LETKF - Properties and Studies

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Motivation I

Let H be the observation operator mapping the state φ onto the measurements f. Then we need to update or find φ using the equation

$$H(\varphi) = f,$$

where H^{-1} is unstable or unbounded. When we have some initial guess $\varphi^{(b)}$, we transform the equation into

$$H(\varphi - \varphi^{(b)}) = f - H\varphi^{(b)},$$

with the incremental form

$$\varphi = \varphi^{(b)} + H^{-1}(f - H\varphi^{(b)}).$$

Least Squares

In order to find out φ we should minimize the functional

$$J(\varphi) := \left\| \varphi - \varphi^{(b)} \right\|^2 + \left\| f - H\varphi^{(b)} \right\|^2.$$

The normal equations are obtained from first order optimality conditions

$$\nabla_{\varphi} J = 0.$$

Usually, the relation between variables at different points is incorporated by using covariances/weighted norms:

$$J(\varphi) := \left\| \varphi - \varphi^{(b)} \right\|^2_{B^{-1}} + \left\| f - H\varphi^{(b)} \right\|^2_{R^{-1}},$$

The variational update formula is now

$$\varphi^{(a)} = \varphi^{(b)} + BH^*(R + HBH^*)^{-1}(f - H\varphi^{(b)})$$

Kalman Filter

In the Kalman filter method we calculate an analysis update by

$$\varphi_k^{(a)} = \varphi_k^{(b)} + B_k^{(b)} H^* (R + HB^{(b)} H^*)^{-1} (f_k - H\varphi_k^{(b)}) \tag{1}$$

and an covariance update by

$$B_k^{(a)} = (I - KH) B_k^{(b)}, \quad k = 1, 2, 3, \dots \tag{2}$$

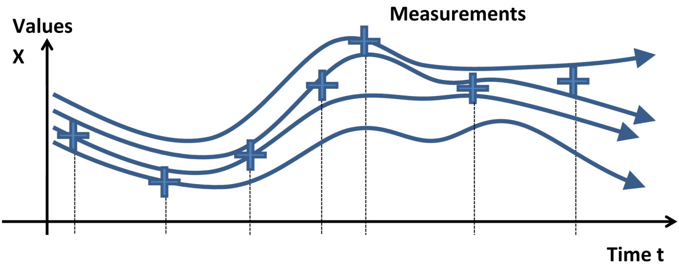
with the *Kalman Gain Matrix*

$$K_k = B_k^{(b)} H^* (R + HB_k^{(b)} H^*)^{-1}$$

and the weight or covariance matrix B evolves with the model dynamics M,

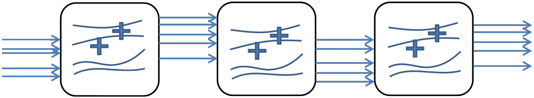
$$B_{k+1}^{(b)} = M_k B_k^{(a)} M_k^*, \quad k = 1, 2, 3, \dots \tag{3}$$

Use Ensembles for Approximation



- Instead of running only one version of our dynamical system, we run *L* different versions of it, which we call **ensembles** or **particles**.
- This is computationally expensive for the forward problem, but we will save on the minimization needed for calculating the analysis.
- With the ensemble we can **capture the uncertainty** both in the model as well as in the analysis!

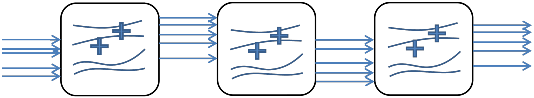
Ensemble Kalman Filter



The main idea of the **Ensemble Kalman Filter** is to approximate the B matrix in all of its steps by an ensemble in the form $B = QQ^*$, when

$$Q := \frac{1}{\sqrt{L-1}} \left(\varphi^{(1)} - \mu, \ldots, \varphi^{(L)} - \mu \right)$$

with ensemble mean $\mu = \sum_{j=1}^{L} \varphi^{(j)}$. This is the standard **unbiased stochastic estimator** for the covariance matrix.



We need to propagate the ensemble through time. Starting with an ensemble $\left\{ \varphi_0^{(l)}, \quad l = 1, ..., L \right\}$, this leads to ensemble members

$$\varphi_{k+1}^{(l)} = M_k \varphi_k^{(l)}, \quad k = 1, 2, 3, ...$$

This means that we solve the equation in a low-dimensional subspace

$$U^{(L)} := \text{span}\{\varphi_k^{(1)} - \mu_k, ..., \varphi_k^{(L)} - \mu_k\}.$$

The **update formula** now is

$$\varphi_k^{(a)} = \varphi_k^{(b)} + Q_k Q_k^* H^* \big(R + H Q_k Q_k^* H^*\big)^{-1} \big(f_k - H\varphi_k^{(b)}\big)$$

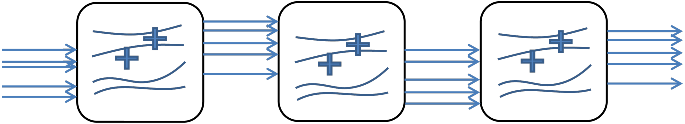
The updates of the EnKF are a linear combination of the columns of Q_k. We can therefore write

$$\varphi_k - \varphi_k^{(b)} = \sum_{l=1}^{L} \gamma_l \frac{1}{\sqrt{L-1}} \left(\varphi_k^{(l)} - \overline{\varphi}_k^{(b)}\right) = Q_k \gamma$$

with coefficient vector $\gamma \in \mathbb{R}^L$. The resulting the expresion to minimize is

$$J(\gamma) := \|Q_k\gamma\|^2_{B_k^{-1}} + \|f_k - H\varphi_k^{(b)} - HQ_k\gamma\|^2_{R^{-1}}.$$

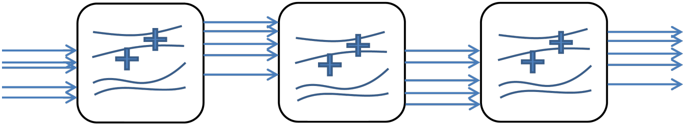
Ensemble updates?



A key question of ensemble methods is how to update the ensemble in the data assimilation step. More precisely:

Given the data f_k at time t_k and an ensemble which approximates the background matrix $B_k^{(b)}$, how do we get an analysis ensemble $Q^{(a)}$ which approximates the analysis matrix $B_k^{(a)}$ in the form $Q^{(a)}Q^{(a),*}$?

Ensemble updates?



