Validation

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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.

Validation must therefore aim primarily at determining, as far as possible, the accuracy with which assimilation reconstructs the state of the flow. In particular, if one wants to compare two different assimilation procedures, the ultimate test lies in the comparison of the accuracies with which those two procedures reconstruct the flow.

Now, the state of the flow is not perfectly known, and the output of an assimilation process is precisely meant to be the best possible estimate of that state. So there is a circular argument there.

But there is another aspect to evaluation of an assimilation process. Does the process make the best possible use of the available information ? This is totally distinct from the accuracy with which the process reconstructs the state of the flow. We will distinguish *numerical accuracy* from *optimality* (the property that the process makes the best possible use of the available information).

Objective validation of assimilation can only be statistical, and must be made against observations (or data) that are unbiased, and are affected by errors that are statistically independent of the errors affecting the data used in the assimilation.

Amplitude of forecast error, if estimated against observations that are really independent of observations used in assimilation, is an objective measure of accuracy of assimilation.

But neither the unbiasedness nor the ‘independence’ of the verifying observations can be objectively verified, at least within the world of data and assimilation. External knowledge must be used.

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, 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*.

Best Linear Unbiased Estimate (continuation 2)

Assume $E(\zeta^b) = 0$, $E(\boldsymbol{\varepsilon}) = 0$
Set $\boldsymbol{d} \equiv \boldsymbol{y} - H\boldsymbol{x}^b$ (innovation vector)

$$\boldsymbol{x}^a = \boldsymbol{x}^b - E(\zeta^b \boldsymbol{d}^{\mathrm{T}}) \, [E(\boldsymbol{d}\boldsymbol{d}^{\mathrm{T}})]^{-1} \, (\boldsymbol{y} - H\boldsymbol{x}^b)$$
$$\boldsymbol{P}^a = E(\zeta^b \zeta^{b\mathrm{T}}) - E(\zeta^b \boldsymbol{d}^{\mathrm{T}}) \, [E(\boldsymbol{d}\boldsymbol{d}^{\mathrm{T}})]^{-1} \, E(\boldsymbol{d}\zeta^{b\mathrm{T}})$$

Assume $E(\zeta^b \boldsymbol{\varepsilon}^{\mathrm{T}}) = 0$ (not restrictive). Set $E(\zeta^b \zeta^{b\mathrm{T}}) = \boldsymbol{P}^b$ (also often denoted $\boldsymbol{B}$), $E(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^{\mathrm{T}}) = \boldsymbol{R}$

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

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

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

Determination of the *BLUE* requires (at least apparently) the *a priori* specification of the expectation and covariance matrix, *i. e.* the statistical moments of orders 1 and 2 of the errors. The expectation is required for unbiasing the data in the first place.

Questions

- Is it possible to objectively evaluate the accuracy of an assimilation system ?

- Is it possible to objectively evaluate the first- and second-order statistical moments of the data errors, whose specification is required for determining the *BLUE* ?

- Is it possible to objectively determine whether an assimilation system is optimal (*i. e.*, in the case of the *BLUE*, whether it uses the correct error statistics) ?

- More generally, how to make the best of an assimilation system ?

$$x^b = x + \zeta^b$$
$$y = Hx + \varepsilon$$

The only combination of the data that is a function of only the error is the innovation vector

$$d = y - Hx^b = \varepsilon - H\zeta^b$$

(if H weakly nonlinear, $d = \varepsilon - H'\zeta^b$,where H' is local jacobian)

Innovation is the only objective source of information on errors. Now innovation is a combination of background and observation errors, while determination of the *BLUE* requires explicit knowledge of the statistics of both observation and background errors.

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

Innovation alone will never be sufficient to determine the required statistics.

With hypotheses made above

$$E(d) = 0 \quad ; \quad E(dd^{\mathrm{T}}) = HP^bH^{\mathrm{T}} + R$$

Possible to check statistical *consistency* between *a priori* assumed and *a posteriori* observed statistics of innovation.

Consistency, which will be considered now, is a different quality than either accuracy or optimality.

Consider assimilation scheme of the form

$$\boldsymbol{x}^a = \boldsymbol{x}^b + K(\boldsymbol{y} - H\boldsymbol{x}^b) \qquad (1)$$

with any (*i. e.* not necessarily optimal) gain matrix K.

(1) $\Leftrightarrow$ if data are perfect, then so is the estimate $\boldsymbol{x}^a$.

Take more general approach.

Data assumed to consist of a vector z, belonging to data space $\mathcal{D}$ ($\dim\mathcal{D} = m$), in the form

$$z = \Gamma x + \zeta$$

where Γ is a known (mxn)-matrix, and ζ an unknown 'error'

For instance

$$z = \begin{pmatrix} x^b = x + \zeta^b \\ y = Hx + \varepsilon \end{pmatrix}$$

which corresponds to

$$\Gamma = \begin{pmatrix} I_n \\ H \end{pmatrix} \qquad\qquad \zeta = \begin{pmatrix} \zeta^b \\ \varepsilon \end{pmatrix}$$

Look for estimated state vector x^a of the form

$$x^a = \alpha + Az$$

subject to

- invariance in change of origin in state space $\Rightarrow$ $A\Gamma = I_m$

- quadratic estimation error $E[(x^a_i - x_i)^2]$ minimum for any component x_i.

Solution

$\boldsymbol{x}^a = (\Gamma^T S^{-1}\Gamma)^{-1}\, \Gamma^T S^{-1} [\boldsymbol{z} - \boldsymbol{\mu}]$

$P^a \equiv E[(\boldsymbol{x}^a - \boldsymbol{x})\, (\boldsymbol{x}^a - \boldsymbol{x})^T] = (\Gamma^T S^{-1}\Gamma)^{-1}$

where $\boldsymbol{\mu} \equiv E(\zeta)$, $S \equiv E(\zeta' \zeta'^T)$, $\zeta' \equiv \zeta - \boldsymbol{\mu}$

Requires (at least apparently) *a priori* explicit knowledge of $E(\zeta)$ and $E(\zeta' \zeta'^T)$

Unambiguously defined iff rank$\Gamma = n$. *Determinacy condition*. Requires $m \geq n$.
We shall set $m = n + p$.

Invariant in any invertible linear change of coordinates, either in data or state space.

