

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 5

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Best Linear Unbiased Estimate

State vector 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

$$x^b = x + \zeta^b$$

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

$$y = Hx + \varepsilon$$

H is known linear observation operator.

Assume probability distribution is known for the couple (ζ^b, ε) .

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

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

Best Linear Unbiased Estimate (continuation 2)

Apply formulæ for Optimal Interpolation

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

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

\mathbf{x}^a is the *Best Linear Unbiased Estimate (BLUE)* of \mathbf{x} from \mathbf{x}^b and \mathbf{y} .

Equivalent set of formulæ

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

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

Vector $\mathbf{d} \equiv \mathbf{y} - H\mathbf{x}^b$ is *innovation vector*

Matrix $\mathbf{K} \equiv P^b H^T [HP^b H^T + R]^{-1} = P^a H^T R^{-1}$ is *gain matrix*.

If probability distributions are *globally gaussian*, *BLUE* achieves bayesian estimation, in the sense that $P(\mathbf{x} | \mathbf{x}^b, \mathbf{y}) = \mathcal{N}[\mathbf{x}^a, \mathbf{P}^a]$.

Best Linear Unbiased Estimate (continuation 3)

H can be any linear operator

Example : (scalar) satellite observation

$\mathbf{x} = (x_1, \dots, x_n)^T$ temperature profile

Observation $y = \sum_i h_i x_i + \varepsilon = \mathbf{H}\mathbf{x} + \varepsilon$, $\mathbf{H} = (h_1, \dots, h_n)$, $E(\varepsilon^2) = r$
 Background $\mathbf{x}^b = (x_1^b, \dots, x_n^b)^T$, error covariance matrix $P^b = (p_{ij}^b)$

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

$$[\mathbf{H} P^b \mathbf{H}^T + R]^{-1} (y - \mathbf{H}\mathbf{x}^b) = (y - \sum_i h_i x_i^b) / (\sum_{ij} h_i h_j p_{ij}^b + r) \equiv \mu \quad \text{scalar !}$$

- - $P^b = p^b \mathbf{I}_n$ $x_i^a = x_i^b + p^b h_i \mu$
- - $P^b = \text{diag}(p_{ii}^b)$ $x_i^a = x_i^b + p_{ii}^b h_i \mu$
- General case $x_i^a = x_i^b + \sum_j p_{ij}^b h_j \mu$

Each level i is corrected, not only because of its own contribution to the observation, but because of the contribution of the other levels to which its background error is correlated.

Best Linear Unbiased Estimate (continuation 4)

Variational form of the *BLUE*

BLUE x^a minimizes following scalar *objective function*, defined on state space

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

- $$\begin{aligned} \mathcal{J}(\xi) &\equiv (1/2) (x^b - \xi)^T [P^b]^{-1} (x^b - \xi) + (1/2) (y - H\xi)^T R^{-1} (y - H\xi) \\ &\equiv \mathcal{J}_b \quad + \quad \mathcal{J}_o \end{aligned}$$

‘3D-Var’

Can easily, and heuristically, be extended to the case of a nonlinear observation operator H .

Used operationally in USA, Australia, China, ...

Best Linear Unbiased Estimate (continuation 4)

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Question. How to introduce temporal dimension in estimation process ?

- Logic of Optimal Interpolation and of *BLUE* can be extended to time dimension.
- But we know much more than just temporal correlations. We know explicit dynamics.

Real (unknown) state vector at time k (in format of assimilating model) x_k . Belongs to state space \mathcal{S} ($\dim \mathcal{S} = n$)

Evolution equation

$$x_{k+1} = M_k(x_k) + \eta_k$$

M_k is (known) model, η_k is (unknown) model error

Sequential Assimilation

- Assimilating model is integrated over period of time over which observations are available. Whenever model time reaches an instant at which observations are available, state predicted by the model is updated with new observations. In the jargon of the trade, *Optimal Interpolation* designates an algorithm for sequential assimilation in which the matrix P^b is constant with time, and *3D-Var* an algorithm in which, in addition, the analysis x^a is obtained through a variational algorithm.

Variational Assimilation

- Assimilating model is globally adjusted to observations distributed over observation period. Achieved by minimization of an appropriate scalar *objective function* measuring misfit between data and sequence of model states to be estimated.

Sequential Assimilation

Optimal Interpolation

- Observation vector at time k

$$y_k = H_k x_k + \varepsilon_k \quad k = 0, \dots, K$$

$$E(\varepsilon_k) = 0 \quad ; \quad E(\varepsilon_k \varepsilon_j^T) = R_k \delta_{kj}$$

H_k linear

- Evolution equation

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

Optimal Interpolation (2)

At time k , background x_k^b and associated error covariance matrix P^b known, assumed to be independent of k .

