Assimilation des Observations et Traitement des Incertitudes en Météorologie

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Purpose of assimilation : reconstruct as accurately as possible the state of the atmospheric or oceanic flow, using all available appropriate information. The latter essentially consists of

- The observations proper, which vary in nature, resolution and accuracy, and are distributed more or less regularly in space and time.

- The physical laws governing the evolution of the flow, available in practice in the form of a discretized, and necessarily approximate, numerical model.

- ‘Asymptotic’ properties of the flow, such as, *e*. *g*., geostrophic balance of middle latitudes. Although they basically are necessary consequences of the physical laws which govern the flow, these properties can usefully be explicitly introduced in the assimilation process.

Difficultés spécifiques :

- Il y a beaucoup plus d'information dans les observations distribuées sur 12 ou 24 heures que dans les observations effectuées à un instant donné $\Rightarrow$ nécessité de prendre en compte l'évolution temporelle du système. *Dynamique est non triviale* !

- Dimensions numériques. *Centre Européen pour les Prévisions Météorologiques à Moyen Terme* (Reading, GB).

  Dimension du vecteur d'état du modèle : $n \approx 2{,}3\ 10^8$

  Nombre d'observations (valeurs scalaires) utilisées sur 24 heures : $1{,}8\ 10^7$

Both observations and 'model' are affected with some uncertainty $\Rightarrow$ uncertainty on the estimate.

For some reason, uncertainty is conveniently described by probability distributions (Jaynes, E. T., 2007, *Probability Theory: The Logic of Science*, Cambridge University Press).

Assimilation is a problem in bayesian estimation.

Determine the conditional probability distribution for the state of the system, knowing everything we know (unambiguously defined if a prior probability distribution is defined; see Tarantola, 2005).

Bayesian estimation

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

Data vector $\boldsymbol{z}$, belonging to *data space* $\mathcal{D}$ ($\dim \mathcal{D} = m$), available.

$$\boldsymbol{z} = \boldsymbol{F}(\boldsymbol{x}, \boldsymbol{\zeta}) \qquad (1)$$

where $\boldsymbol{\zeta}$ is a random element representing the uncertainty on the data (or, more precisely, on the link between the data and the unknown state vector).

For example

$$\boldsymbol{z} = \boldsymbol{\Gamma}\boldsymbol{x} + \boldsymbol{\zeta}$$

Bayesian estimation (continued)

Probability that $x = \xi$ for given ξ ?

$$x = \xi \quad \Rightarrow \quad z = F(\xi, \zeta) \tag{1}$$

$$P(x = \xi \mid z) = P[z = F(\xi, \zeta)] \; / \int_{\xi'} P[z = F(\xi', \zeta)]$$

Unambiguously defined iff, for any ζ, there is at most one ξ such that (1) is verified.

$\Leftrightarrow$ data contain information, either directly or indirectly, on any component of x
$\Leftrightarrow$ rank$DF/Dx = n \;\Rightarrow\; m \geq n$. We set $p \equiv m - n$

Determinacy condition.

Bayesian estimation impossible in practice because

- It is impossible to explicitly describe a probability distribution in a space with dimension even as low as $n \approx 10^3$, not to speak of the dimension $n \approx 10^{6\text{-}8}$ of present NWP models.

- Probability distribution of errors affecting data is very poorly known (errors in assimilating model).

How to define in practice a probability distribution in a very large dimensional space ?

Only possible way seems to be through a finite ensemble, meant to sample the distribution.

$\Rightarrow$ *Ensemble methods* (used also for prediction)

Typical size of ensembles in present meteorological applications : *O*(10-100)

Exist at present in two forms

- *Ensemble Kalman Filter* (*EnKF*).
- *Particle filters.*

Bayesian Linear Estimation (still at the basis of a large part of 'real life' assimilation algorithms)

Data in the form

$$z = \boldsymbol{\Gamma x} + \zeta$$

where $\boldsymbol{\Gamma}$ is a known (mxn)-matrix, and ζ is 'error'