In case ζ is gaussian, $\zeta = \mathcal{N}[\boldsymbol{\mu}, S]$, *BLUE* achieves bayesian estimation in the sense that $P(\boldsymbol{x} \mid \boldsymbol{z}) = \mathcal{N}[\boldsymbol{x}^a, P^a]$

If determinacy condition is verified, it is always possible to decompose data vector $\boldsymbol{z}$ into

$$\boldsymbol{x}^b = \boldsymbol{x} + \boldsymbol{\zeta}^b$$
$$\boldsymbol{y} = \boldsymbol{H}\boldsymbol{x} + \boldsymbol{\varepsilon}$$

with $E(\boldsymbol{\zeta}^b) = 0$; $E(\boldsymbol{\varepsilon}) = 0$; $E(\boldsymbol{\varepsilon}\boldsymbol{\zeta}^{b\mathrm{T}}) = 0$

$\boldsymbol{x}^a$ is the same estimate (*BLUE*) as before, *viz.*,

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

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

Data have been put in the format

$$x^b = x + \zeta^b$$
$$d = y - Hx^b = \varepsilon - H\zeta^b$$

through linear invertible transformation

Assume that, through further linear invertible transformation, I put data in format

$$u = Cx + \beta$$
$$v = \gamma$$

where C is invertible, and β and γ are functions of the original error ζ only

$$u = Bx^b + Dd$$
$$v = Ex^b + Fd$$

with necessarily $EC = 0 \Rightarrow E = 0$

Then $v = Fd$, with F invertible

Conclusion. Innovation is much more than observation-minus-background difference, it is what one obtains by eliminating the unknowns from the data, independently of how elimination is performed.

Conclusion. Innovation is much more than observation-minus-background difference, it is what one obtains by eliminating the unknowns from the data, independently of how elimination is performed.

Extends to nonlinear situations.

One particular form of elimination

Linear analysis (whether optimal or not)

$$\boldsymbol{x}^a = \boldsymbol{x} + \zeta^a$$

Data-minus-analysis difference

$$\delta \equiv z - \Gamma \boldsymbol{x}^a = -\Gamma \zeta^a + \zeta$$

Data-minus-analysis difference is in one-to-one correspondance with the innovation.

It is exactly equivalent to compute statistics on either the innovation d or on the *DmA* difference δ.

For perfectly consistent system (*i. e.*, system that uses the exact error statistics):

$$E(\boldsymbol{d}) = 0 \ (\Leftrightarrow \ E(\boldsymbol{\delta}) = 0)$$

Any systematic bias in either the innovation vector or the DmA difference is the signature of an inappropriately taken into account bias in either the background or the observation (or both).

$$E[(\boldsymbol{x}^b\text{-}\boldsymbol{x}^a)(\boldsymbol{x}^b\text{-}\boldsymbol{x}^a)^{\mathrm{T}}] \ = \ \boldsymbol{P}^b - \boldsymbol{P}^a$$
$$E[(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}^a)(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}^a)^{\mathrm{T}}] \ = \ \boldsymbol{R} - \boldsymbol{H}\boldsymbol{P}^a\boldsymbol{H}^{\mathrm{T}}$$

A perfectly consistent analysis statistically fits the data to within their own accuracy.

If new data are added to (removed from) an optimal analysis system, *DmA* difference must increase (decrease).

Also (Desroziers *et al*., 2006, *QJRMS*)

$$E[\boldsymbol{H}(\boldsymbol{x}^{a}\text{-}\boldsymbol{x}^{b})(\boldsymbol{y}\text{-}\boldsymbol{H}\boldsymbol{x}^{b})^{\mathrm{T}}] = E[\boldsymbol{H}(\boldsymbol{x}^{a}\text{-}\boldsymbol{x}^{b})\boldsymbol{d}^{\mathrm{T}}] = \boldsymbol{H}\boldsymbol{P}^{b}\boldsymbol{H}^{\mathrm{T}}$$

$$E[(\boldsymbol{y}\text{-}\boldsymbol{H}\boldsymbol{x}^{a})(\boldsymbol{y}\text{-}\boldsymbol{H}\boldsymbol{x}^{b})^{\mathrm{T}}] = E[(\boldsymbol{y}\text{-}\boldsymbol{H}\boldsymbol{x}^{a})\boldsymbol{d}^{\mathrm{T}}] = \boldsymbol{R}$$

Assume inconsistency has been found between *a priori* assumed and *a posteriori* observed statistics of innovation or DmA difference.

- What can be done ?

or, equivalently

- Which bounds does the knowledge of the statistics of innovation put on the error statistics whose knowledge is required by the *BLUE* ?

Come back to global data format

$$z = \Gamma x + \zeta$$

where Γ is a known (mxn)-matrix, and ζ an unknown 'error'

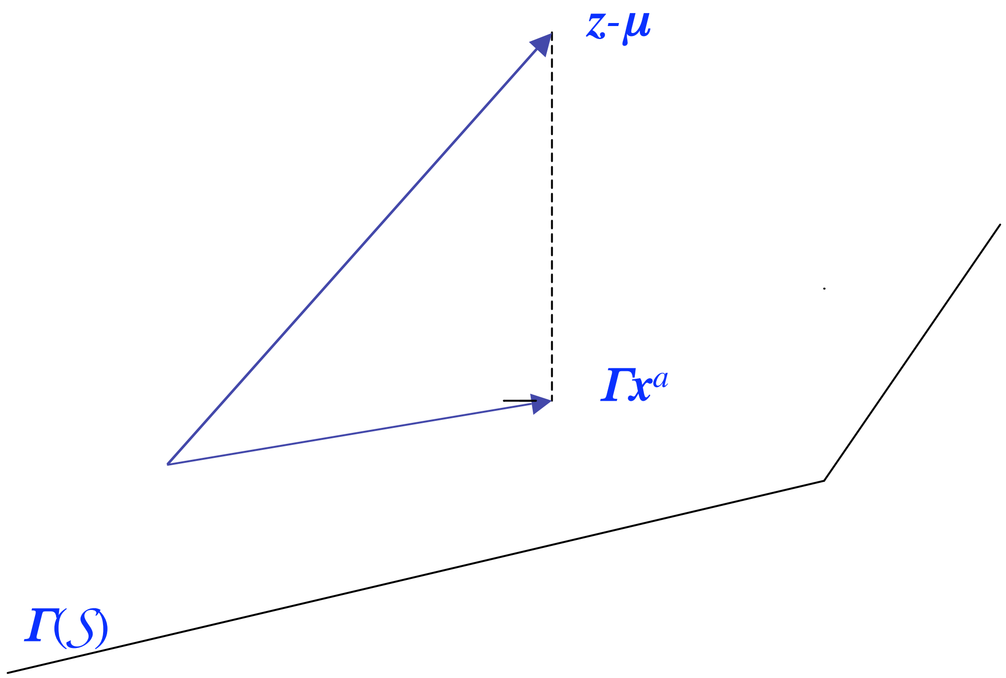
Variational form.

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

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

(Mahalanobis S-metric)

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



Minimizing $\mathcal{J}(\xi)$ amounts to

- unbias z
- project orthogonally onto space $\Gamma(\mathcal{S})$ according to Mahalanobis S-metric
- take inverse through Γ (inverse unambiguously defined through determinacy condition)

Many assimilation methods

- Optimal Interpolation
- 3DVar, either primal or dual
- Kalman Filter, either in its simple or Extended form
- Kalman Smoother
- 4DVar, either in its strong- or weak-constraint form, or in its primal or dual form

are particular cases of that general scheme.

