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Posterior Covariance vs. Analysis Error Covariance in Data Assimilation

F.-X. Le Dimet(1), I. Gejadze(2), V. Shutyaev(3)

(1) Université de Grenoble

(2) University of Strathclyde, Glasgow, UK

(3) Institute of Numerical Mathematics, RAS, Moscow, Russia

ledimet@imag.fr

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- Introduction
- Analysis Error Covariance via Hessian
- Posterior Covariance : A Bayesian approach
- Effective Covariance Estimates
- Implementation : some remarks
- Asymptotic Properties
- Numerical Example
- Conclusion

There are two basic approaches for Data Assimilation:

- Variational Methods
- Kalman Filter

Both lead to minimize a cost function :

$$J(u) = \frac{1}{2}(V_b^{-1}(u - u_b), u - u_b)_X + \frac{1}{2}(V_o^{-1}(C\varphi - y), C\varphi - y)_{Y_o}, \quad (1)$$

where $u_b \in X$ is a prior initial-value function (background state), $y \in Y_o$ is a prescribed function (observational data), Y_o is an observation space, $C : Y \rightarrow Y_o$ is a linear bounded operator.

We get the same optimal solution \bar{u}

\bar{u} is the solution of the Optimality System :

$$\begin{cases} \frac{\partial \varphi}{\partial t} = F(\varphi) + f, & t \in (0, T) \\ \varphi|_{t=0} = u, \end{cases} \quad (2)$$

$$\begin{cases} \frac{\partial \varphi^*}{\partial t} + (F'(\varphi))^* \varphi^* = C^* V_o^{-1}(C\varphi - y), & t \in (0, T) \\ \varphi^*|_{t=T} = 0, \end{cases} \quad (3)$$

$$V_b^{-1}(u - u_b) - \varphi^*|_{t=0} = 0 \quad (4)$$

In an analysis there are two inputs:

- The background u_b
- the observation y

Both have error and the question is what is the impact of these errors on the analysis?

The background can be considered from two different viewpoints:

- Variational viewpoint: the background is a regularization term in the Tykhonov's sense to make the problem well posed
- Bayesian view point: the background is an a priori information on the analysis

In the linear case we get the same covariance error for the analysis : the **inverse of the Hessian** of the cost function.

In the non linear case we get two different items:

- Variational approach : Analysis Error Covariance
- Bayesian Approach : Posterior Covariance

Questions:

- How to compute, approximate, these elements?
- What are the differences?

Analysis Error Covariance 1: True solution and Errors

We assume the existence of a "true" solution u^t and an associated "true" state φ^t verifying:

$$\left\{ \begin{array}{l} \frac{\partial \varphi^t}{\partial t} = F(\varphi^t) + f, \quad t \in (0, T) \\ \varphi^t|_{t=0} = u^t. \end{array} \right. \quad (5)$$

Then the errors are defined by : $u_b = u^t + \xi_b$, $y = C\varphi^t + \xi_o$ with covariances V_b and V_o

Analysis Error Covariance 2: Discrepancy Evolution

Let

$$\delta\varphi = \varphi - \varphi^t, \quad \delta u = u - u^t.$$

Then for regular F there exists $\tilde{\varphi} = \varphi^t + \tau(\varphi - \varphi^t)$, $\tau \in [0, 1]$, such that

$$\begin{cases} \frac{\partial \delta\varphi}{\partial t} - F'(\tilde{\varphi})\delta\varphi = 0, & t \in (0, T), \\ \delta\varphi|_{t=0} = \delta u, \end{cases} \quad (6)$$

$$\begin{cases} \frac{\partial \varphi^*}{\partial t} + (F'(\varphi))^* \varphi^* = C^* V_o^{-1}(C\delta\varphi - \xi_o), \\ \varphi^*|_{t=T} = 0, \end{cases} \quad (7)$$

$$V_b^{-1}(\delta u - \xi_b) - \varphi^*|_{t=0} = 0. \quad (8)$$

Analysis Error Covariance 3: Exact Equation for Analysis Error

Let us introduce the operator $R(\varphi) : X \rightarrow Y$ as follows:

$$R(\varphi)v = \psi, \quad v \in X, \quad (9)$$

where ψ is the solution of the tangent linear problem

$$\frac{\partial \psi}{\partial t} - F'(\varphi)\psi = 0, \quad \psi|_{t=0} = v. \quad (10)$$

