Hybrid Data Assimilation I

A brief recap

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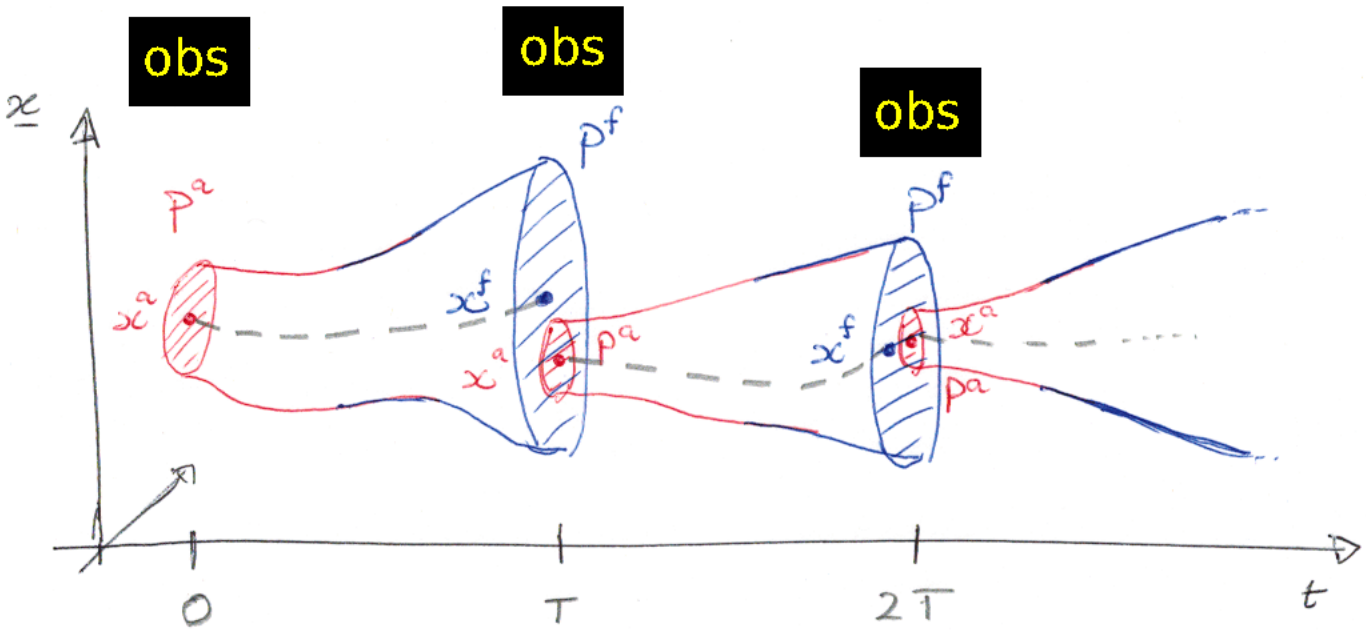
$$p^{\mathrm{a}}(\mathbf{x}|\mathbf{y}) \sim p^{\mathrm{b}}(\mathbf{x}) \times p^{\mathrm{l}}(\mathbf{y}|\mathbf{x})$$

What do we have, and what do we want to improve?

1. Kalman filter



$$\text{forecast state ... } \mathbf{x}^{\mathrm{f}}_{t+1} = \boldsymbol{\mathcal{M}}_t\left(\mathbf{x}^{\mathrm{a}}_t\right)$$

$$\text{... and covariance } \mathbf{P}^{\mathrm{f}}_{t+1} = \mathbf{M}_t\mathbf{P}^{\mathrm{a}}_t\mathbf{M}^{\mathrm{T}}_t + \mathbf{Q}_t$$

$$\text{where } \mathbf{M}_t = \partial\boldsymbol{\mathcal{M}}_t\left(\mathbf{x}\right)/\partial\mathbf{x}\big|_{\mathbf{x}^{\mathrm{a}}_t}$$

$$\text{update state ... } \mathbf{x}^{\mathrm{a}}_t = \mathbf{x}^{\mathrm{f}}_t + \mathbf{K}_t\left(\mathbf{y}_t - \mathbf{h}_t(\mathbf{x}^{\mathrm{f}}_t)\right)$$

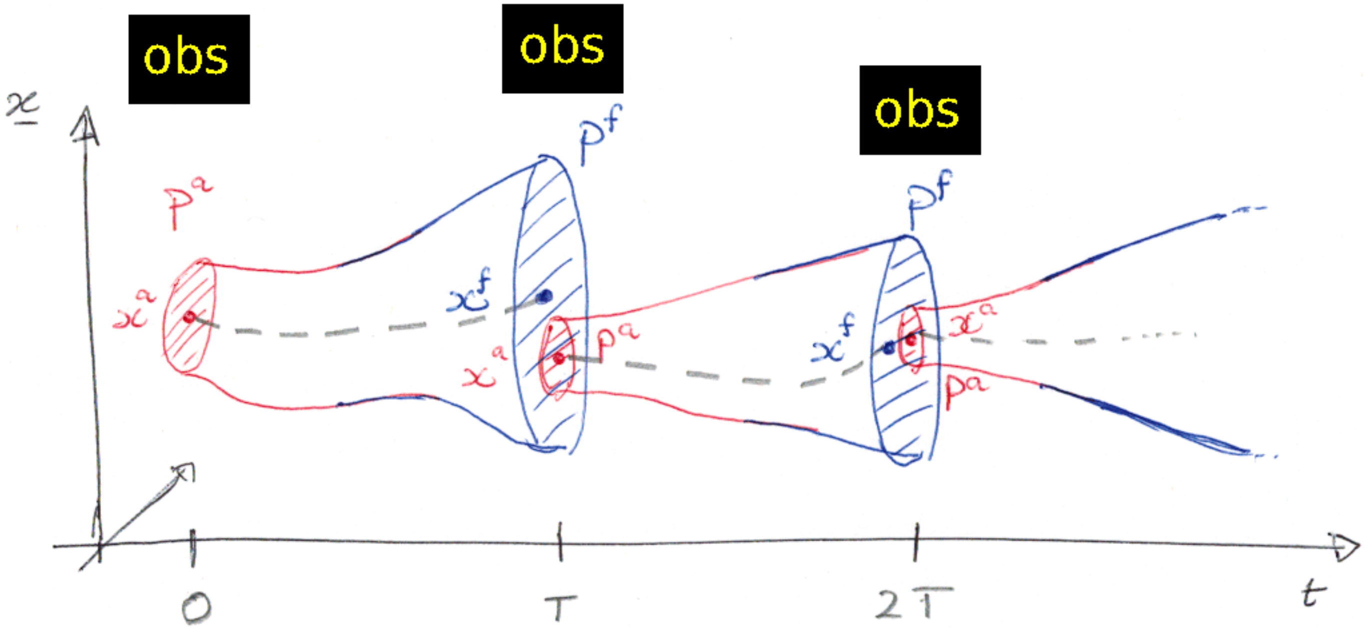
$$\text{... and cov } \mathbf{P}^{\mathrm{a}}_t = \left(\mathbf{I} - \mathbf{K}_t\mathbf{H}_t\right)\mathbf{P}^{\mathrm{f}}_t$$

