Error Analysis and Adaptive Localization for Ensemble Methods in Data Assimilation

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Challenge

- Understand the basic properties of localization in the ensemble Kalman filter scheme.
- Define an adaptive localization depending on the density of data, observation and background error.
- Decomposition of the error sources to determine its effect on the optimal localization length scale.
- Perspective of approximation theory and functional analysis.
- Addressed with numerical experimental results.

Introduction

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:

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

The update formula is now

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

Ensemble Kalman Filter

- In the KF method B evolves with the model dynamics: $B_{k+1} = MB_kM^*$.
- EnKF[1] is a Monte Carlo approximation to the KF.
- EnKF methods use reduced rank estimation techniques to aproximate the classical filters.
- The ensemble matrix $Q_k := \left(\varphi_k^{(1)} - \overline{\varphi}_k^{(b)}, ..., \varphi_k^{(L)} - \overline{\varphi}_k^{(b)}\right)$.
- In the EnKF methods the background convariance matrix is represented by $B := \frac{1}{L-1} Q_k Q_k^*$.
- Update solved in a low-dimensional subspace

$$U^{(L)} := \text{span}\{\varphi_k^{(1)} - \overline{\varphi}_k^{(b)}, ..., \varphi_k^{(L)} - \overline{\varphi}_k^{(b)}\}.$$

[1] Evensen 1994

- The updates of the EnKF are a linear combination of the columns of Q_k.

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

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

- The previous cost function

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

results now in this expresion to minimize:

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

- We denote the analysis error $E_k := \|\varphi^{(a)} - \varphi^{(true)}\|$

Error analysis without background contribution

Lemma

Assume that H is injective, that we study true measurement data $f = H\varphi^{(true)}$ and consider the EnKF with data term only

$$J^{(data)}(\gamma) = \|(f - H\varphi^{(b)}) - HQ_k\gamma\|^2_{R^{-1}}$$

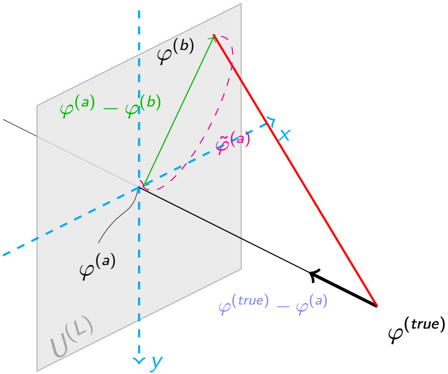
Then, for the analysis $\varphi^{(a)}$ calculated by the EnKF the difference $\varphi^{(a)} - \varphi^{(b)}$ is the orthogonal projection of $\varphi^{(true)} - \varphi^{(b)}$ onto the ensemble space $U_k^{(L)}$ and the analysis error is given by [2]

$$E_k = d_{H^* R^{-1} H}\Big(U_k^{(L)}, \varphi_k^{(true)} - \varphi^{(b)}\Big),$$

where the right-hand side denotes the distance between a point $\psi = \varphi_k^{(true)} - \varphi^{(b)}$ and the subspace $U^{(L)}$ with respect to the norm induced by the scalar product $< ., . >_{H^* R^{-1} H}$.

[2] Proof in Perianez A., Reich H. and Potthast R. *In preparation.*

Illustration of Lemma



Error analysis with background term

Theorem

For H injective, the analysis $\tilde{\varphi}^{(a)}$ generated by the minimization of the whole cost function within the EnKF for perfect data $f^{(true)}$ satisfies the estimate

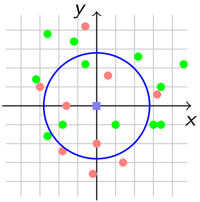
$$\begin{aligned} \left\| \tilde{\varphi}^{(a)} - \varphi^{(true)} \right\|_{HR^{-1}H} &\leq \sqrt{q^2 (E^{(b)})^2 + (1-q^2) E_{min}^2} \\ &= E^{(b)} \sqrt{q^2 + (1-q^2) \frac{E_{min}^2}{(E^{(b)})^2}} \end{aligned}$$

with some constant $q < 1$ depending on B, R and H, where

$$\begin{aligned} E_{min} &:= \min_{\varphi \in U^{(L)}} \left\| \varphi - \varphi^{(true)} \right\|_{H^* R^{-1} H} = \left\| \check{\varphi}^{(a)} - \varphi^{(true)} \right\|_{H^* R^{-1} H}, \\ E^{(b)} &:= \left\| \varphi^{(b)} - \varphi^{(true)} \right\|_{H^* R^{-1} H}. \end{aligned}$$

Localization

- Localization denotes the restriction to a subset of physical space.
- Study the analysis in dependence of the localization radius ρ when the domain D is given by a ball $D = B_\rho(x_0)$.