Only exceptions (so far)

- Ensemble Kalman Filter (which is linear however in its 'updating' phase)
- Particle Filters

Decompose data space $\mathcal{D}$ into image space $\Gamma(\mathcal{S})$ (index 1) and its $\mathcal{S}$-orthogonal space $\perp\Gamma(\mathcal{S})$ (index 2)

$$\Gamma = \begin{pmatrix} \Gamma_1 \\ 0 \end{pmatrix} \qquad \boldsymbol{\Gamma}_1 \text{ invertible} \qquad z = \begin{pmatrix} z_1 = \Gamma_1 x + \zeta_1 \\ z_2 = \zeta_2 \end{pmatrix}$$

Assume $\quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$

Then

$$\boldsymbol{x}^a = \boldsymbol{\Gamma}_1^{-1} [z_1 - \boldsymbol{\mu}_1]$$

$$\boldsymbol{x}^a = \boldsymbol{\Gamma}_1^{-1}\,[\boldsymbol{z}_1 - \boldsymbol{\mu}_1]$$

The probability distribution of the error

$$\boldsymbol{x}^a - \boldsymbol{x} = \boldsymbol{\Gamma}_1^{-1}\,[\boldsymbol{\zeta}_1 - \boldsymbol{\mu}_1]$$

depends on the probability distribution of $\boldsymbol{\zeta}_1$.

On the other hand, the probability distribution of

$$\boldsymbol{\delta} = (\boldsymbol{z}-\boldsymbol{\mu}) - \boldsymbol{\Gamma}\boldsymbol{x}^a = \begin{pmatrix} 0 \\ \zeta_2 - \mu_2 \end{pmatrix}$$

depends only on the probability distribution of $\boldsymbol{\zeta}_2$.

DmA difference, *i. e.* $(z-\mu) - \Gamma x^a$, is in effect 'rejected' by the assimilation. Its expectation and covariance are irrelevant for the assimilation.

Consequence. Any assimilation scheme (*i. e.*, *a priori* subtracted bias and gain matrix K) is compatible with any observed statistics of either *DmA* or innovation. Not only is not consistency between *a priori* assumed and *a posteriori* observed statistics of innovation (or *DmA*) sufficient for optimality of an assimilation scheme, it is not even necessary.

Example

$$z_1 = x + \zeta_1$$
$$z_2 = x + \zeta_2$$

Errors ζ_1 and ζ_2 assumed to be centred ($E(\zeta_1) = E(\zeta_2) = 0$), to have same variance s and to be mutually uncorrelated. Then

$$x^a = (1/2)\,(z_1 + z_2)$$

with expected quadratic estimation error

$$E[(x^a - x)^2] = s/2$$

Innovation is difference $z_1 - z_2$. With above hypotheses, one expects to observe

$$E(z_1 - z_2) = 0 \qquad ; \qquad E[(z_1 - z_2)^2] = 2s$$

Assume one observes

$$E(z_1 - z_2) = b \qquad ; \qquad E[(z_1 - z_2)^2] = b^2 + 2\gamma$$

Inconsistency if $b \neq 0$ and/or $\gamma \neq s$

Inconsistency can always be resolved by assuming that

$$E(\zeta_1) = -E(\zeta_2) = -b/2$$

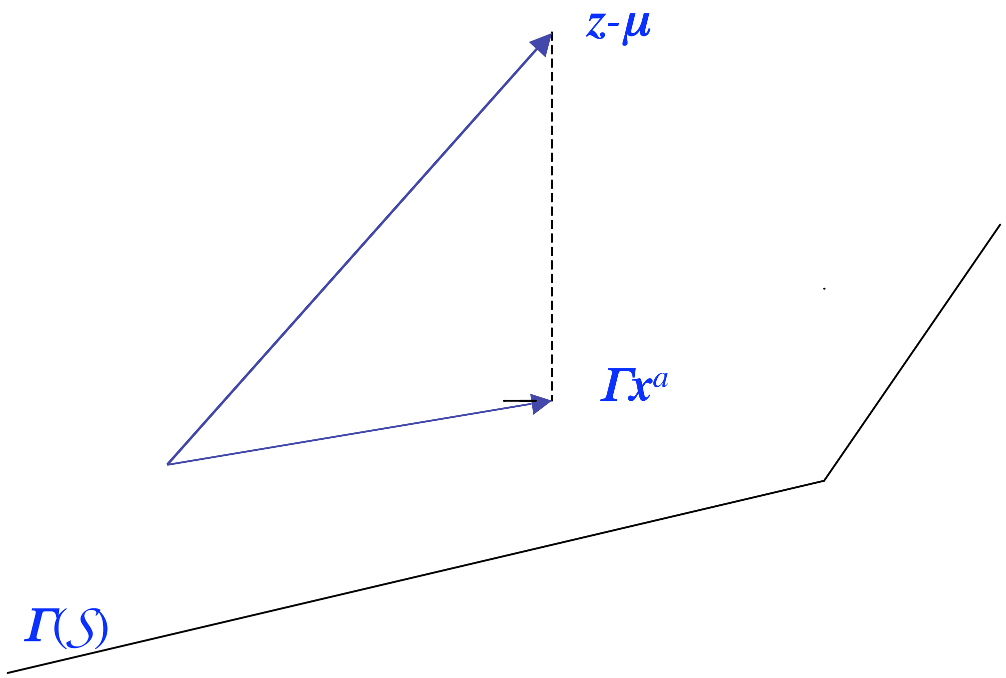
$$E(\zeta'_1{}^2) = E(\zeta'_2{}^2) = (s+\gamma)/2$$
$$E(\zeta'_1\zeta'_2) = (s-\gamma)/2$$

This alters neither the *BLUE* x^a, nor the corresponding quadratic estimation error $E[(x^a-x)^2]$.

Explanation. It is not necessary to know explicitly the complete expectation μ and covariance matrix S in order to perform the assimilation. It is necessary to know the projection of $\boldsymbol{\mu}$ and S onto the subspace $\Gamma(\mathcal{S})$. As for the subspace that is S-orthogonal to $\Gamma(\mathcal{S})$, it suffices to know what it is, but it is not necessary to know the projection of $\boldsymbol{\mu}$ and S onto it. A number of degrees of freedom are therefore useless for the assimilation. The parameters determined by the statistics of $\boldsymbol{d}$ are equal in number to those useless degrees of freedom, to which any inconsistency between *a priori* and *a posteriori* statistics of the innovation can always mathematically be attributed.

However, it may be that resolving the inconsistency in that way requires conditions that are (independently) known to be very unlikely, if not simply impossible. For instance, in the above example, consistency when $\gamma \neq s$ requires the errors ζ_1 and ζ_2 to be mutually correlated, which may be known to be very unlikely.

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



That result, which is purely mathematical, means that the specification of the error statistics required by the assimilation must always be based, in the last resort, on external hypotheses, *i. e.* on hypotheses that cannot be validated on the basis of the innovation alone. Now, such knowledge always exists in practice.

Problem. Identify hypotheses

- That will not be questioned (errors on observations performed a long distance apart by radiosondes made by different manufacturers are uncorrelated)

- That sound reasonable, but may be questioned (observation and background errors are uncorrelated)

- That are undoubtedly questionable (model errors are negligible)

Ideally, define a minimum set of hypotheses such that all remaining undetermined error statistics can be objectively determined from observed statistics of innovation.

