Project V. Ensemble Kalman Filter (EnKF)

- Dates
  - 10min presentation: 2013.04.25 & 04.30 in-class
    - Order to be announced
  - Report: 2013.05.01 5pm by email

- Objectives: Implementation of Ensemble Kalman Filter based on
  - Data Assimilation Framework (Project 1)
  - Ensemble representation of EKF (Project 3)
    - Understanding of dynamic propagation of uncertainty using tangent linear model (EKF) vs nonlinear model (EnKF)
    - Schemes to improve the performance: Inflation and localization
    - Understanding strength & weakness of EnKF as data assimilation method
  - Diagnostic tools (Projects 1-4 and Exercises 2&5)
Project V. Ensemble Kalman Filter (EnKF)

- Project Description (as reference – you are welcome to improvise)
  - Objective:
    - Implementation of at least
      - Perturbed-Observation EnKF
        and only if possible
      - Serial Ensemble square-root KF (EnSRF)
      - [Local] Ensemble Transform KF ([L]ETKF)
    - Verification of ensemble analysis
      - in comparison with “adjusted” EKF analysis, given the choice of the EnKF method (slide 3)
  - Diagnostics: Having successfully implemented the EnKF,
    - Comparison of the results with:
      - EKF (& 3D-Var/OI) and 4D-Var
      - truth: actual error $|\mathbf{x}^b-\mathbf{x}^t|^2$ & $|\mathbf{x}^a-\mathbf{x}^t|^2$ vs estimated error by $\text{var}\{\mathbf{x}_m^b\} & \text{var}\{\mathbf{x}_m^a\}$
    - Study the effects of
      - Size of ensemble (start from $M=N$, and in/decrease)
      - Covariance inflation
      - Covariance localization
    - Case study (not statistics) in which EnKF failed, and identify the cause, for example
      - Observations: Insufficient obs? Too large obs error?
      - Background: Failed forecast due to nonlinearity?
      - Analysis: Inappropriate inflation and Localization?
Schematics of Ensemble Kalman Filter

**Assimilation cycle**

- **Model**
  - Forecast: \( \{x^a_{k,m}\} \)
  - \( \frac{d}{dt} x^b_m = f(x^b_m, t) \)

- **Observation**
  - Measurement: \( (y^o_k, R^o_k) \)
  - \( y^o_k = h_k(x^t_k) + \epsilon^t_k : \epsilon^t_k \sim N(0, R^t_k) \)

- **Optimization**
  - Analysis: \( \{x^a_{k,m}\} \)
  - Several methods exist
  - No one method is the most optimal.

- Ensemble attempts to satisfy (for min. var.)

\[
\begin{align*}
x^a_k &= x^t_k + K_k (y^o_k - h(x^b_k)) \\
K_k &= P_k^b (H_k)^T (R^o_k + H_k P_k^b (H_k)^T)^{-1} \\
H_k &= \frac{\partial}{\partial x} h_k(x^b_k)
\end{align*}
\]

- **Initial ensemble**
- \( \{x^a_{k-1,m}\} \)

- **Forecast ensemble**
- \( \{x^b_{k,m}\} \)

- **Assimilation window**
Basic Ensemble Operations (Notation)

- In $\mathbf{x}$-space based on ensemble $\{\mathbf{x}_m\}$
  - Ensemble $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_M\} \in \mathbb{R}^{N \times M}$
  - Mean $\bar{\mathbf{x}} = \frac{1}{M} \sum_{m=1}^{M} \mathbf{x}_m \in \mathbb{R}^N$
  - Spread $\hat{\mathbf{X}} = \{\mathbf{x}_1 - \bar{\mathbf{x}}, \ldots, \mathbf{x}_M - \bar{\mathbf{x}}\} \in \mathbb{R}^{N \times M}$
  - Covariance $\hat{\mathbf{P}} = \frac{1}{M-1} \hat{\mathbf{X}}\hat{\mathbf{X}}^T \in \mathbb{R}^{N \times N}$

