Introduction to Data Assimilation, Subgrid-scale Parameterization and Predictability

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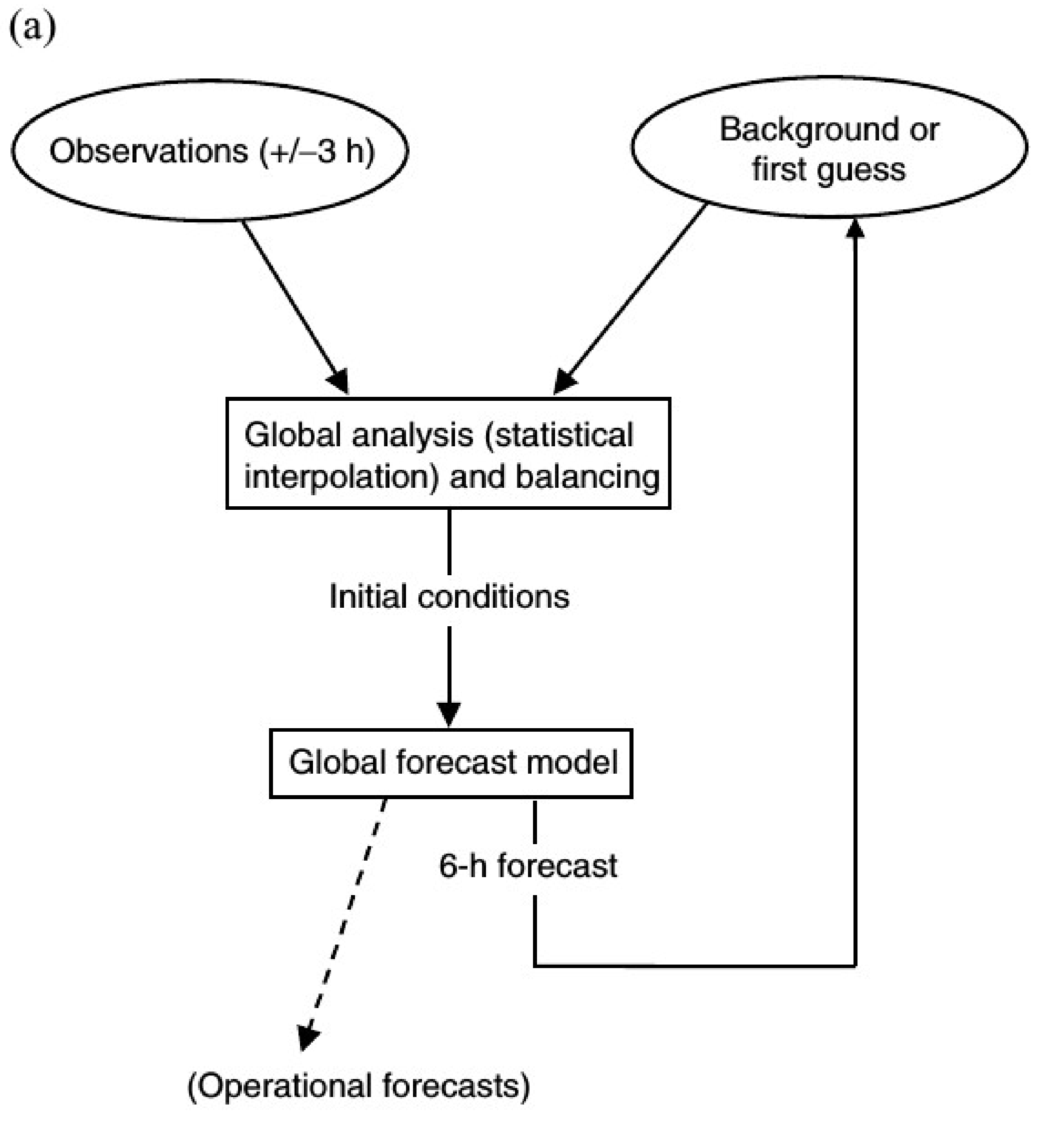
Outline

