Overview of localization techniques for ensemble based Kalman filter algorithms

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Why ensemble Kalman filter

- The Kalman filter is difficult to implement in realistic systems because of:
  - computational costs,
  - the nonlinearity of dynamics and
  - poorly characterized error sources.
- The ensemble Kalamn filter (EnKF) (Evensen 1994) uses ensembles (a sample) to calculate the uncertainty of the background and analysis error covariance.
- Ensembles are propagated with full nonlinear numerical model. This can be done over long time period, and results in flow dependent covariances.

Pros of ensemble Kalman filter

- Cross correlations are represented naturally
- Covariances are flow dependent
- Computationally algorithm is not expensive

Cons of ensemble Kalman filter

- Only small number of ensembles can be evolved due to complexity of the dynamical systems;
- Due to the small ensemble numbers covariances are not representing correctly uncertainty, in particular long-distance correlations.
- The analysis increment is restricted to the r dimensional subspace.

Outline localization

- What is localization?
- Two basic approaches for localization:
  - Covariance localization or direct forecast error localization (used in Houtekamer and Mitchell (1998, 2001))
  - Domain localization (used in Haugen and Evensen 2002; Brusdal et al. 2003; Ott et al. 2004; Hunt et al. 2007; Miyoshi and Yamane 2007)
- Effects of localization on each of the steps of ensemble Kalman filter algorithm
- Simple 1D experiment
- Localization and Balance
- Conclusion

Step 1: Analysis

$$\mathbf{w}_k^a = \mathbf{w}_k^b + \mathbf{K}_k(\mathbf{y}_k^o - \mathbf{H}_k\mathbf{w}_k^b),$$

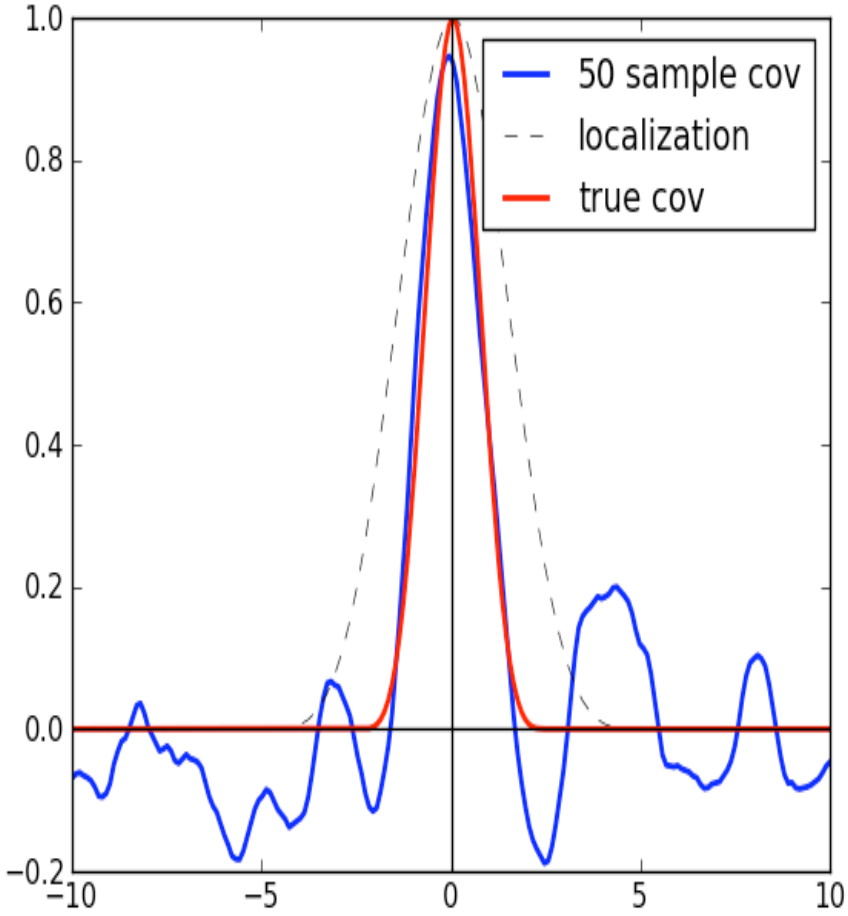
$\mathbf{K}_k$ is taken as

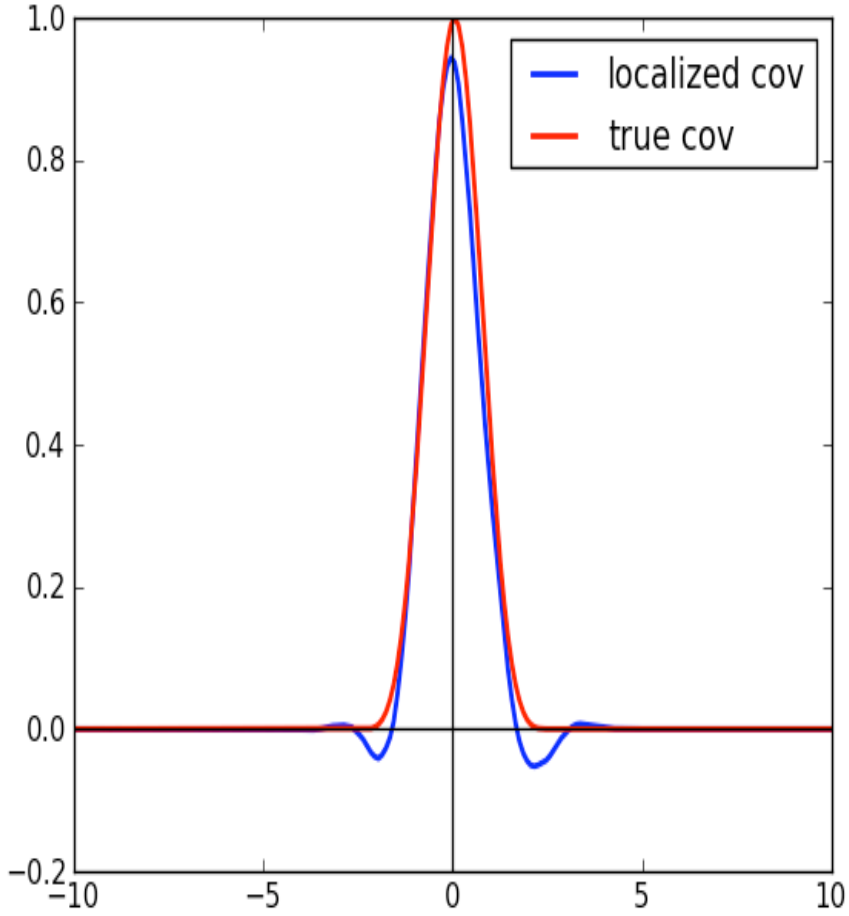
$$\mathbf{K}_k = \mathbf{B}_k^b\mathbf{H}_k^T(\mathbf{H}_k\mathbf{B}_k^b\mathbf{H}_k^T + \mathbf{R}_k)^{-1}$$