$$\text{where } \mathbf{K}_t = \mathbf{P}^{\mathrm{f}}_t\mathbf{H}^{\mathrm{T}}_t\left(\mathbf{H}_t\mathbf{P}^{\mathrm{f}}_t\mathbf{H}^{\mathrm{T}}_t + \mathbf{R}_t\right)^{-1}$$

$$\text{and } \mathbf{H}_t = \partial\mathbf{h}_t(\mathbf{x})/\partial\mathbf{x}\big|_{\mathbf{x}^{\mathrm{f}}_t}$$

What do we have, and what do we want to improve?

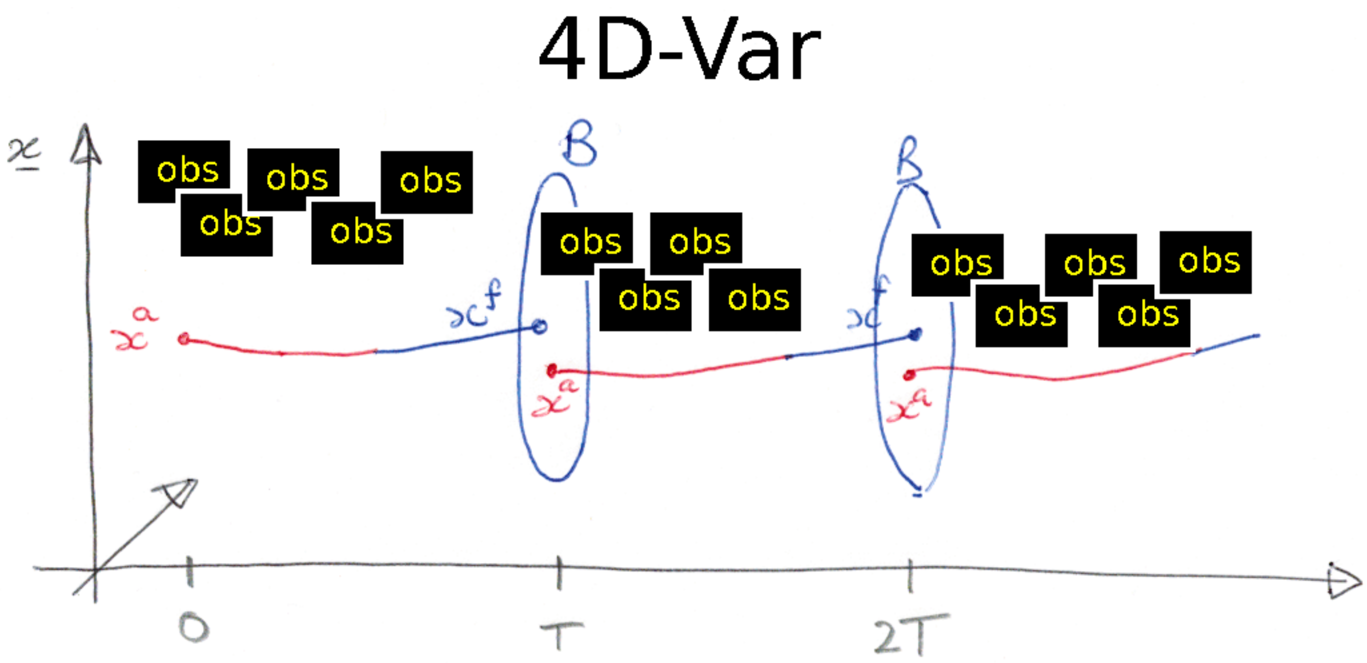
1. Kalman filter (cont.)



- The *state* (1st moments of p^{a} and p^{f}) and *covariance* (2nd moments) are updated and evolved.
- The covariance matrices are potentially *full rank*.
- Gold standard for linear systems.
- Non-linear/non-Gaussian effects are not fully accounted for.
- Restricted to application to small state spaces, n.
- (Be aware of notation: p is a PDF, $\mathbf{P}$ is a covariance.)

What do we have, and what do we want to improve?

2. Variational data assimilation (e.g. strong constraint inc. 4D-Var)



$$
\begin{aligned}
J^{\mathrm{4DVar}}(\delta\mathbf{x}_0) &= \frac{1}{2}\delta\mathbf{x}_0^{\mathrm{T}}\mathbf{B}_0^{-1}\delta\mathbf{x}_0 + \frac{1}{2}\sum_{t=0}^{T}\left(\mathbf{y}_t - \boldsymbol{H}_t(\mathbf{x}_t^{\mathrm{b}}) - \mathbf{H}_t\delta\mathbf{x}_t\right)^{\mathrm{T}}\mathbf{R}_t^{-1}\,(\bullet) \\
\mathbf{x}_t^{\mathrm{b}} &= \boldsymbol{\mathcal{M}}_{0\to t}(\mathbf{x}_0^{\mathrm{b}}) \\
\delta\mathbf{x}_t &\approx \mathbf{M}_{t-1}\mathbf{M}_{t-2}\ldots\mathbf{M}_0\delta\mathbf{x}_0
\end{aligned}
$$

What do we have, and what do we want to improve?