Objective function

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

$$\mathcal{J}_{min} \equiv \mathcal{J}(\boldsymbol{x}^a) = (1/2)\,[\Gamma\boldsymbol{x}^a - \boldsymbol{z}]^{\mathrm{T}}\, S^{-1}\,[\Gamma\boldsymbol{x}^a - \boldsymbol{z}]$$

$$= (1/2)\,\boldsymbol{d}^{\mathrm{T}}\,[E(\boldsymbol{d}\boldsymbol{d}^{\mathrm{T}})]^{-1}\,\boldsymbol{d}$$

$$\Rightarrow \qquad E(\mathcal{J}_{min}) = p/2 \qquad (p = \mathrm{dim}\boldsymbol{y} = \mathrm{dim}\boldsymbol{d})$$

If p is large, a few realizations are sufficient for determining $E(\mathcal{J}_{min})$
Often called χ^2 criterion.

Remark. If in addition errors are gaussian $Var(\mathcal{J}_{min}) = p/2$

Results for ECMWF (January 2003, $n = 8\ 10^6$)

- Operations ($p = 1.4\ 10^6$, has significantly increased since then)

$$2\mathcal{J}_{min}/p \;=\; 0.40 - 0.45$$

Innovation is significantly smaller than implied by $\boldsymbol{P}^b$ and $\boldsymbol{R}$ (a residual bias in $\boldsymbol{d}$ would make $\mathcal{J}_{min}$ too large).

- Assimilation without satellite observations ($p = 2 - 3\ 10^5$)

$$2\mathcal{J}_{min}/p \;=\; 1. - 1.05$$

Similar results obtained at other NWP centres (C. Fischer, W. Sadiki with Aladin model, T. Payne at Meteorological Office, UK).

Probable explanation: error variance of satellite observations overestimated in order to compensate for ignored spatial correlation.

Informative content

Objective function

$$\mathcal{J}(\xi) = \Sigma_k \mathcal{J}_k(\xi)$$

where

$$\mathcal{J}_k(\xi) \equiv (1/2)\,(H_k\boldsymbol{\xi} - \boldsymbol{y}_k)^{\mathrm{T}}\, S_k^{-1}\,(H_k\boldsymbol{\xi} - \boldsymbol{y}_k)$$

with $\quad \dim \boldsymbol{y}_k = m_k$

Accuracy of analysis

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

$$[P^a]^{-1} = \Sigma_k\; H_k^{\mathrm{T}}\, S_k^{-1}\, H_k$$

$$\begin{aligned} 1 &= (1/n)\,\Sigma_k\; \mathrm{tr}(P^a H_k^{\mathrm{T}}\, S_k^{-1}\, H_k) \\ &= (1/n)\,\Sigma_k\; \mathrm{tr}(S_k^{-1/2} H_k\, P^a H_k^{\mathrm{T}}\, S_k^{-1/2}) \end{aligned}$$

Informative content (continuation 1)

$$(1/n)\ \Sigma_k\ \mathrm{tr}(S_k^{-1/2}\, H_k\, P^a\, H_k^{\mathrm{T}}\, S_k^{-1/2}) = 1$$

$I(\boldsymbol{y}_k) \equiv (1/n)\ \mathrm{tr}(S_k^{-1/2}\, H_k\, P^a\, H_k^{\mathrm{T}}\, S_k^{-1/2})$ is a measure of the relative contribution of subset of data $\boldsymbol{y}_k$ to overall accuracy of assimilation. Invariant in linear change of coordinates in data space $\Rightarrow$ valid for *any* subset of data.

In particular

$$I(\boldsymbol{x}^b) = (1/n)\ \mathrm{tr}[P^a\,(P^b)^{-1}] = 1 - (1/n)\ \mathrm{tr}(KH)$$
$$I(\boldsymbol{y}) = (1/n)\ \mathrm{tr}(KH)$$

Rodgers, 2000, calls those quantities *Degrees of Freedom for Signal*, or *for Noise*, depending on whether considered subset belongs to ‘observations’ or ‘background’.

See also papers by C. Cardinali, M. Fisher and others.

