The Error-subspace Transform Kalman Filter

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Introduction

Ensemble square-root Kalman filters are currently the computationally most efficient ensemble-based Kalman filter methods. In particular, the Ensemble Transform Kalman Filter (ETKF) [1] is known to provide a minimum ensemble transformation in a very efficient way. In order to further improve the computational efficiency, the Error-Subspace Transform Kalman Filter (ESTKF) was developed [2]. The ESTKF solves the estimation problem of the Kalman filter directly in the error-subspace that is represented by the ensemble. As the ETKF, the ESTKF provides the minimum ensemble transformation, but at a slightly lower cost. Both, the ETKF and ESTKF are related to the SEIK filter [3]. This filter shows small deviations from the minimum transformation, but is similarly efficient as the ESTKF.

Conclusion

- The Error Subspace Transform Kalman filter (ESTKF) is an efficient ensemble square-root filter that computes the weights for the ensemble transformation directly in the error subspace. The transformations are identical to those of the ETKF.
- The compute performance of the ETKF can be improved by using a projection matrix of size $N \times N$

$$\tilde{\mathbf{T}}_{i,j} = \begin{cases} 1-\frac{1}{N} & \text{for } i=j \\ -\frac{1}{N} & \text{for } i \neq j \end{cases}$$

  to compute $\mathbf{Z}^f = \mathbf{X}^f\tilde{\mathbf{T}}$.
- When the symmetric square root is used, the SEIK filter shows very similar results to those of the ETKF and ESTKF. With Cholesky decompositions, the quality of the SEIK filter deteriorates.
- An implementation of the ESTKF is available in the release of the Parallel Data Assimilation Framework (PDAF) [5, 6].

Representation of the error subspace

ETKF

$$\mathbf{Z}^f = \mathbf{X}^f - \overline{\mathbf{X}^f}, \quad \mathbf{Z}^f \in \mathbb{R}^{n\times N}$$

ESTKF

$$\mathbf{S}^f = \mathbf{X}^f\mathbf{T}, \quad \mathbf{S}^f \in \mathbb{R}^{n\times (N-1)}$$

$$\mathbf{T}_{i,j} = \begin{cases} 1-\frac{1}{N}\frac{1}{\frac{1}{\sqrt{N}}+1} & \text{for } i=j, i<N \\ -\frac{1}{N}\frac{1}{\frac{1}{\sqrt{N}}+1} & \text{for } i\neq j, i<N \\ -\frac{1}{\sqrt{N}} & \text{for } i=N \end{cases}$$

SEIK

$$\mathbf{L}^f = \mathbf{X}^f\hat{\mathbf{T}}, \quad \mathbf{L}^f \in \mathbb{R}^{n\times (N-1)}$$

$$\hat{\mathbf{T}}_{i,j} = \begin{cases} 1-\frac{1}{N} & \text{for } i=j, i<N \\ -\frac{1}{N} & \text{for } i\neq j, i<N \\ -\frac{1}{N} & \text{for } i=N \end{cases}$$

Notation:

State vector $\mathbf{x}^f \in \mathbb{R}^n$; Ensemble of N members $\mathbf{X}^f = \left[\mathbf{x}^{f(1)},\ldots,\mathbf{x}^{f(N)}\right]$; Matrix of ensemble means $\overline{\mathbf{X}^f} = \left[\overline{\mathbf{x}}^f,\ldots,\overline{\mathbf{x}}^f\right]$

The error subspace has a dimension of $N-1$. The ETKF uses an ensemble representation of the error subspace of N ensemble perturbations. The ESTKF and the SEIK filter directly use a basis of the error subspace of dimension $N-1$. The difference between ESTKF and SEIK is caused by the distinct projection matrices $\mathbf{T}$ and $\hat{\mathbf{T}}$.

Ensemble Transformations

ETKF

Analysis covariance matrix

$$\tilde{\mathbf{P}}^a = \mathbf{Z}^f\tilde{\mathbf{A}}(\mathbf{Z}^f)^T$$

with transformation matrix

$$\tilde{\mathbf{A}} \in \mathbb{R}^{N\times N}$$

$$\tilde{\mathbf{A}}^{-1} = (N-1)\mathbf{I} + (\mathbf{H}\mathbf{Z}^f)^T\mathbf{R}^{-1}\mathbf{H}\mathbf{Z}^f$$

Ensemble transformation

$$\tilde{\mathbf{X}}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{Z}^f\tilde{\mathbf{C}}$$

with square-root

$$\tilde{\mathbf{C}}\tilde{\mathbf{C}}^T = \tilde{\mathbf{A}}$$

ESTKF

$$\mathbf{P}^a = \mathbf{S}^f\mathbf{A}(\mathbf{S}^f)^T$$

$$\mathbf{A} \in \mathbb{R}^{(N-1)\times(N-1)}$$

$$\mathbf{A}^{-1} = (N-1)\mathbf{I} + (\mathbf{H}\mathbf{S}^f)^T\mathbf{R}^{-1}\mathbf{H}\mathbf{S}^f$$

$$\mathbf{X}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{S}^f\mathbf{C}\mathbf{T}^T$$