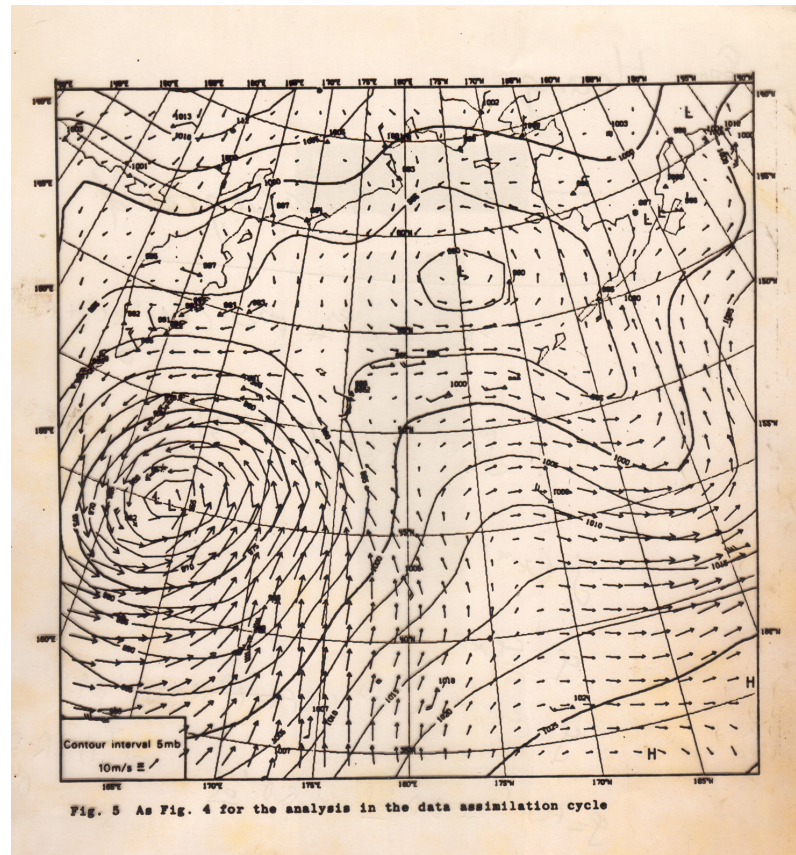
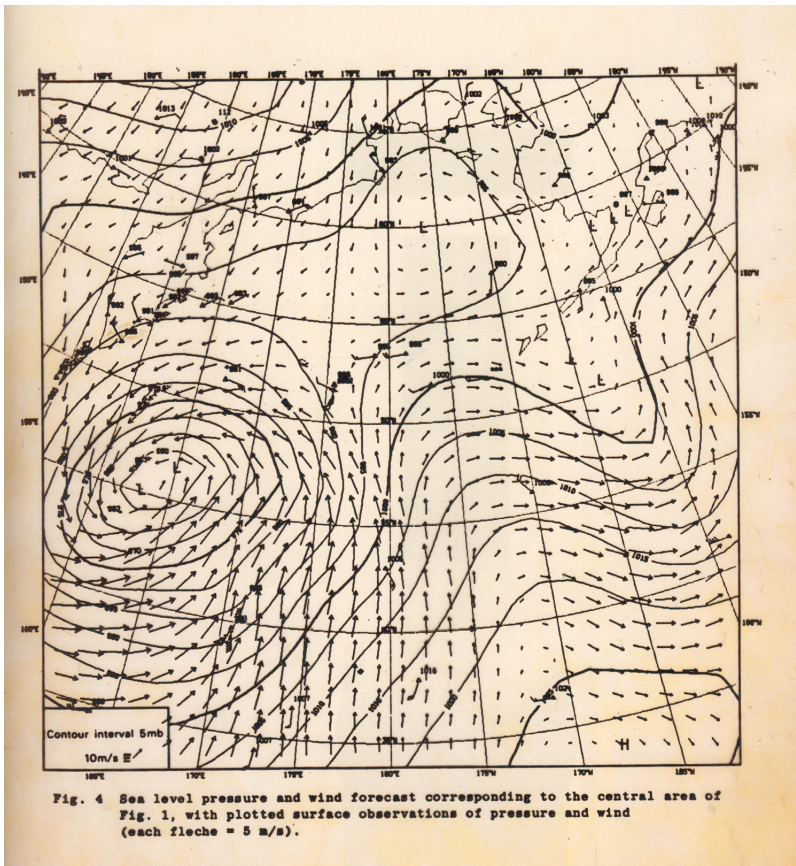
- Analysis step

$$x_k^a = x_k^b + P^b H_k^T [H_k P^b H_k^T + R_k]^{-1} (y_k - H_k x_k^b)$$

In *3D-Var*, x_k^a is obtained by (iterative) minimization of associated objective function

- Forecast step

$$x_{k+1}^b = M_k(x_k^a)$$



After A. Lorenc

Sequential Assimilation. *Kalman Filter*

- Observation vector at time k

$$y_k = H_k x_k + \varepsilon_k \quad k = 0, \dots, K$$

$$E(\varepsilon_k) = 0 \quad ; \quad E(\varepsilon_k \varepsilon_j^T) = R_k \delta_{kj}$$

H_k linear

- Evolution equation

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

$$E(\eta_k) = 0 \quad ; \quad E(\eta_k \eta_j^T) = Q_k \delta_{kj}$$

M_k linear

- $E(\eta_k \varepsilon_j^T) = 0$ (errors uncorrelated in time)