with $\mathbf{B}_k^b$ represented by:

$$\mathbf{B}_k^b = \frac{1}{r-1}\sum_{i=1}^{r}[\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T.$$

What is localization?





Estimates of the covariance from small ensemble size will be noisy, especially signal to noise ratio is large when covariances are small (from Hamill and Whitaker 2009).

Covariance localization

Covariance localization: The ensemble derived forecast error covariance matrix is Schur multiplied with a stationary a priori chosen correlation matrix that is compactly supported.

Let $\mathbf{C}$ be a matrix of rank M that is used for the Schur product.

$$\mathbf{C} \circ \mathbf{B}_k^b$$

Let $\circ$ denotes the element-wise product (Schur product) where

$$[\mathbf{C} \circ \mathbf{B}_k^b]_{ij} = [\mathbf{C}]_{ij}[\mathbf{B}_k^b]_{ij}$$

Covariance localization

Schur product theorem:

If $\mathbf{A}$, $\mathbf{B}$ are positive semi-definite matrices, then $\mathbf{A} \circ \mathbf{B}$ is also positive semi-definite. If $\mathbf{A}$, $\mathbf{B}$ are positive definite matrices, then $\mathbf{A} \circ \mathbf{B}$ is also positive definite.

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Let $\mathbf{C}$ be a matrix of rank M that is used for the Schur product. Let $\mathbf{v}_j$ represent eigenvectors of matrix $\mathbf{C}$ multiplied with the square root of the corresponding eigenvalue.

$$\mathbf{C} = \sum_{j=1}^{M} \mathbf{v}_j \mathbf{v}_j^T.$$

Covariance localization increases the rank of ensemble derived covariances

For any vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and $\mathbf{d}$:

$$(\mathbf{a} \circ \mathbf{c})(\mathbf{b} \circ \mathbf{d})^T = (\mathbf{a}\mathbf{b}^T) \circ (\mathbf{c}\mathbf{d}^T).$$

The localized error covariance $\mathbf{B}_k^b \circ \mathbf{C}$ can be represented as

$$\begin{aligned}
\mathbf{B}_k^b \circ \mathbf{C} &= \frac{1}{r-1} \sum_{i=1}^{r} [\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T \circ \sum_{j=1}^{M} \mathbf{v}_j \mathbf{v}_j^T \\
&= \frac{1}{r-1} \sum_{i,j=1}^{r,M} [\mathbf{w}_k^{b,i} - \mathbf{w}_k^b][\mathbf{w}_k^{b,i} - \mathbf{w}_k^b]^T \circ \mathbf{v}_j \mathbf{v}_j^T \\
&= = \sum_{i,j=1}^{r,M} \mathbf{u}_{i,j} \mathbf{u}_{i,j}^T
\end{aligned}$$

with $\mathbf{u}_{i,j} = \frac{1}{\sqrt{r-1}} [\mathbf{w}^{f,i}(t_k) - \mathbf{w}_k^b] \circ \mathbf{v}_j$

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$$\mathbf{w}_k^a = \mathbf{w}_k^b + \mathbf{K}_k(\mathbf{f}_k^o - \mathbf{H}_k\mathbf{w}_k^b)$$

$$\mathbf{w}_k^a - \mathbf{w}_k^b = \mathbf{W}_k^b\mathbf{T}_k{\mathbf{T}_k}^T(\mathbf{H}_k\mathbf{W}_k^b)^T\mathbf{R}_k^{-1}(\mathbf{f}_k^o - \mathbf{H}_k\mathbf{w}_k^b)$$

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- We have increased the subspace space where the solution is searched for.
- Matrices $\mathbf{W}_k^b$ is of size $n \times Mr$.