Determinacy condition : rank$\boldsymbol{\Gamma} = n$

If $\zeta \sim \mathcal{N}[\boldsymbol{\mu}, \boldsymbol{S}]$, then $P(\boldsymbol{x} \mid z) = \mathcal{N}[\boldsymbol{x}^a, \boldsymbol{P}^a]$ with

$$\boldsymbol{x}^a \equiv (\boldsymbol{\Gamma}^{\mathrm{T}} \boldsymbol{S}^{-1} \boldsymbol{\Gamma})^{-1} \boldsymbol{\Gamma}^{\mathrm{T}} \boldsymbol{S}^{-1} [z - \boldsymbol{\mu}]$$
$$\boldsymbol{P}^a \equiv (\boldsymbol{\Gamma}^{\mathrm{T}} \boldsymbol{S}^{-1} \boldsymbol{\Gamma})^{-1}$$

Even is the error ζ is not gaussian, the estimate $\boldsymbol{x}^a$ still has significance. It is the variance-minimizing, or *Best Linear Unbiased Estimate* (*BLUE*) of $\boldsymbol{x}$ from $\boldsymbol{z}$. $\boldsymbol{P}^a$ is then the covariance matrix of the associated error, averaged on all possible values of ζ (it is no more, as in the gaussian case, the covariance matrix of a probability distribution conditioned to the data $\boldsymbol{z}$).

Variational form.

$\boldsymbol{x}^a$ minimizes following scalar *objective function*, defined on state space $\mathcal{S}$

$$\mathcal{J}(\xi) \equiv (1/2)\,[\Gamma\xi - (z-\mu)]^{\mathrm{T}}\, S^{-1}\, [\Gamma\xi - (z-\mu)]$$

$\boldsymbol{S}$ being a covariance matrix, the quadratic form $\boldsymbol{z}\, \boldsymbol{S}^{-1}\, \boldsymbol{z}$ is a proper (*i. e.*, coordinate-invariant) scalar product on data space $\mathcal{D}$, called the *Mahalanobis scalar product* associated with $\boldsymbol{S}$.

- Observation vector at time k

$$y_k = H_k x_k + \varepsilon_k \qquad\qquad k = 0, \ldots, K$$
$$E(\varepsilon_k) = 0 \quad ; \quad E(\varepsilon_k \varepsilon_j^{\mathrm{T}}) \equiv R_k \, \delta_{kj}$$

- Evolution equation

$$x_{k+1} = M_k x_k + \eta_k \qquad\qquad k = 0, \ldots, K\text{-}1$$
$$E(\eta_k) = 0 \quad ; \quad E(\eta_k \eta_j^{\mathrm{T}}) \equiv Q_k \, \delta_{kj}$$
$$E(\eta_k \varepsilon_j^{\mathrm{T}}) = 0$$

- Background estimate at time 0

$$x^b{}_0 = x_0 + \zeta^b{}_0$$
$$E(\zeta^b{}_0) = 0 \quad ; \quad E(\zeta^b{}_0 \, \zeta^b{}_0{}^{\mathrm{T}}) \equiv P^b{}_0$$
$$E(\zeta^b{}_0 \varepsilon_k{}^{\mathrm{T}}) = 0 \quad ; \quad E(\zeta^b{}_0 \eta_k{}^{\mathrm{T}}) = 0$$

Sequential assimilation assumes the form of *Kalman filter*

Background x^b_k and associated error covariance matrix P^b_k known

- Analysis step

$$x^a_k = x^b_k + P^b_k H_k^{\mathrm{T}} [H_k P^b_k H_k^{\mathrm{T}} + R_k]^{-1} (y_k - H_k x^b_k)$$
$$P^a_k = P^b_k - P^b_k H_k^{\mathrm{T}} [H_k P^b_k H_k^{\mathrm{T}} + R_k]^{-1} H_k P^b_k$$

- Forecast step

$$x^b_{k+1} = M_k x^a_k$$
$$P^b_{k+1} = M_k P^a_k M_k^{\mathrm{T}} + Q_k$$

Kalman Filter produces at every step k the *Best Linear Unbiased Estimate* (*BLUE*) of real unknown state x_k from all data prior to k. In addition, it achieves bayesian estimation when the errors $(\varepsilon_k, \eta_k, \zeta^b_0)$ are globally gaussian.