At time k , background x_k^b and associated error covariance matrix P_k^b known

- Analysis step

$$x_k^a = x_k^b + P_k^b H_k^T [H_k P_k^b H_k^T + R_k]^{-1} (y_k - H_k x_k^b)$$

$$P_k^a = P_k^b - P_k^b H_k^T [H_k P_k^b H_k^T + R_k]^{-1} H_k P_k^b$$

- Forecast step

$$x_{k+1}^b = M_k x_k^a$$

$$P_{k+1}^b = E[(x_{k+1}^b - x_{k+1}^b)(x_{k+1}^b - x_{k+1}^b)^T] = E[(M_k x_k^a - M_k x_k - \eta_k)(M_k x_k^a - M_k x_k - \eta_k)^T]$$

$$= M_k E[(x_k^a - x_k)(x_k^a - x_k)^T] M_k^T - E[\eta_k (x_k^a - x_k)^T] - E[(x_k^a - x_k) \eta_k^T] + E[\eta_k \eta_k^T]$$

$$= M_k P_k^a M_k^T + Q_k$$

At time k , background x_k^b and associated error covariance matrix P_k^b known

- Analysis step

$$x_k^a = x_k^b + P_k^b H_k^T [H_k P_k^b H_k^T + R_k]^{-1} (y_k - H_k x_k^b)$$
$$P_k^a = P_k^b - P_k^b H_k^T [H_k P_k^b H_k^T + R_k]^{-1} H_k P_k^b$$

- Forecast step

$$x_{k+1}^b = M_k x_k^a$$
$$P_{k+1}^b = M_k P_k^a M_k^T + Q_k$$

Kalman filter (KF, Kalman, 1960)

Must be started from some initial estimate (x_0^b, P_0^b)

If all operators are linear, and if errors are uncorrelated in time, Kalman filter produces at time k the *BLUE* x_k^b (resp. x_k^a) of the real state x_k from all data prior to (resp. up to) time k , plus the associated estimation error covariance matrix P_k^b (resp. P_k^a).

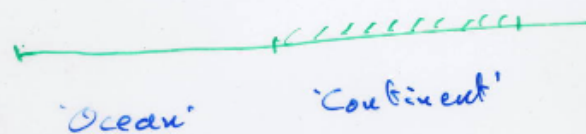
If in addition errors are gaussian, the corresponding conditional probability distributions are the respective gaussian distributions $\mathcal{N}[x_k^b, P_k^b]$ and $\mathcal{N}[x_k^a, P_k^a]$.

A didactic example (Ghil et al.)

Barotropic model

$$\begin{cases} \frac{\partial \varphi}{\partial t} + \operatorname{div}(\varphi \underline{U}) = 0 \\ \frac{\partial \underline{U}}{\partial t} + \operatorname{grad}(\varphi + \frac{1}{2} \underline{U}^2) + \underline{k} \times (\underline{f} + \xi) \underline{U} = 0 \end{cases}$$

One dimension, periodic



Linearized (conserves energy)

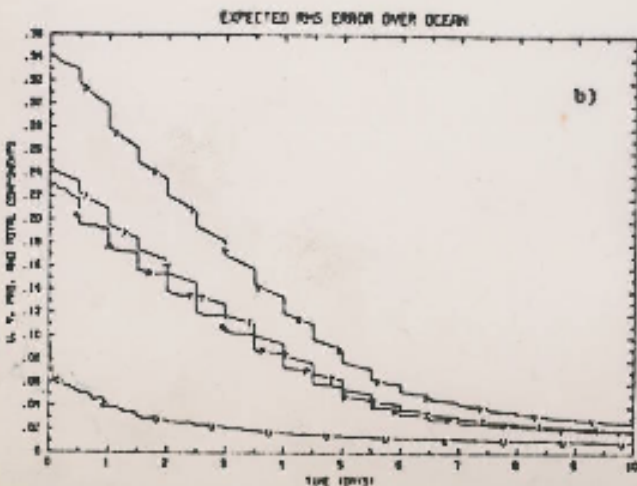
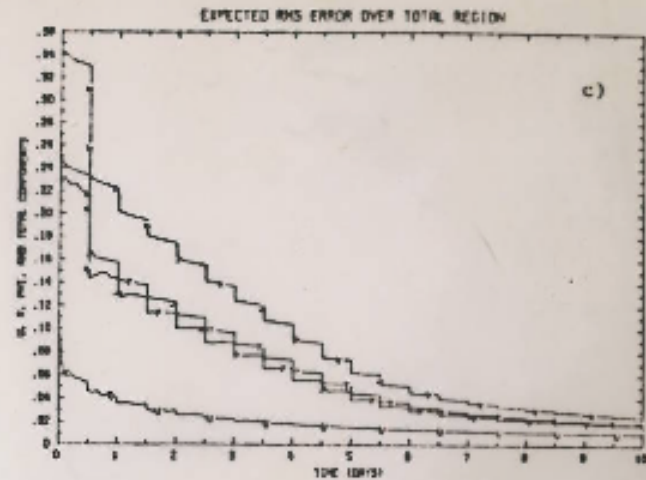
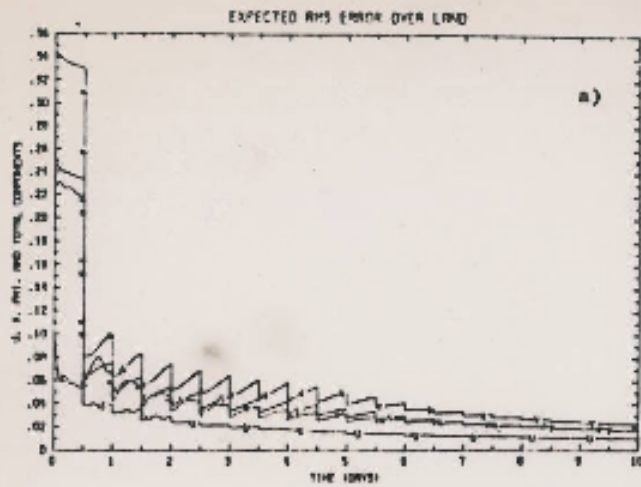
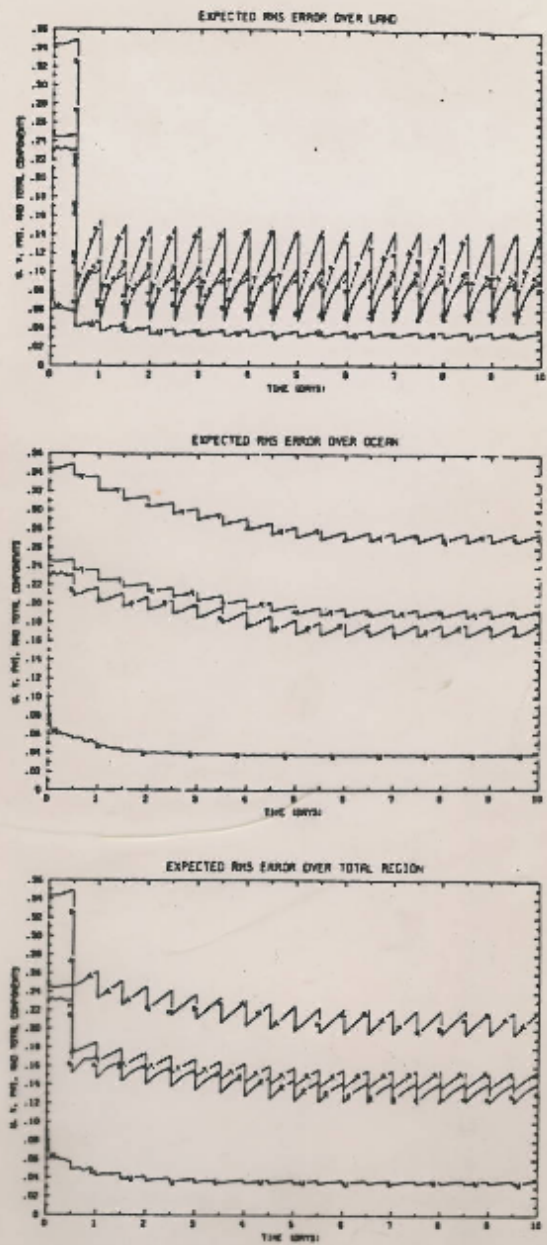