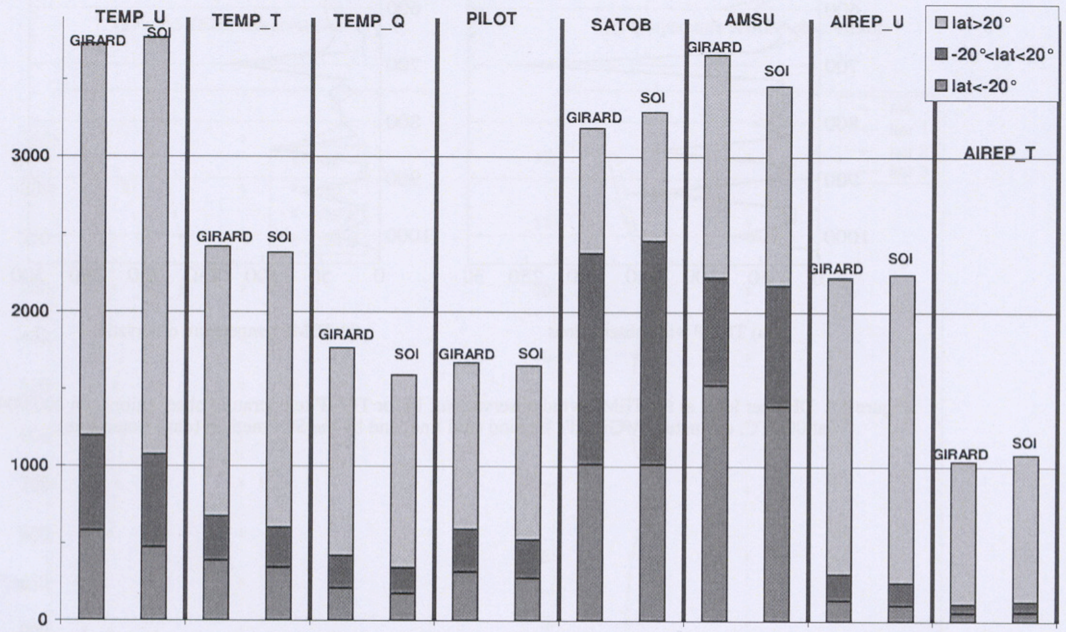
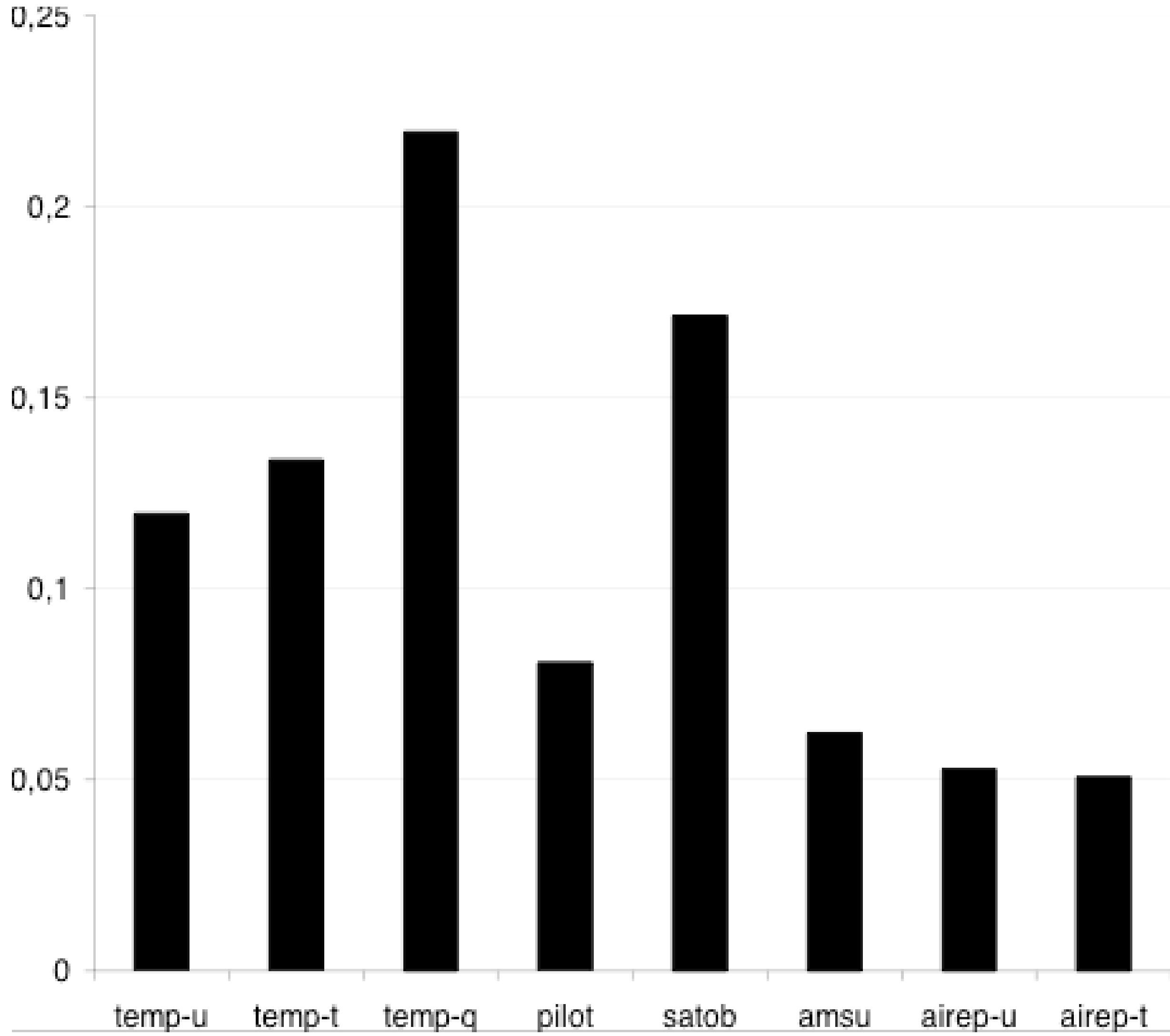


Figure 3. DFS for several subsets of observations. The subsets are separated by thick black lines. For each subset the left hand side bar was computed with Girard's method and the right hand side bar was computed with the SOI method. Each bar is divided into three parts, showing the contribution from the north hemisphere observations, the tropical observations and the southern observations. TEMP U and AIREP U types account for both zonal and

Informative content of subsets of observations (Arpège Assimilation System, Météo-France)

Chapnik *et al.*, 2006, *QJRMS*, **132**, 543-565



Informative content per individual (scalar) observation (courtesy B. Chapnik)

Objective function

$$\mathcal{J}(\xi) \ = \ \Sigma_k \ \mathcal{J}_k(\xi)$$

where

$$\mathcal{J}_k(\xi) \ \equiv \ (1/2)\ (H_k\xi - \boldsymbol{y}_k)^{\mathrm{T}}\ S_k^{-1}\ (H_k\xi - \boldsymbol{y}_k)$$

with $\quad\quad \dim \boldsymbol{y}_k = m_k$

For a perfectly consistent system

$$E[\mathcal{J}_k(x^a)] \ = \ (1/2)\ [m_k \ - \ \mathrm{tr}(S_k^{-1/2}\ H_k\ P^a\ H_k^{\mathrm{T}}\ S_k^{-1/2})]$$

(in particular, $E(\mathcal{J}_{min}) \ = \ p/2$)

For same vector dimension m_k, more informative data subsets lead at the minimum to smaller terms in the objective function.

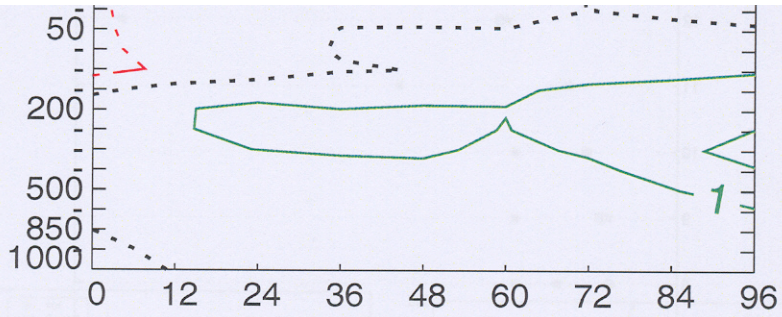
Equality

$$E[\mathcal{J}_k(x^a)] = (1/2)\,[m_k - \mathrm{tr}(S_k^{-1/2}\, H_k\, P^a\, H_k^{\mathrm{T}}\, S_k^{-1/2})] \qquad (1)$$

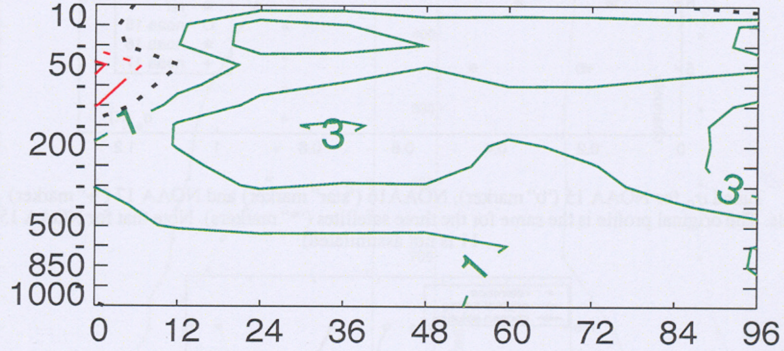
can be objectively checked.

Chapnik *et al*. (2004, 2005). Multiply each observation error covariance matrix S_k by a coefficient α_k such that (1) is verified simultaneously for all observation types.