- Multivariate Data Assimilation
- Ensemble Kalman Filter

Forecast Cycle



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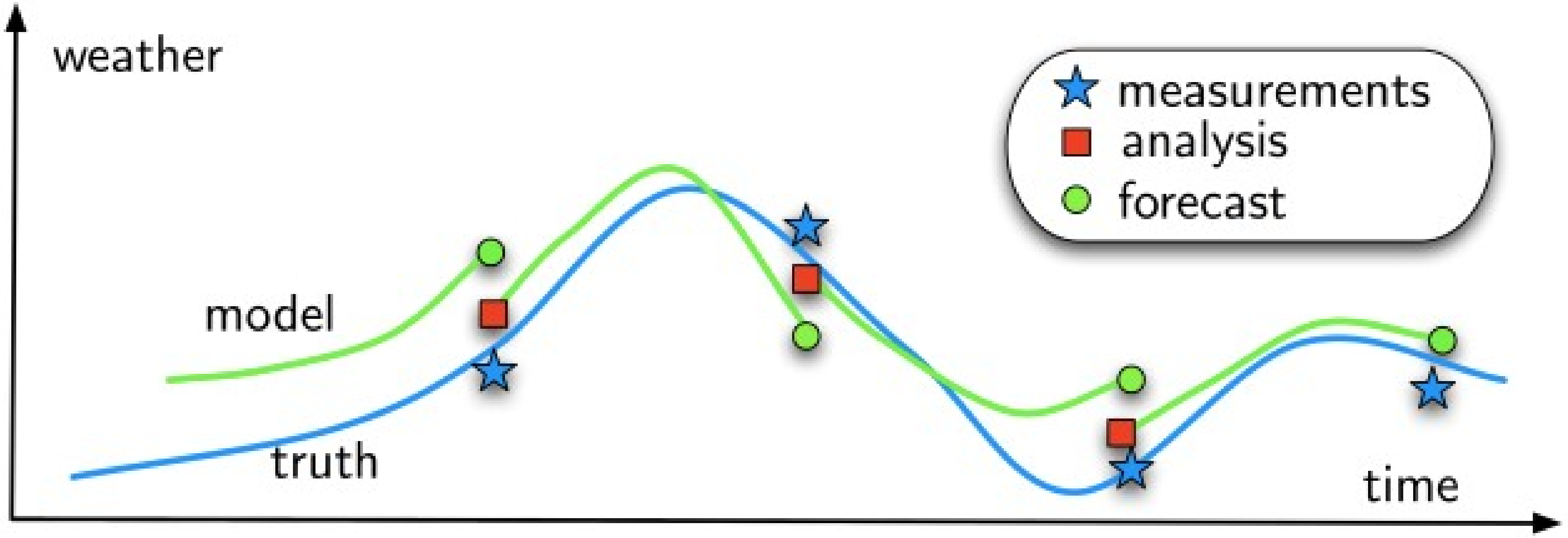
Data Assimilation



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Optimal Interpolation

$$\mathbf{x}_t - \mathbf{x}_b = \mathbf{W}[\mathbf{y}_o - H(\mathbf{x}_b)] - \varepsilon_a = \mathbf{W}\mathbf{d} - \varepsilon_a$$

$$\varepsilon_a = \mathbf{x}_a - \mathbf{x}_t$$

- Truth, analysis and background are vectors of length n
- Weights **W** are (n×p) matrix
- y_0: Observation
- x_t: Truth
- Observations are vector of length p
- Observational operator H can be nonlinear

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Optimal Interpolation

Observational increments vector:

$$\mathbf{d} = \mathbf{y}_o - H(\mathbf{x}_b)$$

We define background and analysis error as:

$$\boldsymbol{\varepsilon}_b(x, y) = \mathbf{x}_b(x, y) - \mathbf{x}_t(x, y)$$

$$\boldsymbol{\varepsilon}_a(x, y) = \mathbf{x}_a(x, y) - \mathbf{x}_t(x, y)$$

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Optimal Interpolation

Observational errors (at irregularly spaced points)

$$\boldsymbol{\varepsilon}_{oi} = \mathbf{y}_o(\mathbf{r}_i) - \mathbf{y}_t(\mathbf{r}_i) = \mathbf{y}_o(\mathbf{r}_i) - H[\mathbf{x}_t(\mathbf{r}_i)]$$

