Diagnosing the optimality of data assimilation systems

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Outline

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1. General framework
2. Lagged innovation covariance
3. «Jmin» diagnostics
4. Observation space diagnostics
5. Ensemble variance diagnostics
6. Observation impact and optimality
7. Conclusion

General formalism

- *Statistical linear estimation* :

$$\mathbf{x}^a = \mathbf{x}^b + \delta\mathbf{x} = \mathbf{x}^b + \mathbf{K}\ \mathbf{d} = \mathbf{x}^b + \mathbf{BH}^T(\mathbf{HBH}^T\mathbf{+R})^{-1}\ \mathbf{d},$$

with $\mathbf{d} = \mathbf{y}^o - H(\mathbf{x}^b)$, *innovation*, **K**, *gain matrix*,

B et **R**, covariances of background and observation errors,

- Solution of the variational problem

$$J(\delta\mathbf{x}) = \delta\mathbf{x}^T\ \mathbf{B}^{-1}\ \delta\mathbf{x} + (\mathbf{d}\mathbf{-H}\ \delta\mathbf{x})^T\ \mathbf{R}^{-1}\ (\mathbf{d}\mathbf{-H}\ \delta\mathbf{x})$$

Non-linear formulation

- *Incremental formulation (Courtier et al, 1994)* : a strategy for minimizing the original non-linear cost-function:

$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + (\mathbf{y}^o - \mathcal{H}(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y}^o - \mathcal{H}(\mathbf{x}))$$

- Even in such a (slightly) non-linear problem, analysis, background and observation errors (or perturbations) are linked:

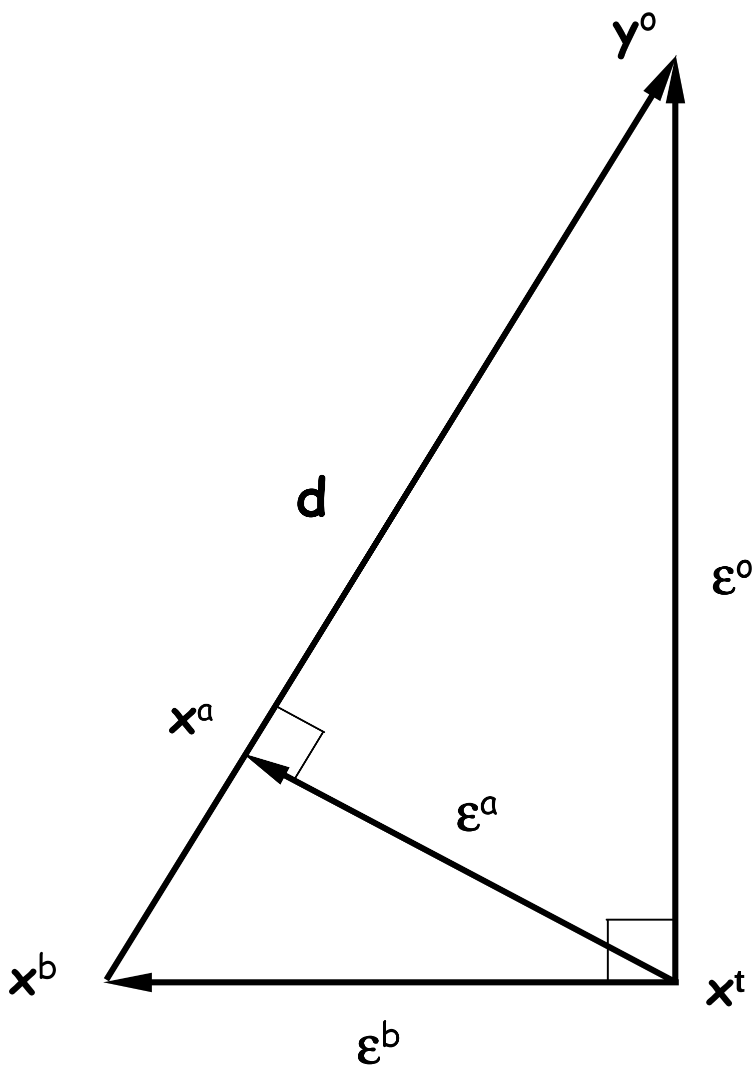
$$\varepsilon^a = (\mathbf{I} - \mathbf{KH})\, \varepsilon^b + \mathbf{K}\, \varepsilon^o \text{, with}$$

$$\varepsilon^a = \mathbf{x}^a - \mathbf{x}^t$$

$$\varepsilon^b = \mathbf{x}^b - \mathbf{x}^t$$

$$\varepsilon^o = \mathbf{y}^o - \mathcal{H}(\mathbf{x}^t)$$

Geometrical interpretation of analysis



$\mathbf{d} = \mathbf{y}^o - H(\mathbf{x}^b)$

Scalar product:

$\langle \varepsilon, \varepsilon' \rangle = E[\varepsilon \ \varepsilon'^T]$

$\langle \varepsilon^a, \mathbf{d} \rangle = E[\varepsilon^a \mathbf{d}^T] = 0$:

- ✓ ε^a and **d** are orthogonal
- ✓ or, in other words, there is no projection of ε^a on **d**

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Lagged innovation covariance

- *Kalman Filter sequence:*

$\mathbf{d}_n = \mathbf{y}^o_n - \mathcal{H}_n(\mathbf{x}^f_n)$
$\mathbf{x}^a_n = \mathbf{x}^f_n + \mathbf{K}_n \mathbf{d}_n$
$\mathbf{x}^f_{n+1} = \mathcal{M}_n(\mathbf{x}^a_n)$

$\mathbf{d}_{n+1} = \mathbf{y}^o_{n+1} - \mathcal{H}_{n+1}(\mathbf{x}^f_{n+1})$
...