2. Variational data assimilation (cont)

- The *state* (1st moment of p^{f} and p^{a} – the forecast\background and analysis) is updated and evolved, but *not the covariances*.
  - I.e. approximation $\mathbf{P}^{\mathrm{f}} \sim \mathbf{B}$ is made.
  - 4D-Var does *implicitly* evolve the covariances to each observation time:
    * $\mathbf{P}^{\mathrm{f}}_t = \mathbf{B}_t = \mathbf{M}_{t-1} \ldots \mathbf{M}_0 \mathbf{B} \mathbf{M}_0^{\mathrm{T}} \ldots \mathbf{M}_{t-1}^{\mathrm{T}}$ for $0 \leq t \leq T$ (not shown).
    * Covariances reset to $\mathbf{B}$ at the start of each cycle.
  - $\mathbf{P}^{\mathrm{a}}_t$ is not normally available *explicitly*.
  - Need to have code for the *tangent linear*, $\mathbf{M}_t$, $\mathbf{H}_t$ and *adjoints*, $\mathbf{M}_t^{\mathrm{T}}$, $\mathbf{H}_t^{\mathrm{T}}$.
- $\mathbf{B}$ is potentially *full rank*.
- Can cope with some non-linearity of the model and observation operators.
- Is efficient for application to systems with large state spaces, n.

Aside: what is the analysis increment produced by 3D-Var due to a single observation of one of the state variables?

Full-fields 3D-Var cost function

$$J^{\mathrm{3DVar}}(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x} - \mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1} \left(\bullet\right) + \frac{1}{2}\left(\mathbf{y} - \mathbf{H}\mathbf{x}\right)^{\mathrm{T}} \mathbf{R}^{-1} \left(\bullet\right)$$

Gradient

$$\nabla_{\mathbf{x}} J \; = \; \mathbf{B}^{-1}\left(\mathbf{x} - \mathbf{x}^{\mathrm{b}}\right) - \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}\right)$$

$$\left.\nabla_{\mathbf{x}} J\right|_{\mathbf{x}^{\mathrm{a}}} \; = \; \mathbf{0}$$

$$\mathbf{B}^{-1}\left(\mathbf{x}^{\mathrm{a}} - \mathbf{x}^{\mathrm{b}}\right) - \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}^{\mathrm{a}}\right) = \mathbf{0}$$

Equivalent explicit answer

$$\mathbf{B}^{-1}\left(\mathbf{x}^{\mathrm{a}}-\mathbf{x}^{\mathrm{b}}\right)-\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{H}\mathbf{x}^{\mathrm{a}}\right)=\mathbf{0}$$

Let $\mathbf{x}^{\mathrm{a}}=\mathbf{x}^{\mathrm{b}}+\Delta\mathbf{x}$:

$$\begin{aligned}\mathbf{B}^{-1}\Delta\mathbf{x}-\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{H}\left[\mathbf{x}^{\mathrm{b}}+\Delta\mathbf{x}\right]\right) &= \mathbf{0}\\ \left(\mathbf{B}^{-1}+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)\Delta\mathbf{x}-\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{H}\mathbf{x}^{\mathrm{b}}\right) &= \mathbf{0}\end{aligned}$$

Use the S-M-W formula (or R-U-F): $\left(\mathbf{B}^{-1}+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)\mathbf{B}\mathbf{H}^{\mathrm{T}}=\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)$:

$$\begin{aligned}\left(\mathbf{B}^{-1}+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)\Delta\mathbf{x}-\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)\left(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1}\left(\mathbf{y}-\mathbf{H}\mathbf{x}^{\mathrm{b}}\right) &= \mathbf{0}\\ \cancel{\left(\mathbf{B}^{-1}+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)}\Delta\mathbf{x}-\cancel{\left(\mathbf{B}^{-1}+\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)}\mathbf{B}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1}\left(\mathbf{y}-\mathbf{H}\mathbf{x}^{\mathrm{b}}\right) &= \mathbf{0}\end{aligned}$$

$$\mathbf{x}^{\mathrm{a}}-\mathbf{x}^{\mathrm{b}}=\Delta\mathbf{x}=\mathbf{B}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1}\left(\mathbf{y}-\mathbf{H}\mathbf{x}^{\mathrm{b}}\right)$$

Compare to the Kalman update formula!

Single observation

$$\mathbf{x}^{\mathrm{a}} - \mathbf{x}^{\mathrm{b}} = \mathbf{B}\mathbf{H}^{\mathrm{T}} \left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)^{-1} \left(\mathbf{y} - \mathbf{H}\mathbf{x}^{\mathrm{b}}\right)$$