Variational form

If model error is ignored

$$\xi_0 \rightarrow$$

$$\mathcal{J}(\xi_0) = (1/2)\,(x_0{}^b - \xi_0)^{\mathrm{T}}\,[P_0{}^b]^{-1}\,(x_0{}^b - \xi_0) + (1/2)\,\Sigma_k[y_k - H_k\xi_k]^{\mathrm{T}}\,R_k{}^{-1}\,[y_k - H_k\xi_k]$$

(*strong constraint*)

If model error is taken into account

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

$$\begin{aligned}\mathcal{J}(\xi_0, \xi_1, \ldots, \xi_K) = {} & (1/2)\,(x_0{}^b - \xi_0)^{\mathrm{T}}\,[P_0{}^b]^{-1}\,(x_0{}^b - \xi_0) \\ & + (1/2)\,\Sigma_{k=0,\ldots,K}[y_k - H_k\xi_k]^{\mathrm{T}}\,R_k{}^{-1}\,[y_k - H_k\xi_k] \\ & + (1/2)\,\Sigma_{k=0,\ldots,K-1}[\xi_{k+1} - M_k\xi_k]^{\mathrm{T}}\,Q_k{}^{-1}\,[\xi_{k+1} - M_k\xi_k]\end{aligned}$$

(*weak constraint*)

Ensemble Kalman filter (*EnKF*, Evensen, 1994, Anderson, …)

Uncertainty is represented, not by a covariance matrix, but by an ensemble of point estimates in state space which are meant to sample the conditional probability distribution for the state of the system (dimension $N \approx O(10\text{-}100)$).

Ensemble is evolved in time through the full model, which eliminates any need for linear hypothesis as to the temporal evolution.

How to update predicted ensemble with new observations ?

Predicted ensemble at time t : $\{x^b_i\}$, $i = 1, \ldots, N$

Observation vector at same time : $y = Hx + \varepsilon$

- Gaussian approach

Produce sample of probability distribution for real observed quantity Hx

$y_i = y - \varepsilon_i$

where ε_i is distributed according to probability distribution for observation error ε.

Then use Kalman formula to produce sample of 'analysed' states

$$x^a_i = x^b_i + P^b H^T [HP^bH^T + R]^{-1} (y_i - Hx^b_i) , \qquad i = 1, \ldots, N \qquad (2)$$

where P^b is 'exact' (not sample) covariance matrix of predicted ensemble $\{x^b_i\}$.

In the linear case, and if errors are gaussian, (2) achieves Bayesian estimation, in the sense that $\{x^a_i\}$ is a sample of conditional probability distribution for x, given all data up to time t.

Ensemble Kalman Filter

- In the forecast phase, ensemble is evolved according to model equations (with possible inclusion of random noise to simulate effect of model errors).

- In the analysis phase, ensemble is updated according to procedure that has just been described (equation 2 on previous slide), the matrix P^b being now the sample covariance matrix of the background ensemble $\{x^b_i\}$.