- The lagged innovations $\mathbf{d}_n$ and $\mathbf{d}_{n+1}$ should be decorrelated.

(Dee, 1983; Daley, 1992)

- Consequence of estimation error and innovation decorrelation.

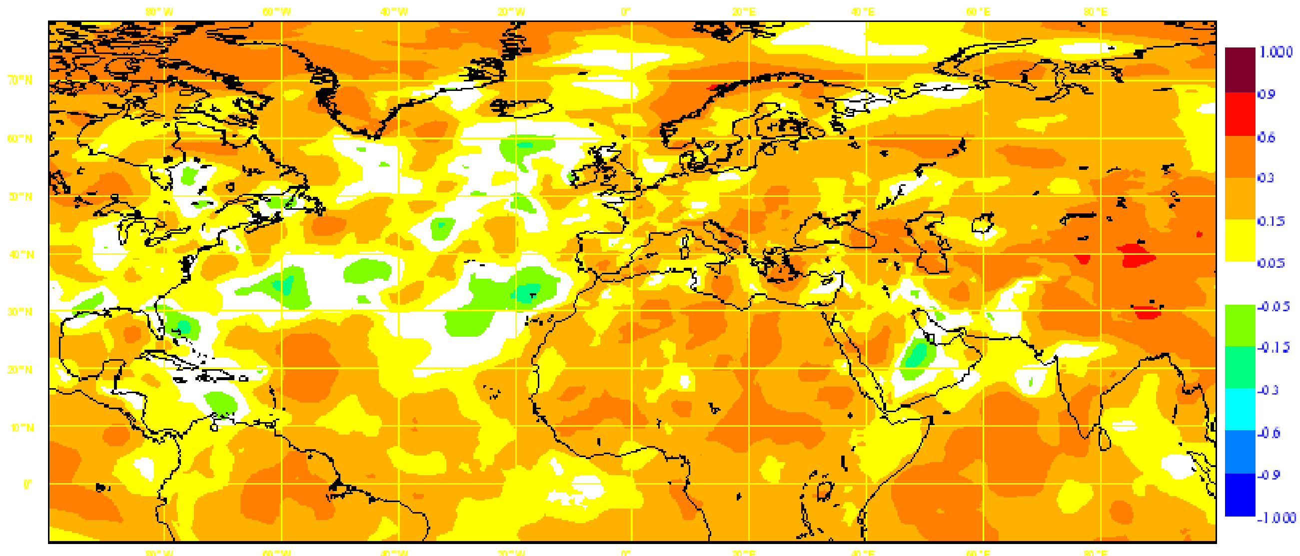
- Translates into $\delta\mathbf{x}_n (\delta\mathbf{x}_{n+1})^T = 0$.

(Chapnik, 2006)

Lagged increment covariance

Fig 4

Correlation of mean sea level pressure increments series.



(from Chapnik, 2006)

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A posteriori « Jmin » diagnostics

- We should have

$$E[J(\mathbf{x}^a)] = p,$$

with p = total number of observations.

(Bennett et al, 1993)

- More precisely

$$E[J_i(\mathbf{x}^a)] = p_i - \mathrm{Tr}(\mathbf{S}_i^{-1/2}\,\Gamma_i\,\mathbf{A}\,\Gamma_i^T\,\mathbf{S}_i^{-1/2}),$$

p_i : number of pieces of information ($\mathbf{x}^b$ or $\mathbf{y}^o$) associated with J_i,

$\mathbf{S}_i$, Γ_i : associated error cov. matrix and « observation » operator.

(Talagrand, 1999)

Particular cases

- Complete background term:

$$\Gamma_i = \mathbf{I}_n,$$
$$\mathbf{S}_i = \mathbf{B},$$
$$E[J^b(\mathbf{x}^a)] = n - Tr(\mathbf{B}^{-1/2}\,\mathbf{I}_n\,\mathbf{A}\,\mathbf{I}_n^T\,\mathbf{B}^{-1/2})$$
$$= Tr(\mathbf{K}\;\mathbf{H})$$

- Complete observation term:

$$\Gamma_i = \mathbf{H},$$
$$\mathbf{S}_i = \mathbf{R},$$
$$E[J^o(\mathbf{x}^a)] = p - Tr(\mathbf{R}^{-1/2}\,\mathbf{H}\,\mathbf{A}\,\mathbf{H}^T\,\mathbf{R}^{-1/2})$$
$$= p - Tr(\mathbf{H}\;\mathbf{K})$$

- Subpart of obs. term:

$$\Gamma_i = \mathbf{H}_i,$$
$$\mathbf{S}_i = \mathbf{R}_i,$$
$$E[J^o_i(\mathbf{x}^a)] = p_i - Tr(\mathbf{R}_i^{-1/2}\,\mathbf{H}_i\,\mathbf{A}\,\mathbf{H}_i^T\,\mathbf{R}_i^{-1/2})$$
$$= p_i - Tr(\mathbf{H}_i\;\mathbf{K}_i),$$

with $\mathbf{H}_i$, $\mathbf{K}_i$ the restrictions of $\mathbf{H}$, $\mathbf{K}$ to subset i.

