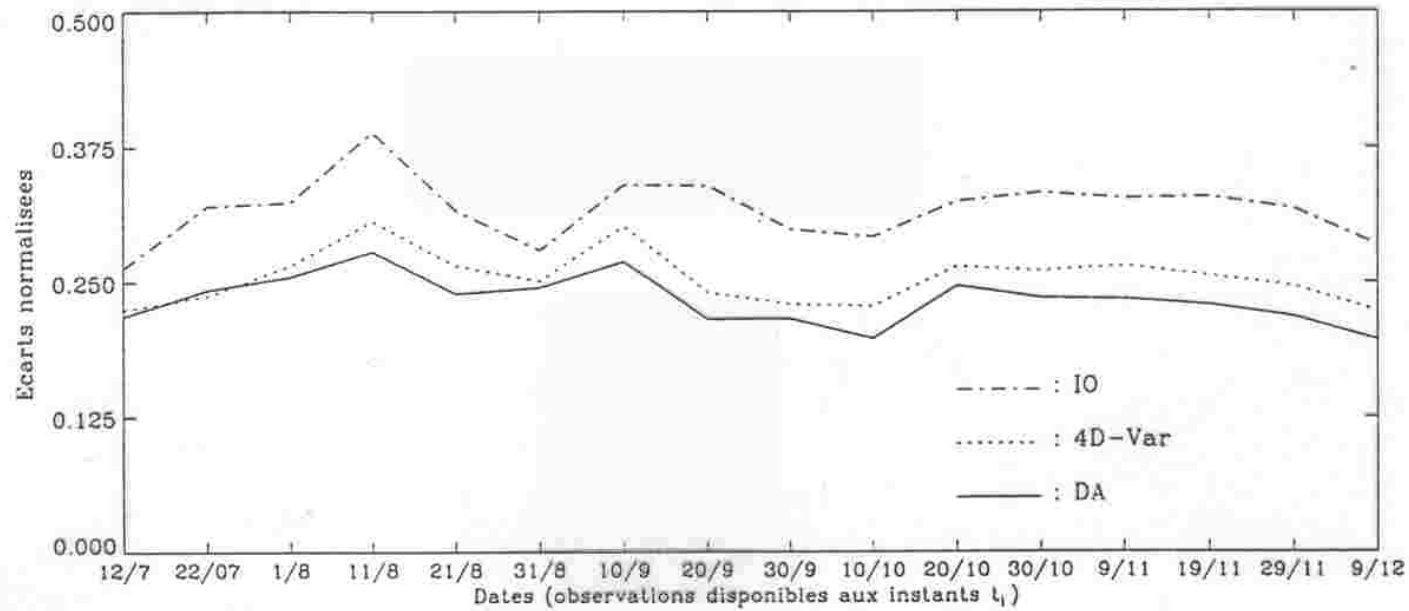


FIG. 9.11 – *Ecartls normalisees prvision/observations sur l'ensemble de la p'riode tudiee*

... pour observer les performances des différentes techniques d'assimilation.

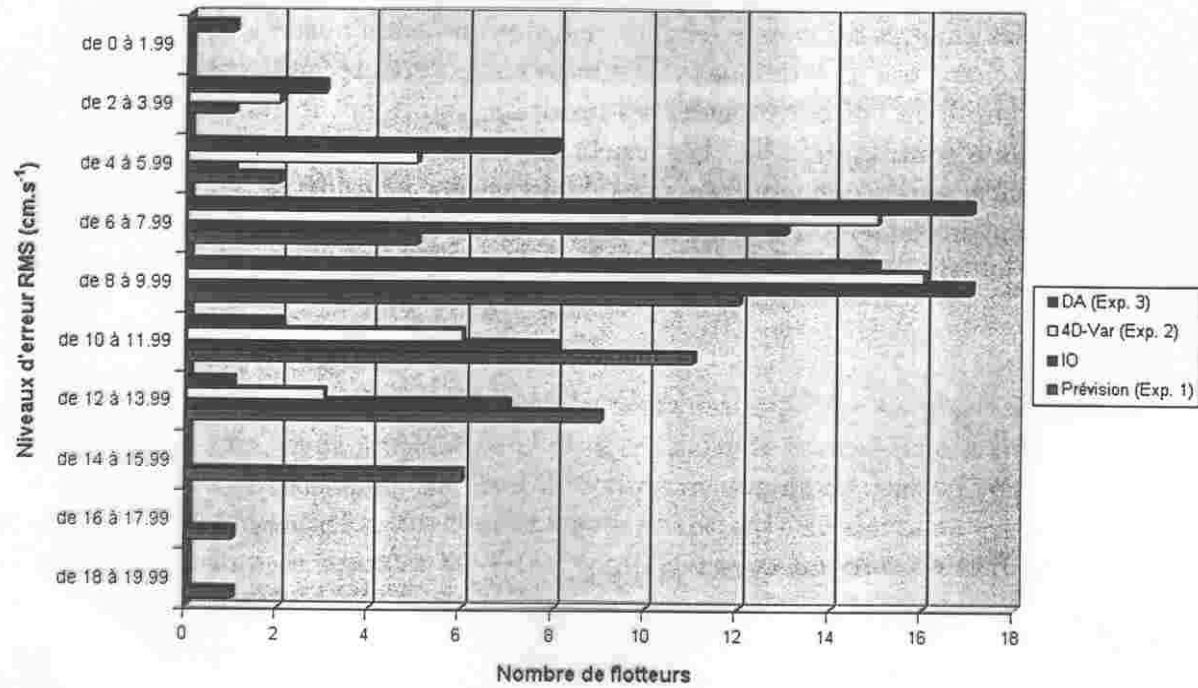


FIG. 9.15 - Description des écarts flotteurs/modèle en terme de vitesse (à 150 m de profondeur) pour les différents algorithmes d'assimilation

Dual Algorithm for Variational Assimilation (continuation)

Requires

- Explicit background (not much of a problem)
- Exact linearity (much more of a problem). Definition of iterative nonlinear procedures is being studied (Auroux, ...)