We know that for the Kalman filter the analysis weight matrix $B_k^{(a)}$ is calculated from $B_k^{(b)}$ by $B^{(a)} = (I - KH)B^{(b)}$. In terms of the ensemble approximations this means

$$Q_k^{(a)}(Q_k^{(a)})^* = (I - K_k H_k) Q_k^{(b)}(Q_k^{(b)})^* \tag{4}$$

with the *ensemble Kalman matrix*

$$K_k := Q_k^{(b)}(Q_k^{(b)})^* H_k^* (R + H_k Q_k^{(b)}(Q_k^{(b)})^* H_k^*)^{-1}, \tag{5}$$

Taking quare roots

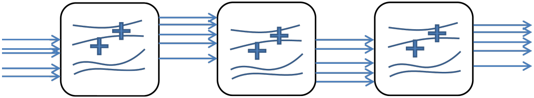
We aim to determine $Q_k^{(a)}$ such that

$$Q_k^{(a)}(Q_k^{(a)})^* = Q_k^{(b)} \Big\{ \underbrace{I - (Q_k^{(b)})^* H_k^* \Big(R + HQ_k^{(b)}(Q_k^{(b)})^* H_k^* \Big)^{-1} H_k Q_k^{(b)}}_{=:A} \Big\} (Q_k^{(b)})^*. \quad (6)$$

The term A in the curly brackets is self-adjoint. Further, it can be seen to be positive, such that there is a square-root, i.e. matrix S with $A = SS^*$. This finally leads to

$$Q_k^{(a)} = Q_k^{(b)} S. \quad (7)$$

Ensemble Kalman Filter: Summary



In the Ensemble Kalman filter method we calculate an analysis update by

$$\varphi_k^{(a)} = \varphi_k^{(b)} + Q_k^{(b)} Q_k^{(b),*} H^* \left(R + H Q_k^{(b)} Q_k^{(b),*} H^*\right)^{-1} \left(f_k - H\varphi_k^{(b)}\right) \quad (8)$$

and a covariance update by $Q_k^{(a)} = Q_k^{(b)} S$ with $S \in \mathbb{R}^{L \times L}$ given by

$$S = \sqrt{I - (Q_k^{(b)})^* H_k^* \left(R + H Q_k^{(b)} (Q_k^{(b)})^* H_k^*\right)^{-1} H_k Q_k^{(b)}} \quad (9)$$

and the ensemble $\{\varphi^{(1)}, \ldots, \varphi^{(L)}\}$ evolves with the model dynamics M by,

$$\varphi_{k+1}^{(b,\ell)} = M_k \varphi_k^{(a,\ell)}, \quad \ell = 1, \ldots, L,\ k = 1, 2, 3, \ldots \quad (10)$$

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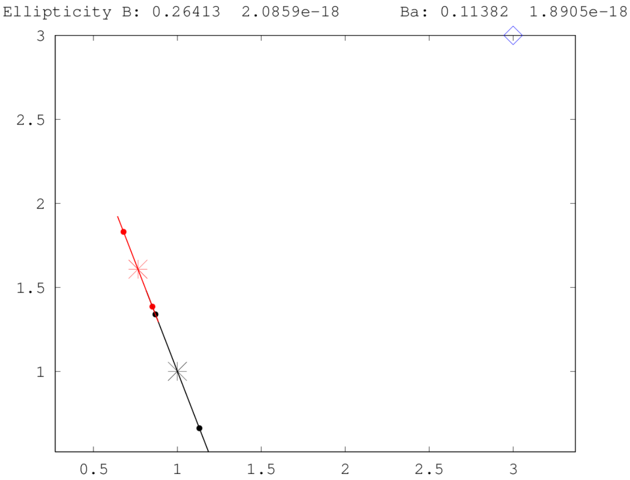
EnKF Extrapolation and Space-Geometry

1. What if all members do not have some particular feature?
2. Can the EnKF do extrapolation?
3. Can we do generic experiments to learn about these two questions?

The answer is:

- The EnKF cannot generate features which are not present at all. We need to take care when we generate our ensemble.
- The EnKF can extrapolate. It will shift the ensemble towards the observation.

Experiments with Lack of Features (Space Dimension)



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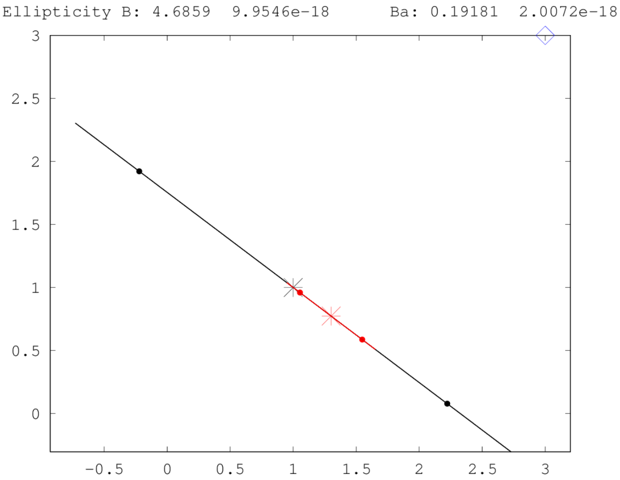

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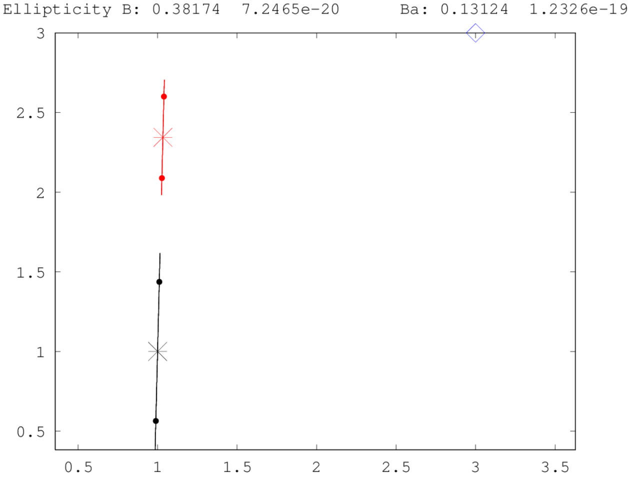

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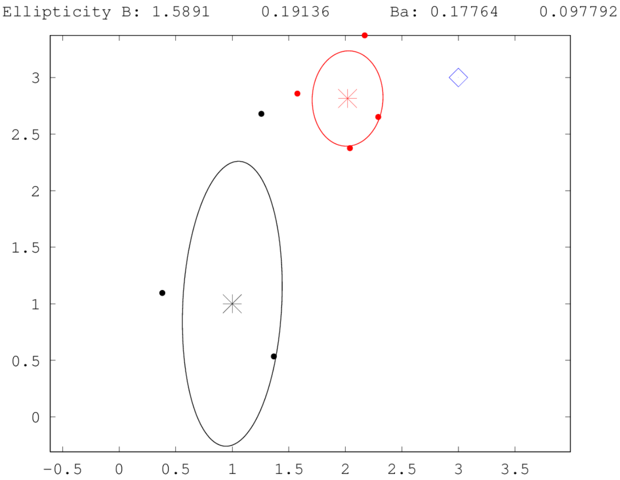

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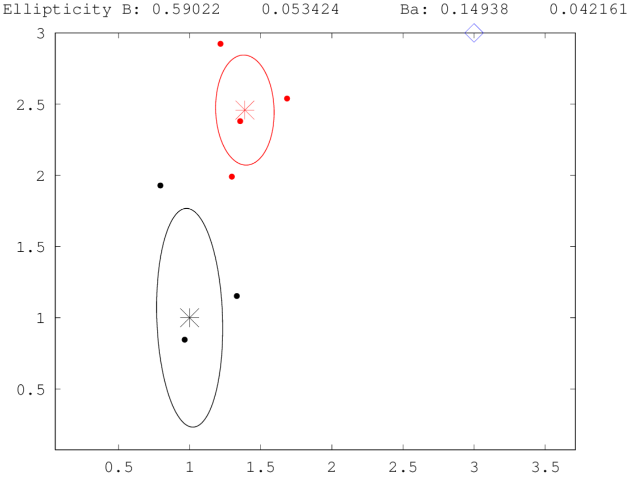


Outline

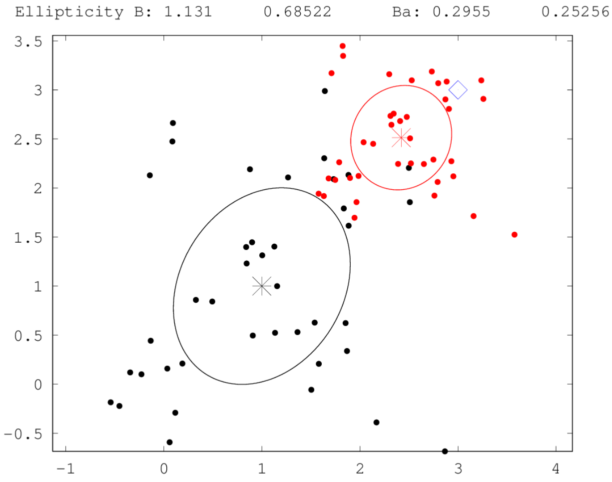
Ensemble Shape and Non-Gaussianity

1. What is the EnKF with Square Root Ensemble Update doing to the particular shape of an ensemble?
2. How is the EnKF treating non-Gaussianity? What happens for example to bi-modal distributions?
3. Can we do generic experiments to learn about these two questions?