- In $\mathbf{y}$-space based on ensemble $\{\mathbf{y}_m\}$
  - Ensemble $\mathbf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_M\} = \{\mathbf{h}(\mathbf{x}_1), \ldots, \mathbf{h}(\mathbf{x}_M)\} \in \mathbb{R}^{L \times M}$
  - Mean $\bar{\mathbf{y}} = \frac{1}{M} \sum_{m=1}^{M} \mathbf{y}_m = \frac{1}{M} \sum_{m=1}^{M} \mathbf{h}(\mathbf{x}_m) \in \mathbb{R}^L$
  - Spread $\hat{\mathbf{Y}} = \{\mathbf{y}_1 - \bar{\mathbf{y}}, \ldots, \mathbf{y}_M - \bar{\mathbf{y}}\} \in \mathbb{R}^{L \times M}$
  - Projection of covariances ("=" holds if linear, i.e., $\mathbf{h}(\mathbf{x}) = \mathbf{Hx}$)
    $\mathbf{P}\mathbf{H}^T \approx \frac{1}{M-1} \hat{\mathbf{X}}\hat{\mathbf{Y}}^T \in \mathbb{R}^{L \times N}$ \& $\mathbf{H}\hat{\mathbf{P}}^T \approx \frac{1}{M-1} \hat{\mathbf{Y}}\hat{\mathbf{Y}}^T \in \mathbb{R}^{L \times L}$

- Essential schemes for analysis
  - Inflation
  - Localization
Formulation: Perturbed observation EnKF & ETKF

- Perturbed observation EnKF
  \[ x^a_m = x^b_m + \hat{K}(y^o_m - y^b_m) \]
  \[ \hat{K} = \frac{1}{M-1} \hat{X}Y^T (\frac{1}{M-1} \hat{Y}Y^T + R)^{-1} \in \mathbb{R}^{N \times L} \]
  \[ y^o_m = y^o + e^o_m \quad e^o_m \text{ is drawn from } \mathcal{N}(0, R^o) \]

- Inflation: common to all EnKF methods
  - For simplicity, multiplicative inflation to background ensemble spread:
    \[ \hat{X}^b \Rightarrow \rho \hat{X}^b \quad \text{with } \rho \geq 1 \]
  - Other approaches to inflation
    - Additive: \[ \hat{X}^b \Rightarrow \hat{X}^b + \hat{X}^r \quad \text{where } \hat{X}^r \in \mathbb{R}^{N \times M} \text{ is small random matrix} \]
    - Relaxation to background:
      \[ \hat{X}^a \Rightarrow \mu \hat{X}^a + (1-\mu) \hat{X}^b \quad \text{with } \mu \subset [0,1] \]


**Formulation: Perturbed observation EnKF**

- Localization: from observations

\[
\hat{X}^b_{(i)}(\hat{Y}^b_{(j)})^T \Rightarrow c(r_{(ij)}) \circ \hat{X}^b_{(i)}(\hat{Y}^b_{(j)})^T
\]

\[
\hat{Y}^b_{(j)}(\hat{Y}^b_{(i)})^T \Rightarrow c(r_{(ij)}) \circ \hat{Y}^b_{(j)}(\hat{Y}^b_{(i)})^T
\]

- Localization:
  - Model dependent scale length
  - Typical localization function: Gaussian

\[
c(r) = \begin{cases} 
\exp(-(r/R)^2) & \text{if } r \leq R_{CS} \sim 3R \\
0 & \text{otherwise}
\end{cases}
\]

- Localization:
  - Distance between:
    - Obs position \( l \): \( Y^b_{(l)} \) [subset of \( Y^b \)]
    - Grid point \( n \): \( X^b_{(i)} \) [subset of \( X^b \)]
    - Obs position \( i \): \( Y^b_{(li)} \) [subset of \( Y^b \)]
    - Obs position \( l \): \( Y^b_{(l)} \) [subset of \( Y^b \)]
Perturbed observation EnKF
\[ x_m^a = x_m^b + \hat{K}(y_m^o - y_m^b) \]
\[ \hat{K} = \frac{1}{M-1} \hat{X}^T (\frac{1}{M-1} \hat{Y}^T + R)^{-1} \in \mathbb{R}^{N \times L} \]
\[ y_m^o = y_m^o + e_m^o \quad e_m^o \text{ is drawn from } \mathcal{N}(0,R^o) \]

ETKF
\[ \bar{x}^a = \bar{x}^a + \hat{X}^b \bar{w}^a \quad \bar{w} \in \mathbb{R}^M \]
\[ \hat{x}^a = \hat{x}^b \bar{W}^a \quad \bar{W} \in \mathbb{R}^{M \times M} \]

where
\[ (\bar{P}^b)^{-1} \equiv (M-1)I \]
\[ \bar{P}^a = ((\bar{P}^b)^{-1} + (\hat{Y}^b)^T (R^o)^{-1} (\hat{Y}^b))^{-1} \]
\[ \bar{w}^a = \bar{P}^a (\hat{Y}^b)^T (R^o)^{-1} (y^o - \bar{y}^b) \]
\[ \bar{W}^a = ((M-1)\bar{P}^a)^{1/2} \]
Formulation: EnSRF