- Localization function χ_ρ depending on ρ such that[3]

$$\chi_\rho(x) := \begin{cases} \chi_\rho(x) & x \in D \\ 0 & \text{otherwise.} \end{cases}$$

- R localization[4] modifies the observation error covariance matrix to suppress the influences of distant observations $\rightarrow R_{loc} := \chi \cdot R$

$$E^{(\rho)}(x_0) := \left\| \check{\varphi}^{(a,\rho)} - \varphi^{(true,\rho)} \right\|_{H^* R_{loc}^{-1} H}$$

[3] Houtekamer et al. 1998

[4] Hunt et al. 2007

Localization. Convergence results.

Theorem

We study assimilation in the case where true data $\varphi^{(true)}$ *are used and* $\hat{\varphi}^{(a,\rho)}$ *is chosen such that* $\hat{\varphi}^{(a,\rho)} - \varphi^{(b)}$ *is the orthogonal projection of* $\varphi^{(true)} - \varphi^{(b)}$ *onto the ensemble space* $U^{(L)}$*. Assume that there is* c, $C > 0$ *such that for all* $x \in D$ *there is* $l \in \{1, ..., L\}$ *such that*

$$|\varphi^{(l)}(x) - \varphi^{(b)}(x)| \geq c,$$

and that the ensemble members are continuously differentiable on D *with*

$$|\nabla(\varphi^{(j)}(x) - \varphi^{(b)}(x))| \leq C, \ \ x \in D, \ \ j \in \{1, ..., L\}.$$

Further assume that $\varphi^{(true)} - \varphi^{(b)}$ *is continuously differentiable on* D*. Then, we have*

$$\sup_{x_0 \in D} E^{\rho}(x_0) \leq \tilde{C}\rho \ \ \to 0, \ \ \rho \to 0$$

with some constant $\tilde{C}$ *depending on* C, H *and* R*.*

Remarks

- Using last two theorems we can derive

$$\left\| \tilde{\varphi}^{(a,\rho)} - \varphi^{(true,\rho)} \right\|_{H^* R_{loc}^{-1} H} \leq \sqrt{E^{(b,\rho)} q^2 + (1-q^2) C \rho^2}.$$

- The first term q^2 in the square root reflects the influence of the *background error*.
- The second *approximation error* term can be made small by reducing the localization radius ρ.
- In a balanced relationship between background and data, q is between 0 and 1.
- *Effective observation error*: With data error, ρ needs to be kept sufficiently large since it also controls the number of observations used for the assimilation.

A one-dimensional example

- Ensemble space given by linear functions $U^{(L)} := \{a + bx : \ \ a, b \in \mathbb{R}\} \subset L^2([0, A])$.
- The truth $\varphi^{(true)}$ given by a quadratic function $\varphi^{(true)}(x) := B \cdot (x - C)^2, \ \ x \in [0, A]$.
- Observations from a Gaussian distribution with variance σ_{obs}.
- Localization by a decomposition of $[0, A]$ into $q \in \mathbb{N}$ subsets $[A_j, A_{j+1}]$ where $A_j := \frac{j \cdot A}{q}, \ \ j = 0, ..., q$.
- Localization radius here $\rho = A/2q$.
- On each subset the analysis is carried out by solving the least squares problem in $U^{(L)}|_{[A_j, A_{j+1}]}$.

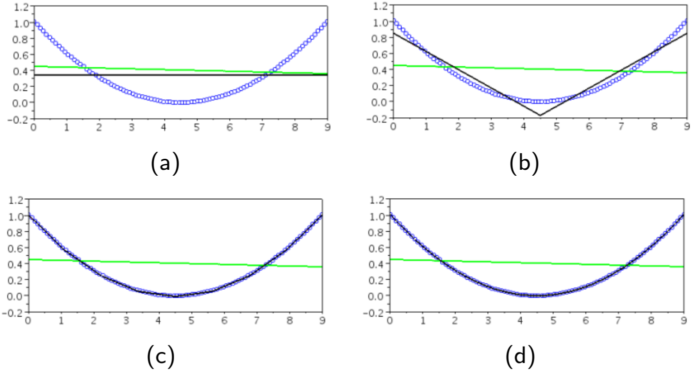


Figure: The truth (blue line) overlaps with the observations (blue circles) due to σ_{obs} takes very small values ($\sigma_{obs} = 0.0005$). The green line shows background information. In (a) we show the analysis without any localization. Localization radii gradually decreases in (b), (c), and (d).