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Optimal Interpolation

We define error covariance matrices:

$$\mathbf{P}_a = \mathbf{A} = E\left\{\boldsymbol{\varepsilon}_a \boldsymbol{\varepsilon}_a^T\right\}$$

$$\mathbf{P}_b = \mathbf{B} = E\left\{\boldsymbol{\varepsilon}_b \boldsymbol{\varepsilon}_b^T\right\}$$

$$\mathbf{P}_o = \mathbf{R} = E\left\{\boldsymbol{\varepsilon}_o \boldsymbol{\varepsilon}_o^T\right\}$$

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Optimal Interpolation

The nonlinear observation operator H that transforms model variables into observed variables can be linearized as:

$$H(\mathbf{x} + \delta \mathbf{x}) = H(\mathbf{x}) + \mathbf{H}\delta \mathbf{x}$$

where **H** is a p×n matrix, denoting the linear observation operator with elements

$$h_{i,j} = \partial H_i / \partial x_j$$

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Optimal Interpolation

We assume that the background is a good approximation of the truth, so that the analysis and the observations are equal to the background values plus small increments

$$\mathbf{d} = \mathbf{y}_o - H(\mathbf{x}_b) = \mathbf{y}_o - H(\mathbf{x}_t + (\mathbf{x}_b - \mathbf{x}_t))$$

$$= \mathbf{y}_o - H(\mathbf{x}_t) - \mathbf{H}(\mathbf{x}_b - \mathbf{x}_t) = \boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b$$

The **H** matrix transforms vectors from model to observation space.
Its transpose or adjoint $\mathbf{H}^T$ transforms vectors from observation to model space.

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Optimal Interpolation

Best unbiased estimation: Least Squares

$$\mathbf{W} = E\left(\mathbf{x}\mathbf{y}^T\right)\left[E\left(\mathbf{y}\mathbf{y}^T\right)\right]^{-1}$$

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How to estimate W?

Multiple Regression

How to estimate W?

Multiple Regression

Assume we have two time series of vectors

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix} \qquad \mathbf{y}(t) = \begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_p(t) \end{bmatrix}$$

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How to estimate W?

Multiple Regression

We now derive the best linear unbiased estimation of **x** in terms of **y**, the optimal value of **W**

$$\mathbf{x}_a(t) = \mathbf{W}\mathbf{y}(t)$$

which approximates the true relationship

$$\mathbf{x}(t) = \mathbf{W}\mathbf{y}(t) - \varepsilon(t)$$

linear regression (analysis) error

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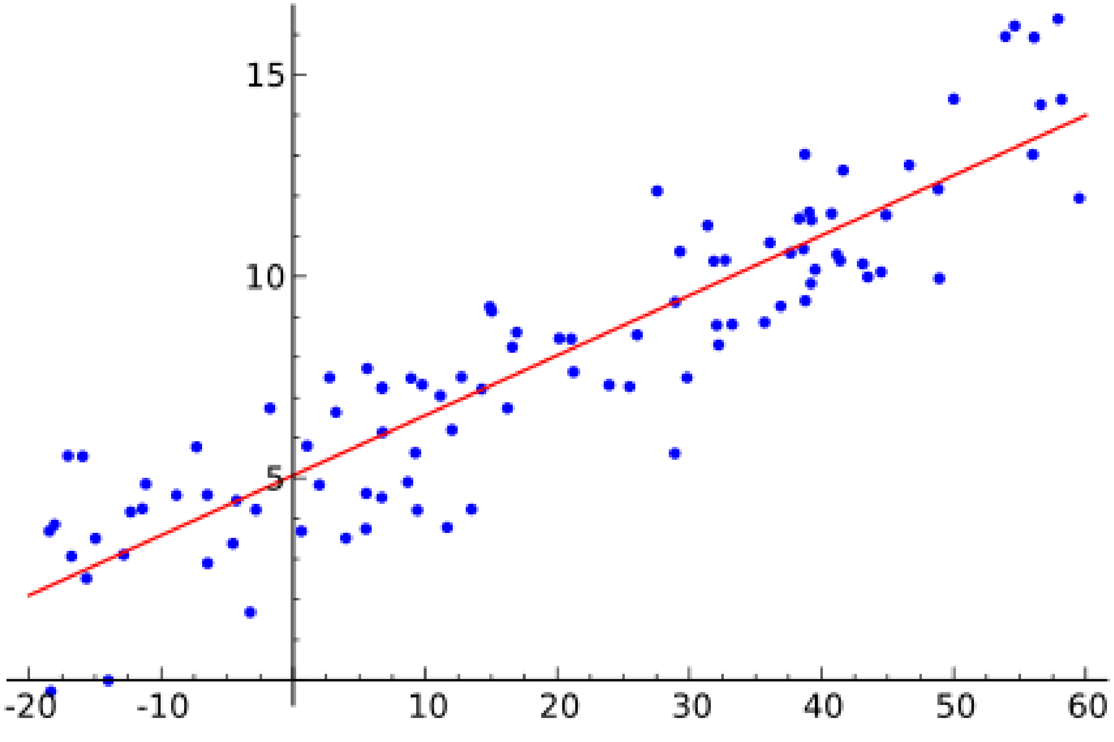
How to estimate W?