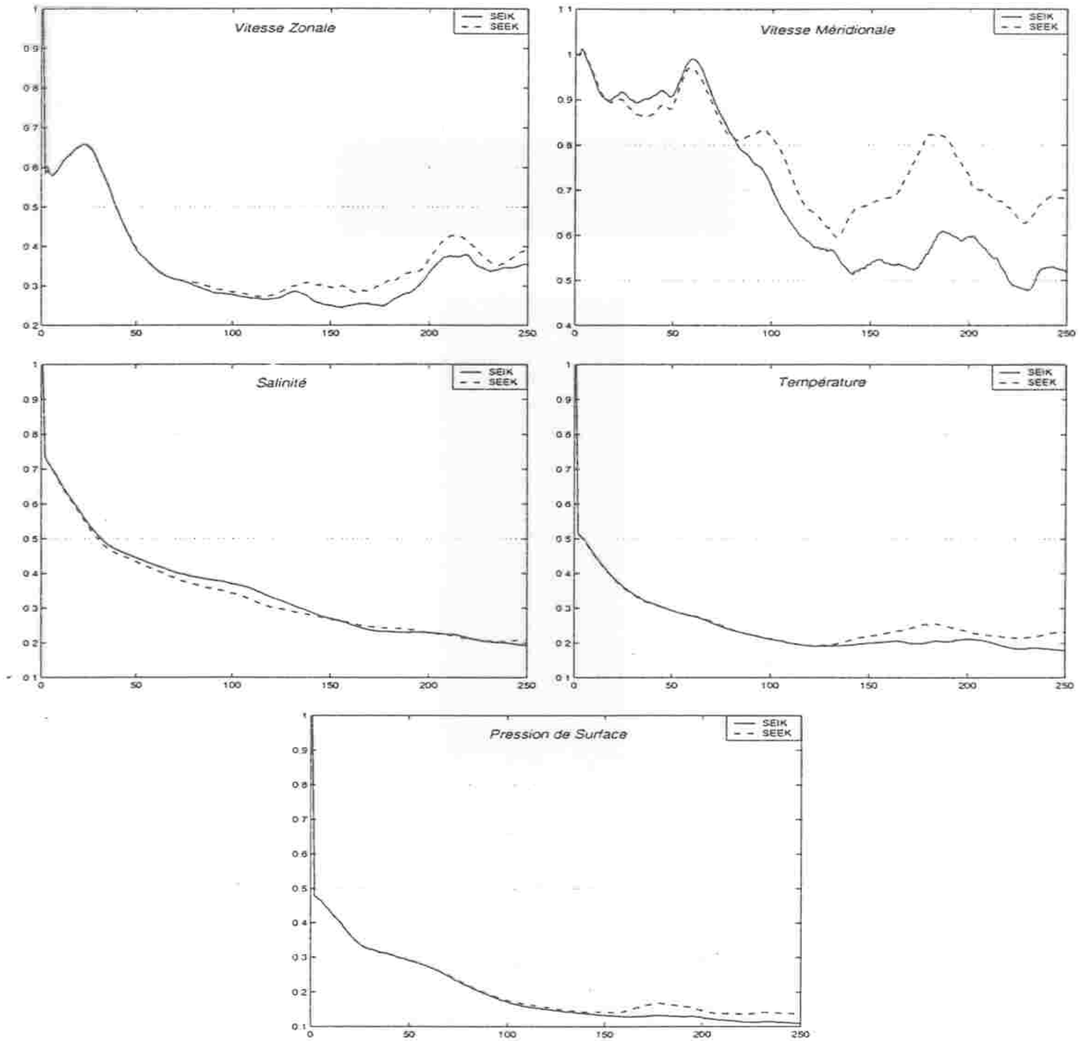


FIG. 5.2 – *Evolution dans le temps de la RRMS des filtres SEIK et SEEK*

I. Hoteit, Doctoral Dissertation, Université Joseph Fourier, Grenoble, 2001

Ensemble Kalman Filter (continuation)

Even if dynamical model is nonlinear, forecast phase is bayesian (provided errors are independent in time). Analysis phase will not in general because of

- Nonlinearity of observation operator

- Non-gaussianity of background and/or observation errors (convergence, but not in general to bayesian estimate, when $N \rightarrow \infty$, F. Le Gland)

- Sampling effects in P^b (but convergence to bayesian estimate in the gaussian case when $N \rightarrow \infty$, F. Le Gland)

Ensemble Kalman Filter is very commonly used in meteorological and oceanographical applications. Many variants exist, some of which do not require perturbations of the observations, but require previous analysis about which ensemble is evolved (Ensemble Transform Kalman Filter, ETKF, Bishop *et al.*, 2001)

A general problem is *collapse of ensemble* in analysis phase. If dimension of ensemble is small (O(10-50)), spread of ensembles decreases in analysis. Since large ensembles are costly, *ad hoc* procedures are used to alleviate that effect :

- *Covariance inflation*. The spread of the ensemble about its mean is increased by an empirically determined numerical factor.

- '*Localization*'. Sampling effects in the background error covariance matrix create unrealistic correlations over large distances in physical space. These unrealistic correlations seem to contribute to the collapse of ensembles. They are eliminated by element-wise multiplication of the sample covariance matrix by another positive-definite matrix with compact support in physical space.

- *Double ensembles*. Two ensembles are evolved in parallel, the background error covariance matrix for updating either ensemble being determined from the other ensemble.

Origin of ensemble collapse ?

Ensemble collapse generally attributed to the fact that ensemble size N is small in comparison with state dimension n (10-100 against $10^{6\text{-}7}$). In particular, corrections made by analysis on background are limited to a space with dimension N.