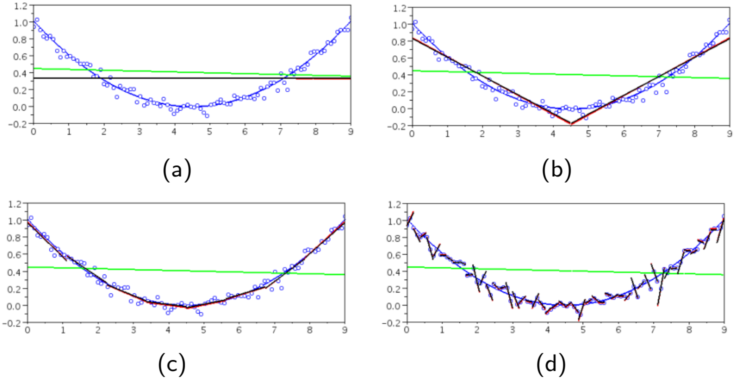


Figure: Observation error $\sigma_{obs} = 0.05$. No localization is applied for (a). In (b), (c) and (d) the localization radii is progressively reduced.

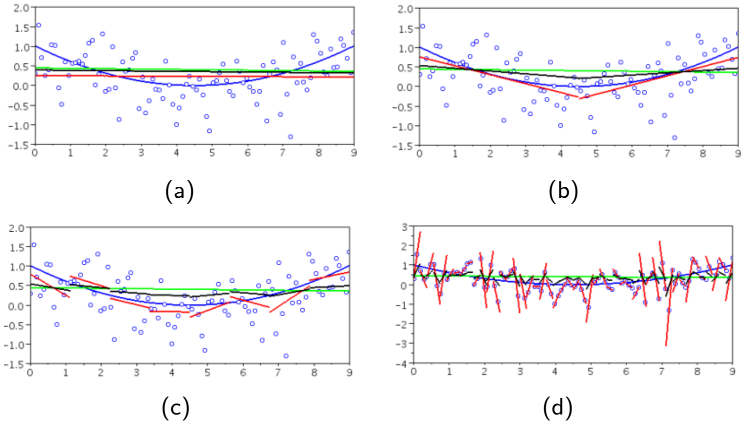


Figure: Higher observation error, $\sigma_{obs} = 0.5$, is provided. The analsyis in (a) is computed with no localization, being progressively smaller in (b), (c) and (d) cases.

Estimating fronts in a 2d example with LETKF [5]

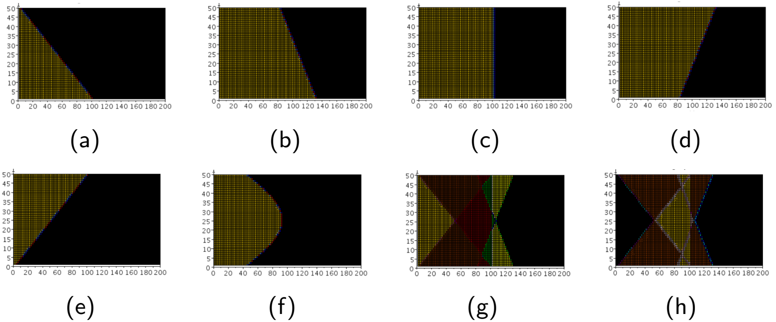


Figure: The different ensemble members are shown in (a)-(e). The truth is displayed in (f). The first guess mean and spread are plotted in (g) and (h), respectively.

[5] Hunt et al. 2007

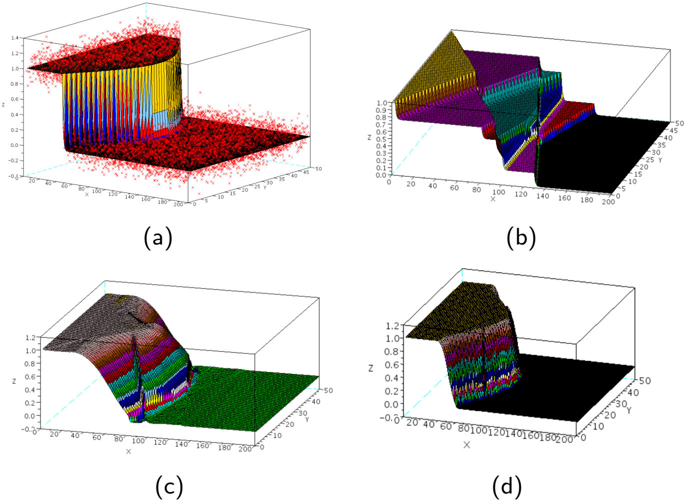


Figure: Truth (front) and observations (red crosses) for $\sigma_{obs} = 0.1$ in (a). Truth (a) is approximated without any localization procedure in (b). In (c) $\rho = 15$, and in (d) $\rho = 5$.