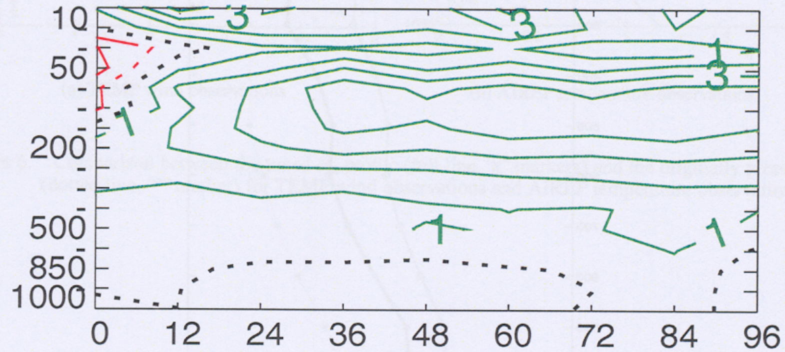
System of equations fot the α_k's solved iteratively.



(a) Northern hemisphere



(b) Southern hemisphere



(c) Subtropical area

Figure 9. Difference between tunned rms (tuned geopotential forecasts - geopotential TEMP obserrvations) and the operational rms computed over 21 siutations. the x axis is the forecast term and the y axis is the vertical pressure level. Dashed lines mean that the tuned forecast is further from the observations than the operational one (degradation), on the contrary the solid lines mean that the tuned forecast is better than the operational. the difference between two colored line is 1 m. Subpanel a is for the northern hemisphere, subpanel b for the southern

Chapnik *et al.*, 2006, *QJRMS*, **132**, 543-565

Informative content (continuation 2)

$$I(\boldsymbol{y}_k) \equiv (1/n)\ \mathrm{tr}(S_k^{-1/2}\, H_k\, P^a\, H_k^{\mathrm{T}}\, S_k^{-1/2})$$

Two subsets of data $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$

If errors affecting $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$ are uncorrelated, then $I(\boldsymbol{z}_1 \cup \boldsymbol{z}_2) \ = \ I(\boldsymbol{z}_1) + I(\boldsymbol{z}_2)$

If errors are correlated $\quad I(\boldsymbol{z}_1 \cup \boldsymbol{z}_2) \neq \ I(\boldsymbol{z}_1) + I(\boldsymbol{z}_2)$

Informative content (continuation 3)

Example 1

$z_1 = x + \zeta_1$

$z_2 = x + \zeta_2$

Errors ζ_1 and ζ_2 assumed to centred, to have same variance and correlation coefficient c.

$$I(z_1) = I(z_2) = (1/2)\,(1 + c)$$

More generally, two sets of data z_1 and z_2 can be said to be positively correlated if $I(z_1 \cup z_2) < I(z_1) + I(z_2)$, and negatively correlated if $I(z_1 \cup z_2) > I(z_1) + I(z_2)$.

Informative content (continuation 4)

Example 2

State vector $\boldsymbol{x}$ evolving in time according to

$$\boldsymbol{x}_2 = \alpha\, \boldsymbol{x}_1$$

Observations are performed at times 1 and 2. Observation errors are assumed centred, uncorrelated and with same variance σ^2. Information contents are then in ratio $(1, \alpha^2)$. For an unstable system ($\alpha > 1$), later observation contains more information (and the opposite for a stable system).

If model error is present, *viz.*

$$\boldsymbol{x}_2 = \alpha\, \boldsymbol{x}_1 + \eta$$

η uncorrelated with observation errors, $E(\eta^2) = \beta\sigma^2$, then informative contents in observation at time 1, observation at time 2 and in model are in the proportion $(1+\beta,\ \alpha^2+\beta,\ 1+\alpha^2)$.

Informative content (continuation 5)

Subset $\boldsymbol{u}_1$ of analyzed fields, $dim\boldsymbol{u}_1 = n_1$. Define relative contribution of subset $\boldsymbol{y}_k$ of data to accuracy of $\boldsymbol{u}_1$?

$\boldsymbol{u}_2$: component of $\boldsymbol{x}$ orthogonal to $\boldsymbol{u}_1$ with respect to Mahalanobis norm associated with P^a (analysis errors on $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ are uncorrelated).

$\boldsymbol{x} = (\boldsymbol{u}_1{}^{\mathrm{T}}, \boldsymbol{u}_2{}^{\mathrm{T}})^{\mathrm{T}}$. In basis $(\boldsymbol{u}_1, \boldsymbol{u}_2)$

$$P^a = \begin{pmatrix} P^a{}_1 & 0 \\ 0 & P^a{}_2 \end{pmatrix}$$

Informative content (continuation 6)

Observation operator H_k decomposes into

$$H_k = (H_{k1}, H_{k2})$$

and expression of estimation error covariance matrix into

$$[P^a{}_1]^{-1} = \Sigma_k \, H_{k1}{}^T S_k{}^{-1} H_{k1}$$

$$[P^a{}_2]^{-1} = \Sigma_k \, H_{k2}{}^T S_k{}^{-1} H_{k2}$$

Same development as before shows that the quantity

$$(1/n_1) \, \mathrm{tr}(S_k{}^{-1/2} H_{k1} P^a{}_1 H_{k1}{}^T S_k{}^{-1/2})$$

is a measure of the relative contribution of subset $\boldsymbol{y}_k$ of data to analysis of subset $\boldsymbol{u}_1$ of state vector.

But can it be computed in practice for large dimension systems (requires the explicit decomposition $\boldsymbol{x} = (\boldsymbol{u}_1{}^T, \boldsymbol{u}_2{}^T)^T$) ?

If we accept to systematically describe uncertainty by probability distributions (see, *e. g.*, Jaynes, 2007), then assimilation can be stated as a problem in *bayesian estimation*

Determine the conditional probability distribution for the state of the system, knowing everything that is known

(unambiguously defined if a prior probability distribution is defined; see Tarantola, 2005).

Questions are now

- Is it possible to objectively evaluate whether the system achieves bayesian estimation ?

- Is it possible to objectively determine the probability distributions which describe the uncertainty on the data ?

‘Bayesianity’ of estimation. Conditional probability distribution that it sought is meant to describe our uncertainty on the state of the system. As such, it depends on elements (such as our present state of knowledge of the physical laws that govern the system) that cannot influence whatever we can observe.