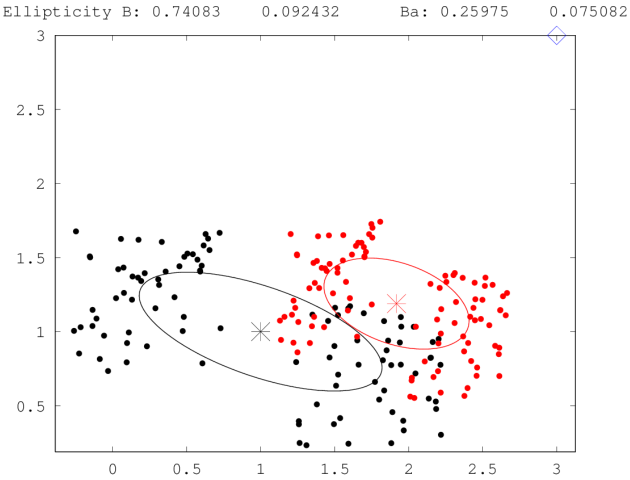
The answer is:

- The EnKF is keeping the shape of the ensemble, it is just scaling it in the directions of the main axis of the B matrix.
- The EnKF can potentially deal well with non-Gaussianity, we need to be careful about the scaling!

Experiments with the Ensemble Shape



Experiments with the Bi-Modal Distributions



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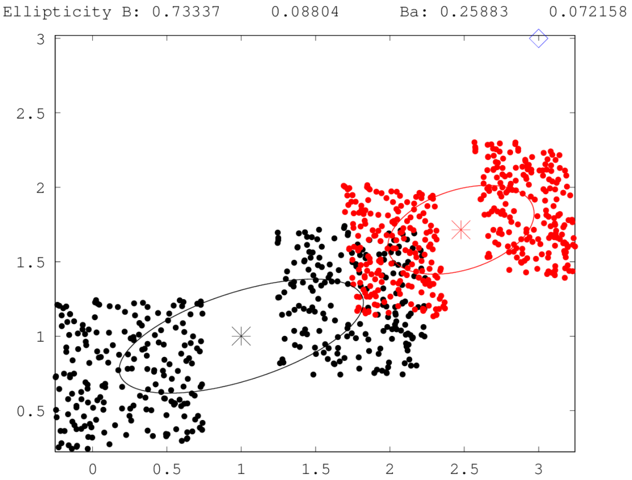
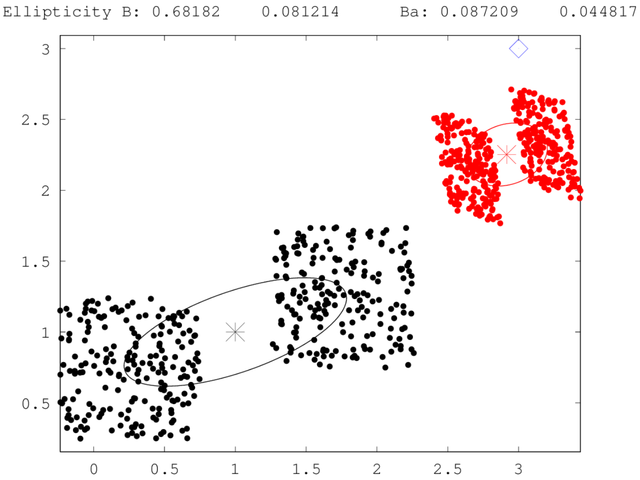
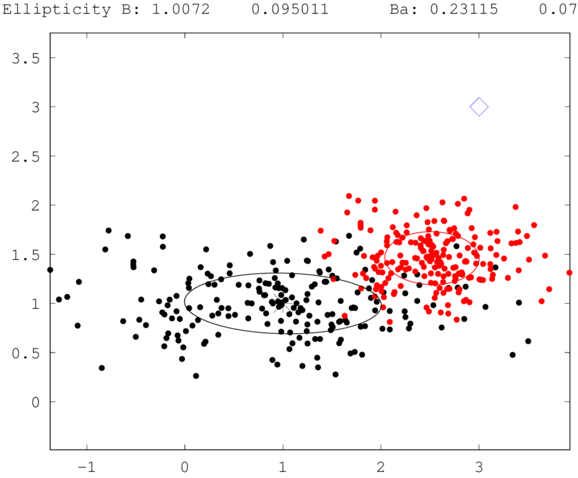


Experiments with the Bi-Modal Distributions

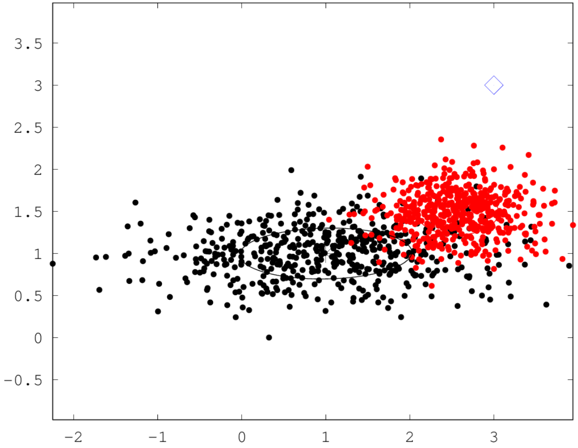


Experiments with the Bi-Modal Distributions

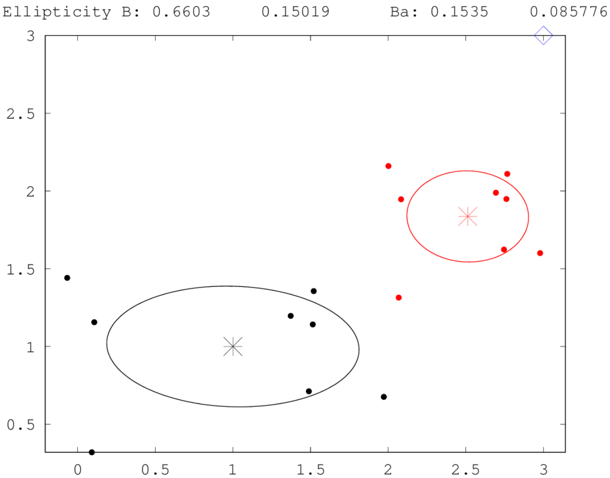


Experiments with the Bi-Modal Distributions

Ellipticity B: 1.0453   0.091188   Ba: 0.2331   0.069931



Experiments with the Bi-Modal Distributions



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Least Squares Analysis Model

To *understand the role of localization*, we study a simplified problem which is characteristic for our analysis step in the EnKF.