Step 2

In resampling step we can not produce an ensemble with size r if we use the analysis error covariance calculated from $\mathbf{W}_k^b = [\mathbf{u}_{1,1} \dots \mathbf{u}_{r,M}]$.

$$\mathbf{w}_k^{a,i} = \mathbf{w}_k^a + \sqrt{r-1}[\mathbf{W}_k^b \mathbf{T}_k \mathbf{U}]_i$$

One approach to limit the ensemble to r ensemble members that we can propagate to time $k+1$ around the newly calculated analysis:

- use instead $\mathbf{W}_k^b = \frac{1}{\sqrt{r-1}}[\mathbf{w}_k^{b,1} - \mathbf{w}_k^b \dots \mathbf{w}_k^{b,r} - \mathbf{w}_k^b]$

Example

The state vector **w** to be estimated will be taken as a realization of normally distributed random function $w(y) \sim \mathcal{N}(0, W(y_1, y_2))$ on the circle of radius $D/2\pi$, where the covariance $W(y_1, y_2)$ is either

$$W(y_1, y_2) = (1 + \frac{|y_1 - y_2|}{L}) e^{\frac{-|y_1 - y_2|}{L}}, \tag{1}$$

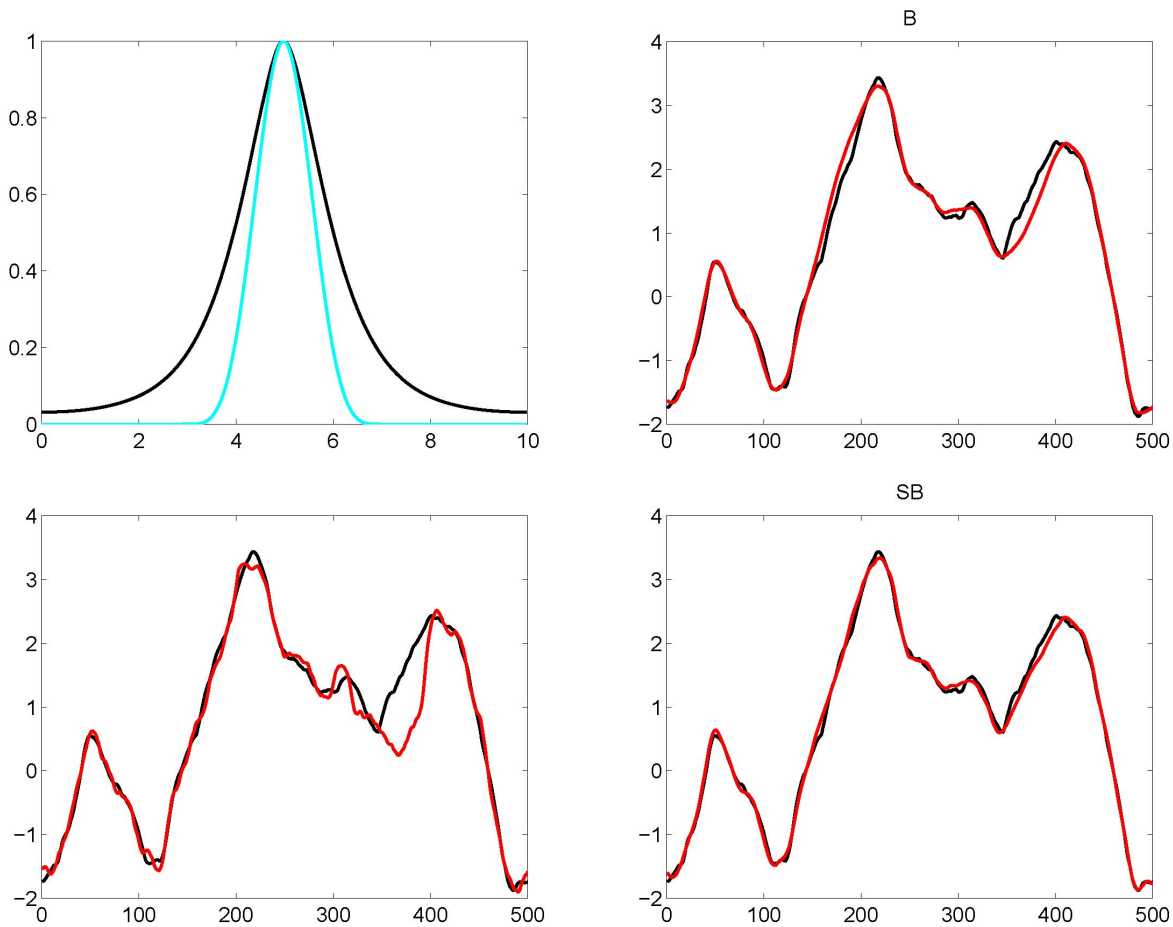
or

$$W(y_1, y_2) = e^{-\frac{|y_1 - y_2|}{L}}. \tag{2}$$

Here, $|y_1 - y_2|$ represents the chord length between the points y_1 and y_2 on the circle of radius $D/2\pi$.