Fig. 2

The components of the total expected rms error (Erms), $(\text{trace } P_k)^{1/2}$, in the estimation of solutions to the stochastic-dynamic system $k(Y, H)$, with Y given by (3.6) and $H \approx (I \ 0)$. System noise is absent, $Q = 0$. The filter used is the standard K-B filter (2.11) for the model.

a) Erms over land; b) Erms over the ocean; c) Erms over the entire L-domain

In each one of the figures, each curve represents one component of the total Erms error. The curves labelled U, V, and P represent the u component, v component and ϕ component, respectively. They are found by summing the diagonal elements of P_k which correspond to u, v, and ϕ , respectively, dividing by the number of terms in the sum, and then taking the square root. In a) the summation extends over land points only, in b) over ocean points only, and in c) over the entire L-domain. The vertical axis is scaled in such a way that 1.0 corresponds to an Erms error of v_{max} for the U and V curves, and of ϕ_0 for the P curve. The observational error level is 0.089 for the U and V curves, and 0.080 for the P curve. The curves labelled T represent the total Erms error over each region. Each T curve is a weighted average of the corresponding U, V, and P curves, with the weights chosen in such a way that the T curve measures the error in the total energy $u^2 + v^2 + \phi^2/4$, conserved by the system (3.1). The observational noise level for the T curve is then 0.088. Notice the immediate error decrease over land and the gradual decrease over the ocean. The total estimation error tends to zero.



M. Ghil *et al.*

Fig. 6 This figure and the following ones show the properties of the estimated algorithms (2.11) in the presence of system noise, $Q \neq 0$. This figure gives the Erms estimation error, and is homologous to Fig. 2. Notice the sharper increase of error over land between synoptic times, and the convergence of each curve to a periodic, nonzero function.

Nonlinearities ?

Model is usually nonlinear, and observation operators (satellite observations) tend more and more to be nonlinear.

- Analysis step

$$x_k^a = x_k^b + P_k^b H_k'{}^T [H_k' P_k^b H_k'{}^T + R_k]^{-1} [y_k - H_k(x_k^b)]$$
$$P_k^a = P_k^b - P_k^b H_k'{}^T [H_k' P_k^b H_k'{}^T + R_k]^{-1} H_k' P_k^b$$

- Forecast step

$$x_{k+1}^b = M_k(x_k^a)$$
$$P_{k+1}^b = M_k' P_k^a M_k'{}^T + Q_k$$

Extended Kalman Filter (EKF, heuristic !)