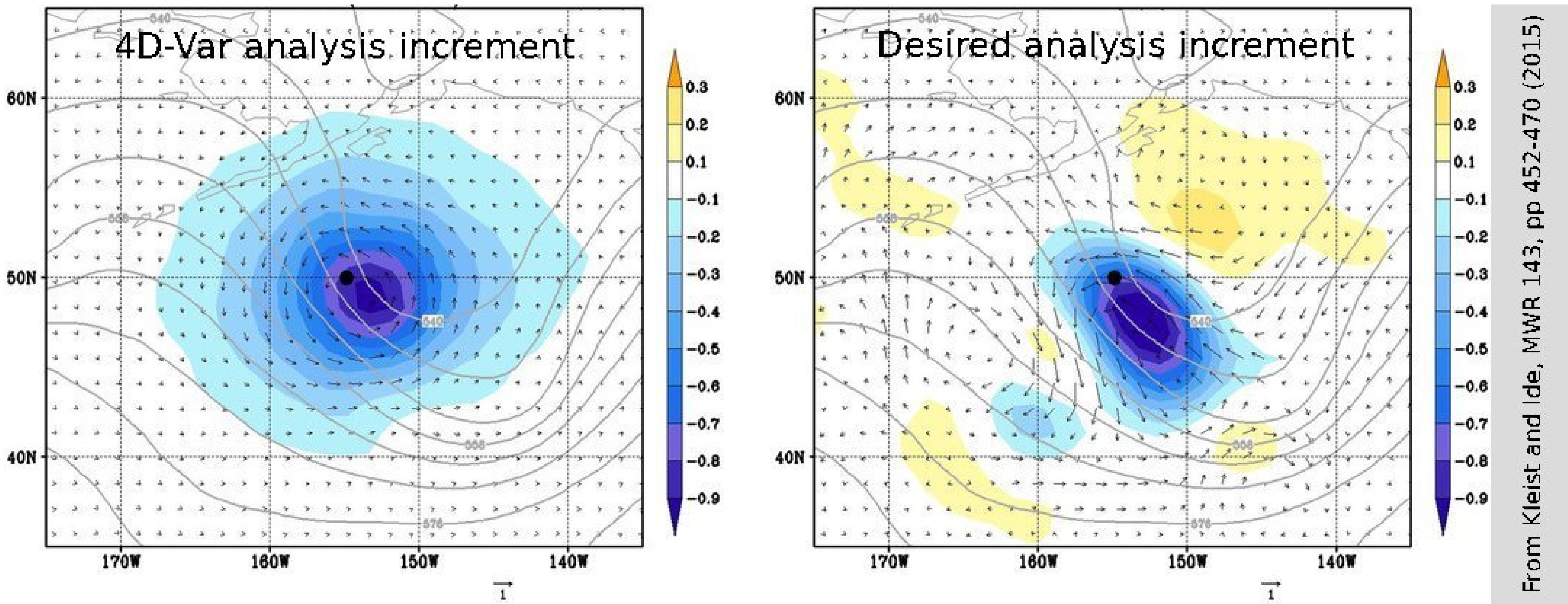
$\mathbf{H} = \begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix}$ (0 in all elements apart from the jth, which is 1)

$$\mathbf{H}\mathbf{x}^{\mathrm{b}} = \mathbf{H} \begin{pmatrix} \mathbf{x}_1^{\mathrm{b}} \\ \vdots \\ \mathbf{x}_j^{\mathrm{b}} \\ \vdots \\ \mathbf{x}_n^{\mathrm{b}} \end{pmatrix} = \mathbf{x}_j^{\mathrm{b}}, \qquad \mathbf{B}\mathbf{H}^{\mathrm{T}} = \begin{pmatrix} \mathbf{B}_{1j} \\ \vdots \\ \mathbf{B}_{jj} \\ \vdots \\ \mathbf{B}_{nj} \end{pmatrix}, \qquad \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} = \mathbf{B}_{jj}$$

$$\Delta\mathbf{x} = \begin{pmatrix} \mathbf{B}_{1j} \\ \vdots \\ \mathbf{B}_{jj} \\ \vdots \\ \mathbf{B}_{nj} \end{pmatrix} \frac{\mathbf{y}_1 - \mathbf{x}_j^{\mathrm{b}}}{\mathbf{R}_{11} + \mathbf{B}_{jj}} = \begin{pmatrix} \text{structure} \\ \\ \text{function} \end{pmatrix} \times \frac{\text{innovation}}{\text{innovation covariance}}$$

What do we have, and what do we want to improve?

2. Variational data assimilation (cont)



Colours: analysis increments of T, arrows: analysis increments of (u, v), contours: background geopotential height. All data are at 500 hPa [2].

Recall, analysis increment: $$\Delta \mathbf{x} = \begin{pmatrix} \mathbf{B}_{1j} \\ \vdots \\ \mathbf{B}_{jj} \\ \vdots \\ \mathbf{B}_{nj} \end{pmatrix} \frac{\mathbf{y}_1 - \mathbf{x}_j^{\mathrm{b}}}{\mathbf{R}_{11} + \mathbf{B}_{jj}}$$

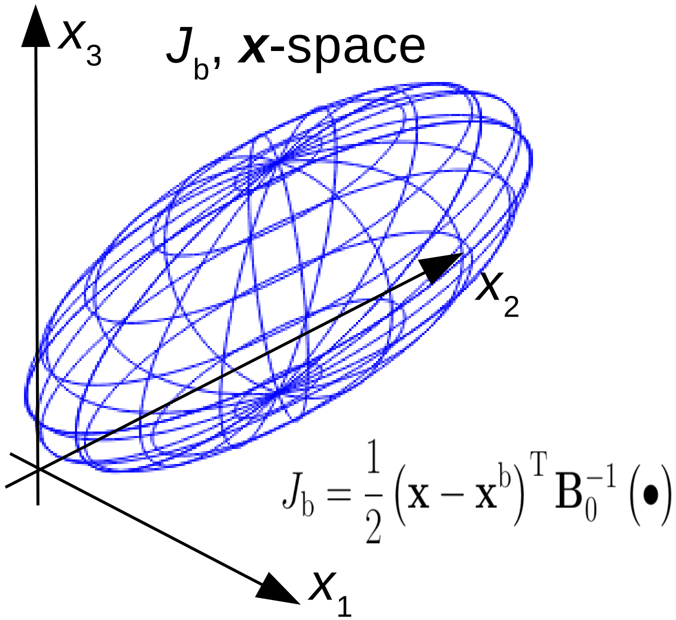
What do we have, and what do we want to improve?