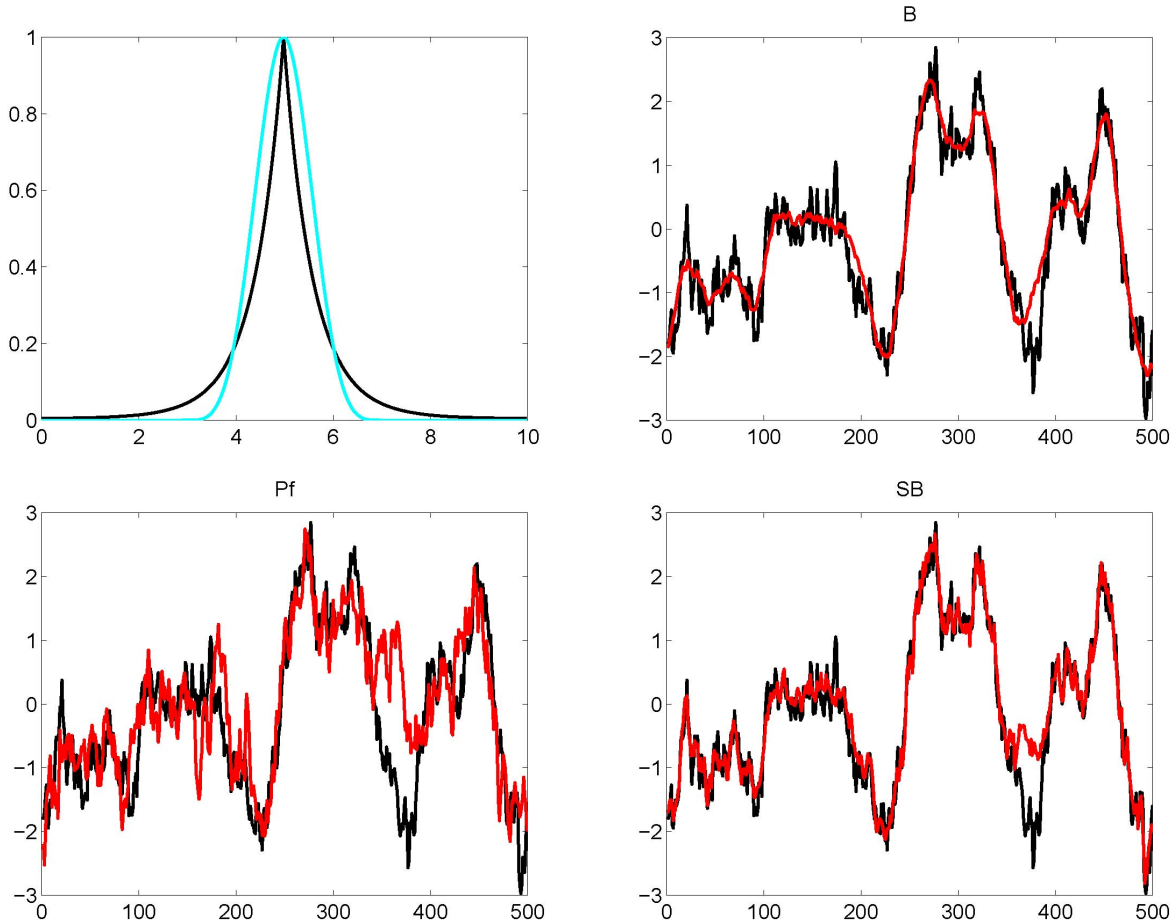
The observations are given as a vector of values of the realization at all grid points contaminated by normally distributed random noise with standard deviation of 0.05, the observations from two subdomains were removed.

Example $W(y_1, y_2) = (1 + \frac{|y_1 - y_2|}{L})e^{\frac{-|y_1 - y_2|}{L}}$



Upper Left: True covariance (black) and approximate C covariance (blue). Upper Right: True state (black) and analysis (red) after one assimilation step with approximate B covariance. Lower Left: True state (black) and analysis (red) after one assimilation step with ensemble covariance from 30 ensemble members. Lower Right: True state (black) and analysis (red) after one assimilation step with localized ensemble covariance.

Example nonsmooth field $W(y_1, y_2) = e^{-\frac{|y_1 - y_2|}{L}}$



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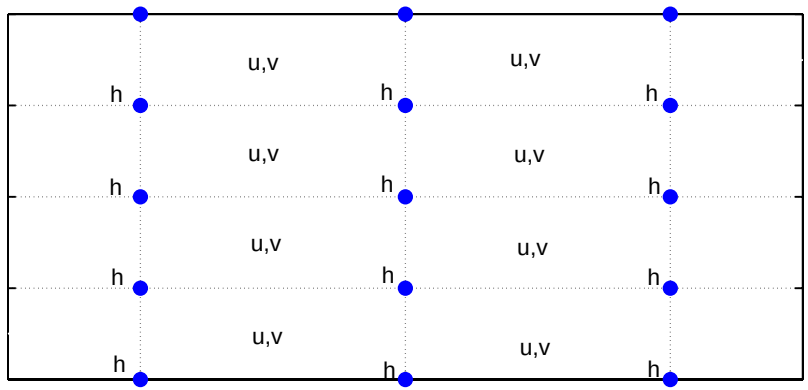
Covariance localization

- Distant correlation are removed
- Positive definite correlation matrix is introduced that increases the rank of forecast error covariance and this way
- increases the space where the solution can be searched for
- usually correlation function $\mathbf{C}$ is chosen full rank, positive definite, isotropic matrix, compactly supported. Usually 5th order polynomial correlation function (Gaspari and Cohn 1999).

Domain localization

Domain localization: Disjoint domains in the physical space are considered as domains on which the analysis is performed. Therefore, for each subdomain an analysis step is performed independently using observations not necessarily belonging only to that subdomain. Results of the local analysis steps are pasted together and then the global forecast step is performed.



Basic properties:

- The localized error covariance is calculated using

$$\mathbf{B}_k^{f,loc} = \sum_{i,j=1}^{r,L} \mathbf{u}_{i,j}\mathbf{u}_{i,j}^T \tag{3}$$

where $\mathbf{u}_{i,j} = \frac{1}{\sqrt{r}}[\mathbf{w}^{f,i}(t_k) - \mathbf{w}_k^b] \circ \mathbf{1}_{Dj}$ with $j = 1, \ldots, L$ and L is the number of subdomains. Here $\mathbf{1}_{Dj}$ is a vector whose elements are 1 if the corresponding point belongs to the domain Dj.

Domain localization

- $\mathbf{C}$ positive semidefinite, has block structure and is the sum of rank one matrices $\mathbf{1}_{Dj}\mathbf{1}_{Dj}^T$. The rank of matrix $\mathbf{C}$ corresponds to the number of subdomains.
- In case that $\text{rank}(\mathbf{C})\text{rank}(\mathbf{B}_k^f) < n$, the matrix $\mathbf{C} \circ \mathbf{B}_k^f$ is singular.
- In domain localization methods, the rank is not increased locally on each subdomain. Accordingly, it is possible to resample exactly on that subdomain in contrast to direct forecast error localization.
- Because the assimilations are performed independently in each local region, the smoothness of the analysis fields is of more concern in domain localization methods than with direct forecast error localization. In particular, two neighboring subdomains might produce strongly different analysis estimates when the assimilated observations have gaps, because distinct sets of observations are used for the analyses.