Then, the system for errors can be represented as a single operator equation for δu :

$$H(\varphi, \tilde{\varphi})\delta u = V_b^{-1}\xi_b + R^*(\varphi)C^*V_o^{-1}\xi_o, \quad (11)$$

where

$$H(\varphi, \tilde{\varphi}) = V_b^{-1} + R^*(\varphi)C^*V_o^{-1}CR(\tilde{\varphi}). \quad (12)$$

Analysis Error Covariance 4 : H Operator

The operator $H(\varphi, \tilde{\varphi}) : X \rightarrow X$ can be defined by

$$\frac{\partial \psi}{\partial t} - F'(\tilde{\varphi})\psi = 0, \quad \psi|_{t=0} = v, \quad (13)$$

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^*\psi^* = -C^*V_o^{-1}C\psi, \quad \psi^*|_{t=T} = 0, \quad (14)$$

$$H(\varphi, \tilde{\varphi})v = V_b^{-1}v - \psi^*|_{t=0}. \quad (15)$$

The operator $H(\varphi, \tilde{\varphi})$ is neither symmetric, nor positive definite.

$\varphi = \tilde{\varphi} = \theta$, it becomes the Hessian $H(\theta)$ of the cost function J_1 in the following auxiliary DA problem: find δu and $\delta \varphi$ such that

$J_1(\delta u) = \inf_V J_1(v)$, where

$$J_1(\delta u) = \frac{1}{2}(V_b^{-1}(\delta u - \xi_b), \delta u - \xi_b)_X + \frac{1}{2}(V_o^{-1}(C\delta\varphi - \xi_o), C\delta\varphi - \xi_o)_{Y_o}, \quad (16)$$

and $\delta\varphi$ satisfies the problem

$$\frac{\partial \delta\varphi}{\partial t} - F'(\theta)\delta\varphi = 0, \quad \delta\varphi|_{t=0} = \delta u. \quad (17)$$

Analysis Error Covariance 5 : Analysis Error Covariance via Hessian

The optimal solution (analysis) error δu is assumed to be unbiased, i.e. $E[\delta u] = 0$, and

$$V_{\delta u} = E[(\cdot, \delta u)_X \delta u] = E[(\cdot, u - u^t)_X (u - u^t)]. \quad (18)$$

The best value of φ and $\tilde{\varphi}$ independent of ξ_o, ξ_b is apparently φ^t and using

$$R(\tilde{\varphi}) \approx R(\varphi^t), \quad R^*(\varphi) \approx R^*(\varphi^t), \quad (19)$$

the error equation reduces to

$$H(\varphi^t)\delta u = V_b^{-1}\xi_b + R^*(\varphi^t)C^*V_o^{-1}\xi_o, \quad H(\cdot) = V_b^{-1} + R^*(\cdot)C^*V_o^{-1}CR(\cdot). \quad (20)$$

We express δu from equation (??)

$$\delta u = H^{-1}(\varphi^t)(V_b^{-1}\xi_b + R^*(\varphi^t)C^*V_o^{-1}\xi_o)$$

and obtain for the **analysis error covariance**

$$V_{\delta u} = H^{-1}(\varphi^t)(V_b^{-1} + R^*(\varphi^t)C^*V_o^{-1}CR(\varphi^t))H^{-1}(\varphi^t) = H^{-1}(\varphi^t). \quad (21)$$

Analysis Error Covariance 6 : Approximations

In practice the 'true' field φ^t is not known, thus we have to use an approximation $\bar{\varphi}$ associated to a certain optimal solution \bar{u} defined by the real data (\bar{u}_b, \bar{y}) , i.e. we use

$$V_{\delta u} = H^{-1}(\bar{\varphi}). \quad (22)$$

In (Rabier and Courtier,1992), the error equation is derived in the form

$$(V_b^{-1} + R^*(\varphi)C^*V_o^{-1}CR(\varphi))\delta u = V_b^{-1}\xi_b + R^*(\varphi)C^*V_o^{-1}\xi_o. \quad (23)$$