- One dimensional model without cycling
- **Least square estimation** to obtain the analysis (LSA) and the truth is given by a high-order function.
- The analysis is obtained using both all available observations and only a **local set**.
- Estimation performed with and without **background terms**.
- Observations are generated from the truth with a specified **observation error** σ_{obs}.
- Analysis approximated by straight lines $a + bx$ (an ensemble of linear functions).

Example

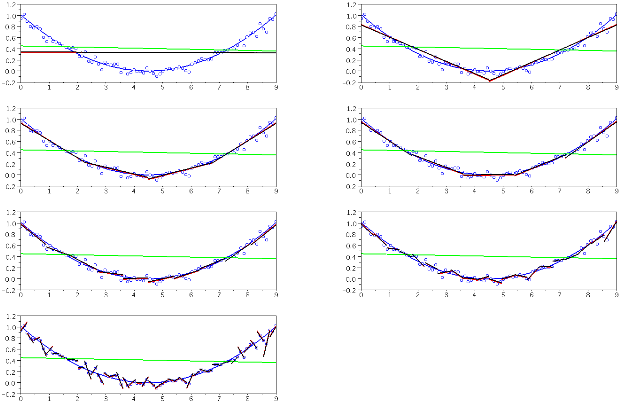


Fig.1: Truth (blue line), observations (blue circles), background (green), no background LSA (red) and background LSA (black) for $\sigma_{obs} = 0.05$ and different localization radii.

Remarks

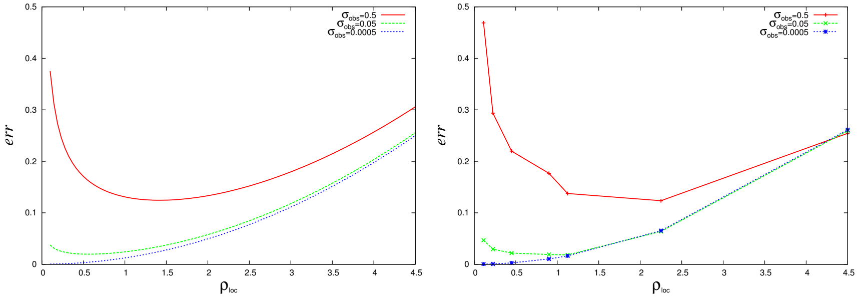
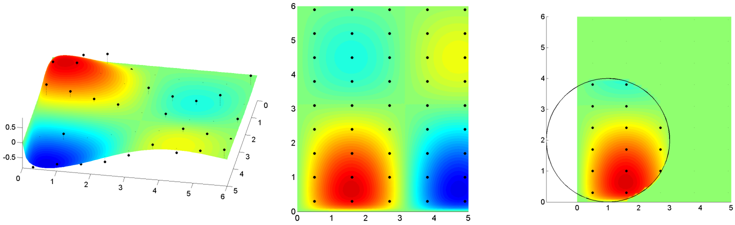


Fig.4: Theoretical and numerical results for error as a function of ρ_{loc}, $\sigma_{obs} = [0.0005\ 0.05\ 0.5]$.

- The optimal value of ρ_{loc} takes smaller values when σ_{obs} decreases.
- For large values of σ_{obs} the analysis without the background correction is clearly worse than analysis considering the background.

Idea of Localization I



- Carry out the ensemble analysis in subsets of the full spatial domain!
- Given a **localization radius** $\rho > 0$ the analysis at a point x this is effectively using only observations at one point y with $\|x - y\| \leq \rho$.

Idea of Localization II

- Localization assumes that every free variable of our state φ is located at some point x in physical space. If φ is a vector

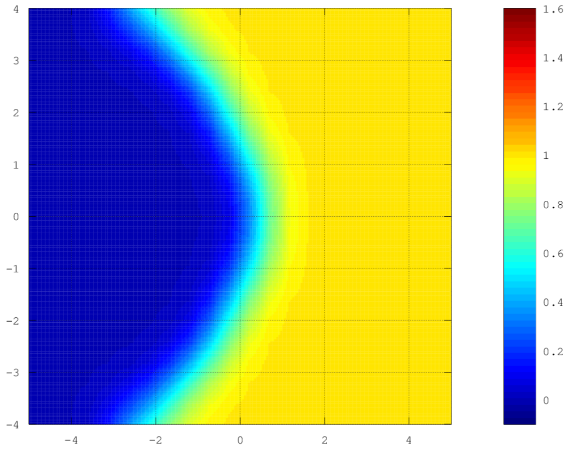
$$\varphi = \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_n \end{pmatrix},$$

and our space is $\mathbb{R}^3$, then this means we have a mapping

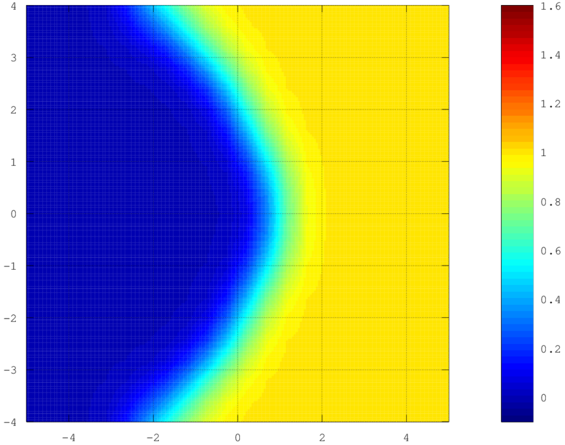
$$\varphi_j \mapsto x_j \in \mathbb{R}^3, \quad j = 1, ..., n$$

- Localization can be carried out in different ways. Here, we consider the **full restriction of the analysis to some subset D**, i.e. we take observations into accout only if they are related to D and we construct a solution only on D.

Instructive Example for the effect of Localization



Instructive Example for the effect of Localization



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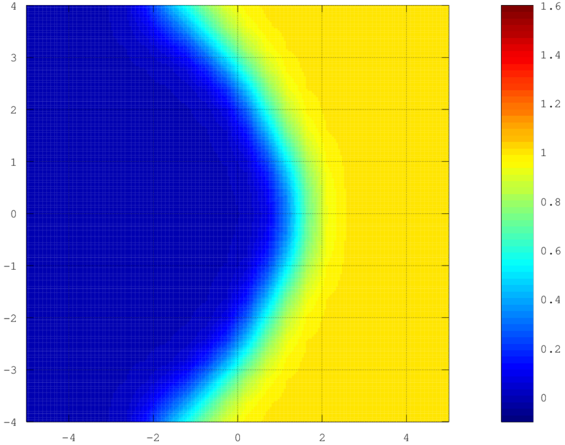
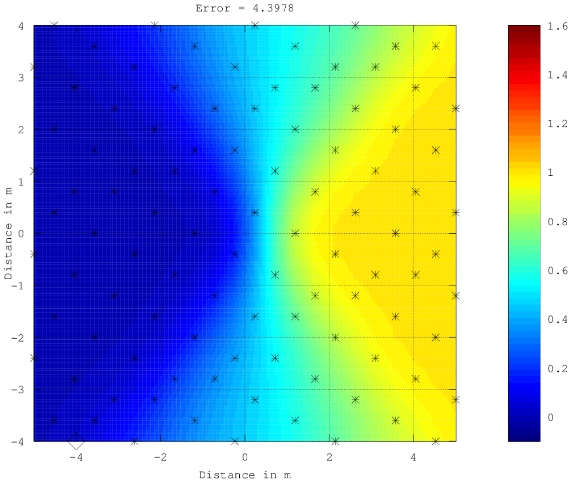
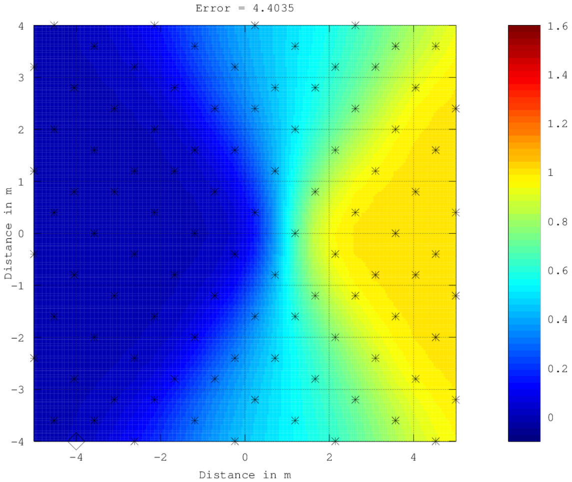