Ensemble based Kalman filters apply the observation operator directly on each ensemble member before localization is applied. The localization is usually performed on the matrices $\mathbf{H_k B}_k^b$ and $\mathbf{H_k B}_k^b \mathbf{H_k}^T$

$$\mathbf{H_k B}_k^b = \frac{1}{r} \sum_{i=1}^{r+1} [\mathbf{H_k}(\mathbf{x}^{f,i}(t_k)) - \mathbf{H_k}(\mathbf{x}_k^b)][\mathbf{x}^{f,i}(t_k) - \mathbf{x}_k^b]^T$$

$$\mathbf{H_k B}_k^b \mathbf{H_k}^T = \frac{1}{r} \sum_{i=1}^{r+1} [\mathbf{H_k}(\mathbf{x}^{f,i}(t_k)) - \mathbf{H_k}(\mathbf{x}_k^b)][\mathbf{H_k}(\mathbf{x}^{f,i}(t_k)) - \mathbf{H_k}(\mathbf{x}_k^b)]^T.$$

Once these matrices are calculated, they are Schur multiplied with the matrices $\mathbf{H_k C}$ and $\mathbf{H_k C H_k}^T$, respectively.

For the domain localization methods, different analysis results can be obtained depending on the treatment of the observations.

If all the observations in the full domain are used for the analysis in each disjoint subdomain, the algorithm without localization is recovered. This follows from

$$\frac{1}{r}\sum_{i=1}^{r+1}\sum_{j=1}^{L}[\mathbf{H_k}(\mathbf{x}^{f,i}(t_k)) - \mathbf{H_k}(\mathbf{x}_k^b)][\mathbf{x}^{f,i}(t_k)\circ\mathbf{1}_{D_j} - \mathbf{x}_k^b\circ\mathbf{1}_{D_j}]^T =$$

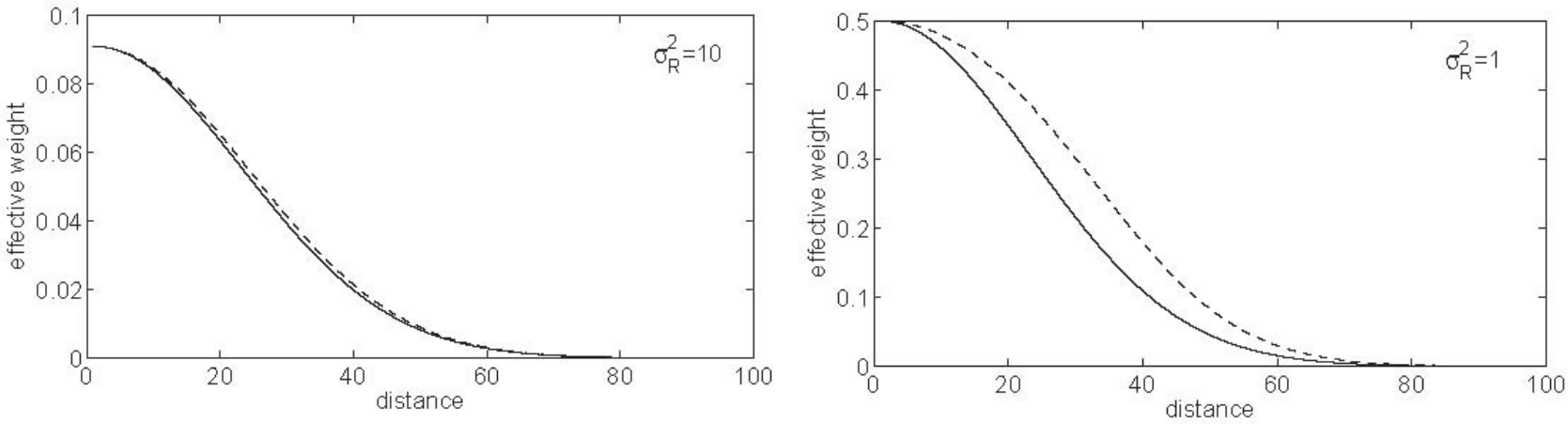
$$\frac{1}{r}\sum_{i=1}^{r+1}[\mathbf{H_k}(\mathbf{x}^{f,i}(t_k)) - \mathbf{H_k}(\mathbf{x}_k^b)][\mathbf{x}^{f,i}(t_k) - \mathbf{x}_k^b]^T = \mathbf{H_k}\mathbf{B}_k^b \ .$$

If, on the other hand, we restrict observations to the local analysis subdomains the covariance matrix is given by (3).