The error due to transitions $R(\tilde{\varphi}) \rightarrow R(\varphi^t)$ and $R^*(\varphi) \rightarrow R^*(\varphi^t)$; we call it the 'linearization' error. The use of $\bar{\varphi}$ instead of φ^t in the Hessian computations leads to another error, which shall be called the 'origin' error.

Posterior Covariance : Bayesian Approach 1

Given $u_b \sim \mathcal{N}(\bar{u}_b, V_b)$, $y \sim \mathcal{N}(\bar{y}, V_o)$, the following expression for the posterior distribution of u is derived from the Bayes theorem:

$$\begin{aligned} p(u|\bar{y}) = C \cdot \exp\left(-\frac{1}{2}(V_b^{-1}(u - \bar{u}_b), u - \bar{u}_b)_X\right) \cdot \\ \exp\left(-\frac{1}{2}(V_o^{-1}(C\varphi - \bar{y}), C\varphi - \bar{y})_{Y_o}\right). \end{aligned} \tag{24}$$

The solution to the variational DA problem with the data $y = \bar{y}$ and $u_b = \bar{u}$ is equal to the mode of $p(u, \bar{y})$ (see e.g. Lorenc, 1986; Tarantola, 1987). Accordingly, the Bayesian posterior covariance is defined by :

$$\mathcal{V}_{\delta u} \cdot = E[(\cdot, u - E[u])_X (u - E[u])] \tag{25}$$

with $u \sim p(u|\bar{y})$.

Posterior Covariance : Bayesian Approach 2

In order to compute $\mathcal{V}_{\delta u}$ by the Monte Carlo method, one must generate a sample of pseudo-random realizations u_i from $p(u|\bar{y})$. We will consider u_i to be the solutions to the DA problem with the perturbed data $u_b = \bar{u}_b + \xi_b$, and $y = \bar{y} + \xi_o$, where $\xi_b \sim \mathcal{N}(0, V_b)$, $\xi_o \sim \mathcal{N}(0, V_o)$. Further we assume that $E[u] = \bar{u}$, where \bar{u} is the solution to the unperturbed problem in which case $\mathcal{V}_{\delta u}$ can be approximated as follows

$$\mathcal{V}_{\delta u} = E[(\cdot, u - \bar{u})_X (u - \bar{u})] = E[(\cdot, \delta u)_X \delta u]. \quad (26)$$

Posterior Covariance : O.S. for Errors

Unperturbed O.S. with $u_b = \bar{u}_b$, $y = \bar{y}$:

$$\frac{\partial \bar{\varphi}}{\partial t} = F(\bar{\varphi}) + f, \quad \varphi|_{t=0} = \bar{u}, \quad (27)$$

$$\frac{\partial \bar{\varphi}^*}{\partial t} + (F'(\bar{\varphi}))^* \bar{\varphi}^* = C^* V_o^{-1} (C \bar{\varphi} - \bar{y}), \quad \bar{\varphi}^*|_{t=T} = 0, \quad (28)$$

$$V_b^{-1} (\bar{u} - \bar{u}_b) - \bar{\varphi}^*|_{t=0} = 0 \quad (29)$$

With perturbations : $u_b = \bar{u}_b + \xi_b$, $y = \bar{y} + \xi_o$, where $\xi_b \in X$, $\xi_o \in Y_o$.