Sewaqu 2010

How to estimate W?

W minimizes mean squared error $E(\varepsilon^T \varepsilon)$

$$x_i(t) = \sum_{k=1}^{p} w_{ik} y_k(t) - \varepsilon_i(t)$$

$$\longrightarrow \quad \sum_{i=1}^{n} \varepsilon_i^2(t) = \sum_{i=1}^{n} \left[\sum_{k=1}^{p} w_{ik} y_k(t) - x_i(t) \right]^2$$

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How to estimate W?

Derivative with respect to weight matrix

$$\frac{\partial \sum_{i=1}^{n} \varepsilon_i^2(t)}{\partial w_{ij}} = 2\left[\sum_{k=1}^{p} w_{ik} y_k(t) - x_i(t)\right]\left[y_j(t)\right]$$

$$= 2\left[\sum_{k=1}^{p} w_{ik} y_k(t) y_i(t) - x_i(t) y_j(t)\right]$$

in Matrix form

$$\frac{\partial \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}}{\partial w_{ij}} = 2\left\{\left[\mathbf{W}\mathbf{y}(t)\mathbf{y}^T(t)\right]_{ij} - \left[\mathbf{x}(t)\mathbf{y}^T(t)\right]_{ij}\right\}$$

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How to estimate W?

We get the normal equations

$$\mathbf{W}E\left(\mathbf{y}\mathbf{y}^T\right) - E\left(\mathbf{x}\mathbf{y}^T\right) = 0$$

or

$$\mathbf{W} = E\left(\mathbf{x}\mathbf{y}^T\right)\left[E\left(\mathbf{y}\mathbf{y}^T\right)\right]^{-1}$$

which gives the best unbiased estimation

$$\mathbf{x}_a(t) = \mathbf{W}\mathbf{y}(t)$$

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Optimal Interpolation

Best unbiased estimation: Least Squares

$$\mathbf{W} = E\left(\mathbf{x}\mathbf{y}^T\right)\left[E\left(\mathbf{y}\mathbf{y}^T\right)\right]^{-1}$$

Estimate of weight matrix:

$$\begin{aligned}\mathbf{W} &= E\{(\mathbf{x}_t - \mathbf{x}_b)[\mathbf{y}_o - H(\mathbf{x}_b)]^T\}(E\{[\mathbf{y}_o - H(\mathbf{x}_b)][\mathbf{y}_o - H(\mathbf{x}_b)]^T\})^{-1} \\ &= E[(-\boldsymbol{\varepsilon}_b)(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T]\{E[(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T]\}^{-1}\end{aligned}$$

$$\mathbf{W} = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$$

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Optimal Interpolation

The analysis covariance matrix is:

$$\mathbf{P}_a = E\{\boldsymbol{\varepsilon}_a \boldsymbol{\varepsilon}_a^T\} = E\{\boldsymbol{\varepsilon}_b \boldsymbol{\varepsilon}_b^T + \boldsymbol{\varepsilon}_b(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T \mathbf{W}^T$$
$$+\mathbf{W}(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)\boldsymbol{\varepsilon}_b^T + \mathbf{W}(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T \mathbf{W}^T\}$$
$$= \mathbf{B} - \mathbf{B}\mathbf{H}^T\mathbf{W}^T - \mathbf{W}\mathbf{H}\mathbf{B} + \mathbf{W}\mathbf{R}\mathbf{W}^T + \mathbf{W}\mathbf{H}\mathbf{B}\mathbf{H}^T\mathbf{W}^T$$