Observational error localization: Method (SD+ObLoc)

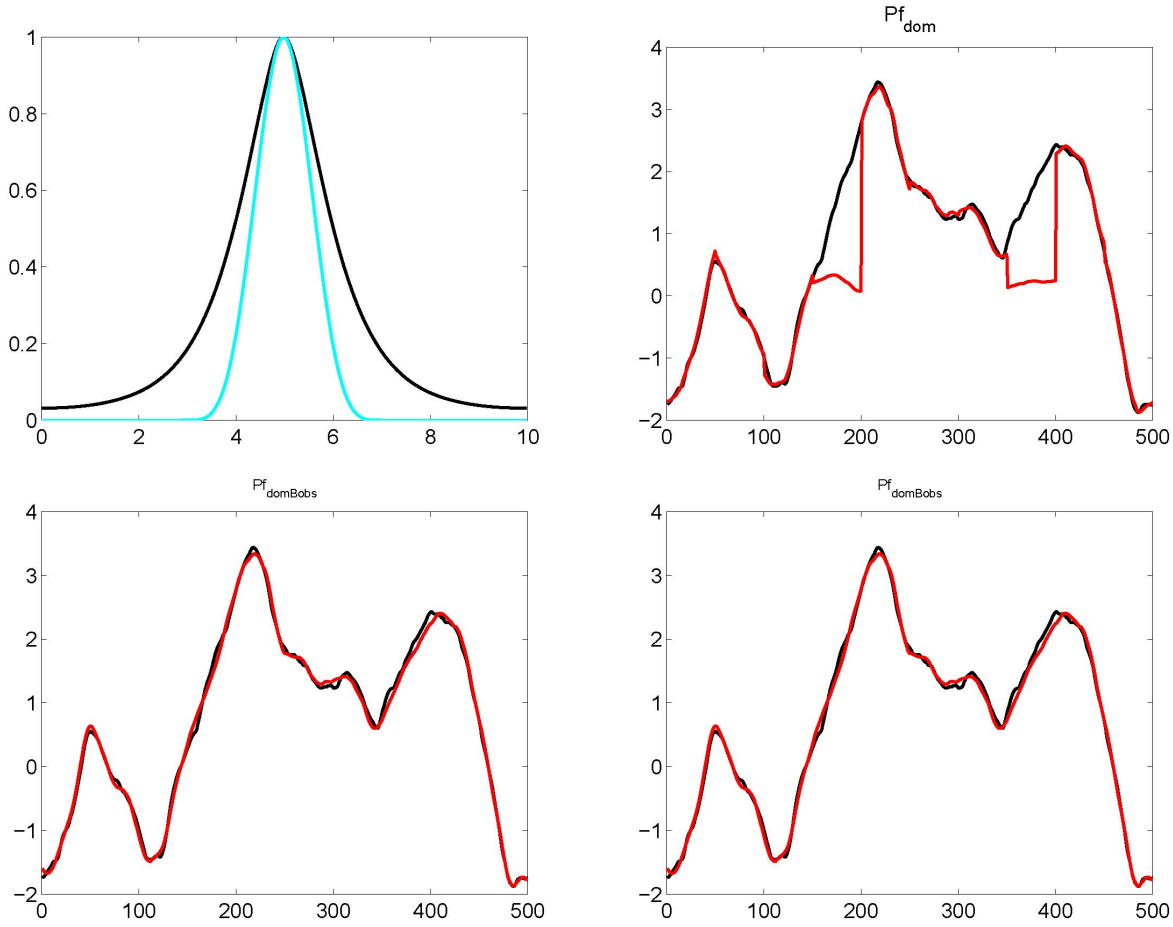
The observation localization method modifies the observational error covariance matrix **R**.

Let us consider a single observation example, in observation error localization method, the observation error σ^2_{obs} is modified to $\sigma^2_{obs}/weight_d$ where $weight_d$ can be calculated using any of the correlation functions.



Resampling step includes modification of **R**.

Example domain localization cont.



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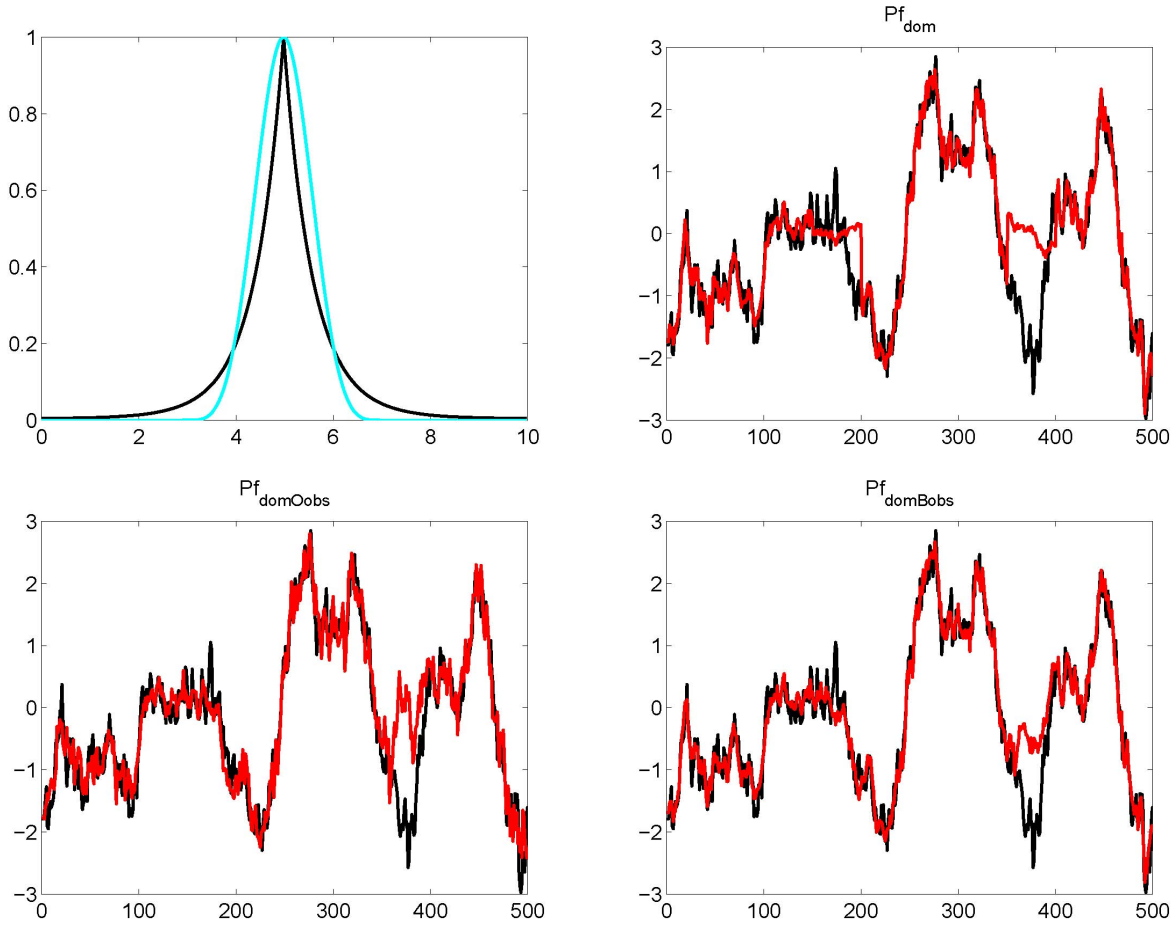