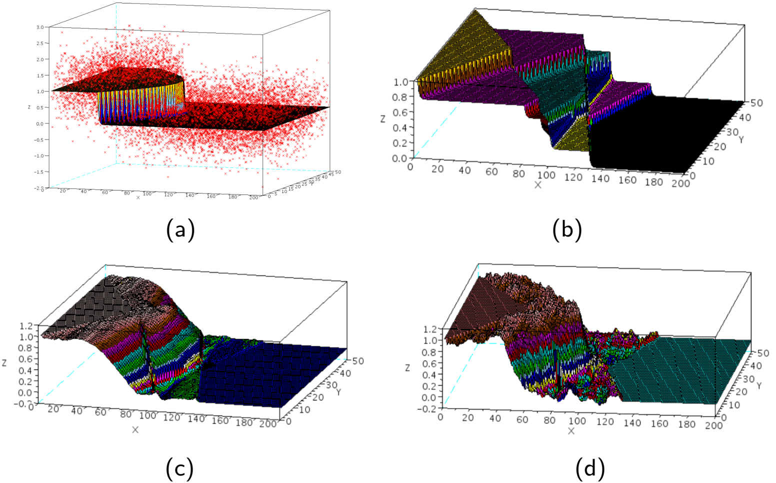


Figure: Truth and observations for $\sigma_{obs} = 0.5$. (a) is approximated without any localization in (b), with $\rho = 15$ in (c) and $\rho = 5$ in (d).

Optimal localization radius

- Estimation of ρ_{loc} as a function of σ_{obs} and observation density μ.
- **Approximation error** (or undersampling error[6]) decreases with smaller localization radius.
- **Effective observation error** decreases with a larger ρ, as a larger number of observations gives a better statistical estimation.
- This leads to the *error asymptotics*

$$E(\rho) = \alpha\rho^p + \frac{\beta\sigma_{obs}}{\sqrt{\mu}}\rho^{-\frac{d}{2}}, \quad \rho > 0,$$

- The minimum of $E(\rho) \quad \rightarrow \quad \rho_{min} = c\left(\frac{d}{p}\right)^{\frac{2}{d+2p}}$

[6] Oke et al. 2007

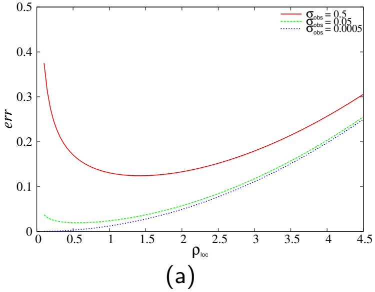


Figure: In (a) we show the theoretical error curve for the case $d = 1$ and $p = 1$. The numerical results (similar curves shown in Greybush et al. 2011) are shown in (b). Here, we display three curves for $\sigma_{obs} \in \{0.0005 \;\; 0.05 \;\; 0.5\}$.

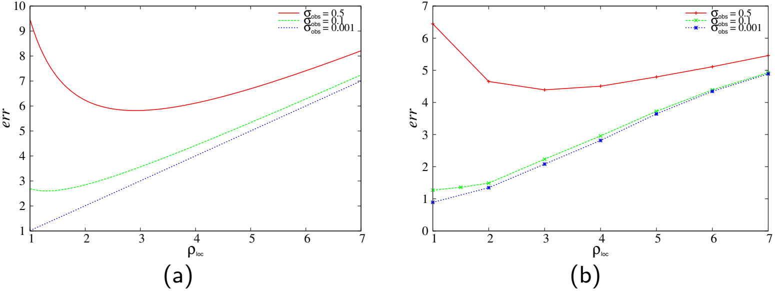


Figure: In (a) we show the theoretical error curve for the case $d = 2$ and $p = 1$. Here, we display three curves for $\sigma_{obs} \in \{0.0001 \;\; 0.1 \;\; 0.5\}$.

Outlook / Conclusion

- Optimal localization length ρ_{loc} depending on σ_{obs} and density of observation. These results are analogous for the L95-LETKF.
- For fixed ρ_{loc} in LETKF: $N_{obs} > (N_{ens} - 1)$ gives better results only if ensemble-subspace is appropiated.
- Next steps: Error analysis for **two-step analysis** with different localization radius for each kind of observation assimilated

$$\begin{aligned}
\varphi_1^{(a)} &= \varphi^{(b)} + BH_1^*(R_{1,\rho_1} + H_1 BH_1^*)^{-1}(f_1 - H_1\varphi^{(b)}) \\
\varphi_2^{(a)} &= \varphi_1^{(a)} + B_1 H_2^*(R_{2,\rho_2} + H_2 B_1 H_2^*)^{-1}(f_2 - H_2\varphi_1^{(a)}) \\
\varphi_{total}^{(a)} &= \varphi_2^{(a)}
\end{aligned}$$

- Two-step analysis gives better results if the two observation types have $\sigma_{obs}^1 >> \sigma_{obs}^2$.

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Deutscher Wetterdienst
Wetter und Klima aus einer Hand