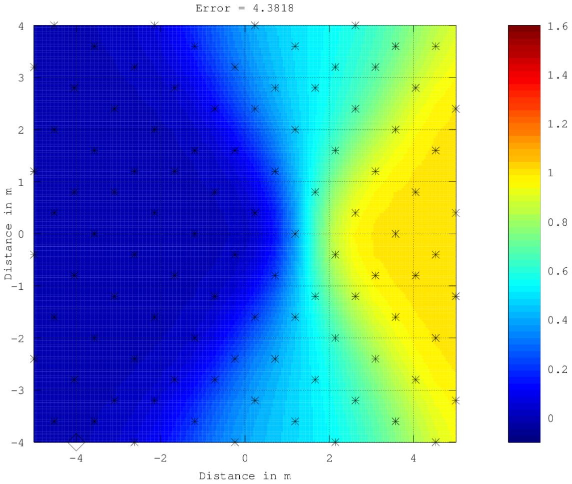
No Localization



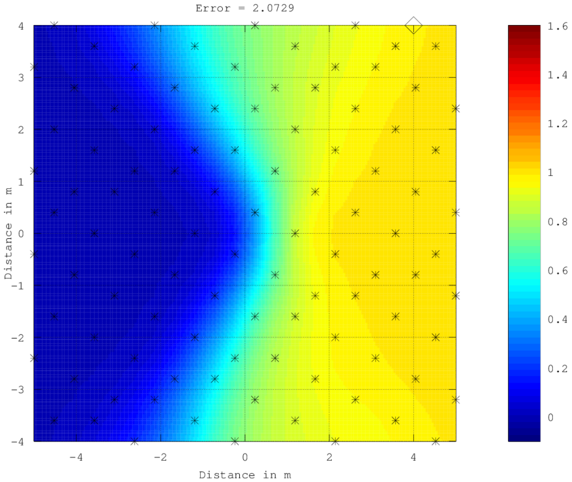
No Localization



No Localization



With Localization, $\rho = 2$



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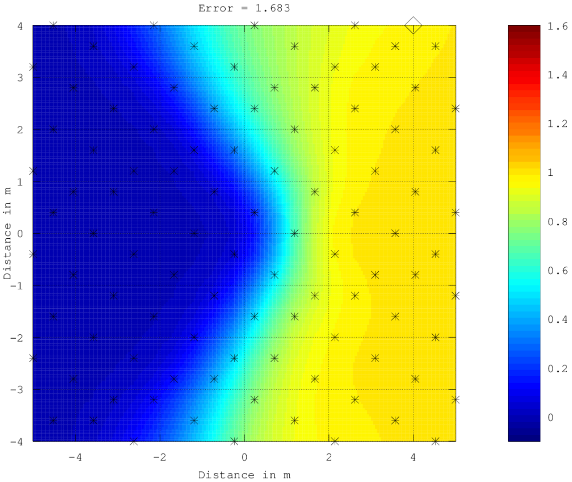
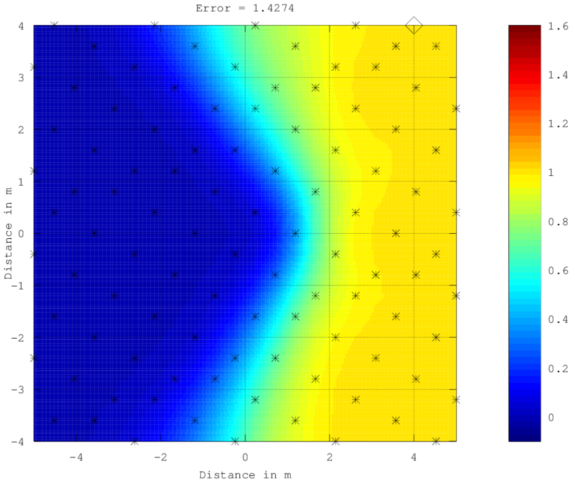
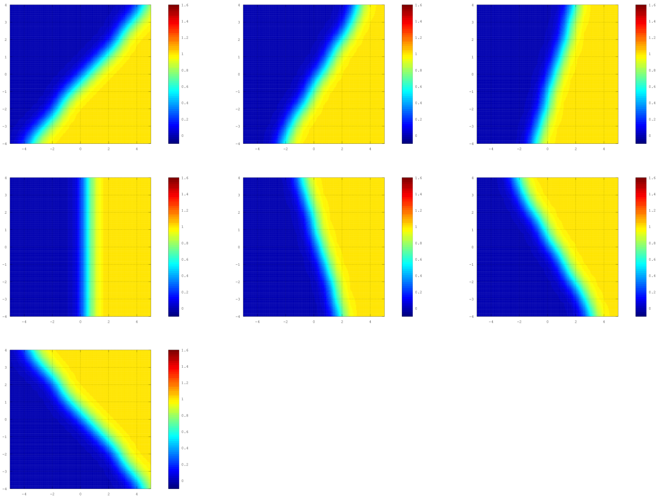


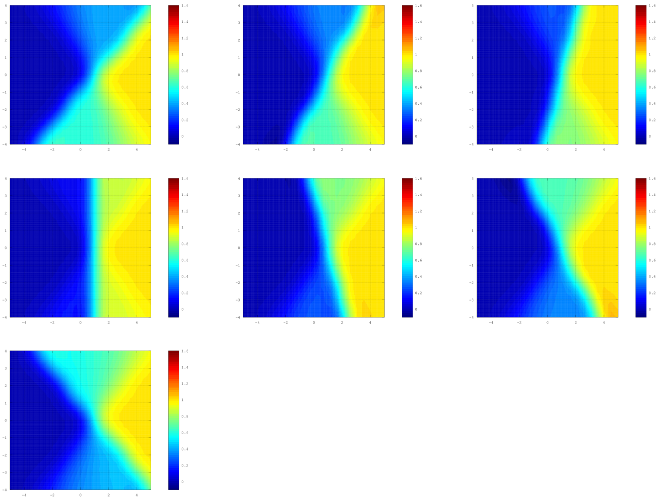
With Localization, $\rho = 2$



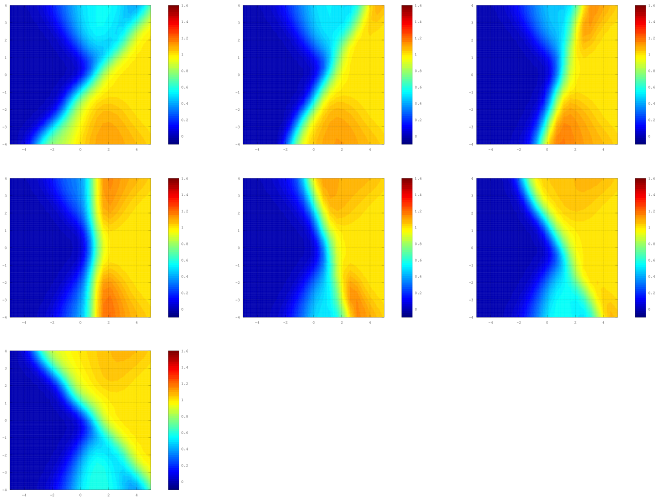
Ensemble at Beginning



Ensemble after 2 steps without Localization



Ensemble after 2 steps with Localization



Localization for Non-Local Operators?