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Domain localization conclusion

- It was shown that domain localization is equivalent to direct forecast error localization with a Schur product matrix that has a block structure and is not isotropic.
- The rank of the matrix corresponding to the domain localization depends on the number of subdomains that are used in the assimilation.
- This matrix is positive semidefinite.
- Inclusion of positive definite matrix through method SD+ObsLoc further increases the rank in domain localization methods.
- Allowing for the results of comparable accuracy as with covariance localization.

Localization and balance

Assume we have two variables h and v defined at the model grid points, i.e. $\mathbf{h}$ and $\mathbf{v}$:

$$\mathbf{P}_{\mathbf{k}}^{\mathbf{b}} \equiv \begin{bmatrix} cov(\mathbf{h},\mathbf{h}) & cov(\mathbf{h},\mathbf{v}) \\ cov(\mathbf{v},\mathbf{h}) & cov(\mathbf{v},\mathbf{v}) \end{bmatrix}$$

Let us assume that we want to apply direct forecast error localization with diagonal matrix then

$$\mathbf{P}_{\mathbf{k}}^{\mathbf{b}} \circ \mathbf{I} \equiv \begin{bmatrix} cov(h_1,h_1) & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & 0 & cov(h_n,h_n) & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0\cdots 0 & cov(v_n,v_n) \end{bmatrix}$$

Example 2: How good are our unobserved variables?

$$\frac{\partial h}{\partial t} + c\frac{\partial h}{\partial x} = 0$$
$$u(x,t) = -\frac{1}{c}\frac{\partial h}{\partial x}$$
$$h(x,0) = sin(x)$$

Solution is given by $h^t(x,t) = sin(x - ct), u^t(x,t) = cos(x - ct)$.

- We observe only h as in Example 1.
- Our $\mathbf{w}_k = \begin{bmatrix} \mathbf{h} \\ \mathbf{u} \end{bmatrix}$
- Field u should be corrected through the background error covariance!

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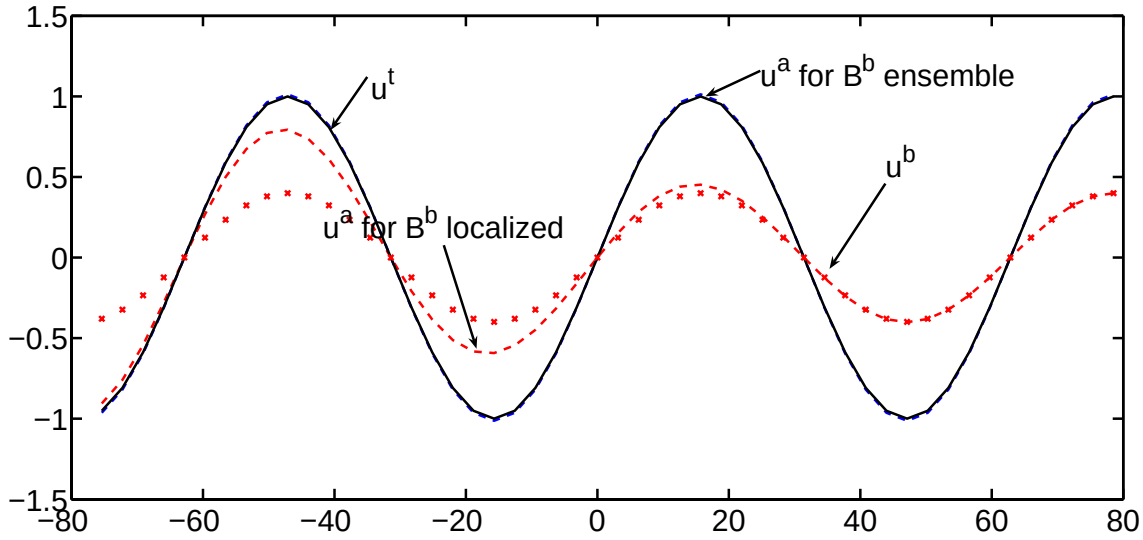

- Diagonal covariance matrix does not correct u since u is not observed.
- Field u was corrected through the ensemble background error covariance using the cross correlations between variables u and h as given by model dynamics!
- Once we localize the covariances we will loose the cross correlations specified by the model.