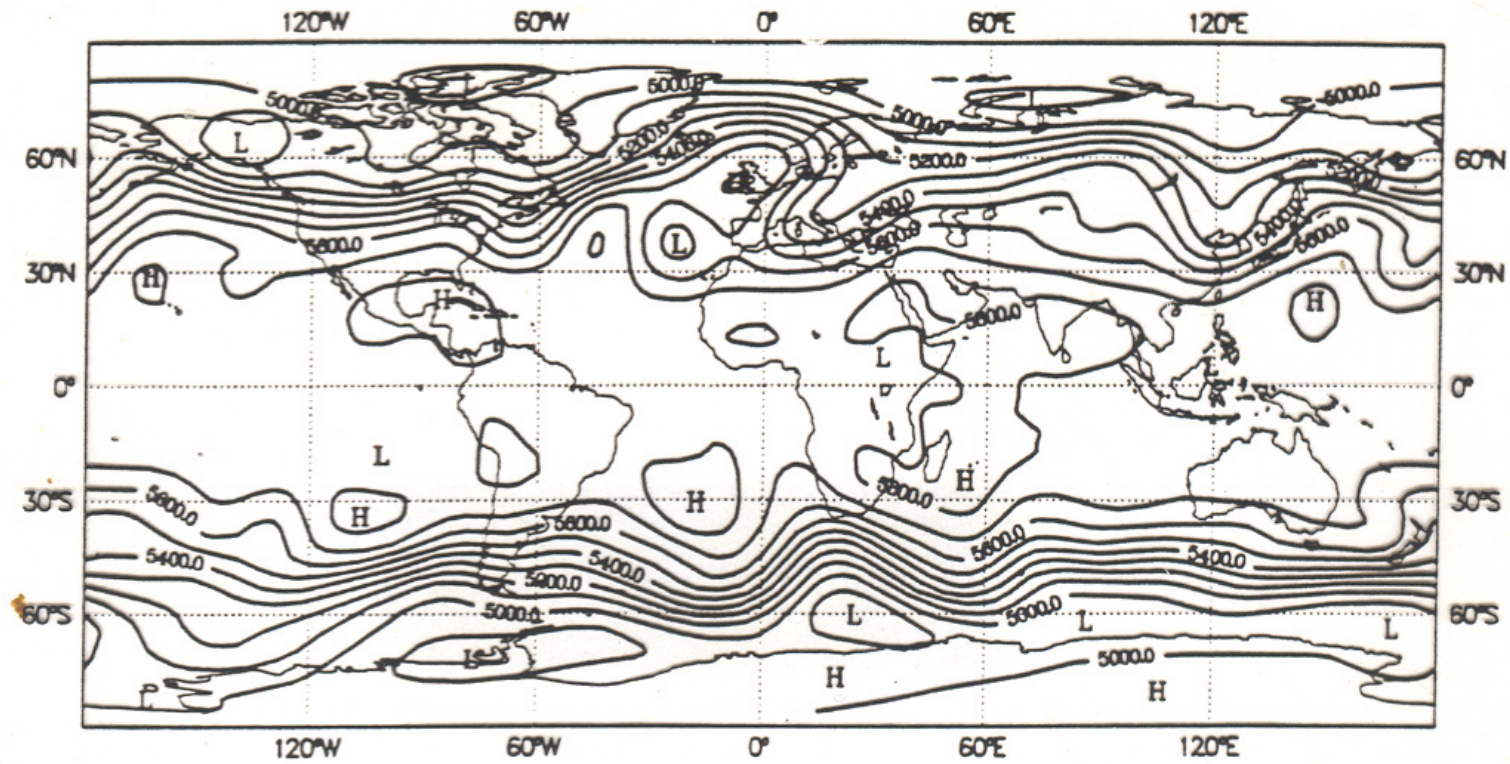
Costliest part of computation

$$P_{k+1}^b = M_k P_k^a M_k^T + Q_k$$

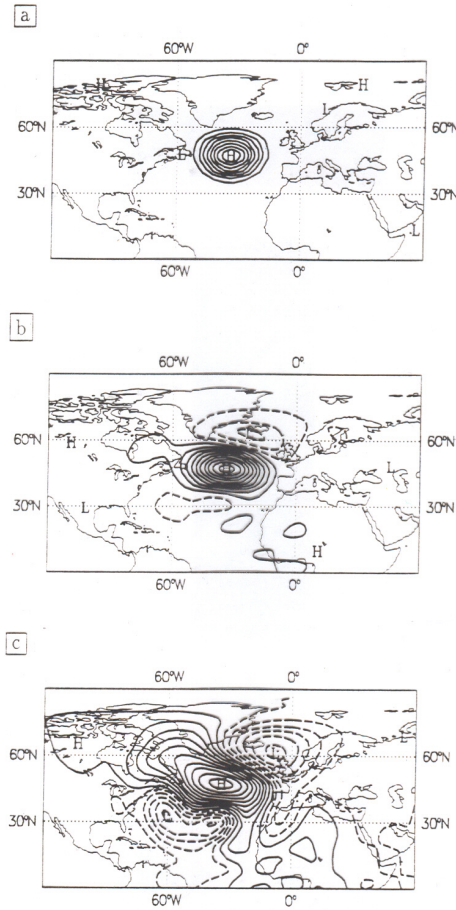
Multiplication by M_k = one integration of the model between times k and $k+1$.

Computation of $M_k P_k^a M_k^T \approx 2n$ integrations of the model

Need for determining the temporal evolution of the uncertainty on the state of the system is the major difficulty in assimilation of meteorological and oceanographical observations



Analysis of 500-hPa geopotential for 1 December 1989, 00:00 UTC (ECMWF, spectral truncation T21, unit *m*. After F. Bouttier)



Temporal evolution of the 500-hPa geopotential autocorrelation with respect to point located at 45N, 35W. From top to bottom: initial time, 6- and 24-hour range. Contour interval 0.1. After F. Bouttier.