- Localization in state space cannot be good for **non-local operators** such as

$$(H\varphi)(\nu) = \int_a^b k(\nu, z)\varphi(z)dz \tag{11}$$

- Use a **transformation** of the spaces to make operators **more local**:

$$\tilde{\varphi} = Tx, \quad \tilde{y} = Sy, \quad \tilde{H} = SHT^{-1} \tag{12}$$

to transform $Hx = y$ into

$$\tilde{H}\tilde{\varphi} = SHT^{-1}Tx = SHx = Sy = \tilde{y}. \tag{13}$$

How does the LETKF behave under transformation?

Lemma

The transformed analysis increment $\tilde{K}_k(\tilde{y}_k - \tilde{H}\tilde{\varphi}_k^{(b)})$ *of the Ensemble Kalman Filter for the transformed ensembles* $\tilde{Q}$ *is given by*

$$\tilde{K}_k(\tilde{y}_k - \tilde{H}\tilde{\varphi}^{(b)}) = TK(y_k - Hx_k^b). \tag{14}$$

The analysis ensemble *is given by*

$$\tilde{Q}_k^{(a)} = \tilde{Q}_k^{(b)}\tilde{L} \tag{15}$$

with a matrix $\tilde{L}$ *which is the same as the update matrix* L *from the non-transformed case, i.e. we have*

$$\tilde{L} = L. \tag{16}$$

Transformed Localization

If we denote the localized transformed matrix by $\tilde{B}_{gl}$, this means we calculate

$$\tilde{\varphi}_{gl}^{(a)} := \tilde{\varphi}^{(b)} + \tilde{K}_{k,gl}(\tilde{y}_k - \tilde{H}\tilde{\varphi}_k^{(b)}), \tag{17}$$

with

$$\tilde{K}_{k,gl} := \tilde{B}_{gl}\tilde{H}^*\big(\tilde{R} + \tilde{H}\tilde{B}_{gl}\tilde{H}^*\big)^{-1}. \tag{18}$$

According to our Transformation Lemma it is equivalent to

$$x_{gl}^{(a)} := x^{(b)} + K_{k,gl}(y_k - Hx_k^{(b)}), \tag{19}$$

with

$$K_{k,gl} = B_{gl}H^*\big(R + HB_{gl}H^*\big)^{-1} \tag{20}$$

for $B_{gl} = T^{-1}\tilde{B}_{gl}(T^*)^{-1}$ in the original space, transformed into each other by T and S.

Generalized Localization

- Understand localization as a **projection method**:

$$Hx = y$$

is replaced by

$$P_j Hx = P_j y$$

- Now employ a different family of **projection operators** P_j, where a projection $\tilde{P}_j$ is combined with a transformation:

$$P_j := S^{-1} \tilde{P}_j S, \qquad P_j Hx = P_j y$$

If S is orthonormal, P_j is clearly a projection operator.

Generalized Localization

- This leads to the equivalence

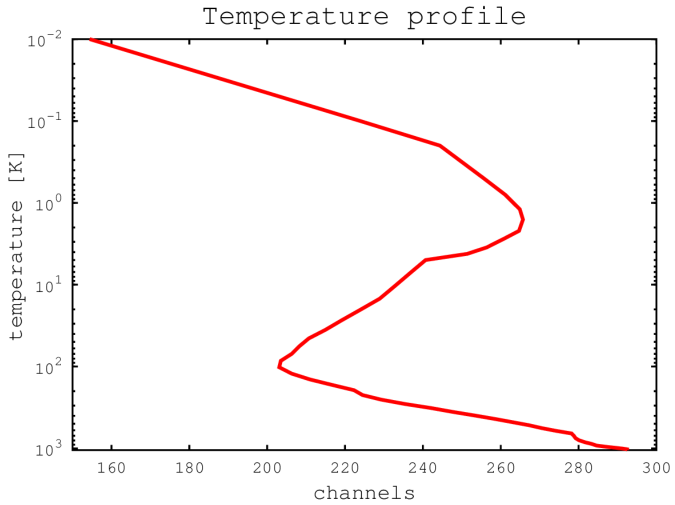
$$
\begin{aligned}
& \tilde{P}_j \tilde{H} \tilde{\varphi} = \tilde{P}_j \tilde{y} \\
\Leftrightarrow \quad & S^{-1} \tilde{P}_j (S H T^{-1})(T x) = S^{-1} \tilde{P}_j (S y) \\
\Leftrightarrow \quad & P_j H x = P_j y
\end{aligned}
$$

Theorem

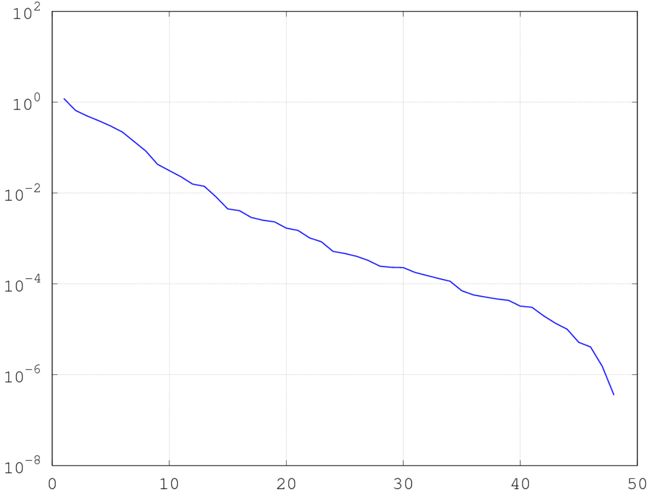
If the transformations S and T are orthonormal transformations of the space X and Y, then the transformed localization and the generalized localization by projection methods are equivalent.

Outline

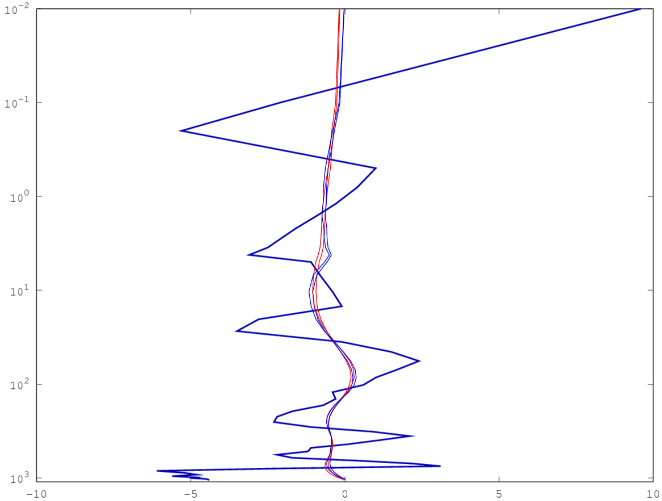
Atmospheric Temperature Profile ...