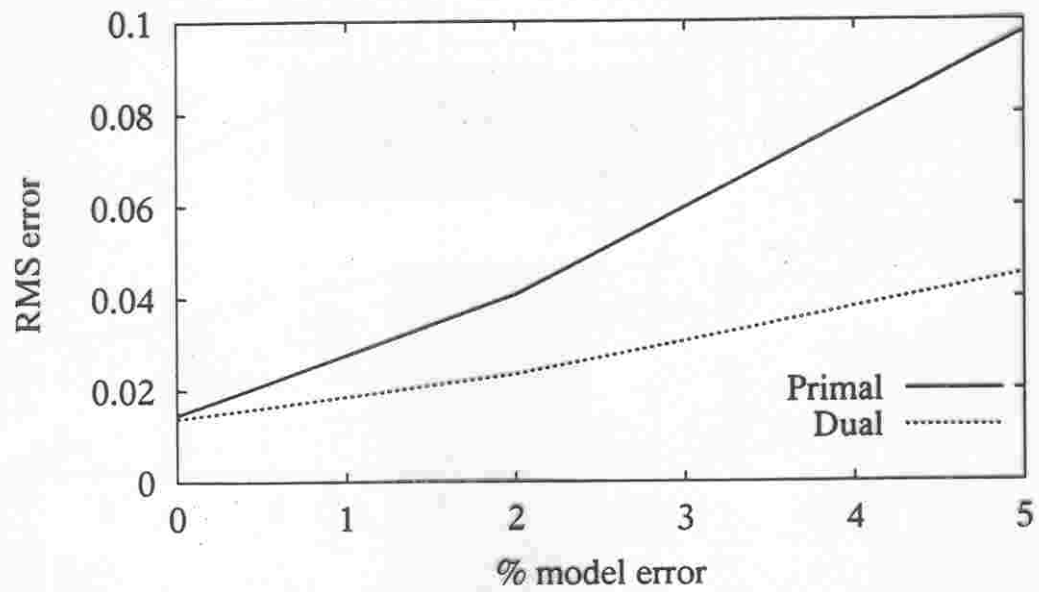


FIG. 6.13 – Normes RMS des erreurs d'assimilation obtenues pour les deux méthodes en fonction de l'erreur introduite dans le modèle au cours de la période d'assimilation.

Dual Algorithm for Variational Assimilation is now used, in the weak-constraint form, at *Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS)* in Toulouse (A. Weaver, S. Gürol) for assimilation of oceanographical observations.

Conclusion on Sequential Assimilation

Pros

‘Natural’, and well adapted to many practical situations

Provides, at least relatively easily, explicit estimate of estimation error

Cons

Carries information only forward in time (of no importance if one is interested only in doing forecast)

In a strictly sequential assimilation (*i.e.*, any individual piece of information is discarded once it has been used), optimality is possible only if errors are uncorrelated in time.

Conclusion on Variational Assimilation

Pros

Carries information both forward and backward in time (important for reassimilation of past data).

Can easily take into account temporal statistical dependence (Järvinen *et al.*)

Does not require explicit computation of temporal evolution of estimation error

Very well adapted to some specific problems (*e. g.*, identification of tracer sources)

Cons

Does not readily provide estimate of estimation error

Requires development and maintenance of adjoint codes. But the latter can have other uses (sensitivity studies).

- Dual approach seems most promising. But little used.
- Can be implemented in ensemble form (see course 8).

Variational assimilation has been extended to non Gaussian probability distributions (lognormal distributions), the unknown being the mode of the conditional distribution (M. Zupanski, Fletcher).

Bayesian character of variational assimilation ?

- If everything is linear and gaussian, ready recipe for obtaining bayesian sample

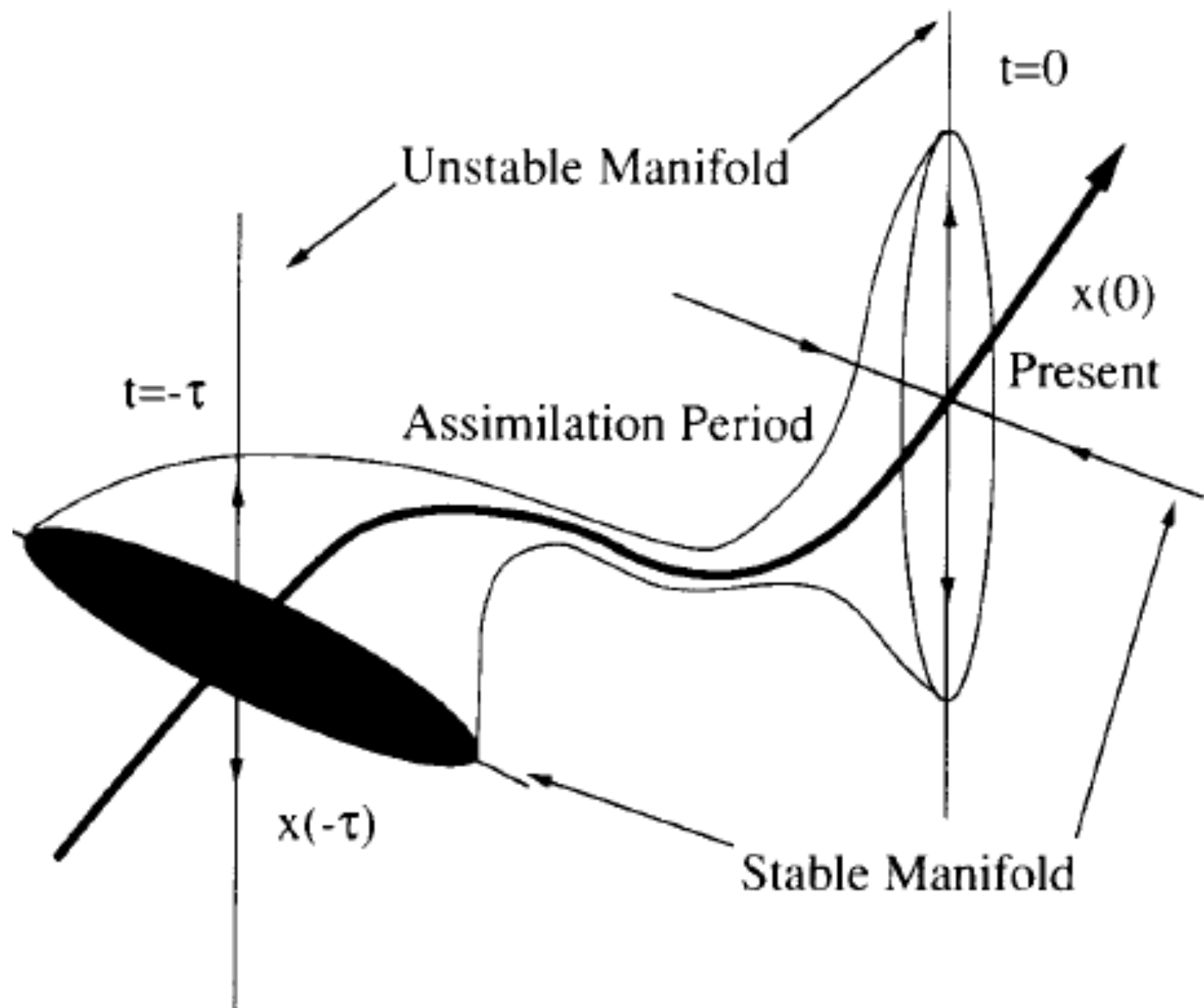
Perturb data (background, observations and model) according to their error probability distributions, do variational assimilation, and repeat process