Two solutions :

- *Low-rank filters*

Use low-rank covariance matrix, restricted to modes in state space on which it is known, or at least assumed, that a large part of the uncertainty is concentrated (this requires the definition of a norm on state space).

Reduced Rank Square Root Filters (RRSQRT, Heemink)

Singular Evolutive Extended Kalman Filter (SEEK, Pham)

....

Reduced Rank Square Root Kalman Filter (RRSQRT, Verlaan and Heemink, 1997)

A covariance matrix P can be written as

$$P = S S^T$$

where the column vectors of S are the (orthogonal) principal components (eigenvectors) of P (the modulus of each vector is the square root of the associated eigenvalue).

The principle of *RRSQRT* is to restrict the background error covariance matrix P^b to $r \ll n$ principal components, thereby approximating P^b by (the time index k is dropped)

$$P^b \approx S^b S^{bT}$$

where S^b has dimensions $n \times r$.

RRSQRT (continuation 1)

Setting $\Psi \equiv (HS^b)^T$, the gain matrix of the Kalman filter and the analysis error covariance matrix respectively become

$$K = S^b \Psi (\Psi^T \Psi + R)^{-1}$$

and

$$P^a = S^a S^{aT}$$

with

$$S^a = S^b [I_r - \Psi (\Psi^T \Psi + R)^{-1} \Psi^T]^{1/2}$$

RRSQRT (continuation 2)

In the prediction phase, the column vectors of S^a are evolved by the tangent linear model (an evolution of a perturbed state by the full model is also possible). If a model error is to be introduced, that is done by reducing the order r of S^a to $r-q$, and introducing q new column vectors meant to represent the model error.

Orthogonality of the column vectors is lost in the prediction, and has to be reestablished. And, even if process is started from dominant column vectors, that dominance may of course be lost.

Advantages : in addition to reduced computational cost, numerical errors are reduced when dealing with square root covariance matrices, as done here, than with full matrices (better conditioning).

Singular Evolutive Extended Kalman Filter (SEEK, Pham, 1996)

Based on the fact that, because of the linearity of Kalman Filter, the rank of the covariance matrix P^a or P^b cannot increase in either the update or the model evolution. SEEK performs a linear filter starting from a low rank P^b_0 , and so runs the exact Kalman filter in the case of a perfect model. The algorithmic implementation takes advantage of the rank-deficiency of the covariance matrix. The rank of the latter is conserved (or decreased), but the subspace spanned by the directions with non-zero error evolves, in both the update and the dynamic evolution.

In case model error is present, corresponding covariance matrix Q_k is projected onto the directions with non-zero error (this is of course an approximation).

Singular Evolutive Interpolated Kalman Filter (SEIK, Pham, 2001)

Non-trivial extension of SEEK to nonlinear model or observation operators. Rank deficiency is now forced.

Second solution :

- *Ensemble filters*

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

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

Ensemble Kalman Filter (EnKF, Evensen, Anderson, ...)

How to update predicted ensemble with new observations ?

Predicted ensemble at time k : $\{x^b_l\}$, $l = 1, \dots, L$

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

- Gaussian approach

Produce sample of probability distribution for real observed quantity Hx

$$y_l = y - \varepsilon_l$$

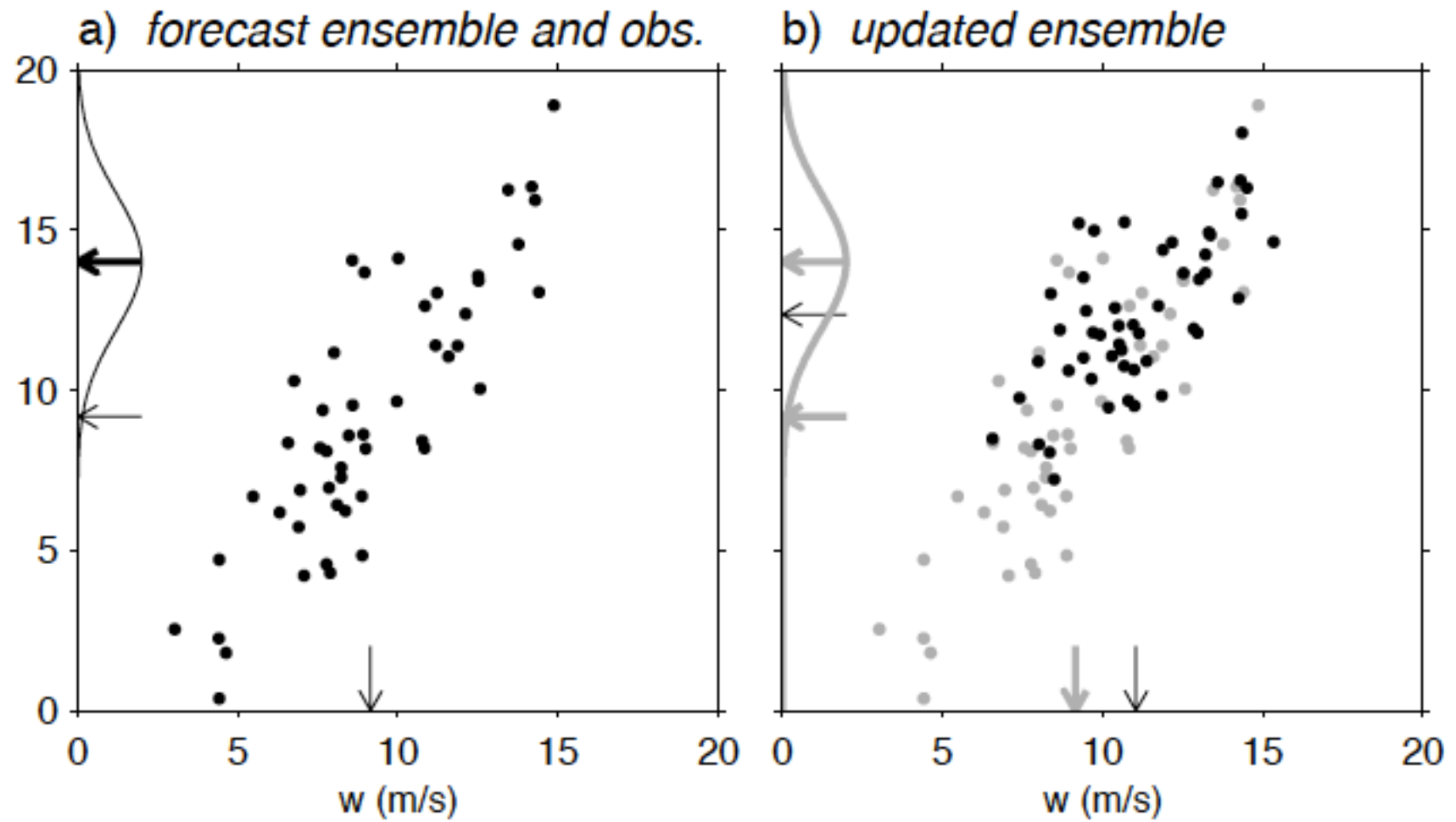
where ε_l is distributed according to probability distribution for observation error ε .