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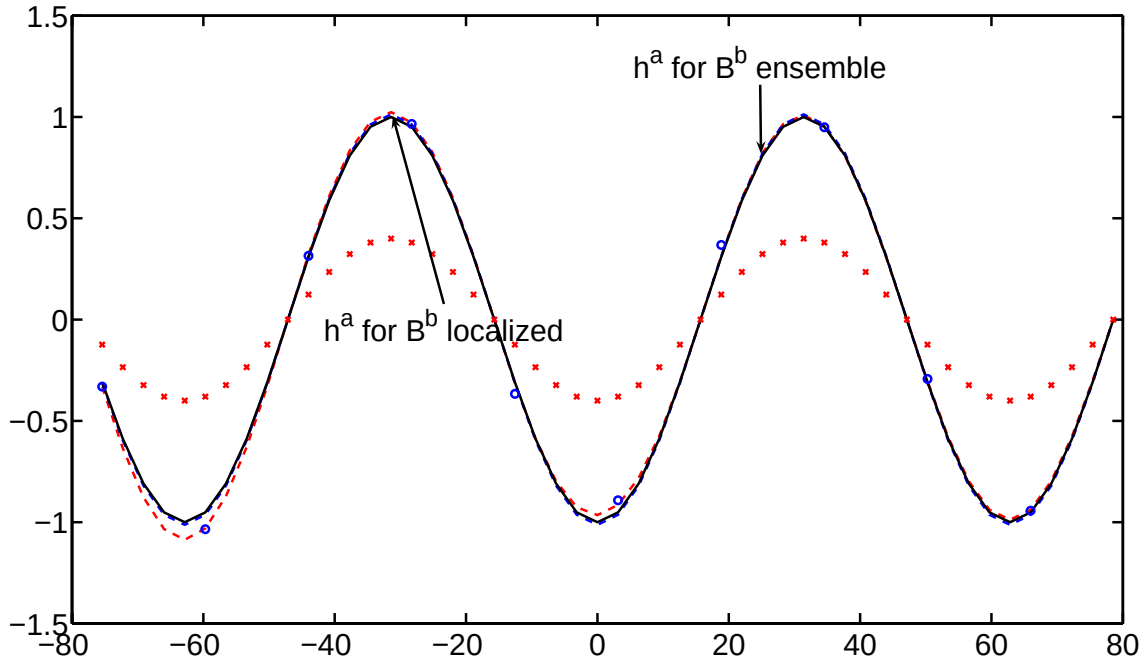

- In the field which is observed we can fit the data better by localizing.
- RMS error calculations against data that is assimilated. In this case: RMS $= 0.0083$ for localized $\mathbf{B}_k^b$, RMS $= 0.0132$ for 5 ensemble members.

Localization and Balance

- By applying localization we destroy correlation given by numerical model between two fields.
- In Greybush et al. MWR 2011 methods (SD+ObsLoc) and direct forecast error localization with exp $\frac{-d(i,j)^2}{2L^2}$ were compared in order to investigate the effects on geostrophic balance
- It was shown that the observational error localization preserves better balance then the direct covariance error localization.

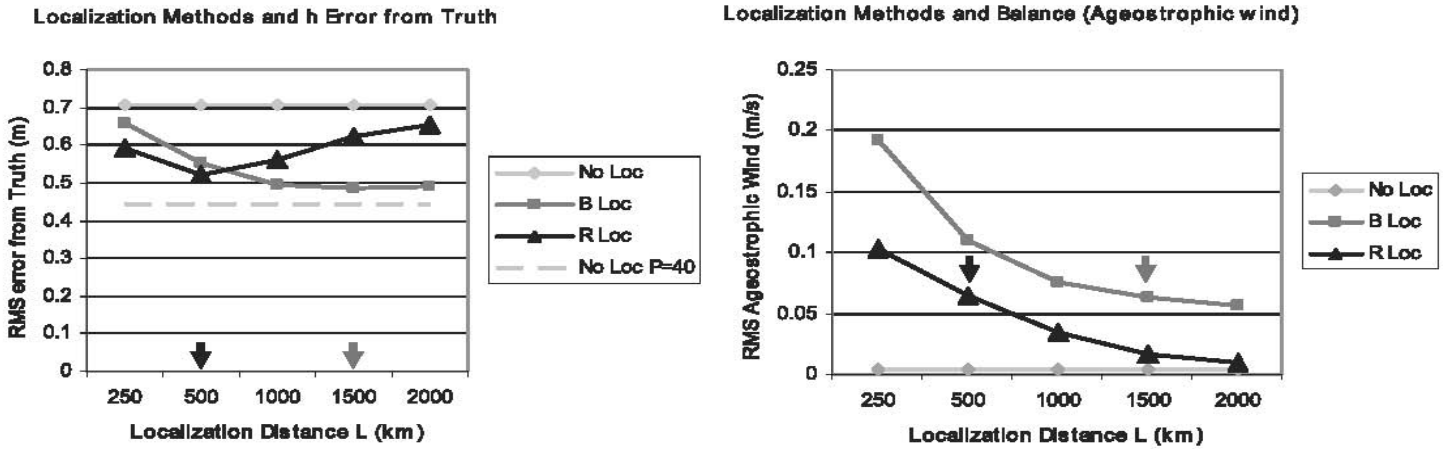

FIG. 3. (left) RMS error of the analysis from the truth for height (m) and (right) RMS ageostrophic wind (m s^{-1}) using no localization, B localization, and R localization for five ensemble members and a variety of localization distances L. For comparison, an analysis with no localization and 40 ensemble members is also plotted. Arrows depict optimum values of L.

Conclusion

- Localization is necessary for application of ensemble Kalman filter algorithms for large scale probelms.
- Several localization techniques are in use.
- Localization removes spurious long range correlations, but it also introduces an ad hoc procedure that requires tuning in ensemble Kalman filter methods.
- Localization is topic of active research especially concerning the effect of localization on balance.
- Proper ways of performing multivariate localization are still not fully understood.
- Proper localization scales depend on the properties of dynamical system and observations.