Computation of $\mathrm{Tr}(\mathbf{H}_i \mathbf{K}_i)$ in a variational scheme

- **K** unknown, but relation between errors (or perturbations) still holds:

$$\varepsilon^a = (\mathbf{I} - \mathbf{KH})\, \varepsilon^b + \mathbf{K}\, \varepsilon^o$$

- For observation subset i:

$$\mathbf{H}_i\, \varepsilon^a = \mathbf{H}_i (\mathbf{I} - \mathbf{KH})\, \varepsilon^b + \mathbf{H}_i \mathbf{K}\, \varepsilon^o$$
$$= \mathbf{H}_i (\mathbf{I} - \mathbf{KH})\, \varepsilon^b + \mathbf{H}_i \Sigma_j \mathbf{K}_j\, \varepsilon^o_j$$

- Linear regression:

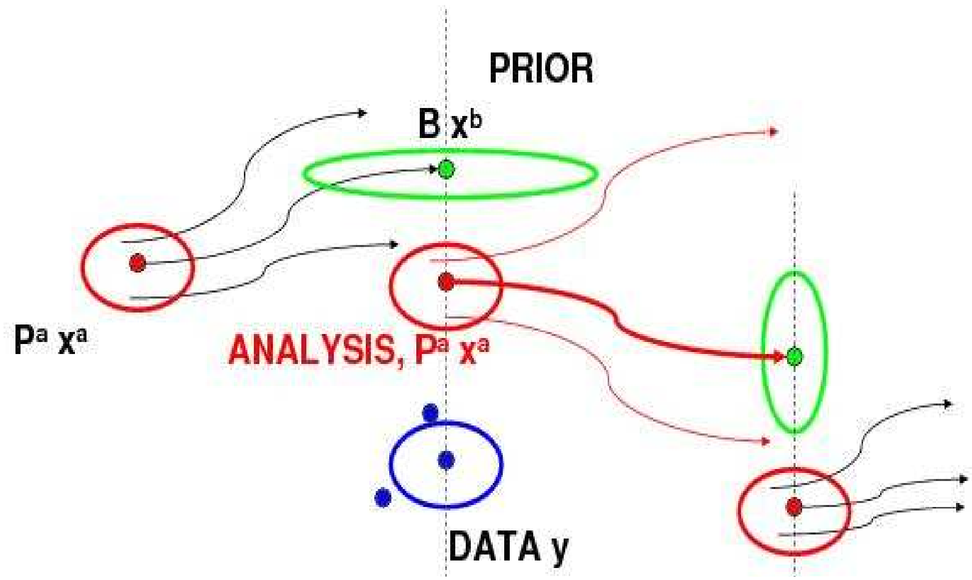
$$\mathbf{H}_i \mathbf{K}_i = \mathrm{cov}(\mathbf{H}_i\, \varepsilon^a, \varepsilon^o_i) / \mathrm{cov}(\varepsilon^o_i, \varepsilon^o_i)$$
$$= \mathrm{cov}(\mathbf{H}_i\, \varepsilon^a, \varepsilon^o_i) / \mathbf{R}_i$$

- Or:

$$\mathrm{Tr}(\mathbf{H}_i \mathbf{K}_i) = {\varepsilon^o_i}^T \mathbf{R}_i^{-1} \mathbf{H}_i\, \varepsilon^a$$

(Desroziers and Ivanov, 2001)

Computation from an ensemble of perturbed assimilations



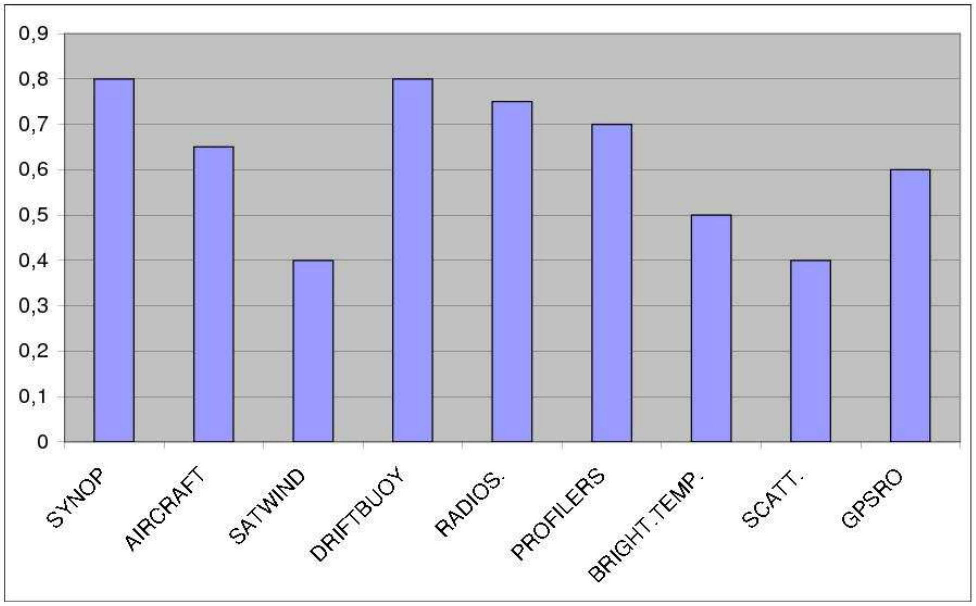
(from Ehrendorfer, 2006)

- Ensemble assimilation : simulation of the joint evolution of analysis, background and observation errors.

- $E[J^o_i(\mathbf{x}^a)] = Tr(\mathbf{H}_i\,\mathbf{K}_i)$ are sub-products of an ensemble of perturbed analyses.

(Desroziers et al, 2009)

Application : optimization of R



Normalization of $\mathbf{R}_i$:

$s^o_i \, \mathbf{R}_i$

Coef. s^o_i diagnosed with

$s^o_i = E[J^o_i(\mathbf{x}^a)]/(E[J^o_i(\mathbf{x}^a)])^{opt}$.

Normalization coefficients of σ^o_i in the French Arpège 4D-Var

(Chapnik, et al, 2004; Buehner, 2005; Desroziers et al, 2009)

Application : normalization of $\mathbf{B}$

- Normalization of $\mathbf{B}$: $s^b\,\mathbf{B}$.