Singular Values of *H* ...



Reconstruction of Profile Difference, Different α ...



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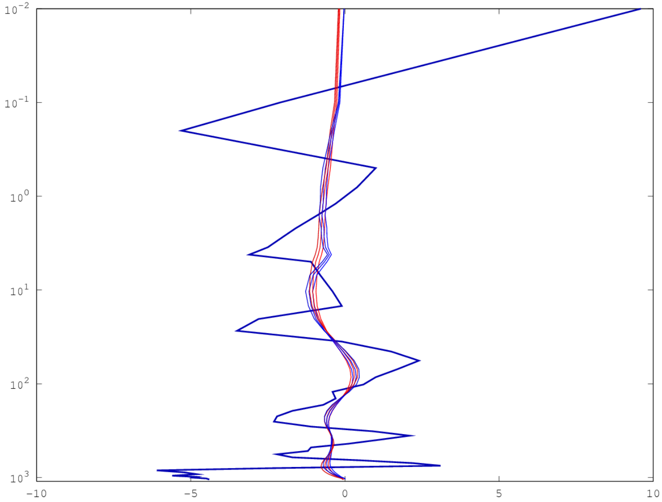

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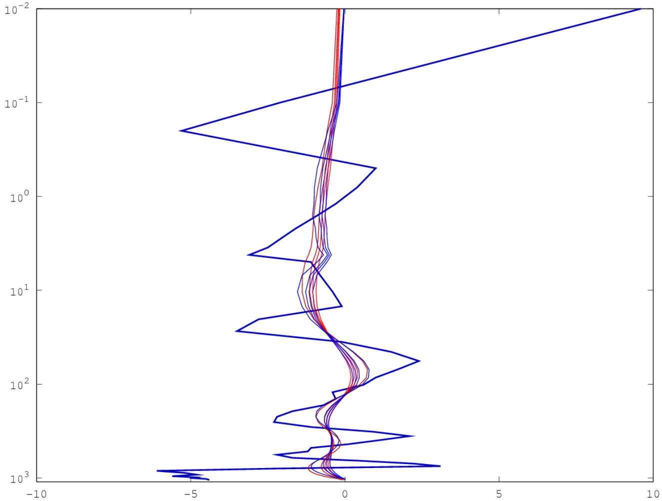
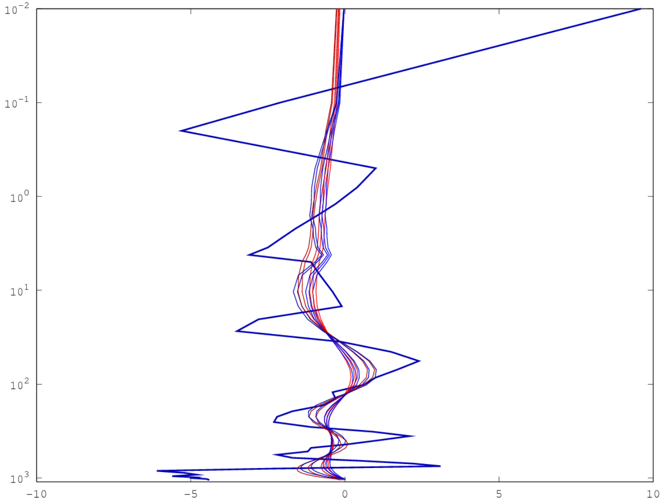
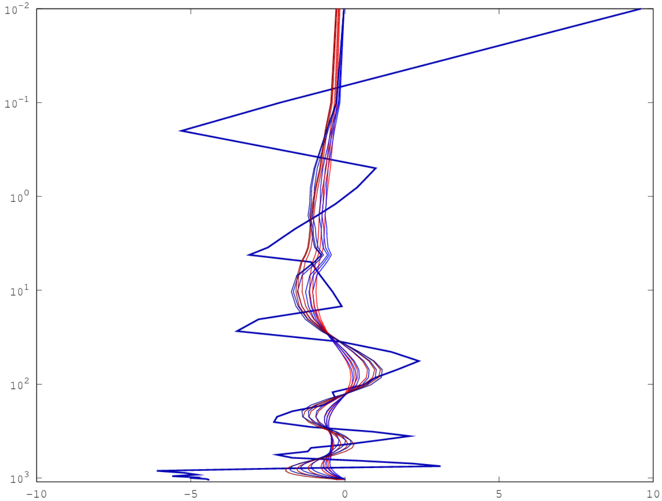


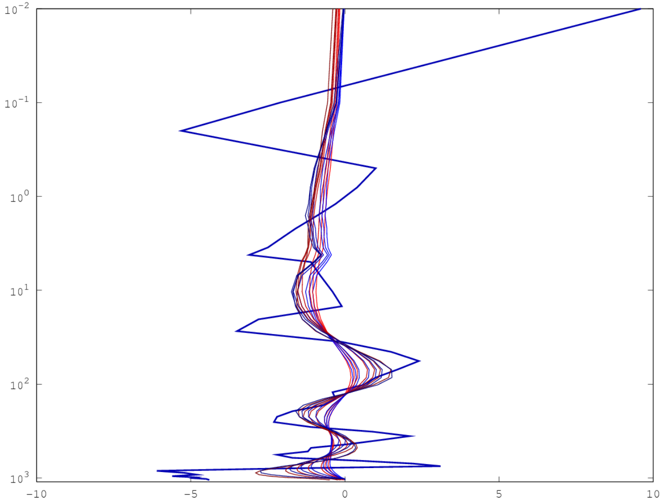
Reconstruction of Profile Difference, Different α ...



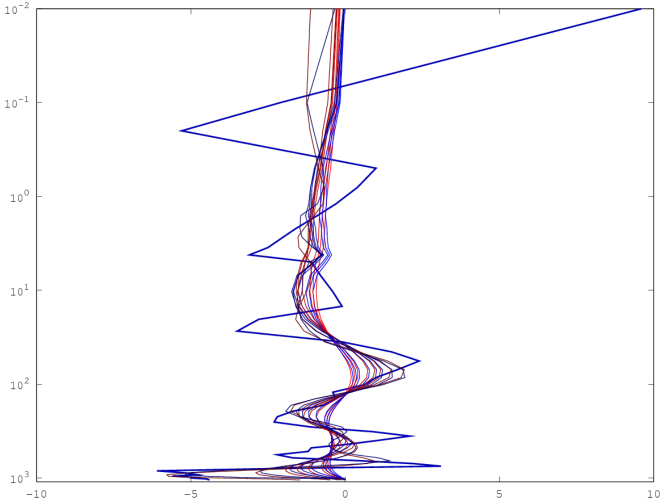
Reconstruction of Profile Difference, Different α ...