Descamps (2007) has observed that collapse occurs in small dimension (n=1) with N>n. Sampling effects in the background error covariance matrix play a role.

Buehner (Canadian Meteorological Service, 2008) has performed clean comparison between 4D-variational assimilation and EnKF. For same numerical cost, quality of ensuing forecasts is very similar.

Exact bayesian estimation

Particle filters

Predicted ensemble at time t : $\{x^b{}_n, n = 1, \ldots, N\}$, each element with its own weight (probability) $P(x^b{}_n)$
Observation vector at same time : $y = Hx + \varepsilon$

Bayes' formula

$$P(x^b{}_n \mid y) \sim P(y \mid x^b{}_n)\, P(x^b{}_n)$$

Defines updating of weights

Remarks

- Many variants exist, including possible 'regeneration' of ensemble elements
- If errors are correlated in time, explicit computation of $P(y \mid x^b{}_n)$ will require using past data that are correlated with y (same remark for evolution of ensemble between two observation times)

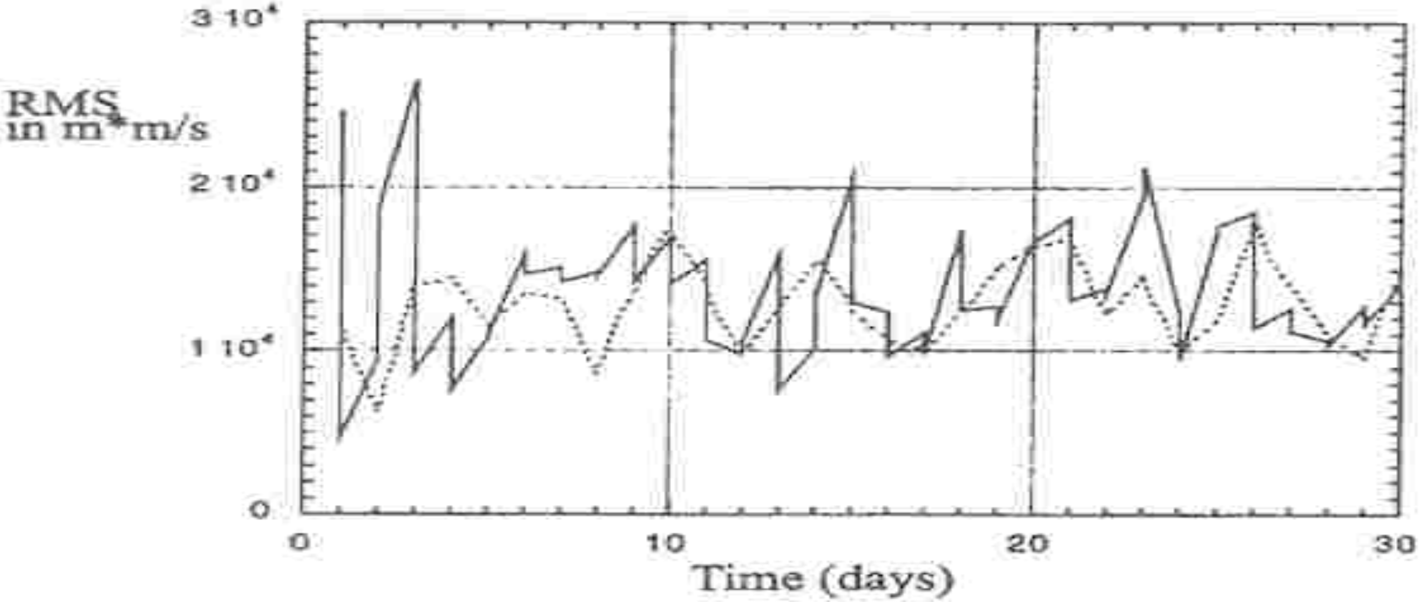


FIG. 12. Comparison of rms error ($m^2 s^{-1}$) between ensemble mean and independent observations (dotted line) and the std dev in the ensemble (solid line). The excellent agreement shows that the SIRF is working correctly.

van Leeuwen, 2003, *Mon. Wea. Rev.*, **131**, 2071-2084

According to Snyder, dimensions required by particle filters for meteorological and oceanographical applications are prohibitive.