- Coefficient s^b diagnosed with $s^b = E[J^b(\mathbf{x}^a)]/(E[J^b(\mathbf{x}^a)])^{opt}$.

- $(E[J^b(\mathbf{x}^a)])^{opt}$ given by $(E[J^b(\mathbf{x}^a)])^{opt} = Tr(\mathbf{HK}) = \Sigma_i\, Tr(\mathbf{H}_i\,\mathbf{K}_i)$.

- Allows the global inflation of background error variances given by an ensemble of perturbed assimilations.

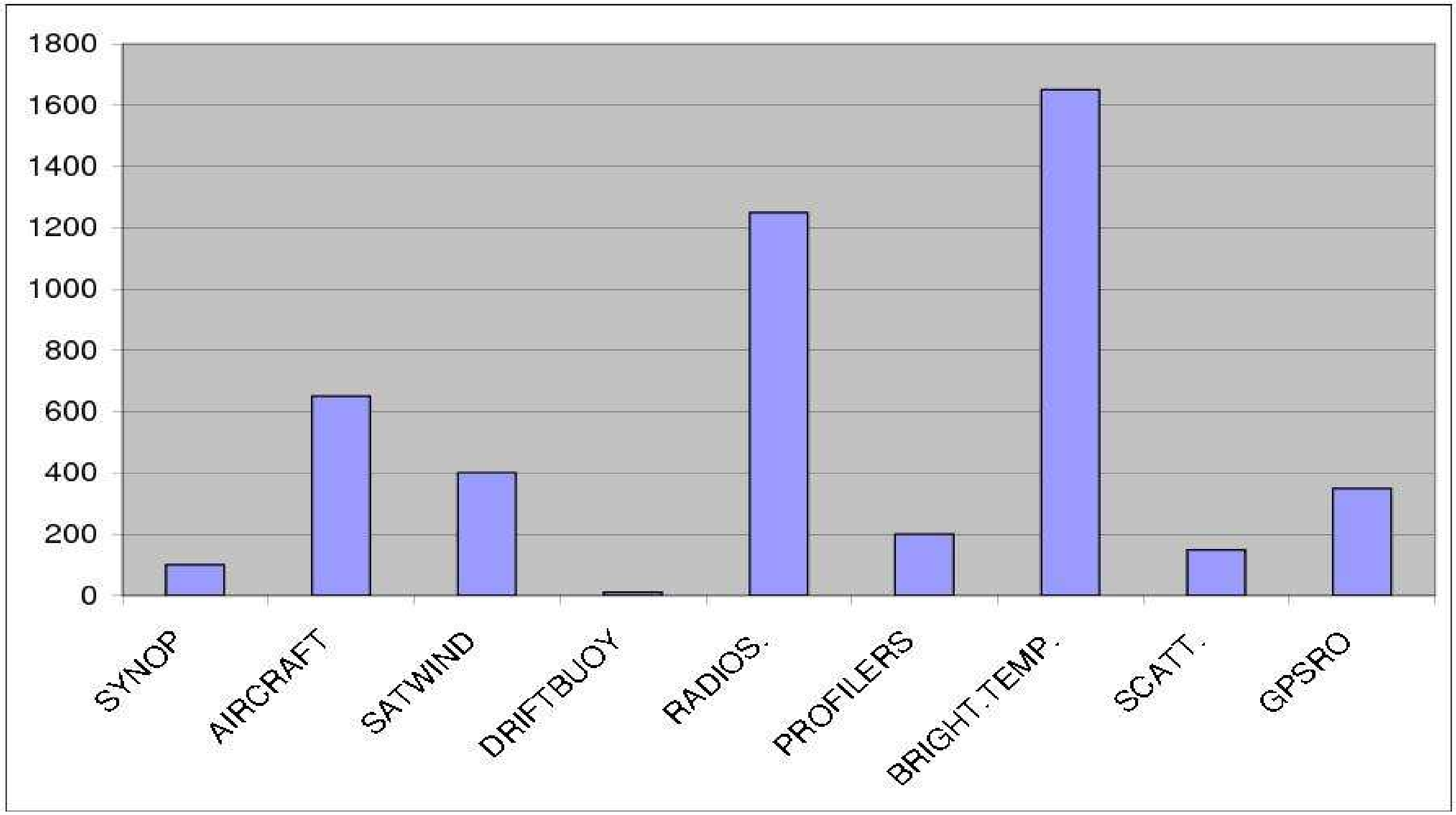
Link with different measures of the impact of independent observations

- $\mathbf{A}^{-1} = \mathbf{B}^{-1} + \Sigma_i \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i$ — $\mathbf{A}^{-1}$ = background « precision » + obs. « precisions »
- $\mathbf{I}_n = \mathbf{A}\ \mathbf{B}^{-1} + \Sigma_i \mathbf{A}\ \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i = (\mathbf{I}_n - \mathbf{KH}) + \Sigma_i \mathbf{K}_i \mathbf{H}_i$ — $\mathbf{I}_n$ = background ponderation + obs. ponderations
- $n = \mathrm{Tr}(\mathbf{I}_n - \mathbf{KH}) + \Sigma_i \mathrm{Tr}(\mathbf{K}_i \mathbf{H}_i)$ — n = DFS background + DFS observations
- $\mathbf{B} = \mathbf{A} + \Sigma_i \mathbf{A}\ \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{B} = \mathbf{A} + \Sigma_i \mathbf{K}_i \mathbf{H}_i \mathbf{B}$ — bg error cov. = res. error cov. + explained error cov.

DFS: Degrees of Freedom for Signal : Information content.