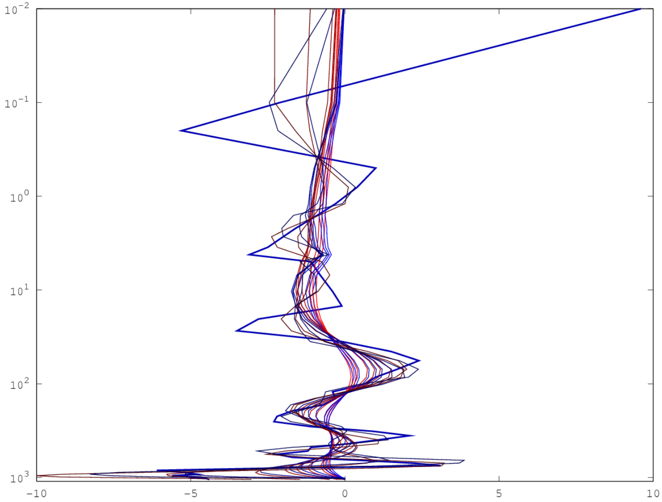
Reconstruction of Profile Difference, Different α ...



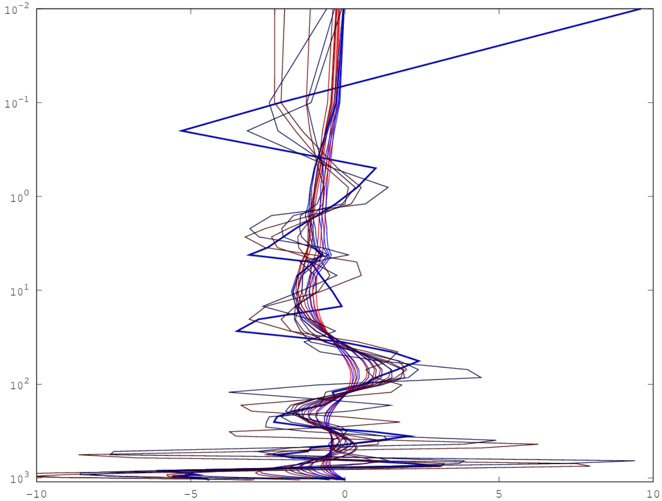
Reconstruction of Profile Difference, Different α ...



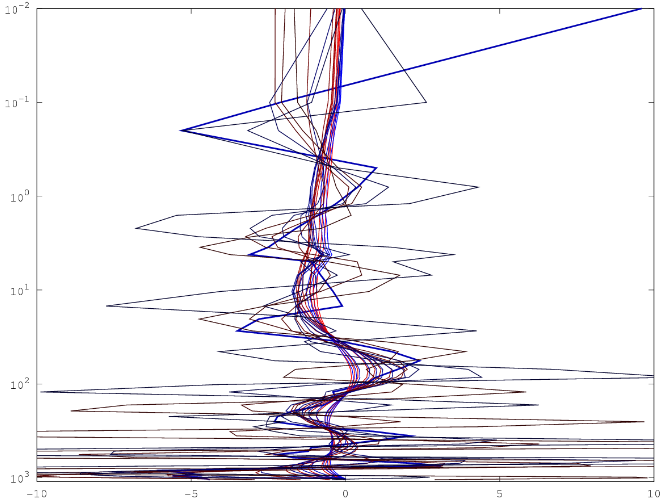
Reconstruction of Profile Difference, Different α ...



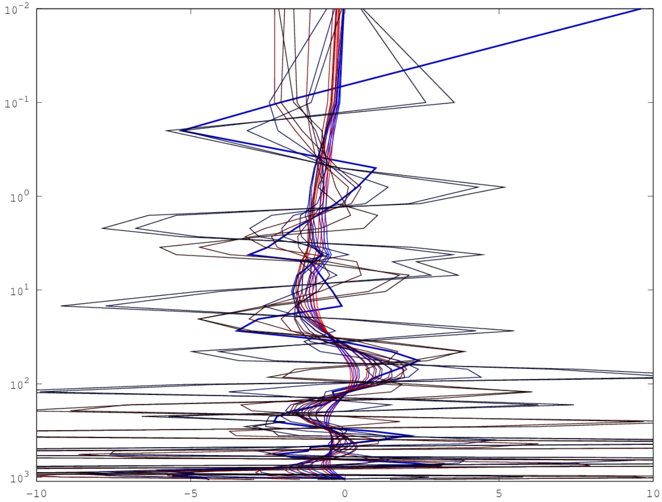
Reconstruction of Profile Difference, Different α ...



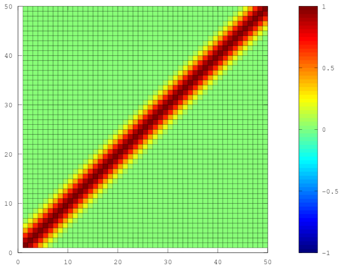
Reconstruction of Profile Difference, Different α ...

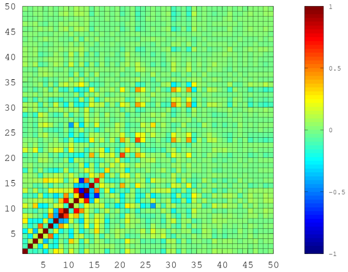


Reconstruction of Profile Difference, Different α ...



Numerics for Gaussian B Matrix ...

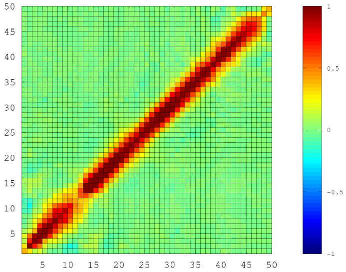


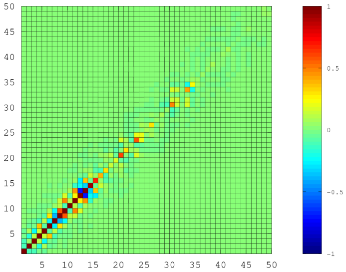


left: B Matrix from global LETKF,

right: **transformed** B matrix

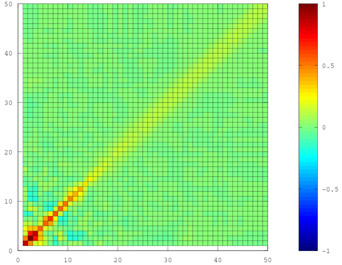
Numerics for Global LETKF of DWD ...

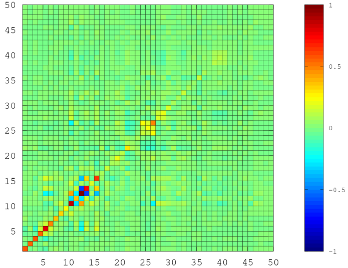




left: retransformed localized B matrix , right: **localized transformed** B matrix

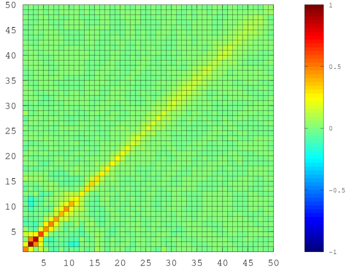
Numerics for Global LETKF of DWD ...

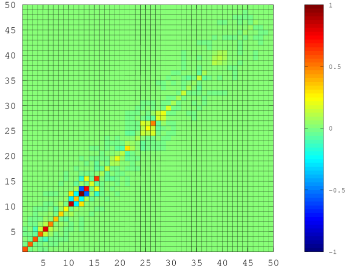




left: B Matrix from global LETKF, right: **transformed** B matrix

Numerics for Global LETKF of DWD ...





left: retransformed localized B matrix , right: **localized transformed** B matrix

Reconstruction without and with Transformation ...