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Optimal Interpolation

The analysis covariance matrix is:

$$\begin{aligned}\mathbf{P}_a = E\{\boldsymbol{\varepsilon}_a\boldsymbol{\varepsilon}_a^T\} = E\{&\boldsymbol{\varepsilon}_b\boldsymbol{\varepsilon}_b^T + \boldsymbol{\varepsilon}_b(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T\mathbf{W}^T \\ &+\mathbf{W}(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)\boldsymbol{\varepsilon}_b^T + \mathbf{W}(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b)^T\mathbf{W}^T\} \\ = \mathbf{B} - \mathbf{B}\mathbf{H}^T\mathbf{W}^T - \mathbf{W}\mathbf{H}\mathbf{B} + \mathbf{W}\mathbf{R}\mathbf{W}^T + \mathbf{W}\mathbf{H}\mathbf{B}\mathbf{H}^T\mathbf{W}^T&\end{aligned}$$

This can be written as:

$$\mathbf{P}_a = (\mathbf{I} - \mathbf{W}\mathbf{H})\mathbf{B}$$

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Summary of OI

Basic equations of OI:

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{W}[\mathbf{y}_o - H(\mathbf{x}_b)] = \mathbf{x}_b + \mathbf{W}\mathbf{d}$$

$$\mathbf{W} = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$$

$$\mathbf{P}_a = (\mathbf{I}_n - \mathbf{W}\mathbf{H})\mathbf{B}$$

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Summary of OI

Interpretation

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{W}[\mathbf{y}_o - H(\mathbf{x}_b)] = \mathbf{x}_b + \mathbf{W}\mathbf{d}$$

The analysis is obtained by adding to the first guess the product of the optimal weight matrix and the innovation (difference between observation and first guess).

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Summary of OI

Interpretation

$$\mathbf{W} = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$$

The optimal weight matrix is given by the background error covariance in the observation space ($\mathbf{BH}^T$) multiplied by the inverse of the total error covariance.

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Summary of OI

Interpretation

$$\mathbf{P}_a = (\mathbf{I}_n - \mathbf{WH})\mathbf{B}$$

The error covariance of the analysis is given by the error covariance of the background, reduced by a matrix equal to the identity matrix minus the optimal weight matrix.

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3D-VAR ~ OI

- OI: Find optimal weight matrix **W** that minimizes the analysis error covariance

- 3D-VAR: Find optimal analysis field that minimizes a cost function

$$2J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + [\mathbf{y}_o - H(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y}_o - H(\mathbf{x})]$$