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

$$x^a_l = x^b_l + P^b H^T [HP^b H^T + R]^{-1} (y_l - Hx^b_l), \quad l = 1, \dots, L \quad (2)$$

where P^b is the sample covariance matrix of predicted ensemble $\{x^b_l\}$.

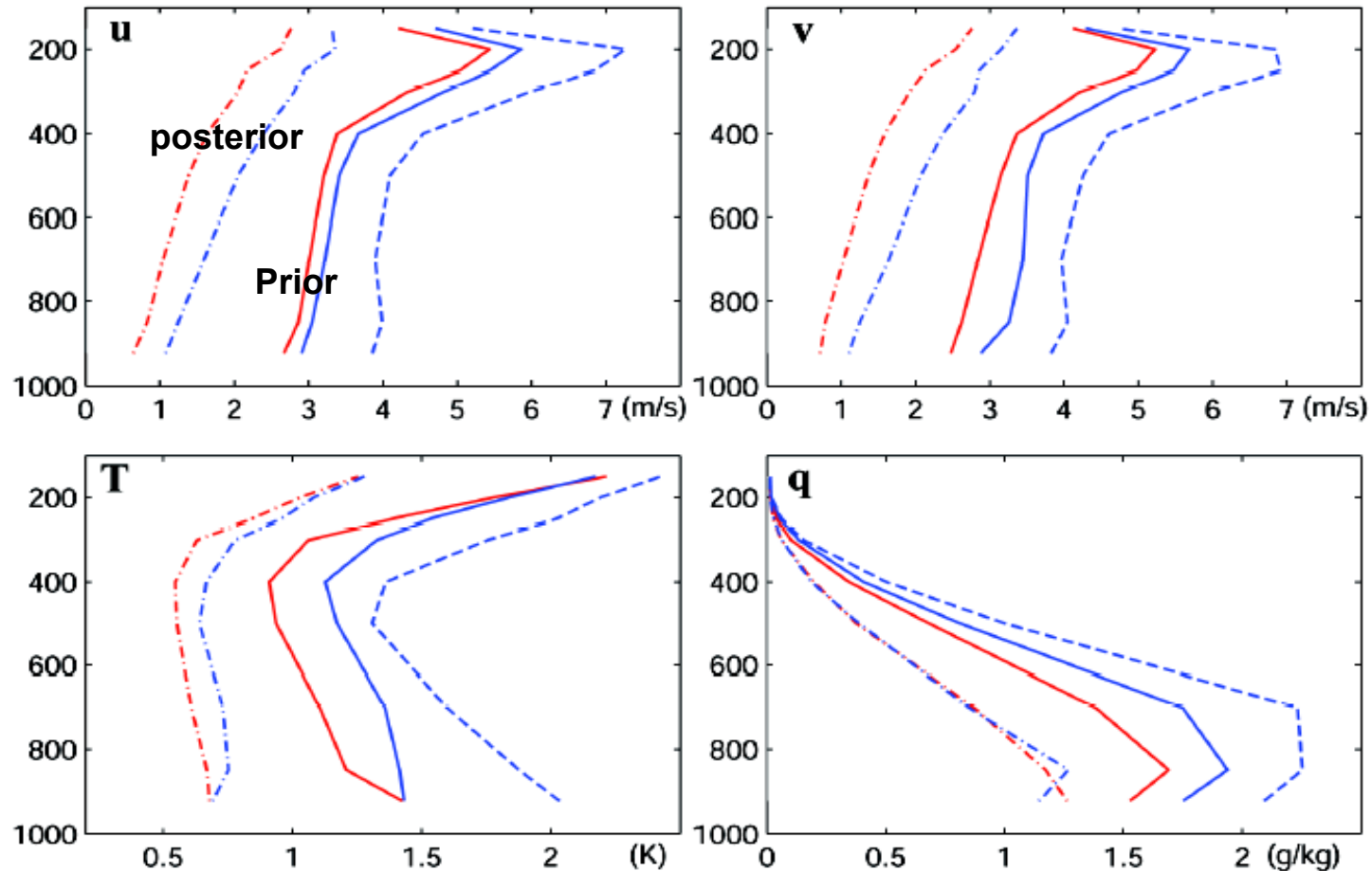
Remark. In case of Gaussian errors, if P^b was exact covariance matrix of background error, (2) would achieve Bayesian estimation, in the sense that $\{x^a_l\}$ would be a sample of conditional probability distribution for x , given all data up to time k .