$\delta u = u - \bar{u}$, $\delta \varphi = \varphi - \bar{\varphi}$, $\delta \varphi^* = \varphi^* - \bar{\varphi}^*$.

$$\frac{\partial \delta \varphi}{\partial t} = F(\varphi) - F(\bar{\varphi}), \quad \delta \varphi|_{t=0} = \delta u, \quad (30)$$

$$\frac{\partial \delta \varphi^*}{\partial t} + (F'(\varphi))^* \delta \varphi^* = [((F'(\bar{\varphi}))^* - F'(\varphi))^*] \bar{\varphi}^* + C^* V_o^{-1} (C \delta \varphi - \xi_o), \quad (31)$$

$$V_b^{-1} (\delta u - \xi_b) - \delta \varphi^*|_{t=0} = 0. \quad (32)$$

Posterior Covariance : Exact Errors Equations

Introducing $\tilde{\varphi}_1 = \bar{\varphi} + \tau_1 \delta\varphi$, $\tilde{\varphi}_2 = \bar{\varphi} + \tau_2 \delta\varphi$, $\tau_1, \tau_2 \in [0, 1]$, we derive the exact system for errors:

$$\frac{\partial \delta\varphi}{\partial t} = F'(\tilde{\varphi}_1) \delta\varphi, \quad \delta\varphi|_{t=0} = \delta u, \quad (33)$$

$$\frac{\partial \delta\varphi^*}{\partial t} + (F'(\varphi))^* \delta\varphi^* = [(F'(\tilde{\varphi}_2))^* \bar{\varphi}^*]' \delta\varphi + C^* V_o^{-1} (C \delta\varphi - \xi_o), \quad (34)$$

$$V_b^{-1} (\delta u - \xi_b) - \delta\varphi^*|_{t=0} = 0, \quad (35)$$

equivalent to a single operator equation for δu :

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) \delta u = V_b^{-1} \xi_b + R^*(\varphi) C^* V_o^{-1} \xi_o, \quad (36)$$

where

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) = V_b^{-1} + R^*(\varphi) (C^* V_o^{-1} C - [(F'(\tilde{\varphi}_2))^* \bar{\varphi}^*]') R(\tilde{\varphi}_1). \quad (37)$$

Posterior Covariance : Operator \mathcal{H}

$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) : X \rightarrow X$ is defined by solving:

$$\frac{\partial \psi}{\partial t} = F'(\tilde{\varphi}_1)\psi, \quad \psi|_{t=0} = v, \quad (38)$$

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^* \psi^* = [(F'(\tilde{\varphi}_2))^* \tilde{\varphi}^*]' \psi - C^* V_o^{-1} C \psi, \quad (39)$$

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)v = V_b^{-1}v - \psi^*|_{t=0}. \quad (40)$$

If we had $\varphi = \tilde{\varphi}_1 = \tilde{\varphi}_2$, $\mathcal{H}(\varphi)$ becomes the Hessian of the cost function in the original DA problem, it is symmetric and positive definite if u is a minimum of $J(u)$. The equation is often referred as the 'second order' adjoint (Le Dimet et al., 2002).

As above, we assume that $E(\delta u) \approx 0$, and we consider the following approximations

$$R(\tilde{\varphi}_1) \approx R(\bar{\varphi}), \quad R^*(\varphi) \approx R^*(\bar{\varphi}), \quad [(F'(\tilde{\varphi}_2))^* \tilde{\varphi}^*]' \approx [(F'(\bar{\varphi}))^* \bar{\varphi}^*]'. \quad (41)$$

Posterior Covariance via Hessian

The exact error equation (??) is approximated as follows

$$\mathcal{H}(\bar{\varphi})\delta u = V_b^{-1}\xi_b + R(\bar{\varphi})^* C^* V_o^{-1}\xi_o, \quad (42)$$

where

$$\mathcal{H}(\cdot) = V_b^{-1} + R^*(\cdot)(C^* V_o^{-1} C - [(F'(\cdot))^* \bar{\varphi}^*]') R(\cdot). \quad (43)$$

Now, we express δu :

$$\delta u = \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1}\xi_b + R(\bar{\varphi})^* C^* V_o^{-1}\xi_o),$$

and obtain an approximate expression for the **posterior error covariance**

$$\mathcal{V}_1 = \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1} + R^*(\bar{\varphi})V_o^{-1}R(\bar{\varphi}))\mathcal{H}^{-1}(\bar{\varphi}) = \mathcal{H}^{-1}(\bar{\varphi})H(\bar{\varphi})\mathcal{H}^{-1}(\bar{\varphi}), \quad (44)$$

where $H(\bar{\varphi})$ is the Hessian of the cost function J_1 computed at $\theta = \bar{\varphi}$.