Sample of system orbits thus obtained is bayesian

- If not, very little can be said at present

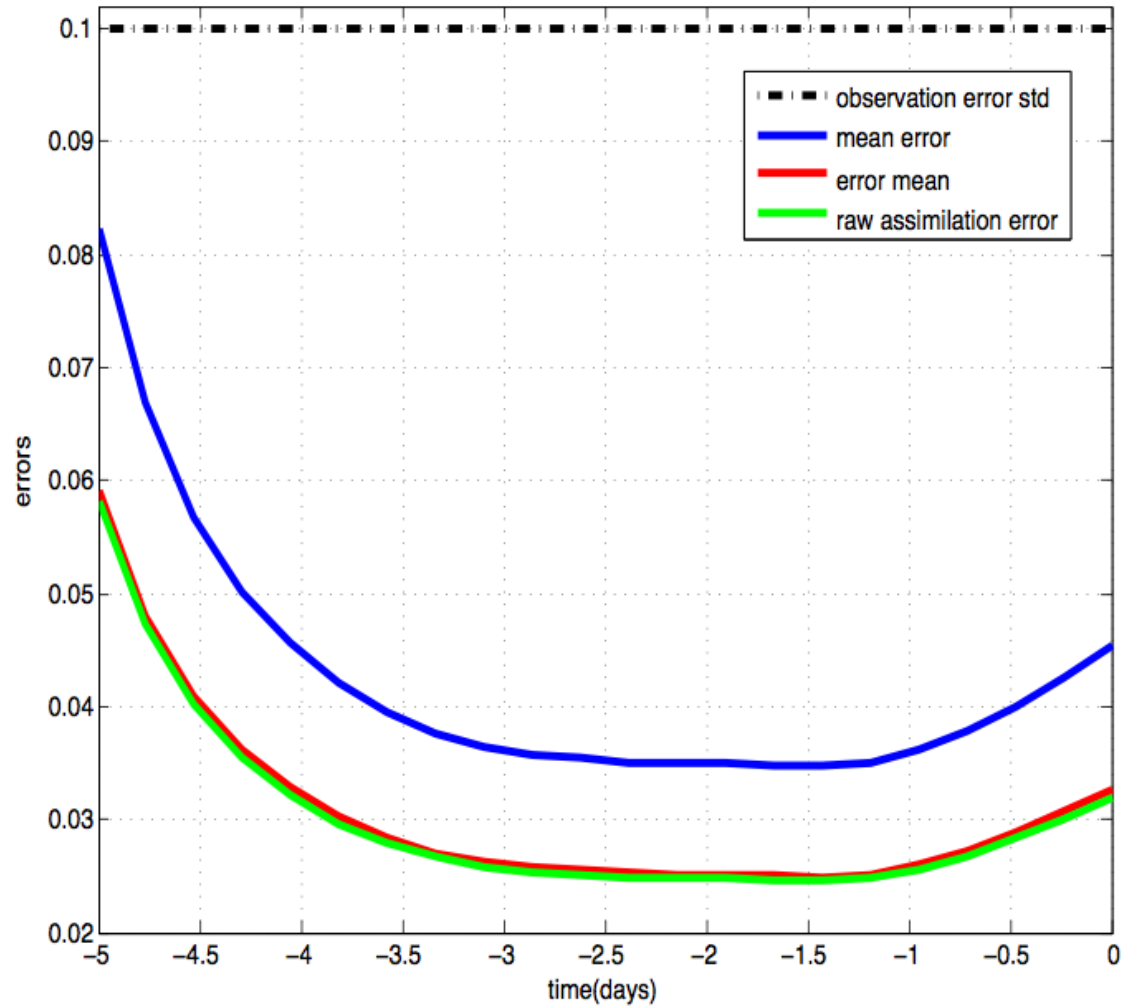
If there is uncertainty on the state of the system, and dynamics of the system is perfectly known, uncertainty on the state along stable modes decreases over time, while uncertainty along unstable modes increases.

Stable (unstable) modes : perturbations to the basic state that decrease (increase) over time.



Consequence : Consider 4D-Var assimilation, or any form of smoother, which carries information both forward and backward in time, performed over time interval $[t_0, t_1]$ over uniformly distributed noisy data. If assimilating model is perfect, estimation error is concentrated in stable modes at time t_0 , and in unstable modes at time t_1 . Error is smallest somewhere within interval $[t_0, t_1]$.

Similar result holds true for Kalman filter (or more generally any form of sequential assimilation), in which estimation error is concentrated in unstable modes at any time.