(Cardinali, 2004)

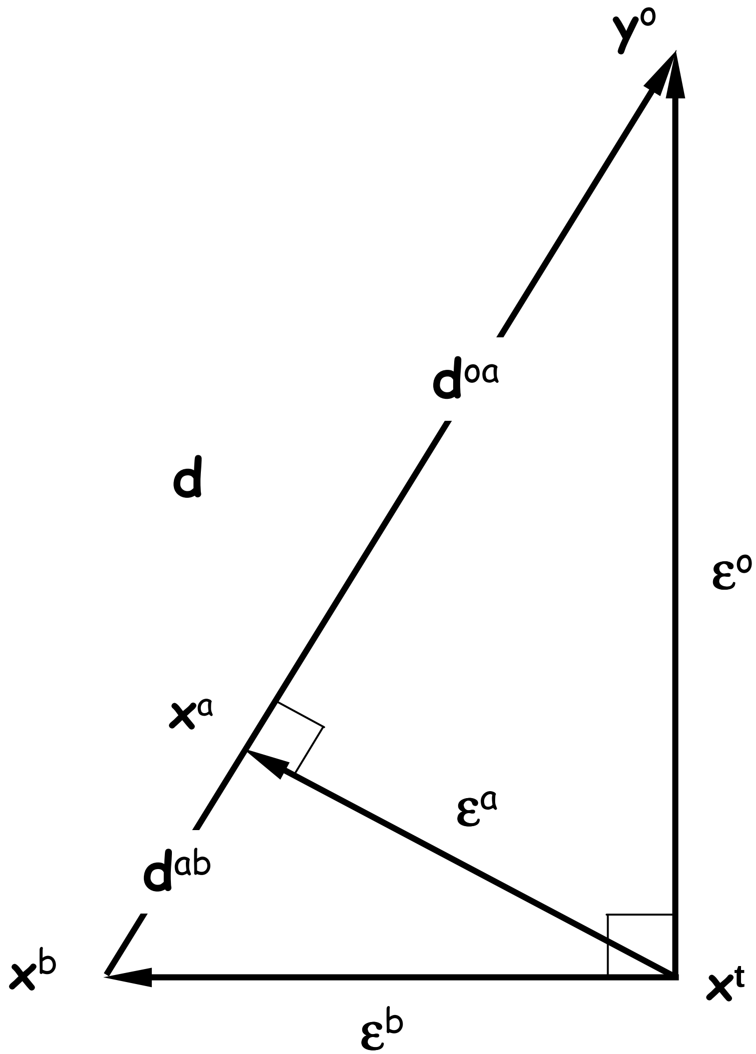
Degrees of Freedom for Signal



Information content of observations in the French Arpège 4D-Var

Outline

Diagnostics in observation space



(Desroziers et al, 2005)

$\mathbf{d} = \mathbf{y}^o - H(\mathbf{x}^b)$

$\mathbf{d}^{oa} = \mathbf{y}^o - H(\mathbf{x}^a)$

$\mathbf{d}^{ab} = H(\mathbf{x}^a) - H(\mathbf{x}^b)$

$E[\mathbf{d}^{oa}\ \mathbf{d}^T] = \mathbf{R}$

$E[\mathbf{d}^{ab}\ \mathbf{d}^T] = \mathbf{HBH}^T$

$\langle \varepsilon, \varepsilon' \rangle = E[\varepsilon\ \varepsilon'^T]$

Practical implementation

- For any subset i with p_i observations, simply compute

$$(\sigma^o_i)^2 = \Sigma_{j=1,pi} (y^o_j - \mathcal{H}_j(\mathbf{x}^a)) (y^o_j - \mathcal{H}_j(\mathbf{x}^b)) / p_i$$