Evaluation of assimilation ensembles

Ensembles must be evaluated as descriptors of probability distributions (and not for instance on the basis of properties of individual elements). This implies, among others

- Validation of the expectation of the ensembles

- Validation of the spread *(spread-skill relationship)*

Reduced Centred Random Variable (RCRV, Candille *et al.*, 2006)

For some scalar variable x, ensemble has mean μ and standard deviation σ. Ratio

$$s = \frac{\xi - \mu}{\sigma}$$

where ξ is verifying observation. Over a large number of realizations

$$E(s) = 0 \quad , \quad E(s^2) = 1$$

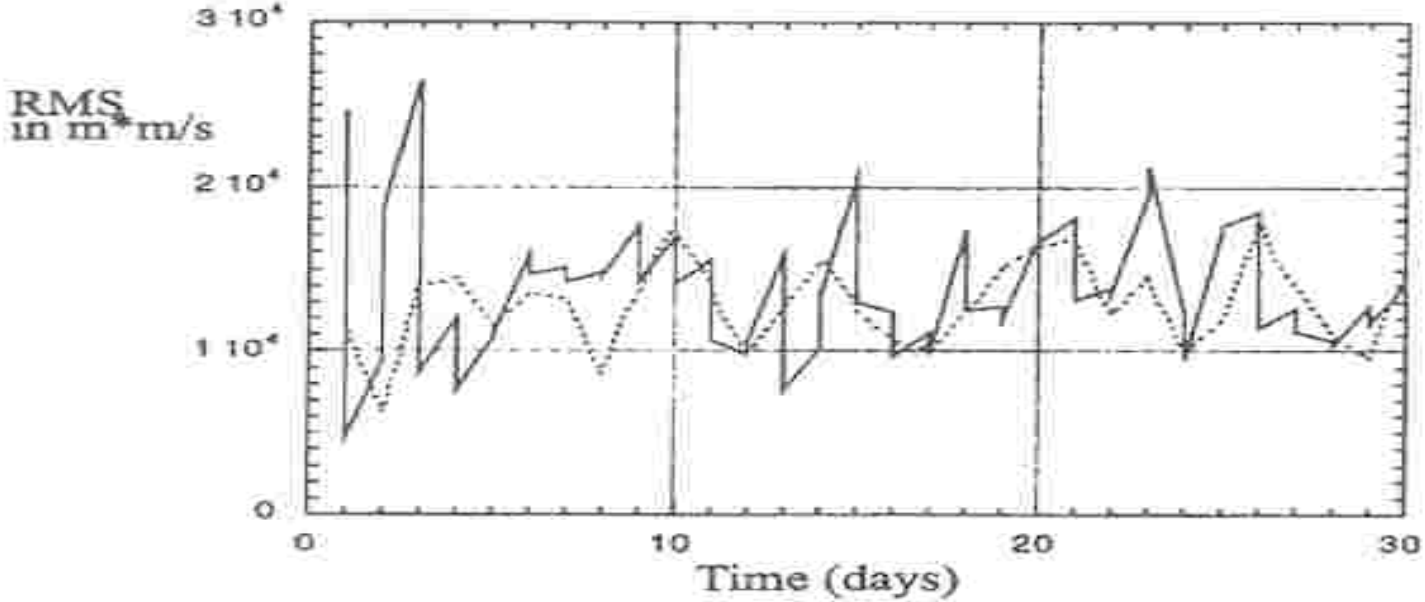


FIG. 12. Comparison of rms error ($m^2 s^{-1}$) between ensemble mean and independent observations (dotted line) and the std dev in the ensemble (solid line). The excellent agreement shows that the SIRF is working correctly.

van Leeuwen, 2003, *Mon. Wea. Rev.*, **131**, 2071-208
(see also presentation by P. Houtekamer)

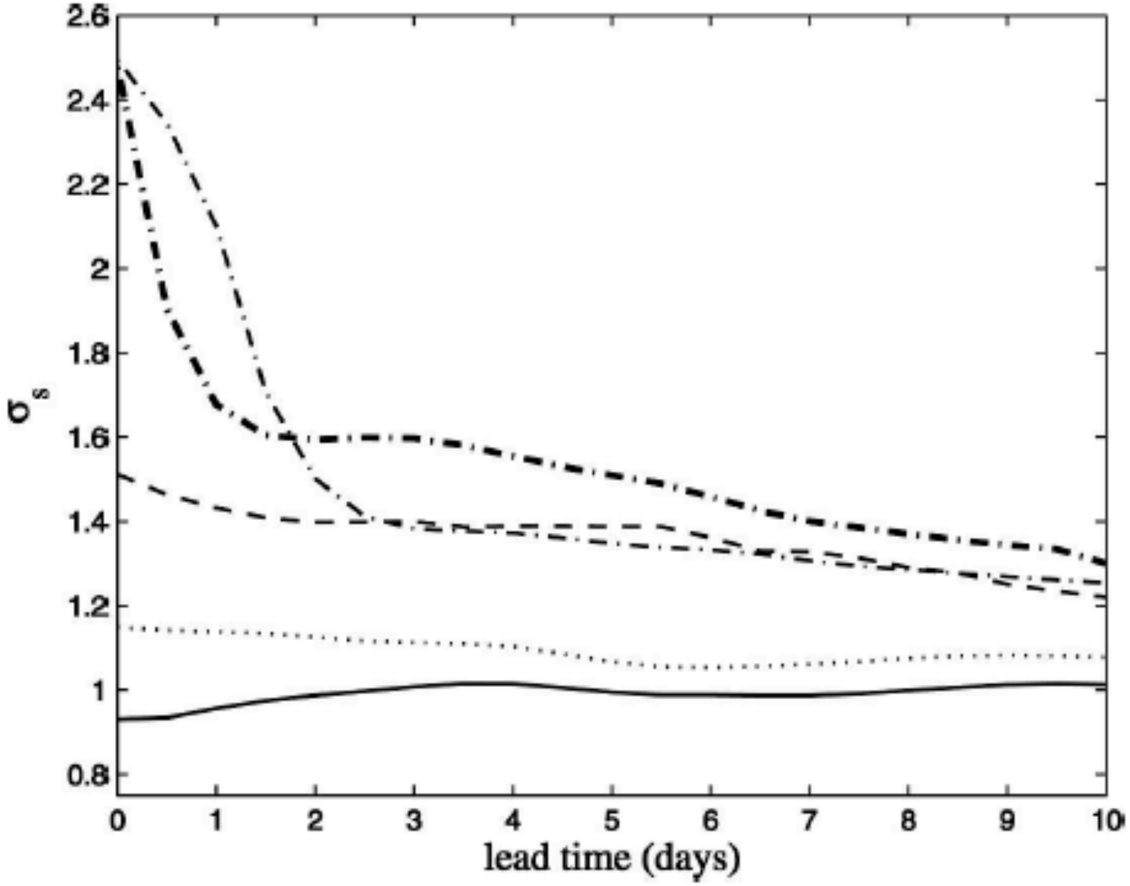


FIG. 4. Evolution of the std dev of the RCRV, as a function of lead time, for the four different methods: EnKF (solid line), ETKF (dotted line), BM (dashed line), and SV computed over a 24-h optimization period (heavy dashed–dotted line) and SV computed over a 48-h optimization period (thin dashed–dotted line).

Descamps and Talagrand, *Mon. Wea. Rev.*, 2007

Two properties make the value of an ensemble estimation system (either for assimilation or for prediction)

Reliability is statistical consistency between estimated probability distributions and verifying observations. Is objectively and quantitatively measured by a number of standard diagnostics (among which Reduced Centred Random Variable and Rank Histograms, reliability component of Brier and Brier-like scores).