Linearized Lorenz'96. 5 days

Jardak and Talagrand

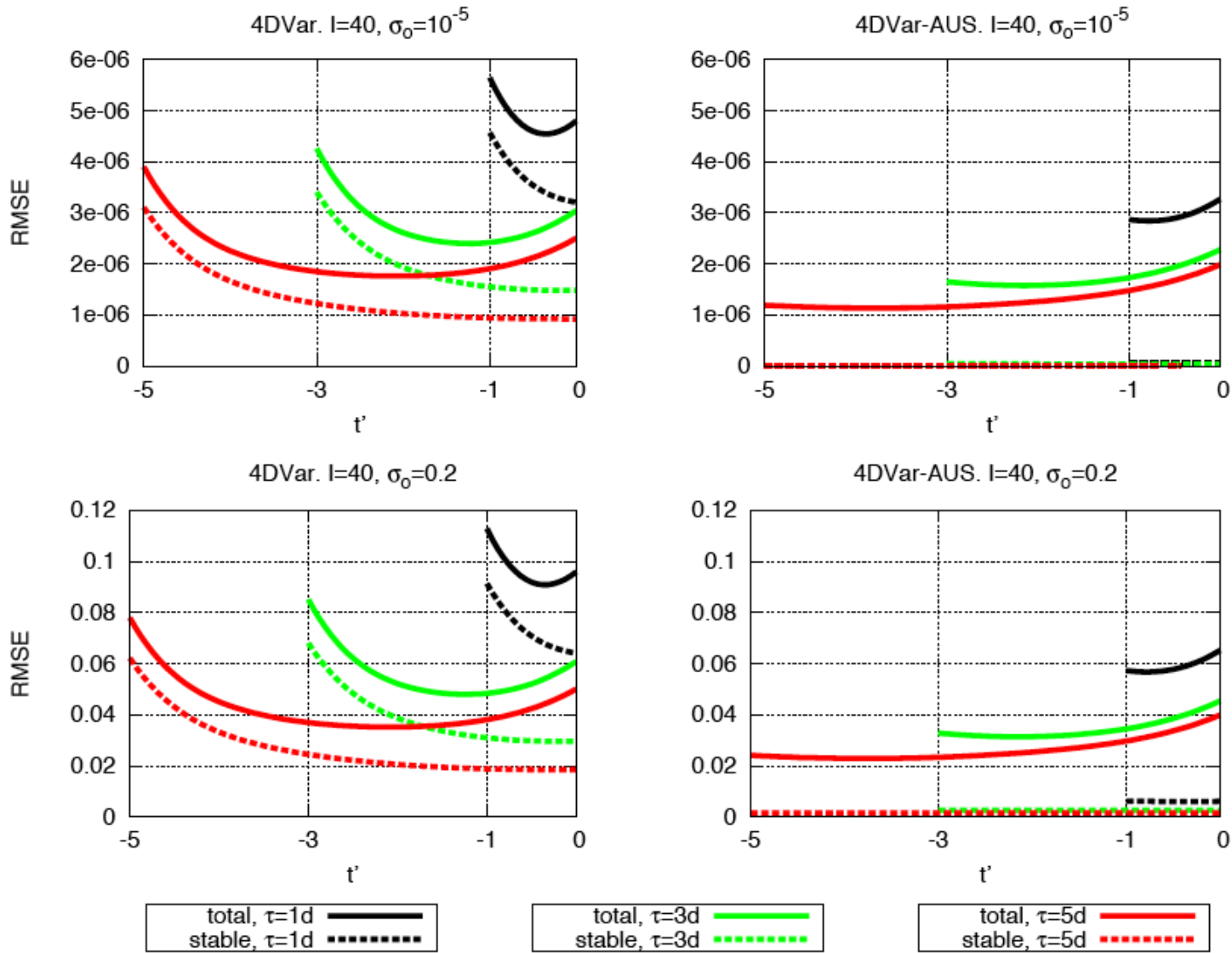


Figure 3. Time average RMS error within 1, 3, 5 days assimilation windows as a function of $t' = t - \tau$, with $\sigma_0 = .2, 10^{-5}$ for the model configuration $I = 40$. Left panel: 4DVar. Right panel: 4DVar-AUS with $N = 15$. Solid lines refer to total assimilation error, dashed lines refer to the error component in the stable subspace e_{16}, \dots, e_{40} .

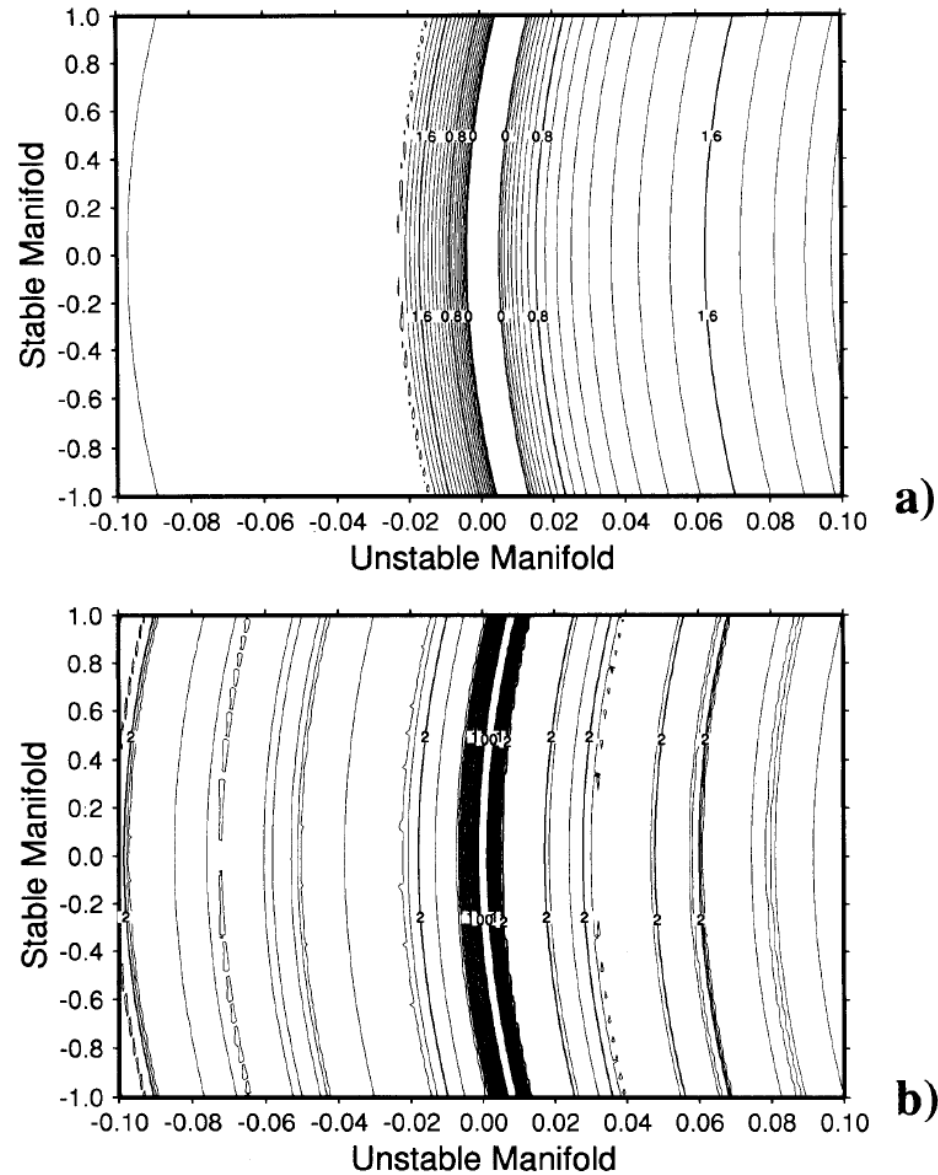


Fig. 3. Variations of the error-free forward cost-function $J'_e(\tau, \hat{x}, x)$ (Lorenz system) in the plane spanned by the stable and unstable directions, as determined from the tangent linear system (see text), and for $\tau = 6$ (panel (a)) and $\tau = 8$ (panel (b)) respectively. The metric has been distorted in order to make the stable and unstable manifolds orthogonal to each other in the figure. The scale on the contour lines is logarithmic (decimal logarithm). Contour interval: 0.1. For clarity, negative contours, which would be present only in the central “valley” directed along the stable manifold, have not been drawn.