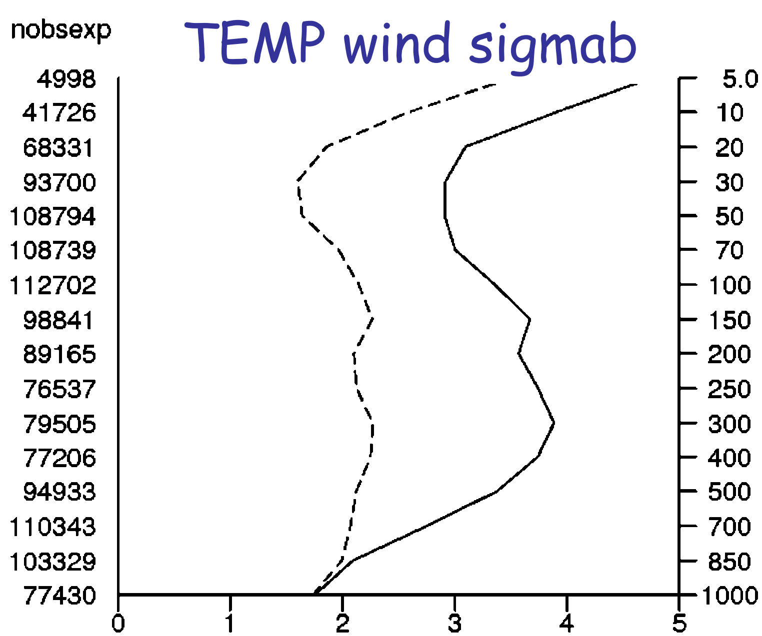
and

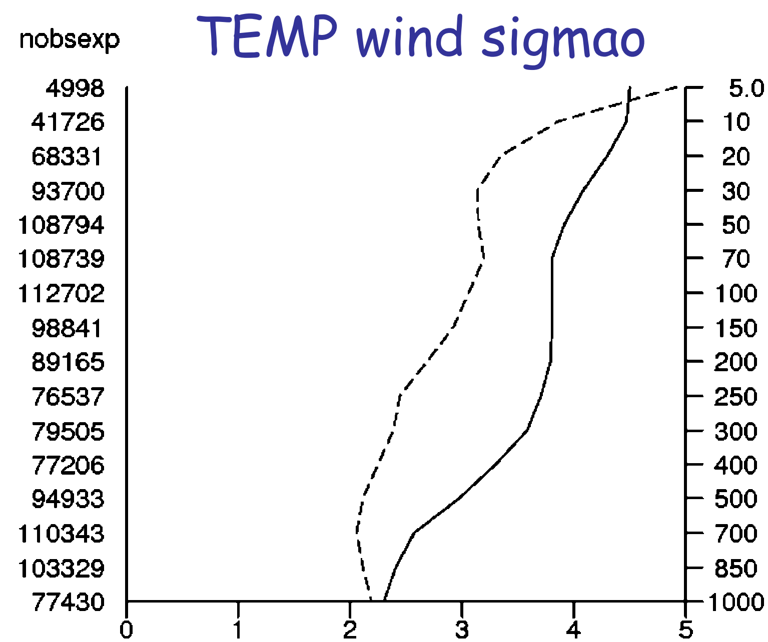
$$(\sigma^b_i)^2 = \Sigma_{j=1,pi} (\mathcal{H}_j(\mathbf{x}^b) - \mathcal{H}_j(\mathbf{x}^a)) (y^o_j - \mathcal{H}_j(\mathbf{x}^b)) / p_i$$

- This is nearly cost-free and can be computed

✓ a posteriori,
✓ over one or several analyses,
✓ in any data assimilation scheme (including 4D-Var).

Practical implementation



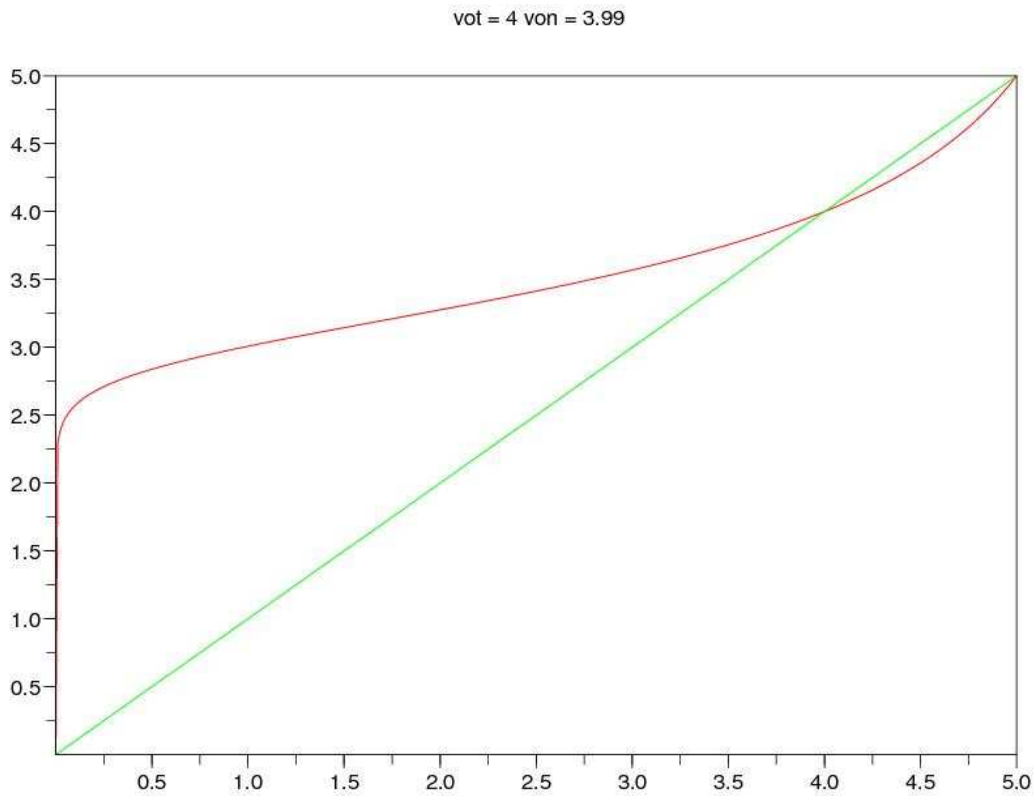


___ specified in Arpège 4D-Var

--- diagnosed in observation space

(20081127 00H – 20081228 18H)