Other approximations of the posterior covariance:

$$\mathcal{V}_2 = \mathcal{H}^{-1}(\bar{\varphi}), \quad \mathcal{V}_3 = H^{-1}(\bar{\varphi}). \quad (45)$$

Posterior Covariance : "Effective" Estimates

To suppress the linearization errors, the 'effective' inverse Hessian may be used for estimating the analysis error covariance (see Gejadze et al., 2011):

$$V_{\delta u} = E [H^{-1}(\varphi)] . \quad (46)$$

The same is true for the posterior error covariance $\mathcal{V}_{\delta u}$:

$$\mathcal{V}_{\delta u} = E [\mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) H(\varphi) \mathcal{H}^{-1}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)] .$$

First, we substitute a possibly asymmetric and indefinite operator $\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)$ by $\mathcal{H}(\varphi)$:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_1^e = E [\mathcal{H}^{-1}(\varphi) H(\varphi) \mathcal{H}^{-1}(\varphi)] . \quad (47)$$

Next, by assuming $H(\varphi)\mathcal{H}^{-1}(\varphi) \approx I$ we get

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_2^e = E [\mathcal{H}^{-1}(\varphi)] . \quad (48)$$

Finally, by assuming $\mathcal{H}^{-1}(\varphi) \approx H^{-1}(\varphi)$ we obtain yet another approximation

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_3^e = E [H^{-1}(\varphi)] . \quad (49)$$

Numerical Example

$\varphi(x, t)$ is governed by the 1D Burgers equation with a nonlinear viscous term :

$$\frac{\partial \varphi}{\partial t} + \frac{1}{2} \frac{\partial(\varphi^2)}{\partial x} = \frac{\partial}{\partial x} \left(\nu(\varphi) \frac{\partial \varphi}{\partial x} \right), \quad (50)$$

$$\varphi = \varphi(x, t), \quad t \in (0, T), \quad x \in (0, 1),$$

with the Neumann boundary conditions

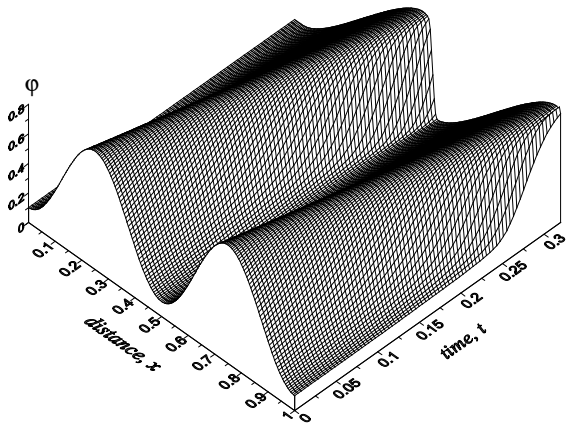
$$\frac{\partial \varphi}{\partial x} \Big|_{x=0} = \frac{\partial \varphi}{\partial x} \Big|_{x=1} = 0 \quad (51)$$

and the viscosity coefficient

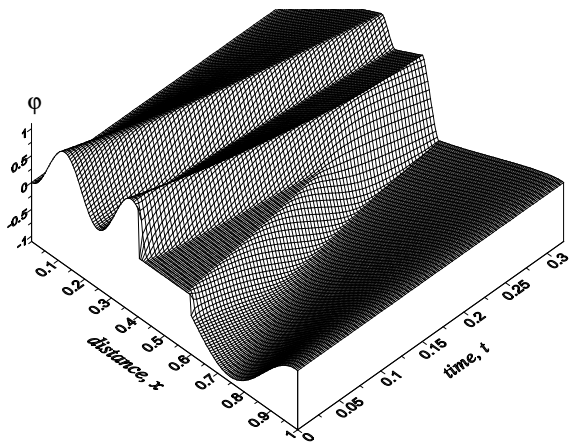
$$\nu(\varphi) = \nu_0 + \nu_1 \left(\frac{\partial \varphi}{\partial x} \right)^2, \quad \nu_0, \nu_1 = \text{const} > 0. \quad (52)$$