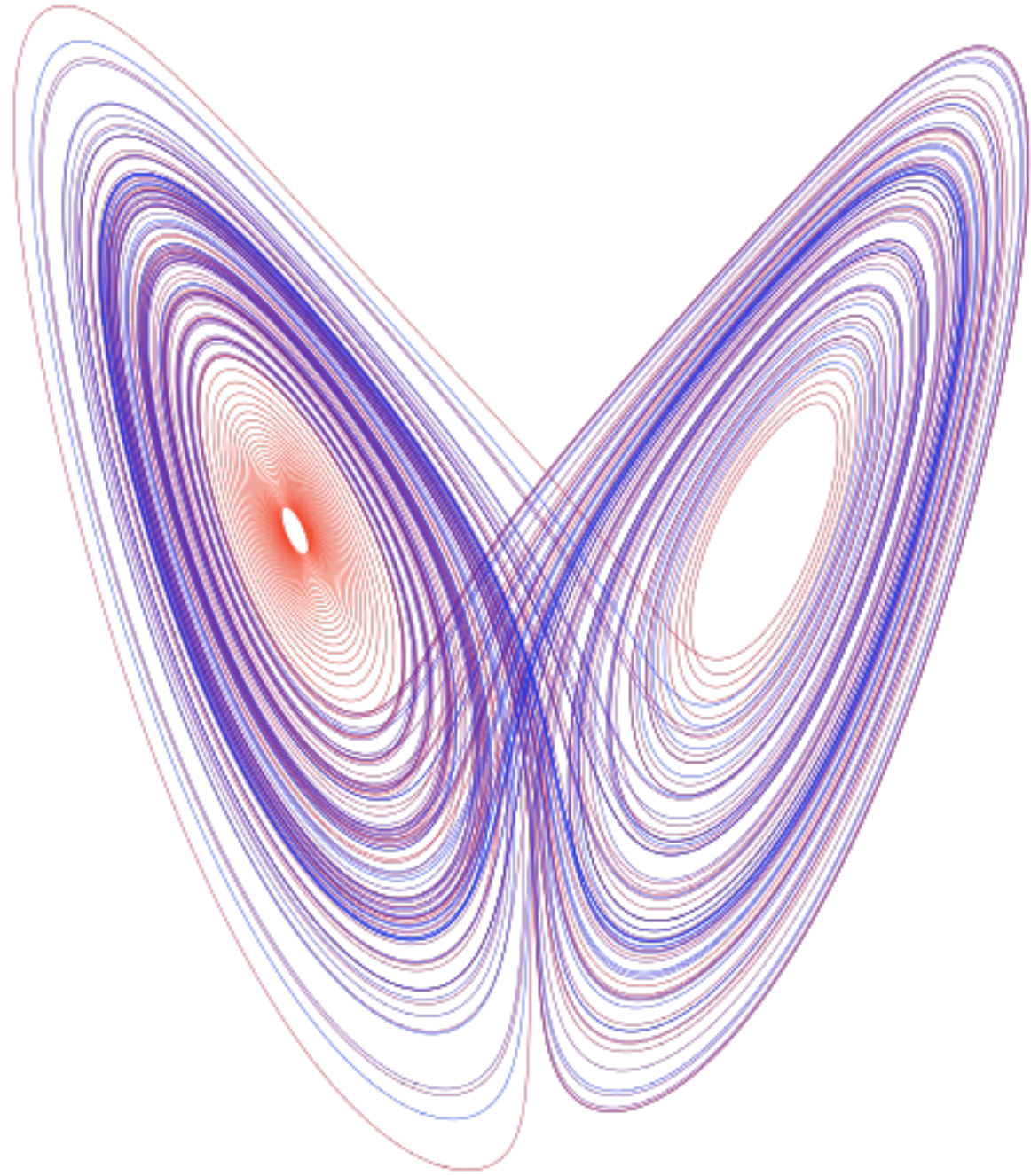
Lorenz (1963)

$$dx/dt = \sigma(y-x)$$

$$dy/dt = \rho x - y - xz$$

$$dz/dt = -\beta z + xy$$

with parameter values $\sigma = 10$, $\rho = 28$, $\beta = 8/3 \Rightarrow$ chaos



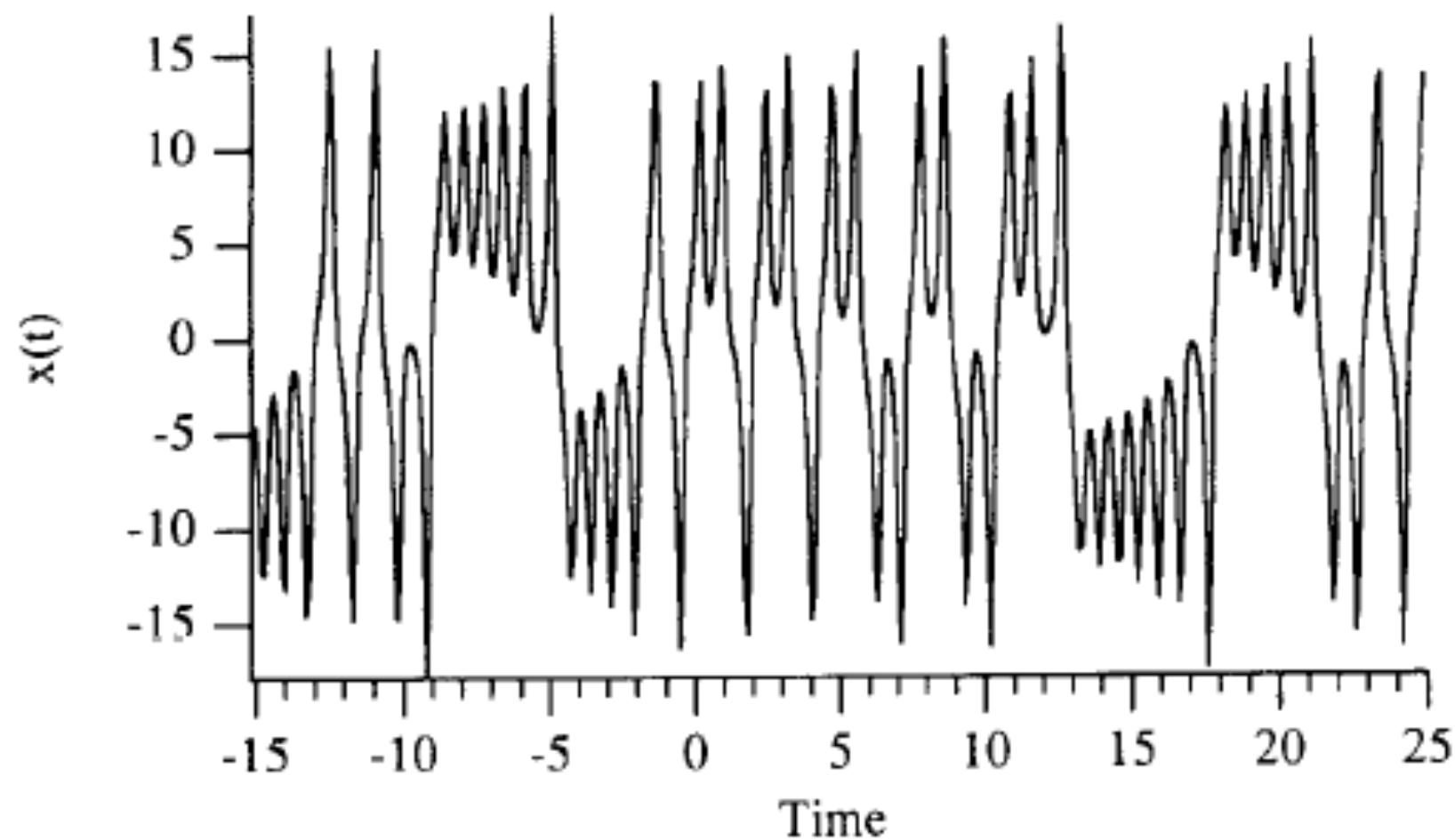


Fig. 2. Time variations, along the reference solution, of the variable $x(t)$ of the Lorenz system.