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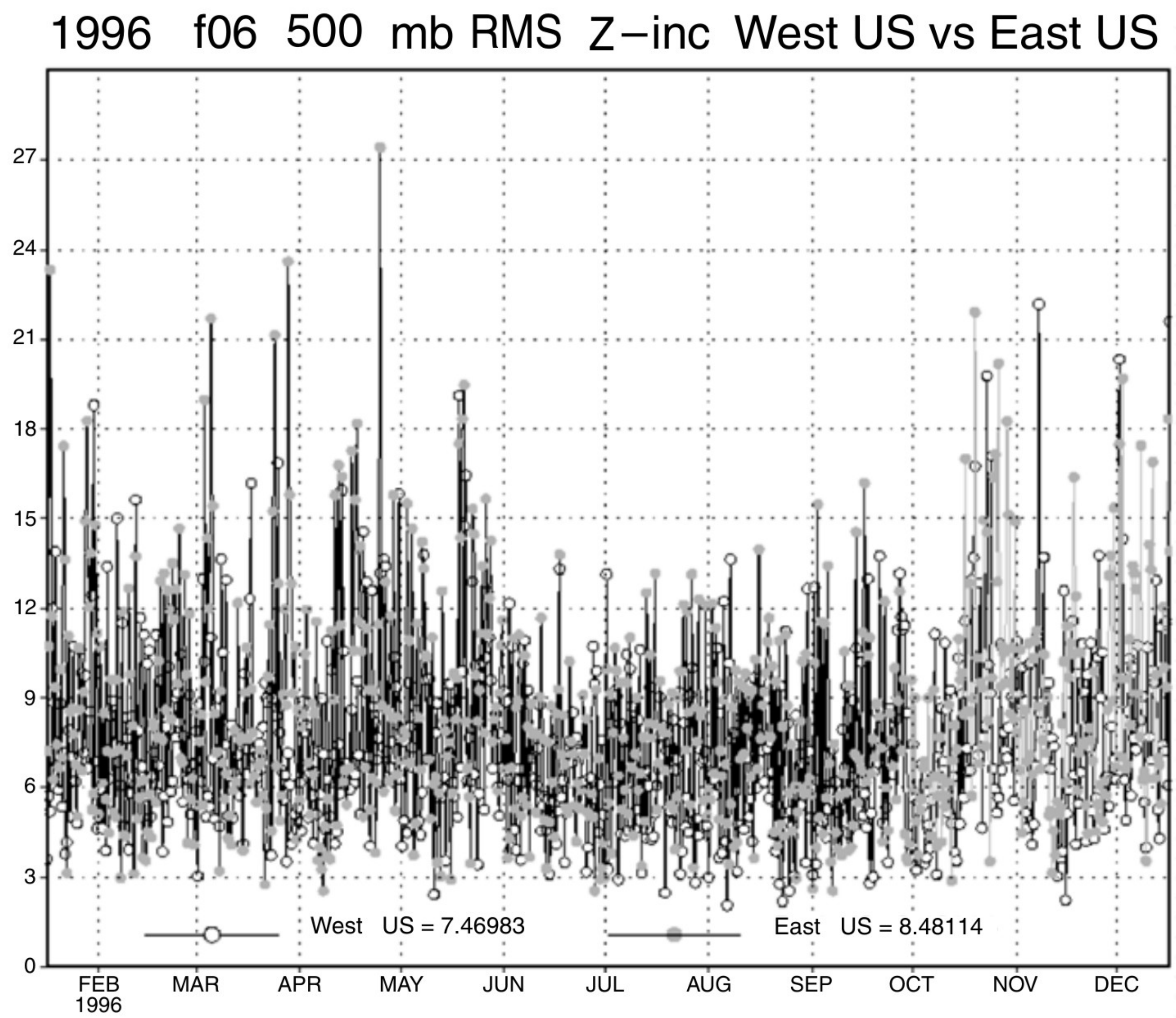
DA with evolving error covariance



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3D-VAR ~ 4D-VAR

3D-VAR

$$2J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + [\mathbf{y}_o - H(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y}_o - H(\mathbf{x})]$$

4D-VAR

$$J[\mathbf{x}(t_0)] = \frac{1}{2}[\mathbf{x}(\mathrm{t}_0) - \mathbf{x}^b(t_0)]^T \mathbf{B}_0^{-1} [\mathbf{x}(\mathrm{t}_0) - \mathbf{x}^b(t_0)] + \frac{1}{2}\sum_{i=0}^{N} \left[H(\mathbf{x}_i) - \mathbf{y}_i^0\right]^T \mathbf{R}_i^{-1} \left[H(\mathbf{x}_i) - \mathbf{y}_i^o\right]$$

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4D-VAR

$$J[\mathbf{x}(t_0)] = \frac{1}{2}[\mathbf{x}(\mathrm{t}_0) - \mathbf{x}^b(t_0)]^T \mathbf{B}_0^{-1}[\mathbf{x}(\mathrm{t}_0) - \mathbf{x}^b(t_0)] + \frac{1}{2}\sum_{i=0}^{N}\left[H(\mathbf{x}_i) - \mathbf{y}_i^0\right]^T \mathbf{R}_i^{-1}\left[H(\mathbf{x}_i) - \mathbf{y}_i^o\right]$$

The cost function includes a term measuring the distance to the background at the beginning of the interval and a summation over time of the cost function for each observation increment

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4D-VAR

4D-Var seeks an initial condition such that the forecast best fits the observations within the assimilation interval.