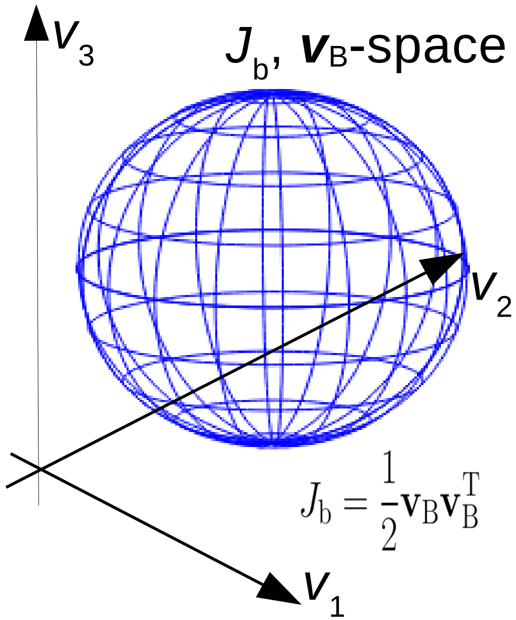
2. Variational data assimilation (cont)

Control variable transforms (CVTs) are used to model the B-matrix.

$$\delta\mathbf{x} = \mathbf{U}\mathbf{v}_\mathrm{B}$$

$$\left.\begin{array}{l}\text{if } \left\langle \delta\mathbf{x}\delta\mathbf{x}^\mathrm{T} \right\rangle_\mathrm{f} = \mathbf{B} \\ \text{and } \left\langle \mathbf{v}_\mathrm{B}\mathbf{v}_\mathrm{B}^\mathrm{T} \right\rangle_\mathrm{f} = \mathbf{I}\end{array}\right\} \quad \text{then} \quad \begin{aligned} \left\langle \delta\mathbf{x}\delta\mathbf{x}^\mathrm{T} \right\rangle_\mathrm{f} &= \left\langle \mathbf{U}\mathbf{v}_\mathrm{B}\mathbf{v}_\mathrm{B}^\mathrm{T}\mathbf{U}^\mathrm{T} \right\rangle_{p_t^\mathrm{f}} \\ &= \mathbf{U}\left\langle \mathbf{v}_\mathrm{B}\mathbf{v}_\mathrm{B}^\mathrm{T} \right\rangle_\mathrm{f} \mathbf{U}^\mathrm{T} \\ &= \mathbf{U}\mathbf{U}^\mathrm{T} \end{aligned}$$





- Minimise the variational cost function with respect to $\mathbf{v}_\mathrm{B}$ instead of with respect to $\delta\mathbf{x}$:

$$\text{e.g. } J^{\mathrm{3DVar}}(\mathbf{v}_\mathrm{B}) = \frac{1}{2}\mathbf{v}_\mathrm{B}^\mathrm{T}\mathbf{v}_\mathrm{B} + \frac{1}{2}\left(\mathbf{y} - \boldsymbol{\mathcal{H}}(\mathbf{x}^\mathrm{b}) - \mathbf{H}\mathbf{U}\mathbf{v}_\mathrm{B}\right)^\mathrm{T}\mathbf{R}^{-1}\left(\bullet\right).$$

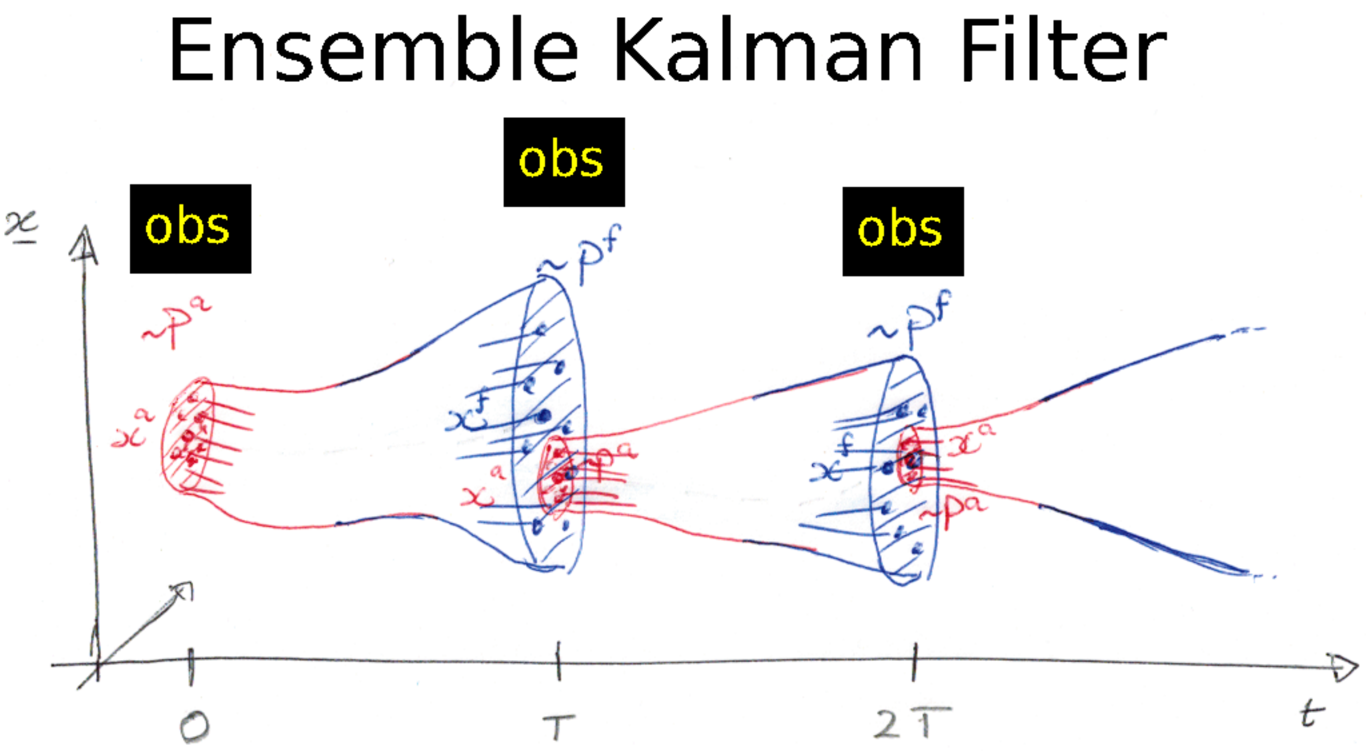
- Equivalent to minimising original incremental cost function with $\mathbf{B} = \mathbf{U}\mathbf{U}^\mathrm{T}$:

$$J^{\mathrm{3DVar}}(\delta\mathbf{x}) = \frac{1}{2}\delta\mathbf{x}^\mathrm{T}\mathbf{B}^{-1}\delta\mathbf{x} + \frac{1}{2}\left(\mathbf{y} - \boldsymbol{\mathcal{H}}(\mathbf{x}^\mathrm{b}) - \mathbf{H}\delta\mathbf{x}\right)^\mathrm{T}\mathbf{R}^{-1}\left(\bullet\right).$$

- $\mathbf{B} = \mathbf{U}\mathbf{U}^\mathrm{T}$ is the *implied covariance.*
- $\mathbf{U} = \mathbf{B}^{1/2}$.
- $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{v}_\mathrm{B} \in \mathbb{R}^{n_v}$, $\mathbf{U} \in \mathbb{R}^{n \times n_v}$.
  - Can have $n_v < n, \quad n_v = n, \quad$ or $n_v > n$.
- $J^{\mathrm{3DVar}}(\mathbf{v}_\mathrm{B})$ is numerically better conditioned than $J^{\mathrm{3DVar}}(\delta\mathbf{x})$.
- Applies equally well to 4D-Var.

What do we have, and what do we want to improve?

3. Ensemble data assimilation



mean: $\overline{\mathbf{x}_t^{\mathrm{f}}} \approx \frac{1}{N}\sum_{\ell=1}^{N}\mathbf{x}_t^{\mathrm{f}(\ell)}$

perturbation: $\mathbf{x}_t^{\mathrm{f}(\ell)} - \overline{\mathbf{x}_t^{\mathrm{f}}}$

covariance: $\left[\mathbf{P}_t^{\mathrm{f}}\right]_{ij} \approx \frac{1}{N-1}\sum_{\ell=1}^{N}\left(\left[\mathbf{x}_t^{\mathrm{f}(\ell)}\right]_i - \overline{\left[\mathbf{x}_t^{\mathrm{f}}\right]_i}\right)\left(\left[\mathbf{x}_t^{\mathrm{f}(\ell)}\right]_j - \overline{\left[\mathbf{x}_t^{\mathrm{f}}\right]_j}\right)$

$$\mathbf{P}_t^{\mathrm{f}} \approx \frac{1}{N-1}\sum_{\ell=1}^{N}\left(\mathbf{x}_t^{\mathrm{f}(\ell)} - \overline{\mathbf{x}_t^{\mathrm{f}}}\right)\left(\mathbf{x}_t^{\mathrm{f}(\ell)} - \overline{\mathbf{x}_t^{\mathrm{f}}}\right)^{\mathrm{T}}$$

matrix of ens perts: $\mathbf{X}_t'^{\mathrm{f}} = \frac{1}{\sqrt{N-1}}\begin{pmatrix} \uparrow & & \uparrow & & \uparrow \\ \mathbf{x}_t^{\mathrm{f}(1)} - \overline{\mathbf{x}_t^{\mathrm{f}}} & \cdots & \mathbf{x}_t^{\mathrm{f}(\ell)} - \overline{\mathbf{x}_t^{\mathrm{f}}} & \cdots & \mathbf{x}_t^{\mathrm{f}(N)} - \overline{\mathbf{x}_t^{\mathrm{f}}} \\ \downarrow & & \downarrow & & \downarrow \end{pmatrix}$

$$\left[\mathbf{X}_t'^{\mathrm{f}}\right]_{i\ell} = \frac{\left[\mathbf{x}_t^{\mathrm{f}(\ell)}\right]_i - \left[\overline{\mathbf{x}_t^{\mathrm{f}}}\right]_i}{\sqrt{N-1}}$$

$$\mathbf{P}_t^{\mathrm{f}} \approx \mathbf{X}_t'^{\mathrm{f}}\mathbf{X}_t'^{\mathrm{f}\,\mathrm{T}}$$

What do we have, and what do we want to improve?

3. Ensemble data assimilation (cont)

The Ensemble Kalman Filter (stochastic EnKF)

- Evaluate one update equation per ensemble member, $\mathbf{x}_t^{\mathrm{a}(\ell)}$, $\ell = 1, \ldots, N$.
- Ensemble members ‘interact’ via covariances, $\mathbf{P}_t^{\mathrm{f}} \approx \mathbf{X'}_t^{\mathrm{f}} \mathbf{X'}_t^{\mathrm{f}\,\mathrm{T}}$.
- Update equation derived directly from the Kalman update equation.
- Update each ensemble member separately:

$$
\begin{aligned}
\mathbf{x}_t^{\mathrm{a}(\ell)} &= \mathbf{x}_t^{\mathrm{f}(\ell)} + \mathbf{X'}_t^{\mathrm{f}} \mathbf{S'}_t^{\mathrm{T}} \left(\mathbf{S'}_t \mathbf{S'}_t^{\mathrm{T}} + \mathbf{R}_t \right)^{-1} \left(\mathbf{y}_t - \mathbf{h}_t(\mathbf{x}_t^{\mathrm{f}(\ell)}) - \boldsymbol{\epsilon}^{(\ell)} \right) \\
\mathbf{S'}_t &= \mathbf{H}_t \mathbf{X'}_t^{\mathrm{f}} \\
\boldsymbol{\epsilon}^{(\ell)} &\sim N(\mathbf{0}, \mathbf{R})
\end{aligned}
$$

What do we have, and what do we want to improve?