Twin (strong constraint) experiment. Observations $y_k = H_k x_k + \varepsilon_k$ at successive times k , and objective function of form

$$J(\xi_0) = (1/2) \sum_k [y_k - H_k \xi_k]^T R_k^{-1} [y_k - H_k \xi_k]$$

x_k denotes here the complete state vector, and H_k is the unit operator (all three components of x_k are observed)

No 'background' term from the past, but observation y_0 at time $k = 0$.

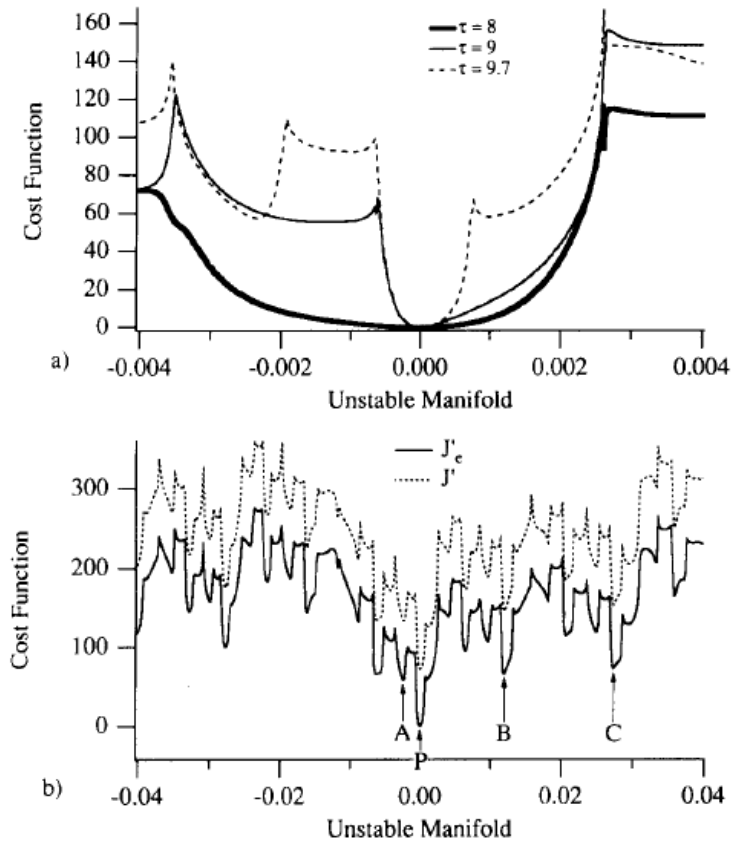


Fig. 4. Panel (a): Cross-section of the error-free forward cost-function $J'_e(\tau, \hat{x}, x)$ along the unstable manifold, for various values of τ . Panel (b). As in panel (a), for $\tau = 9.7$, and with a display interval ten times as large, respectively for the error-free forward cost-function $J'_e(\tau, \hat{x}, x)$ (solid curve) and for the error-contaminated cost-function $J_e(\tau, \hat{x}, x)$ (dashed curve). In the latter case, the total variance of the observational noise is $E^2 = 75$.

Pires *et al.*, *Tellus*, 1996 ; Lorenz system (1963)