4D-Var assumes **perfect model**
→ Big disadvantage

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Kalman Filter ~ OI

In OI the forecast error covariance is computed once and for all.
Assumption: Forecast errors are statistically stationary

Kalman filter propagates error covariance forward
→ State-dependent error covariance

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Extended Kalman Filter

Forecast step:

Nonlinear model

$$\mathbf{x}^f(t_i) = M_{i-1}[\mathbf{x}^a(t_{i-1})]$$

$$\mathbf{P}^f(t_i) = \mathbf{L}_{i-1}\mathbf{P}^a(t_{i-1})\mathbf{L}_{i-1}^T + \mathbf{Q}(t_{i-1})$$

Tangent linear

Analysis step:

$$\mathbf{x}^a(t_i) = \mathbf{x}^f(t_i) + \mathbf{K}_i\mathbf{d}_i$$

$$\mathbf{P}^a(t_i) = (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\mathbf{P}^f(t_i)$$

$$\mathbf{d}_i = \mathbf{y}_i^o - H[\mathbf{x}^f(t_i)]$$

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Kalman Filter

1) Define ensemble of observations

$y^o_j = y^o + \varepsilon_j$

Kalman Filter

1) Define ensemble of observations

$y^o_j = y^o + \varepsilon_j$

2) Define ensemble covariance matrix

$R_e = \overline{\varepsilon\varepsilon^T}$

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Kalman Filter

1) Define ensemble of observations

$$y^o_j = y^o + \varepsilon_j$$

2) Define ensemble covariance matrix

$$R_e = \overline{\varepsilon\varepsilon^T}$$

3) Analysis step

$$y^a_j = y^f_j + P^f_e H^T (H P^f_e H^T + R_e)^{-1} (y^o_j - H y^f_j)$$

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Kalman Filter

3) Analysis step

$$y^a_j = y^f_j + P^f_e H^T (H P^f_e H^T + R_e)^{-1} (y^o_j - H y^f_j)$$

4) Analysis and ensemble mean are identical

$$\overline{y}^a_j = \overline{y}^f_j + P^f_e H^T (H P^f_e H^T + R_e)^{-1} (\overline{y}^o_j - H \overline{y}^f_j)$$

5) Kalman gain (Optimal weight) matrix

$$K_e = P^f_e H^T (H P^f_e H^T + R_e)^{-1}$$

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Kalman Filter

5) Kalman gain (Optimal weight) matrix

$$K_e = P^f_e H^T (H P^f_e H^T + R_e)^{-1}$$

6) Error covariance

$$P^a_e = (I - K_e H) P^f_e$$

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Kalman Filter

5) Kalman gain (Optimal weight) matrix

$$K_e = P^f_e H^T (H P^f_e H^T + R_e)^{-1}$$

6) Error covariance

$$P^a_e = (I - K_e H) P^f_e$$

7) Model error covariance Q

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Kalman Filter

5) Kalman gain (Optimal weight) matrix

$$K_e = P^f_e H^T (H P^f_e H^T + R_e)^{-1}$$

6) Error covariance

$$P^a_e = (I - K_e H) P^f_e$$

7) Model error covariance Q

8) Ensemble error covariance evolves as

$P^{k+1}_e = F P^k_e F^T + Q + \text{n.l.}$ (F: tangent linear operator)

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Ensemble Kalman Filter

- An ensemble of K data assimilation cycles is carried out simultaneously
- All cycles assimilate the same observations
- Different perturbations are added to observations → ensemble forecasts
- This ensemble is used to estimate forecast error covariance

Ensemble mean

$$\mathbf{P}^f \approx \frac{1}{K-1}\sum_{k=1}^{K}\left(\mathbf{x}_k^f - \overline{\mathbf{x}}^f\right)\left(\mathbf{x}_k^f - \overline{\mathbf{x}}^f\right)^T$$

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Ensemble Kalman Filter

- Evolve each ensemble member forward using the nonlinear model perturbed by noise
  $y^a = M(y^f) + \varepsilon$
- Compute ensemble mean and covariance
  $\overline{y^f} = 1/N\boldsymbol{\Sigma} y^f$
  $P^f = y^f (y^f)^T = 1/(N-1)\boldsymbol{\Sigma}(y^f - \overline{y^f})(y^f - \overline{y^f})^T$
- Update analysis
  $y^a = y^f + P^f K(y^o - Hy^f)$

  $K = P^f H^T (HP^f H^T + R)^{-1}$
  Where R is the covariance from the observations

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Excercise

Write a Ensemble Kalman Filter for Lorenz 96