3. Ensemble data assimilation (cont)

The Ensemble Transform Kalman Filter (ETKF, a square-root filter)

- Evaluate mean via one update equation, $\overline{\mathbf{x}_t^{\mathrm{a}}}$.
- Ensemble perturbations computed to have the correct covariance, $\mathbf{P}_t^{\mathrm{a}} \approx \mathbf{X}_t'^{\mathrm{a}} \mathbf{X}_t'^{\mathrm{aT}}$.
- Update equations derived from the Kalman update equation.
- Solve an eigenvalue equation in N-dimensional space.

$$
\begin{aligned}
\text{update mean: } \overline{\mathbf{x}_t^{\mathrm{a}}} &= \overline{\mathbf{x}_t^{\mathrm{f}}} + \mathbf{X}_t'^{\mathrm{f}} \mathbf{Z} \mathbf{\Lambda}^{-1} \mathbf{Z}^{\mathrm{T}} \mathbf{S}_t'^{\mathrm{T}} \mathbf{R}_t^{-1} \left(\mathbf{y}_t - \mathbf{h}_t(\overline{\mathbf{x}_t^{\mathrm{f}}}) \right) \\
\text{perts: } \mathbf{X}_t'^{\mathrm{a}} &= \mathbf{X}_t'^{\mathrm{f}} \mathbf{T} \\
\mathbf{T} &= \mathbf{Z} \mathbf{\Lambda}^{-1/2} \mathbf{Z}^{\mathrm{T}} \\
\mathbf{Z} \mathbf{\Lambda} \mathbf{Z}^{\mathrm{T}} &= \mathbf{I} + \mathbf{S}_t'^{\mathrm{T}} \mathbf{R}_t^{-1} \mathbf{S}_t' \\
\mathbf{S}_t' &= \mathbf{H}_t \mathbf{X}_t'^{\mathrm{f}}
\end{aligned}
$$

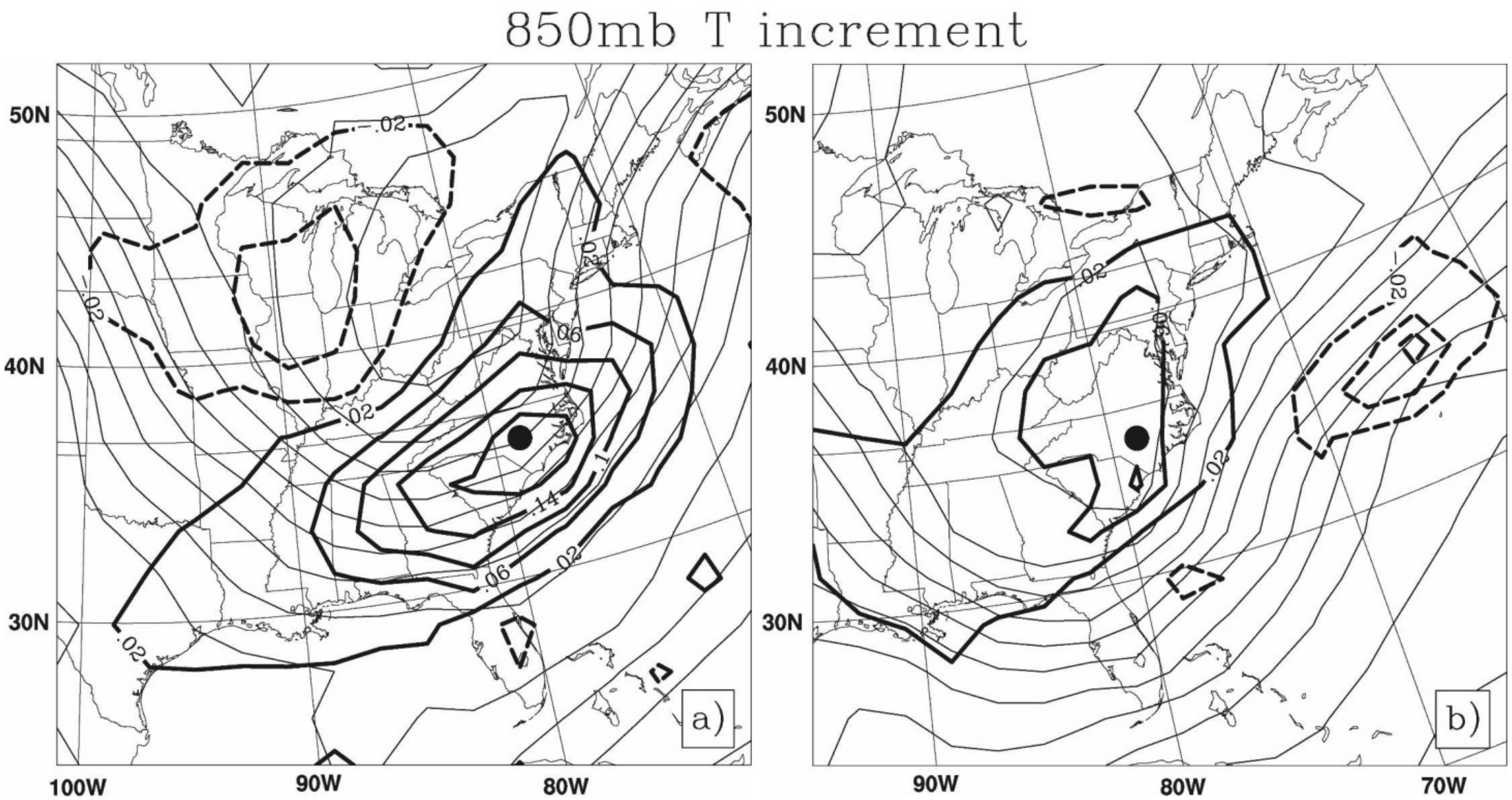
What do we have, and what do we want to improve?