Resolution (aka *sharpness*) is the property that reliably predicted probability distributions are useful (essentially have small spread). Also measured by a number of standard diagnostics (resolution component of Brier and Brier-like scores).

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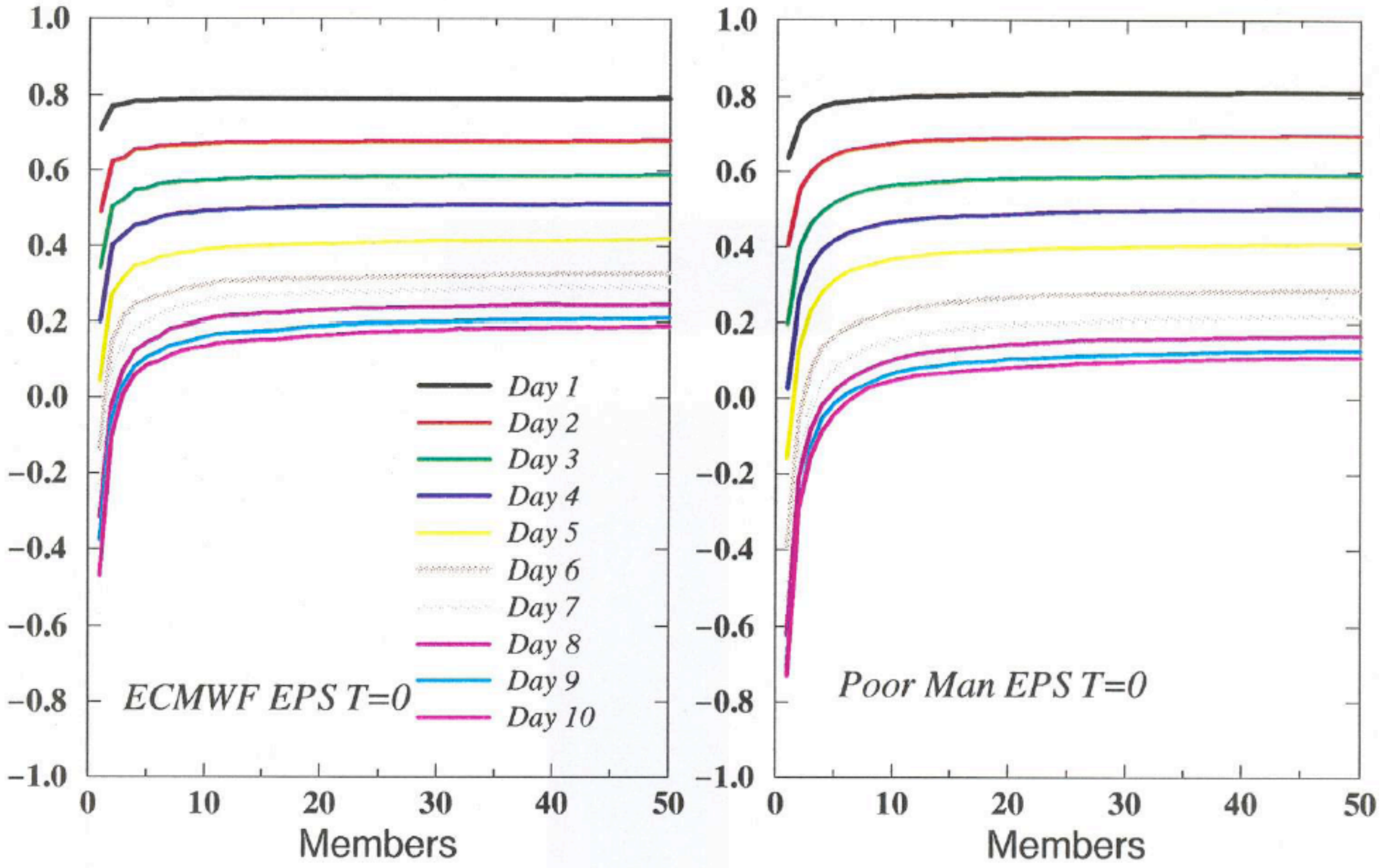
Size of Ensembles ?

- Observed fact : in ensemble prediction, present scores saturate for value of ensemble size N in the range 30-50, independently of quality of score.



Impact of ensemble size on Brier Skill Score
ECMWF, event $T_{850} > T_c$ Northern Hemisphere

(Talagrand *et al.*, ECMWF, 1999)

Theoretical estimate (raw Brier score)

$$B_N = B_\infty + \frac{1}{N}\int_0^1 p(1-p)g(p)dp$$

Question. Why do scores saturate so rapidly ?

Numerical stability of ensemble assimilation, especially of particle filters, seems to require much larger ensembles ($N \approx 100$-200) (presentation by M. Bocquet)

What must determine the size of assimilation ensembles ?

Conclusions

- **Absolute evaluation of analysis schemes, and comparison between different schemes**

  Accuracy can be evaluated only against independent unbiased data (independence and unbiasedness cannot be objectively checked). Fundamental, but not much to say.

- **Determination of required statistics**

  Impossible to achieve in a purely objective way. Will always require physical knowledge, educated guess, interaction with instrumentalists and modelers, and the like.

  Inconsistencies in specification of statistics can be objectively diagnosed, and can help in improving assimilation.

  For given error statistics, possible to quantify relative contribution of each subset of data to analysis of each subset of state vector.

  (and also Generalized Cross-Validation, Adaptive Filtering)

- **Ensemble Assimilation**

  Specific diagnostics are required, which seem to saturate rapidly with ensemble size.

Optimality

Equation

$$\boldsymbol{x}^a = \boldsymbol{x}^b - E(\boldsymbol{\zeta}^b \boldsymbol{d}^{\mathrm{T}}) \, [E(\boldsymbol{d}\boldsymbol{d}^{\mathrm{T}})]^{-1} \, (\boldsymbol{y} - H\boldsymbol{x}^b)$$

means that estimation error $\boldsymbol{x} - \boldsymbol{x}^a$ is uncorrelated with innovation $\boldsymbol{y} - H\boldsymbol{x}^b$ (if it was not, it would be possible to improve on $\boldsymbol{x}^a$ by statistical linear estimation).

Independent unbiased observation

$$\boldsymbol{v} = C\boldsymbol{x} + \boldsymbol{\gamma}$$

Fit to analysis $\quad \boldsymbol{v} - C\boldsymbol{x}^a = C(\boldsymbol{x} - \boldsymbol{x}^a) + \boldsymbol{\gamma}$

$$E[(\boldsymbol{v} - C\boldsymbol{x}^a) \, \boldsymbol{d}^{\mathrm{T}}] = CE[(\boldsymbol{x} - \boldsymbol{x}^a) \, \boldsymbol{d}^{\mathrm{T}}] + E(\boldsymbol{\gamma} \boldsymbol{d}^{\mathrm{T}})$$

First term is 0 if analysis is optimal, second is 0 if observation $\boldsymbol{v}$ is independent from previous data.

Daley (1992)