Convergence : $v^o_{diag}(v^o)$

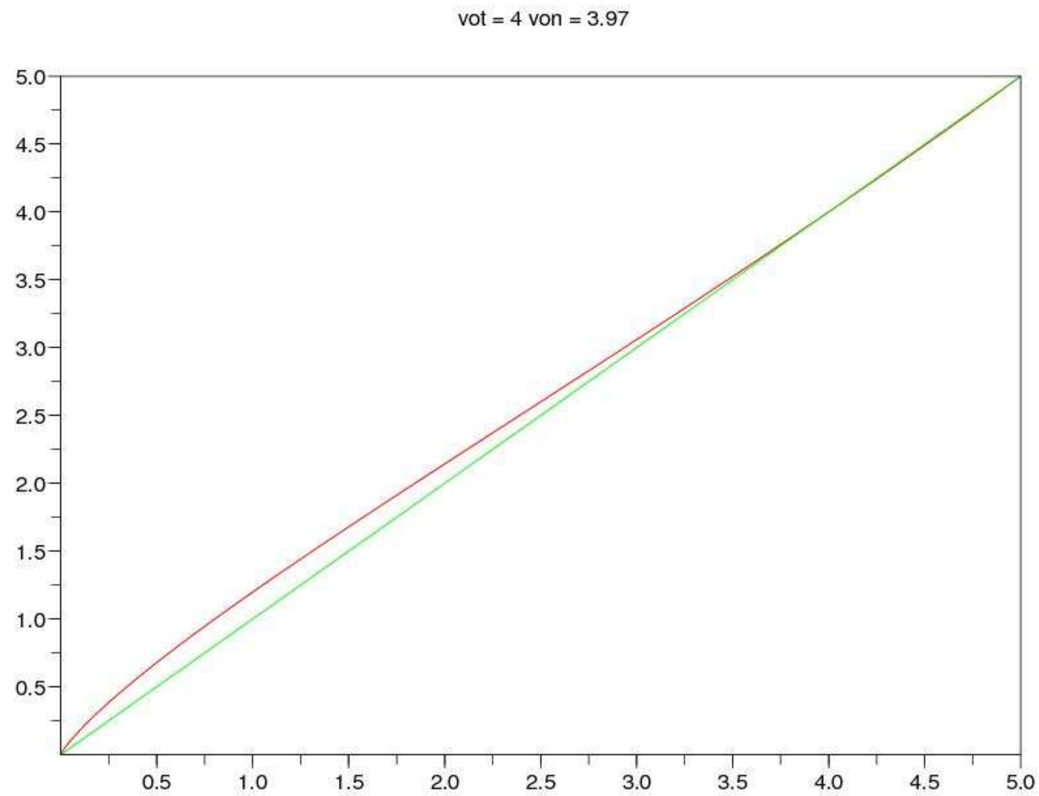


Idealized case: analysis on an equatorial circle (40 000km).

$v^o_{true} = 4.$

L^b = 300 km / L^0= 0 km.

Convergence : $v^o_{diag}(v^o)$



Idealized case: analysis on an equatorial circle (40 000km).

$v^o_{true} = 4$.

L^b = 300 km / L^0= 200 km.

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Ensemble/diagnosed variances in observation space

- Ensemble variances can be computed at observation locations i with

$$(\sigma^{be}_i)^2 = \Sigma_{j=1,ne} (\mathbf{h}_j \, \varepsilon^b)^2 / ne,$$

where ne is the ensemble size.

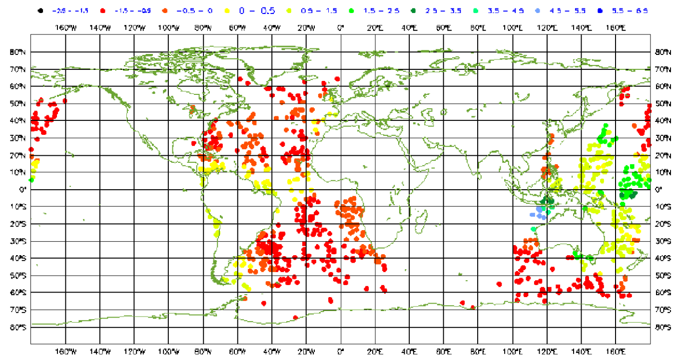
- Can be compared to diagnosed errors

$$(\sigma^{bd}_i)^2 = \Sigma_{j=1,pa} (h_j (\mathbf{x}^b) - h_j (\mathbf{x}^a)) (y^o_j - h_j (\mathbf{x}^b)) / pa,$$

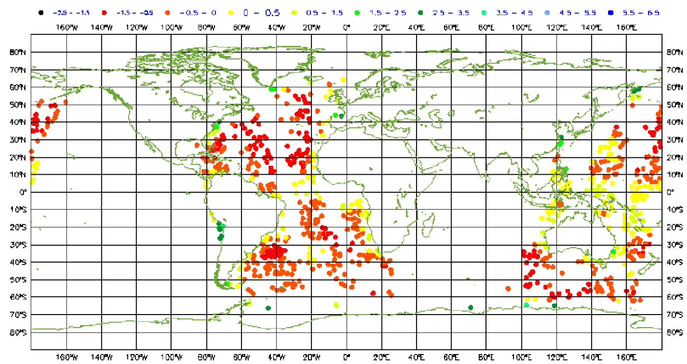
where pa is the number of obs. taken around each obs. location i.

- pa is optimized to maximize the correlation between $(\sigma^{be}_i)^2$ and $(\sigma^{bd}_i)^2$

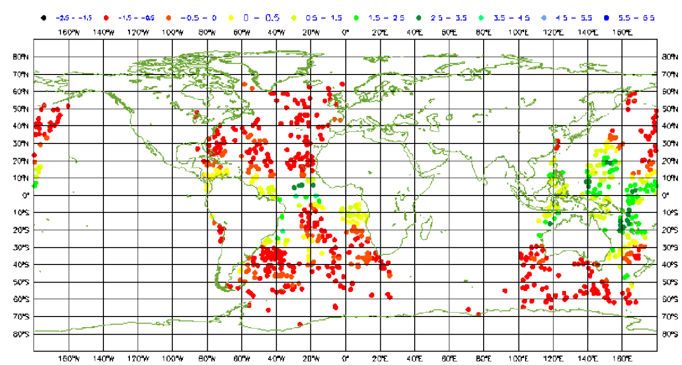
Ensemble / diagnosed background errors in HIRS-7 space