3. Ensemble data assimilation (cont)

- The *state* (1st moments of p_t^{a} and p_t^{f}) and the *approximate covariances* (2nd moments) are updated and evolved via the ensemble.
  - Done approximately, according to number of ensemble members and appropriateness of the spread of the ensemble.
  - $\mathbf{P}_t^{\mathrm{a}}$ and $\mathbf{P}_t^{\mathrm{f}}$ are approximated (<u>and are not computed explicitly</u>).
  - Automatically flow-dependent.
- Can cope with some non-linearity of the model and observation operators.
- Is efficient for application to systems with large state spaces, n.
- Suffers from statistical problems due to finite n:
  - $\mathbf{P}_t^{\mathrm{f}}$ and $\mathbf{P}_t^{\mathrm{a}}$ are rank deficient.
  - Analysis increments lie in the subspace of the forecast perturbation ensemble.
  - The covariances are subject to sampling error (variance deficiency, spurious correlations).
  - Need to employ mitigation techniques (e.g. localisation, inflation).

What do we have, and what do we want to improve?

3. Ensemble data assimilation (cont)

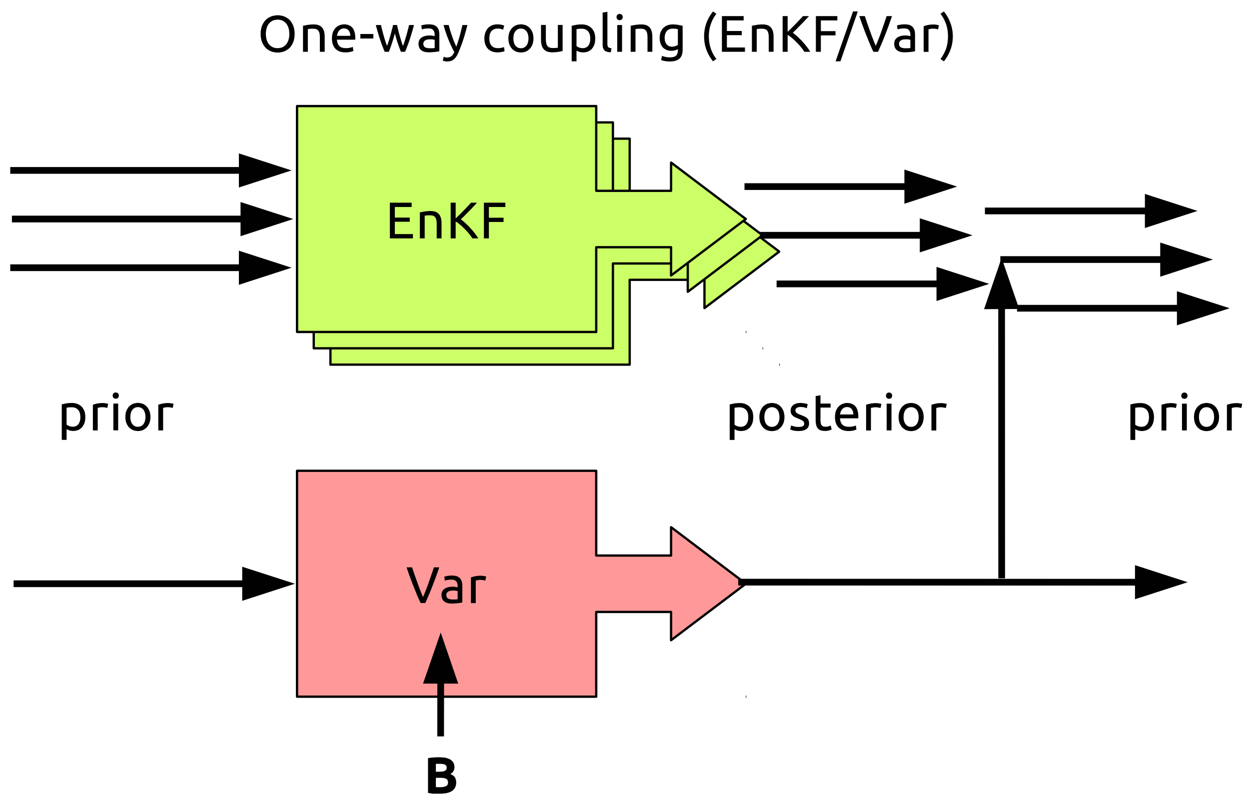


Wang et al., MWR 136, 5116-5131 (2008)

Thick contours: temperature increments after assimilating a single temperature ob. Thin contours: background temperature [3].

(a) 0000 UTC 14 Jan 2003, (b) 0000 UTC 24 Jan 2003

How to combine Ens and Var in a simple way? [1]



How do we combine the properties of ‘flow-dependentness’ of ensemble methods with the ‘full-rankness’ of variational methods?

Quiz: Which of the following is a definition of a hybrid data assimilation method?

A. An ensemble DA method that uses a variational solution?

B. A method that combines the $\mathbf{B}$-matrix of Var with the $\mathbf{P}^{\mathrm{f}}$-matrix of the EnKF?

C. A method that takes the arithmetic average of the analysis increments of Var and EnKF?

D. A method that takes the geometric average of the analysis increments of Var and EnKF?

Bibliography

[1] Neill E Bowler, Alberto Arribas, Kenneth R Mylne, Kelvyn B Robertson, and Sarah E Beare. The MOGREPS short-range ensemble prediction system. *Quarterly Journal of the Royal Meteorological Society*, 134(632):703–722, 2008.

[2] Daryl T Kleist and Kayo Ide. An OSSE-based evaluation of hybrid variational–ensemble data assimilation for the NCEP GFS. Part II: 4DEnVar and hybrid variants. *Monthly Weather Review*, 143(2):452–470, 2015.

[3] Xuguang Wang, Dale M Barker, Chris Snyder, and Thomas M Hamill. A hybrid ETKF-3DVar data assimilation scheme for the WRF model. Part I: Observing system simulation experiment. *Monthly Weather Review*, 136(12):5116–5131, 2008.