C. Snyder

Month-long Performance of EnKF vs. 3Dvar with WRF

— EnKF — 3DVar (prior, solid; posterior, dotted)



Better performance of EnKF than 3DVar also seen in both 12-h forecast and posterior analysis in terms of root-mean square difference averaged over the entire month

(Meng and Zhang 2007c, MWR, in review)

The case of a nonlinear observation operator ?

Predicted ensemble at time k : $\{\mathbf{x}^b_l\}$, $l = 1, \dots, L$

Observation vector at same time : $\mathbf{y} = H(\mathbf{x}) + \boldsymbol{\varepsilon}$ H nonlinear

Two possibilities

1. Take tangent linear approximation (as in Extended KF) and introduce jacobian H'
2. Come back to original formula

$$\mathbf{x}^a = E(\mathbf{x}) + C_{xy} [C_{yy}]^{-1} [\mathbf{y} - E(\mathbf{y})]$$

That formula does not require any other link between \mathbf{x} and \mathbf{y} than the one defined by the covariances matrices C_{xy} and C_{yy} .

Here, as shown on the occasion of the derivation of the *BLUE*, $E(\mathbf{x})$ is the background \mathbf{x}^b , and $\mathbf{y} - E(\mathbf{y})$ is the innovation $\mathbf{y} - H(\mathbf{x}^b)$

Solution. Compute C_{xy} and C_{yy} as sample covariances matrices of the ensembles $\{\mathbf{x}^b_l\}$ and $\{\mathbf{y}_l - H(\mathbf{x}^b_l)\}$, where the \mathbf{y}_l 's are, as before, the perturbed observations $\mathbf{y}_l = \mathbf{y} - \boldsymbol{\varepsilon}_l$.

But problems

- Collapse of ensemble for small ensemble size (less than a few hundred). Collapse originates in the fact that gain matrix $P^b H^T [HP^b H^T + R]^{-1}$ is nonlinear wrt background error matrix P^b , resulting in a systematic sampling effect. Solution : empirical ‘covariance inflation’.
- Spurious correlations appear at large geographical distances. Empirical ‘localization’ (see Gaspari and Cohn, 1999, *Q. J. R. Meteorol. Soc.*)
- In formula

$$x_l^a = x_l^b + P^b H^T [HP^b H^T + R]^{-1} (y_l - Hx_l^b) , \quad l = 1, \dots, L$$

P^b , which is covariance matrix of an L -size ensemble, has rank $L-1$ at most. This means that corrections made on ensemble elements are contained in a subspace with dimension $L-1$. Obviously very restrictive if $L \ll p$, $L \ll n$.

Houtekamer and Mitchell (1998) use two ensembles, the elements of each of which are updated with covariance matrix of other ensemble.

There exist many variants of Ensemble Kalman Filter

Ensemble Transform Kalman Filter (ETKF, Bishop et al., Mon. Wea. Rev., 2001)

Requires a prior ‘control’ analysis x_c^a , emanating from a background x_c^b . An ensemble is evolved about that control without explicit use of the observations (and without feedback to control)

More precisely, define $L \times L$ matrix T such that, given $P^b = ZZ^T$, then $P^a = ZTT^TZ^T$ (not trivial, but possible). Then the background deviations $x_l^b - x_c^b$ are transformed through $Z \rightarrow ZT$ into an ensemble of analysis deviations $x_l^a - x_c^a$.

(does not avoid collapse of ensembles)

Local Ensemble Transform Kalman Filter (LETKF, Hunt et al., Physica D, 2007)

Each gridpoint is corrected only through the use of neighbouring observations.

Other variants of Ensemble Kalman Filter

'Unscented' Kalman Filter (Wan and van der Merve, 2001, Wiley Publishing)

Weighted Kalman Filter (Papadakis *et al.*, 2010, *Tellus A*)

Inflation-free Ensemble Kalman Filters (Bocquet and Sakov, 2012, *Nonlin. Processes Geophys.*)

Bayesian properties of Ensemble Kalman Filter ?

Very little is known.

Le Gland *et al.* (2011). In the linear and gaussian case, the discrete pdf defined by the filter, in the limit of infinite sample size L , tends to the bayesian gaussian pdf.

No result for finite size (note that ensemble elements are not mutually independent)

In the nonlinear case, the discrete pdf tends to a limit which is in general not the bayesian pdf.

Situation still not entirely clear.

In any case, optimality always requires errors to be independent in time. In order to relax that constraint, it is necessarily to augment the state vector in the temporal dimension.