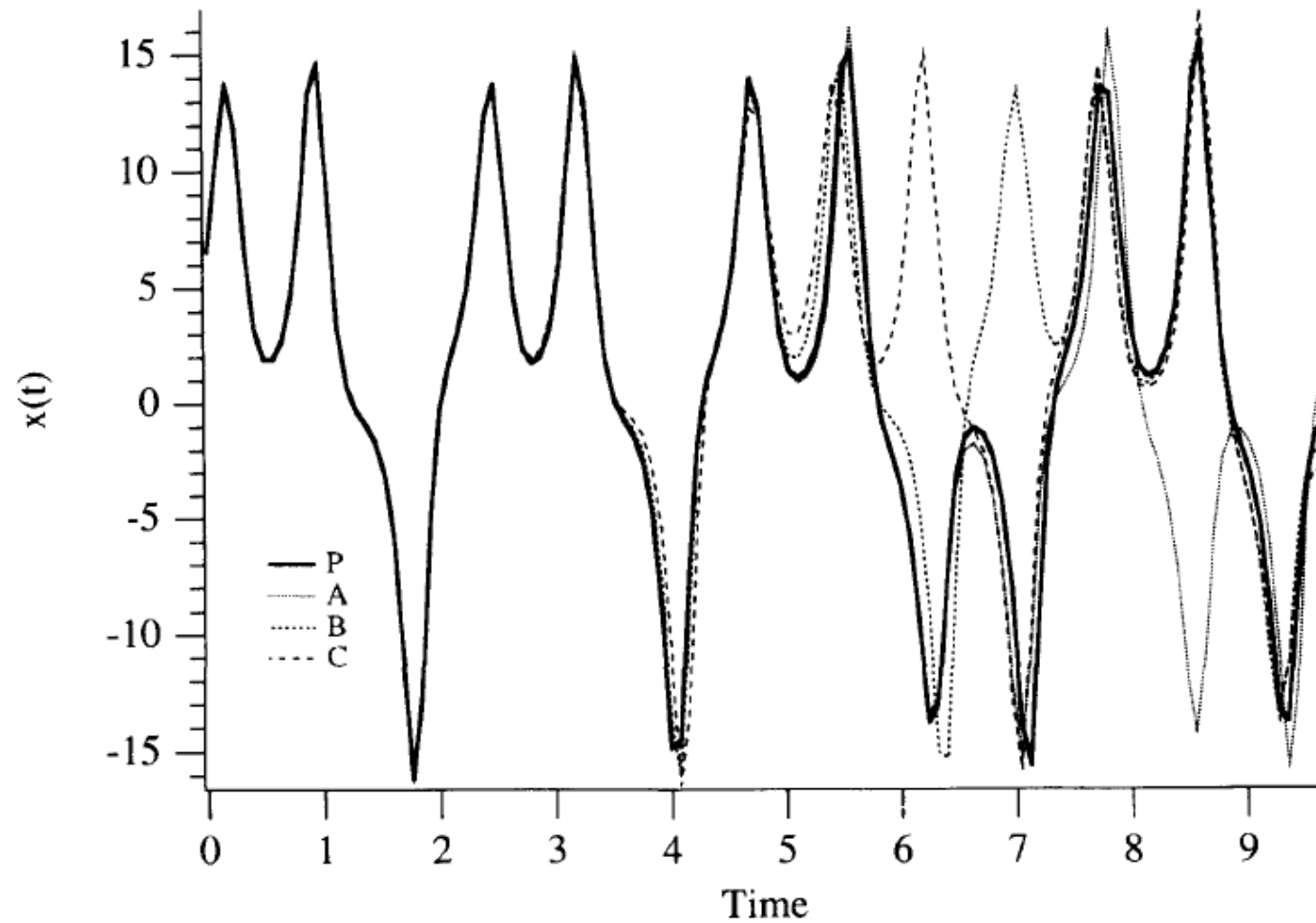


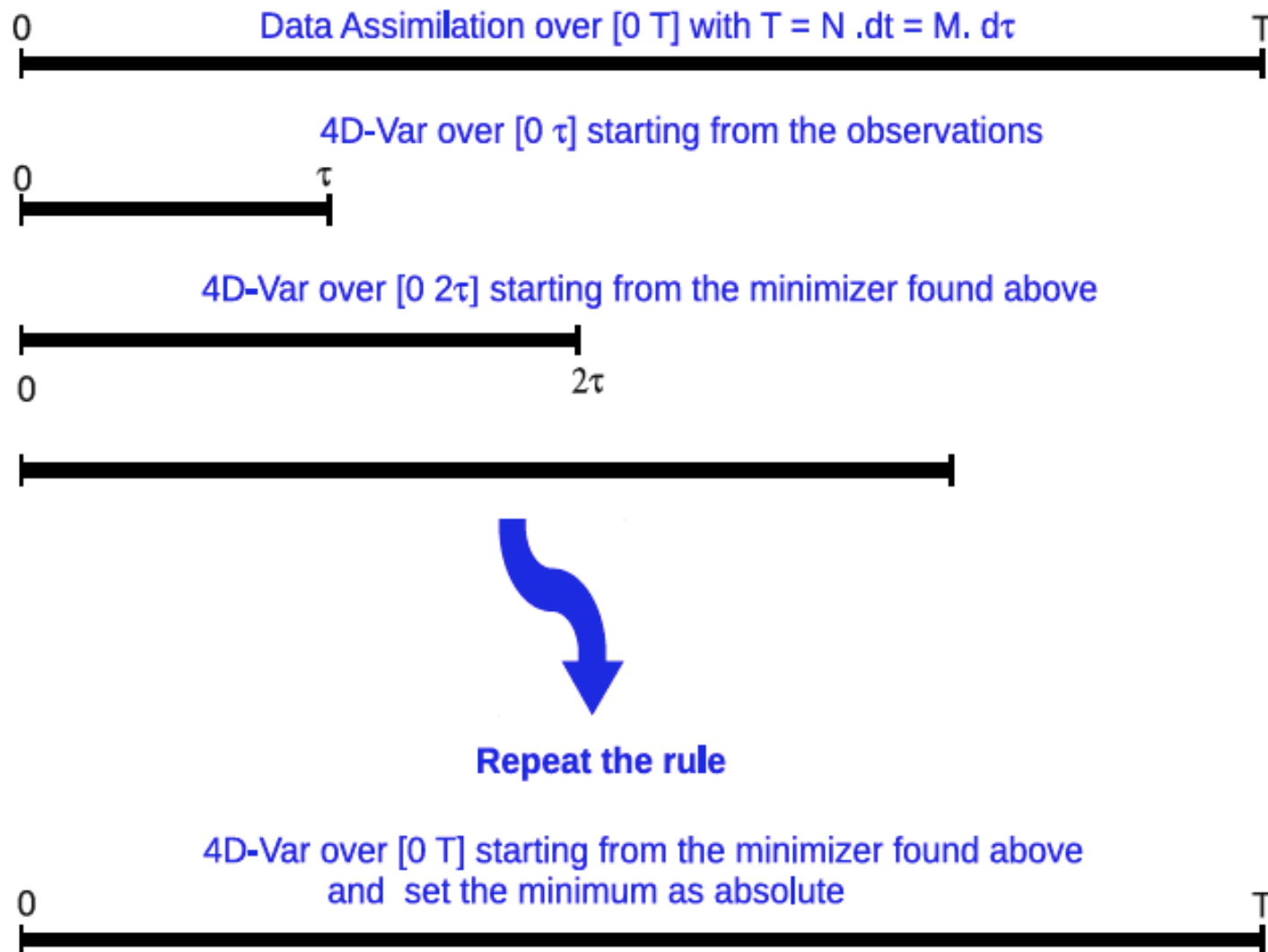
Fig. 5. Variations of the coordinate x along the orbits originating from the minima P , A , B , C (indicated in Fig. 4b) of the error-free cost-function.

Minima in the variations of objective function correspond to solutions that have bifurcated from the observed solution, and to different folds in state space.

Quasi-Static Variational Assimilation (QSVA). Increase progressively length of the assimilation window, starting each new assimilation from the result of the previous one. This should ensure, at least if observations are in a sense sufficiently dense in time, that current estimation of the system always lies in the attractive basin of the absolute minimum of objective function (Pires *et al.*, Swanson *et al.*, Luong, Järvinen *et al.*)

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Quasi-Static Variational Assimilation (QSVA)



$\mu(C(\tau, x))$	Cloud of points QSVA	Cloud of points raw assimilation	Linear tangent system	Upper bound
$\tau = 0$	1	1	1	1
$\tau = 1$	0.36	0.37	0.39	0.46
$\tau = 2$	5.9×10^{-2}	5.74	4.5×10^{-2}	0.401
$\tau = 3$	3.3×10^{-2}	29.4	2.9×10^{-2}	0.397
$\tau = 8$	1.4×10^{-2}	59.9	*	0.396

In the left column, the estimates are calculated from the ensemble of 100 assimilations (see also Fig. 7). The 2nd column contains the values obtained from the raw assimilation. In the 3rd column, the estimates are obtained from the tangent linear system and eqs. (3.5–3.9) (the star indicates a computational overflow). The estimates in the right-hand column are the upper bounds defined by eq. (3.13).