- EnSRF by serial assimilation
  - Starting from $\hat{x}^{(0)} = \hat{x}^b$
    
    $$\bar{x}^{(l)} = x^{(l-1)} + \hat{K}^{(l)}(y^l_h - h_j(x^{(l-1)}))$$
  
  - For $l=1,...,L$:
    $$\hat{x}^{(l)} = \hat{x}^{(l-1)} - \beta^{(l)}\hat{K}^{(l)}\hat{Y}^{(l-1)}$$
    
    $$[=(I-\beta^{(l)}\hat{K}^{(l)}H_j)\hat{x}^{(l-1)} \text{ if } h_j(x) \text{ is linear } ]$$

where

$$\bar{Y}^{(l-1)} = \frac{1}{M} \sum_{m=1}^{M} h_j(x_m^{(l-1)})$$

$$\hat{Y}^{(l-1)} = \{h_j(x_m^{(l-1)}) - \bar{Y}^{(l-1)}\} \in \mathbb{R}^{1 \times M}$$

$$(\gamma^{(l)}, \alpha^{(l)}, \beta^{(l)}) = (\hat{Y}^{(l-1)}(\hat{Y}^{(l-1)})^T / (M - 1), \gamma^{(l)}, \gamma^{(l)} + R^0, (1 + \sqrt{R^0 / \alpha^{(l)}})^{-1} )$$

$$\hat{K}^{(l)} = (M - 1)^{-1} \alpha^{-1} \hat{x}^{(l-1)}(\hat{Y}^{(l-1)})^T \in \mathbb{R}^{N \times 1}$$

- At $l=L$

$$\bar{x}^a = \bar{x}^{(L)}$$

$$\hat{x}^a = \hat{x}^{(L)}$$
Essential Schemes: Inflation & Localization

- Inflation: common to all EnKF methods
  - For simplicity, multiplicative inflation to background ensemble spread:
    \[ \hat{X}^b \rightarrow \rho \hat{X}^b \quad \text{with } \rho \geq 1 \]

- Other approaches to inflation
  - Additive:
  - Relaxation to background:
    \[ \hat{X}^r \Rightarrow \mu \hat{X}^b + (1-\mu) \hat{X}^b \quad \text{with } \mu \subset [0,1] \]

- Localization:
  - Model dependent (Lorenz 3 variable model does not require localization)
  - Typical localization function: Gaussian
    \[ c(r) = \begin{cases} 
    \exp\left(-\left(\frac{r}{R}\right)^2\right) & \text{if } r \leq R_{cs} (\sim 3R) \\
    0 & \text{otherwise}
    \end{cases} \]
Essential Schemes: Localization Based on Observation

- For Perturbed Observation EnKF & EnSRF:
  \[
  K = \frac{\mathbf{X}^b (\mathbf{Y}^b)^T}{(M - 1)} \left( \frac{\mathbf{Y}^b (\mathbf{Y}^b)^T}{(M - 1)} + R^o \right)^{-1}
  \]

  \( \hat{\mathbf{X}}^b (\hat{\mathbf{Y}}^b)^T \) and \( \hat{\mathbf{Y}}^b (\hat{\mathbf{Y}}^b)^T \)

- Spurious correlation in
- Localization is imposed based on distance from observation.

\( r_{(il)} \): distance between
  - obs position \( l \) : \( \mathbf{Y}^b_{(l)} \) [subset of \( \mathbf{Y}^b \)]
  - grid point \( n \) : \( \mathbf{X}^b_{(n)} \) [subset of \( \mathbf{X}^b \)]

\( r_{(jl)} \): distance between
  - obs position \( l \) : \( \mathbf{Y}^b_{(l)} \) [subset of \( \mathbf{Y}^b \)]
  - obs position \( i \) : \( \mathbf{Y}^b_{(il)} \) [subset of \( \mathbf{Y}^b \)]
Essential Schemes: Localization Based on Observation

- For ETKF (becomes LETKF)

\[
\tilde{P}^a = ((\tilde{P}^b)^{-1} + (\hat{Y}^b)^T (R^o)^{-1} (\hat{Y}^b))^{-1}
\]

- ETKF is performed at each grid point \( i \)
- Inverse of observation error covariance \( R^o \) for observation \( l \) used are weighted based on distance from the grid point

\[
(R^o_j)^{-1} \Rightarrow c(r_{ij})(R^o_j)^{-1}
\]