Two initial conditions $u^t = \varphi^t(x, 0)$ are considered (case A and case B),

Numerical Example : Cas A



Numerical Example : Cas B

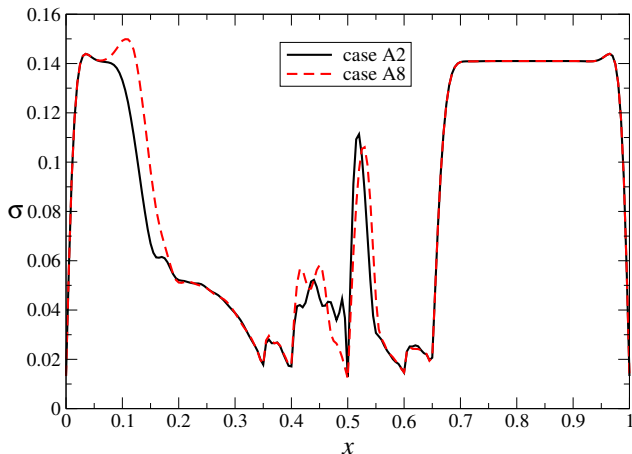


Numerical Example : Squared Riemann distance

$$\mu(A, B) = \left(\sum_{i=1}^M \ln^2 \gamma_i \right)^{1/2}.$$

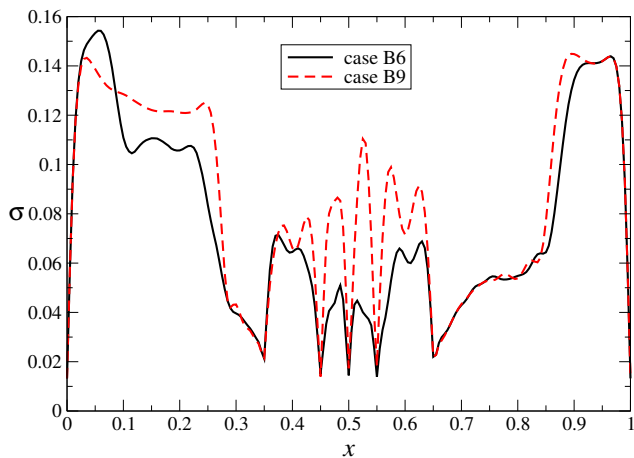
Case	$\mu^2(\mathcal{V}_3, \hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2, \hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1, \hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_3^e, \hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2^e, \hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1^e, \hat{\mathcal{V}})$
A1	3.817	3.058	4.738	2.250	1.418	1.151
A2	17.89	18.06	21.50	2.535	1.778	1.602
A5	5.832	5.070	5.778	3.710	2.886	2.564
A7	20.21	19.76	22.24	4.290	3.508	3.383
A8	1.133	0.585	1.419	1.108	0.466	0.246
A9	20.18	20.65	24.52	2.191	1.986	1.976
A10	10.01	8.521	8.411	3.200	2.437	2.428
B1	7.271	6.452	6.785	2.852	1.835	1.476
B2	16.42	14.89	14.70	15.61	14.11	13.77
B3	9.937	10.70	17.70	4.125	3.636	3.385
B4	6.223	5.353	11.50	2.600	1.773	1.580
B5	10.73	9.515	9.875	4.752	3.178	2.530
B6	6.184	4.153	8.621	4.874	2.479	1.858

The reference mean deviation $\hat{\sigma}(x)$ (related to $\hat{\nu}$). Cases A2, A8.