Possibility of developing more efficient algorithms ? The question is open.

Exact bayesian estimation

Acceptation-rejection

Bayes' formula

$$f(x) \equiv \mathrm{P}(x \mid y) = P(y \mid x)\, P(x) \,/\, P(y)$$

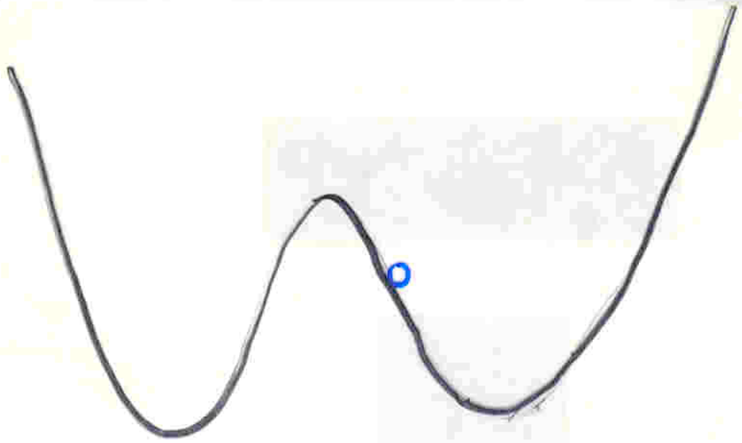
defines probability density function for x.

Construct sample of that pdf as follows.

Draw randomly couple $(\xi, \psi) \in \mathcal{S} \times [0, \sup f]$.

Keep ξ if $\psi < f(\xi)$. ξ is then distributed according to $f(x)$.

Miller, Carter and Blue, Tellus, 1999



$$\frac{d^2x}{dt^2} = -\frac{d\phi}{dx} - \alpha \frac{dx}{dt} + \text{Noise}$$

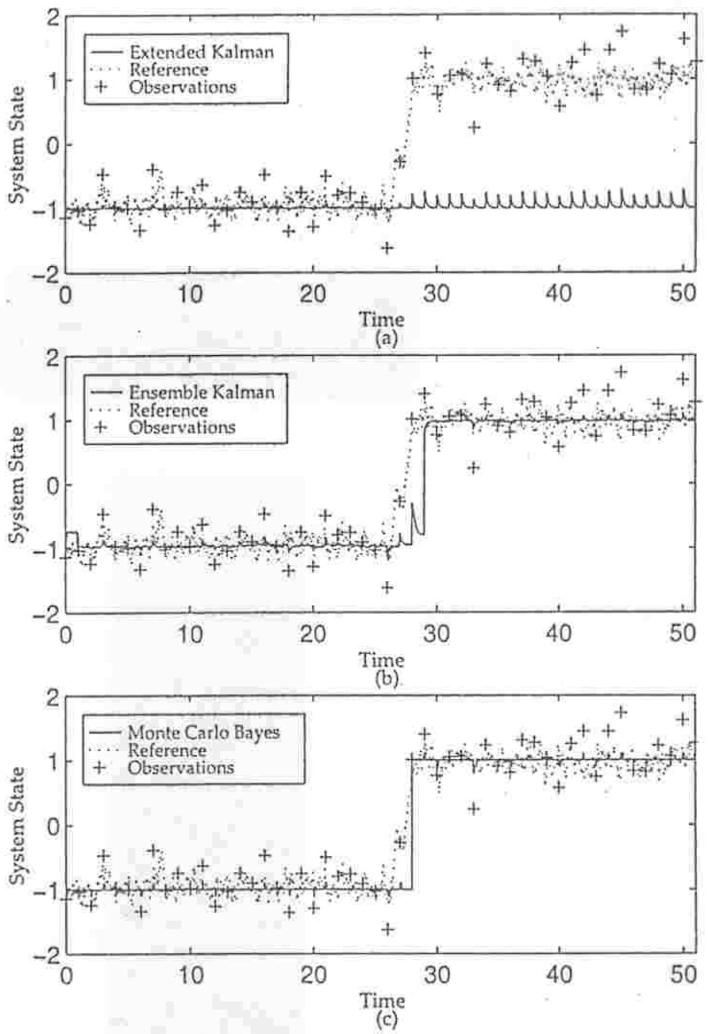


Fig. 4. Comparison of the EKF, the ensemble method and nonlinear filtering by Bayes' theorem for the double-well problem.