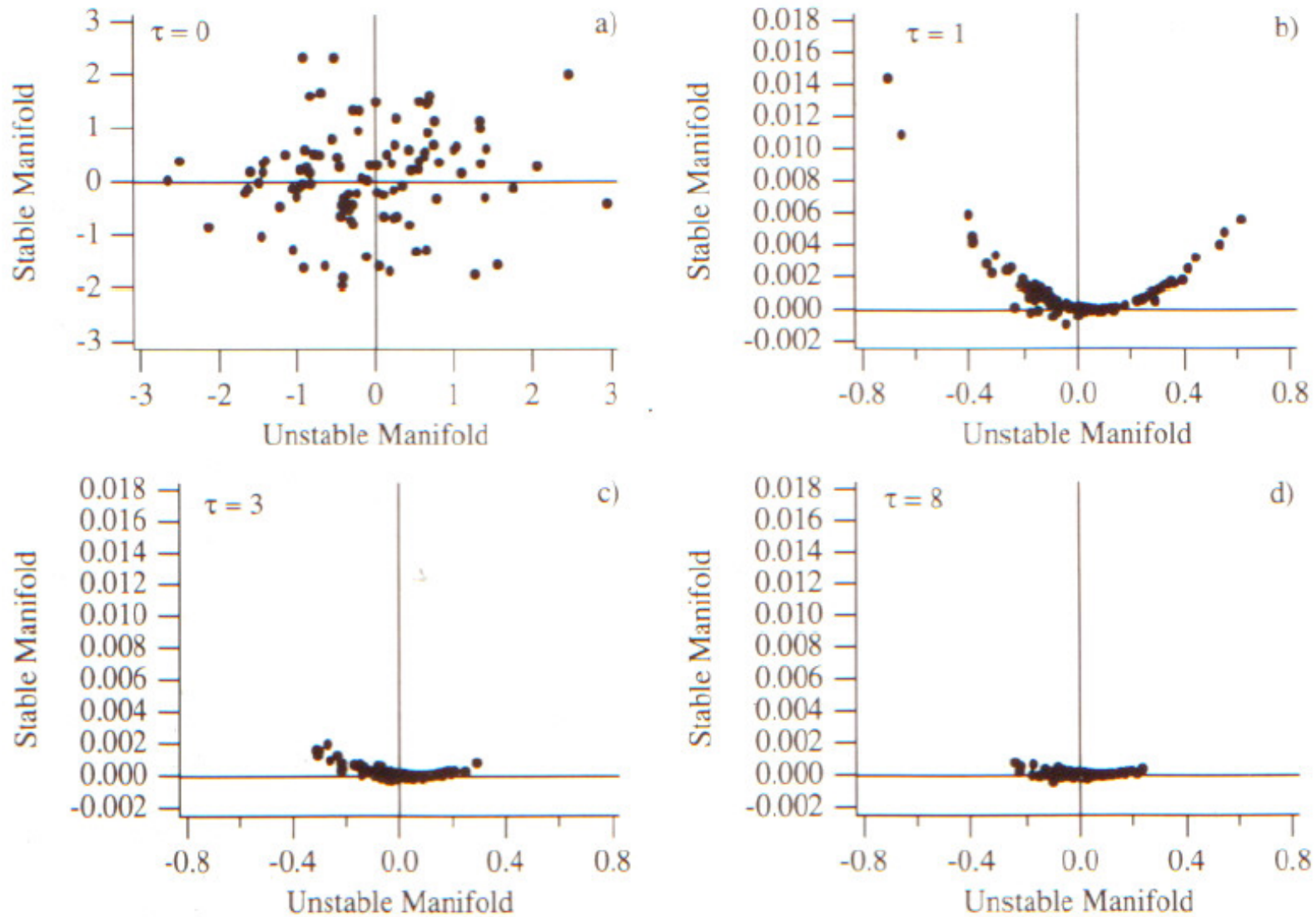


Fig. 7. Projection of the 100 minimizing solutions, at the end of the assimilation period, onto the plane spanned by the stable and unstable directions, defined as in Fig. 3. Values of τ are indicated on the panels. The projection is not an orthogonal projection, but a projection parallel to the local velocity vector $(dx/dt, dy/dt, dz/dt)$ (central manifold).

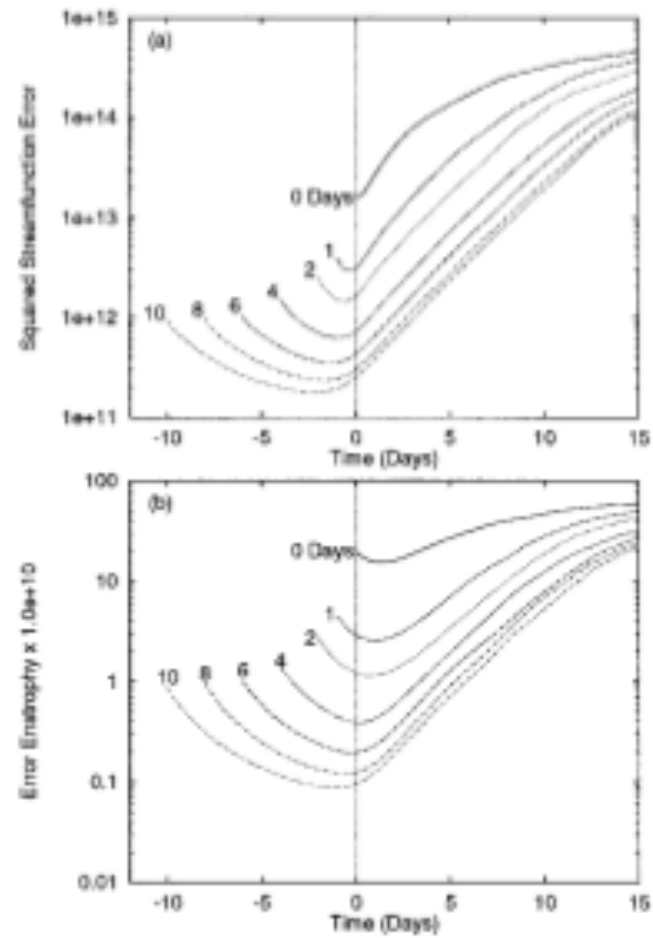


Fig. 5. Median values of the (a) streamfunction squared error, and (b) enstrophy error for the 200 forecast set as a function of forecast time and of the assimilation time T_a .

Swanson, Vautard and Pires, 1998, *Tellus*, **50A**, 369-390

Cours à venir

~~Vendredi 26 mars~~

~~Vendredi 2 avril~~

~~Vendredi 9 avril~~

~~Vendredi 16 avril~~

~~Vendredi 7 mai~~

~~Vendredi 14 mai~~

~~Vendredi 21 mai~~

Vendredi 28 mai