(a) HIRS7-diagnostic



(b) HIRS7-63HE-HR



(c) HIRS7-63QH

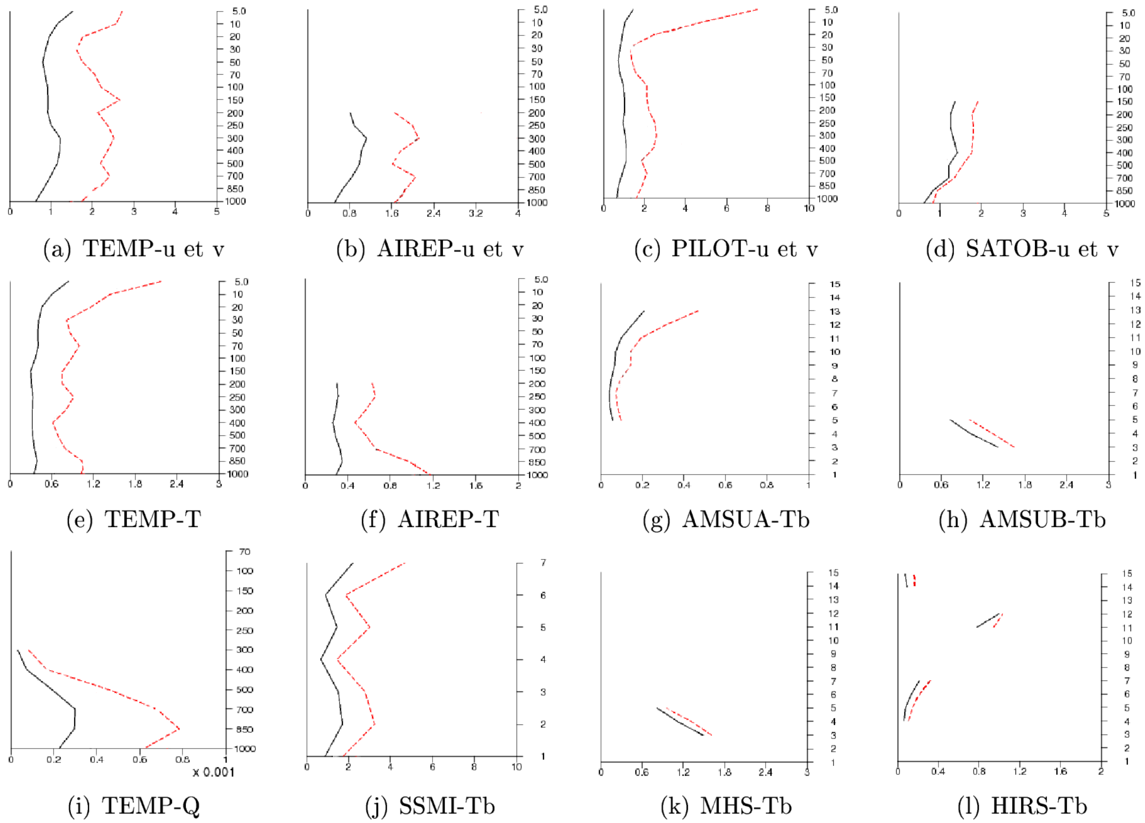
(from Gibier, 2009)

✓Diagnosed 4D-Var background errors

✓3D-Var FGAT ensemble

✓4D-Var ensemble

Ensemble / diagnosed background errors



__ ensemble

--- diagnosed

(from Gibier, 2009)

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Impact of observations on forecasts

- Measure of the quality of a forecast $\mathbf{x}^f = M(\mathbf{x})$:

$$J(\mathbf{x}) = (M(\mathbf{x})-\mathbf{x}^v)^T \boldsymbol{C} (M(\mathbf{x})-\mathbf{x}^v),$$

with, for example, $\boldsymbol{C}$ = energy norm.
and $\mathbf{x}^v$ the verifying analysis at final time t^f.

(Langland et Baker, 2004; Gelaro and Zhu, 2009)

- Expression in terms of initial error:

$$J(\varepsilon) = (\mathbf{M}\ \varepsilon)^T \boldsymbol{C}\ (\mathbf{M}\ \varepsilon),$$

with $\varepsilon = \mathbf{x}-\mathbf{x}^t$ the error at initial time t^i.

Impact of observations on forecasts / optimality

- Taylor expansion at ε^a:

$$J(\varepsilon^b) = J(\varepsilon^a) + (\varepsilon^b - \varepsilon^a)^T J'(\varepsilon^a) + \tfrac{1}{2} (\varepsilon^b - \varepsilon^a)^T J''(\varepsilon^a) (\varepsilon^b - \varepsilon^a)$$
$$= J(\varepsilon^a) + 2 (\varepsilon^b - \varepsilon^a)^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, \varepsilon^a + (\varepsilon^b - \varepsilon^a)^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, (\varepsilon^b - \varepsilon^a)$$
$$= J(\varepsilon^a) + 2\, \mathbf{d}^T \mathbf{K}^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, \varepsilon^a + \mathbf{d}^T \mathbf{K}^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, (\varepsilon^b - \varepsilon^a)$$

First order term = 0 in an optimal system ($<\mathbf{d}, \varepsilon^a> = 0$)! (Cardinali, 2008)

- Taylor expansion at ε^b:

$$J(\varepsilon^a) = J(\varepsilon^b) + 2 (\varepsilon^a - \varepsilon^b)^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, \varepsilon^b + (\varepsilon^a - \varepsilon^b)^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, (\varepsilon^a - \varepsilon^b)$$
$$= J(\varepsilon^b) + 2\, \mathbf{d}^T \mathbf{K}^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, \varepsilon^b + \mathbf{d}^T \mathbf{K}^T \mathbf{M}^T \mathbf{C}\, \mathbf{M}\, (\varepsilon^a - \varepsilon^b)$$

First order term = $- 2\, \mathrm{Tr}(\mathbf{M}^T \mathbf{C}\, \mathbf{M}\, \mathbf{K}\, \mathbf{H}\, \mathbf{B})$ = twice the optimal value of error reduction by observations!

- 2nd order expansion required. (Errico, 2007)

Conclusion

- Wide range of diagnostics, linked with Extended KF formalism.

- Useful to keep in mind.

- Applicable to a slightly non-linear scheme such as incremental 4D-Var.

- *A posteriori* diagnostics are quite useful
  - ✓ to diagnose and tune background and observation error variances,
  - ✓ to measure information content of observations.

- Might be also useful to diagnose model error.