Miller, Carter and Blue, 1999, *Tellus*, **51A**, 167-194

Acceptation-rejection

Seems costly.

Requires capability of permanently interpolating probability distribution defined by finite sample to whole state space.

Time-correlated Errors

Sequential methods, whether of the Kalman or particle filter type cannot be Bayesian if errors are not independent in time. This extends to 'smoothers', in which updating by new observation is performed, not only on estimate at observation time, but also on estimates at previous times.

Time-correlated Errors

Example of time-correlated observation errors

$z_1 = x + \zeta_1$

$z_2 = x + \zeta_2$

$E(\zeta_1) = E(\zeta_2) = 0$; $E(\zeta_1{}^2) = E(\zeta_2{}^2) = s$; $E(\zeta_1 \zeta_2) = 0$

BLUE of x from z_1 and z_2 gives equal weights to z_1 and z_2.

Additional observation then becomes available

$z_3 = x + \zeta_3$

$E(\zeta_3) = 0$; $E(\zeta_3{}^2) = s$; $E(\zeta_1 \zeta_3) = cs$; $E(\zeta_2 \zeta_3) = 0$

BLUE of x from (z_1, z_2, z_3) has weights in the proportion $(1,\ 1{+}c,\ 1)$

Time-correlated Errors (continuation 1)

Example of time-correlated model errors

Evolution equation

` $x_{k+1} = x_k + \eta_k$ $\quad E(\eta_k^{\,2}) = q$

Observations

$y_k = x_k + \varepsilon_k\,,$ $\quad k = 0, 1, 2$ $\quad E(\varepsilon_k^{\,2}) = r$, errors uncorrelated in time

Sequential assimilation. Weights given to y_0 and y_1 in analysis at time 1 are in the ratio $r/(r+q)$. That ratio will be conserved in sequential assimilation. All right if model errors are uncorrelated in time.

Assume $E(\eta_0\eta_1) = cq$

Weights given to y_0 and y_1 in estimation of x_2 are in the ratio

$$\rho = \frac{r - qc}{r + q + qc}$$

Time-correlated Errors (continuation 2)

Moral. If data errors are correlated in time, it is not possible to discard observations as they are used while preserving optimality of the estimation process. In particular, if model error is correlated in time, all observations are liable to be reweighted as assimilation proceeds.

Variational assimilation can take time-correlated errors into account.

Example of time-correlated observation errors. Global covariance matrix

$$\mathcal{R} = (R_{kk'} = E(\varepsilon_k \varepsilon_{k'}^{\mathrm{T}}))$$

Objective function

$$\xi_0 \in \mathcal{S} \rightarrow$$

$$\mathcal{J}(\xi_0) = (1/2)\,(x_0^{\,b} - \xi_0)^{\mathrm{T}}\,[P_0^{\,b}]^{-1}\,(x_0^{\,b} - \xi_0) + (1/2)\,\Sigma_{kk'}[y_k - H_k \xi_k]^{\mathrm{T}}\,[\mathcal{R}^{-1}]_{kk'}\,[y_{k'} - H_{k'} \xi_{k'}]$$

where $[\mathcal{R}^{-1}]_{kk'}$ is the kk'-subblock of global inverse matrix $\mathcal{R}^{-1}$.

Similar approach for time-correlated model error.

Time-correlated Errors (continuation 3)

Time correlation of observational error has been introduced by ECMWF (Järvinen *et al.*, 1999) in variational assimilation of high-frequency surface pressure observations (correlation originates in that case in representativeness error).

Identification and quantification of temporal correlation of errors, especially model errors ?

Q. Is it possible to have at the same time the advantages of both ensemble estimation and variational assimilation (propagation of information both forward and backward in time, and, more importantly, possibility to take temporal dependence into account) ?

Same approach that underlies EnKF. Perturb all data (model and observations) according to the corresponding error probability distribution and, for each set of perturbed data, perform a variational assimilation. In the linear and gaussian case, this will produce a sample of conditional probability distribution for the orbit of the system, subject to the data.

Still to be done.

Works by Liu C. and A. Trevisan

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