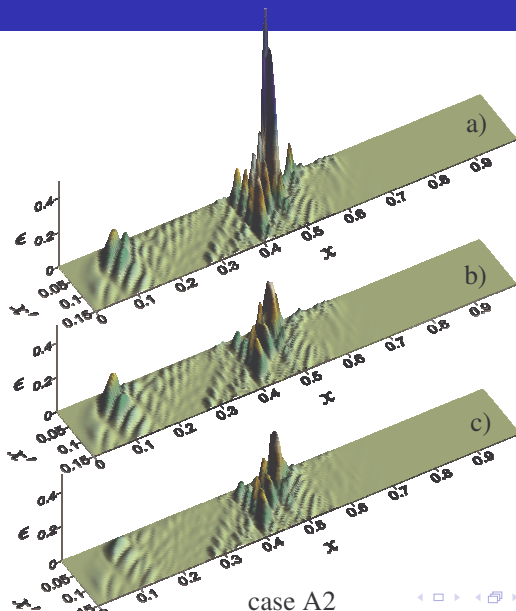


The mean deviation vector σ is defined as follows: $\sigma(i) = \mathcal{V}^{1/2}(i, i)$.

The reference mean deviation $\hat{\sigma}(x)$ (related to $\hat{\nu}$). Cases B6, B9.

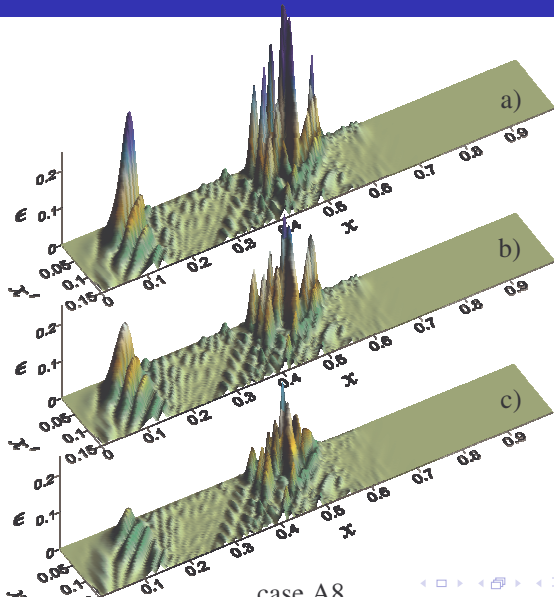


Absolute errors in the correlation matrix: ϵ_3 , ϵ_3^e , ϵ_1^e (case A2)

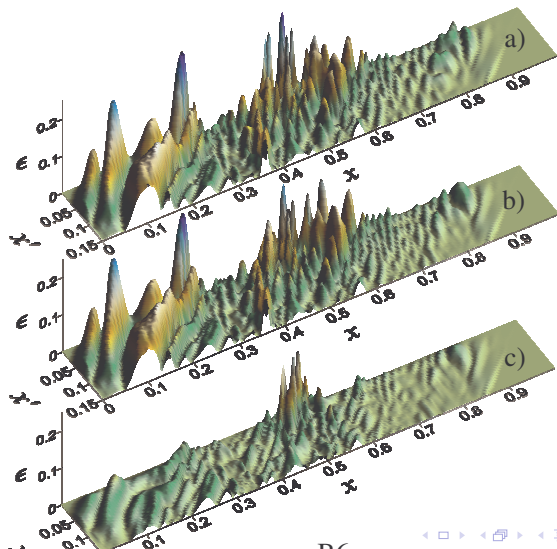


case A2

Absolute errors in the correlation matrix: ϵ_3 , ϵ_3^e , ϵ_1^e (case A8)



Absolute errors in the correlation matrix: ϵ_3 , ϵ_3^e , ϵ_1^e (case B6)



- Variational and Bayesian approaches of DA lead to the minimization of the same function
- For Error Estimation we obtain two different concepts
 - Analysis Error Covariance for the Variational Approach
 - Posterior Covariance for the Bayesian Approach
- In the linear case the covariances coincide
- In the nonlinear case strong discrepancies can occur.
- Algorithms for the estimation and the approximation of these covariances are proposed.

Gejadze, I., Shutyayev, V., Le Dimet, F.-X. **Analysis error covariance versus posterior covariance in variational data assimilation problems.** *Q.J.R.Meteorol. Soc.* (2013).