$$\mathbf{C}\mathbf{C}^T = \mathbf{A}$$

SEIK

$$\hat{\mathbf{P}}^a = \mathbf{L}^f\hat{\mathbf{A}}(\mathbf{L}^f)^T$$

$$\hat{\mathbf{A}} \in \mathbb{R}^{(N-1)\times(N-1)}$$

$$\hat{\mathbf{A}}^{-1} = (N-1)\hat{\mathbf{T}}^T\hat{\mathbf{T}} + (\mathbf{H}\mathbf{L}^f)^T\mathbf{R}^{-1}\mathbf{H}\mathbf{L}^f$$

$$\hat{\mathbf{X}}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{L}^f\hat{\mathbf{C}}\mathbf{T}^T$$

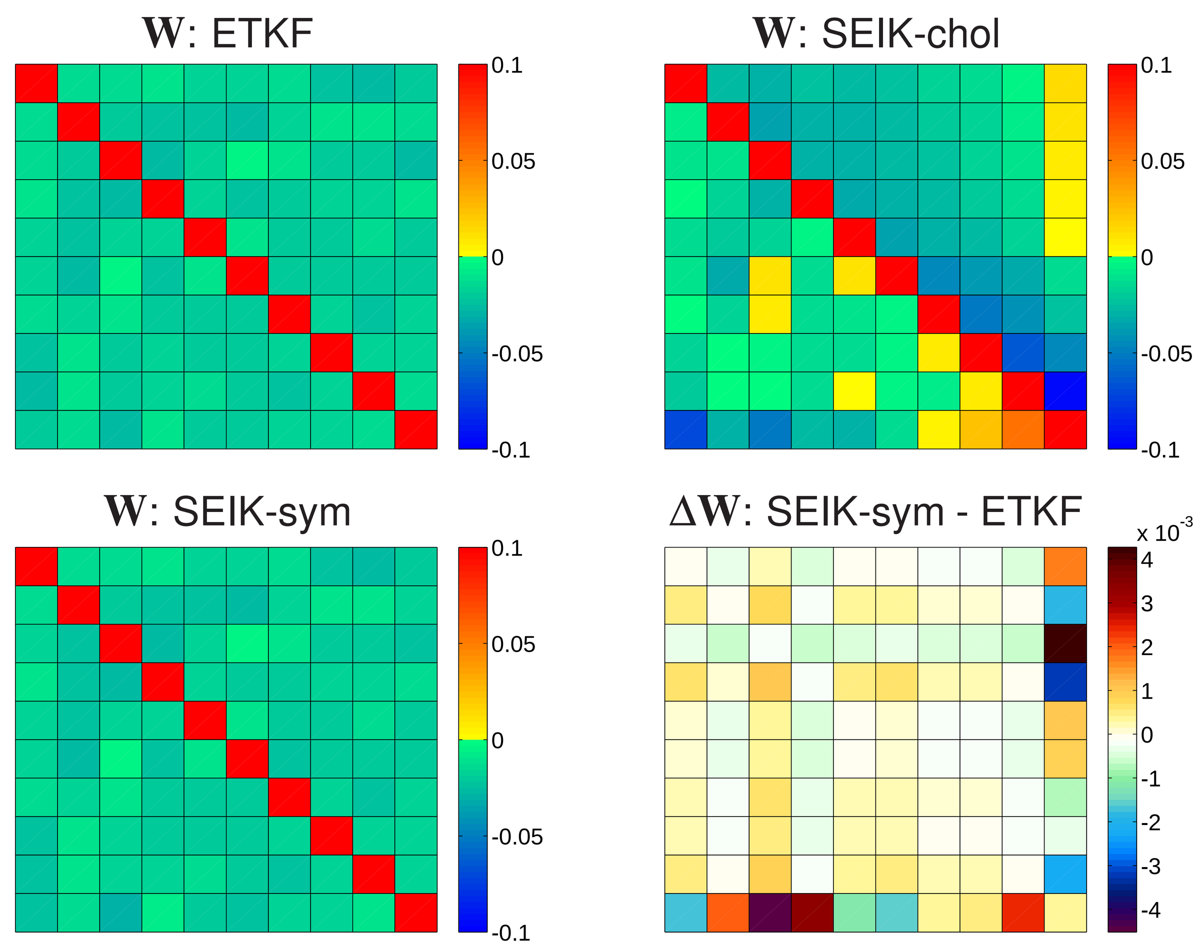
$$\hat{\mathbf{C}}\hat{\mathbf{C}}^T = \hat{\mathbf{A}}$$

The symmetric square root $\mathbf{C} = \mathbf{U}\Lambda^{-1/2}\mathbf{U}^T$ from the singular value decomposition $\mathbf{U}\Lambda\mathbf{V}^T = \mathbf{A}^{-1}$ can be used in all cases.

All filters compute a square root of the transform matrix ($\tilde{\mathbf{A}}$, $\mathbf{A}$, $\hat{\mathbf{A}}$). These matrices are distinct, but the ensemble transformations in ETKF and ESTKF are identical if the symmetric square root is used for both filters.

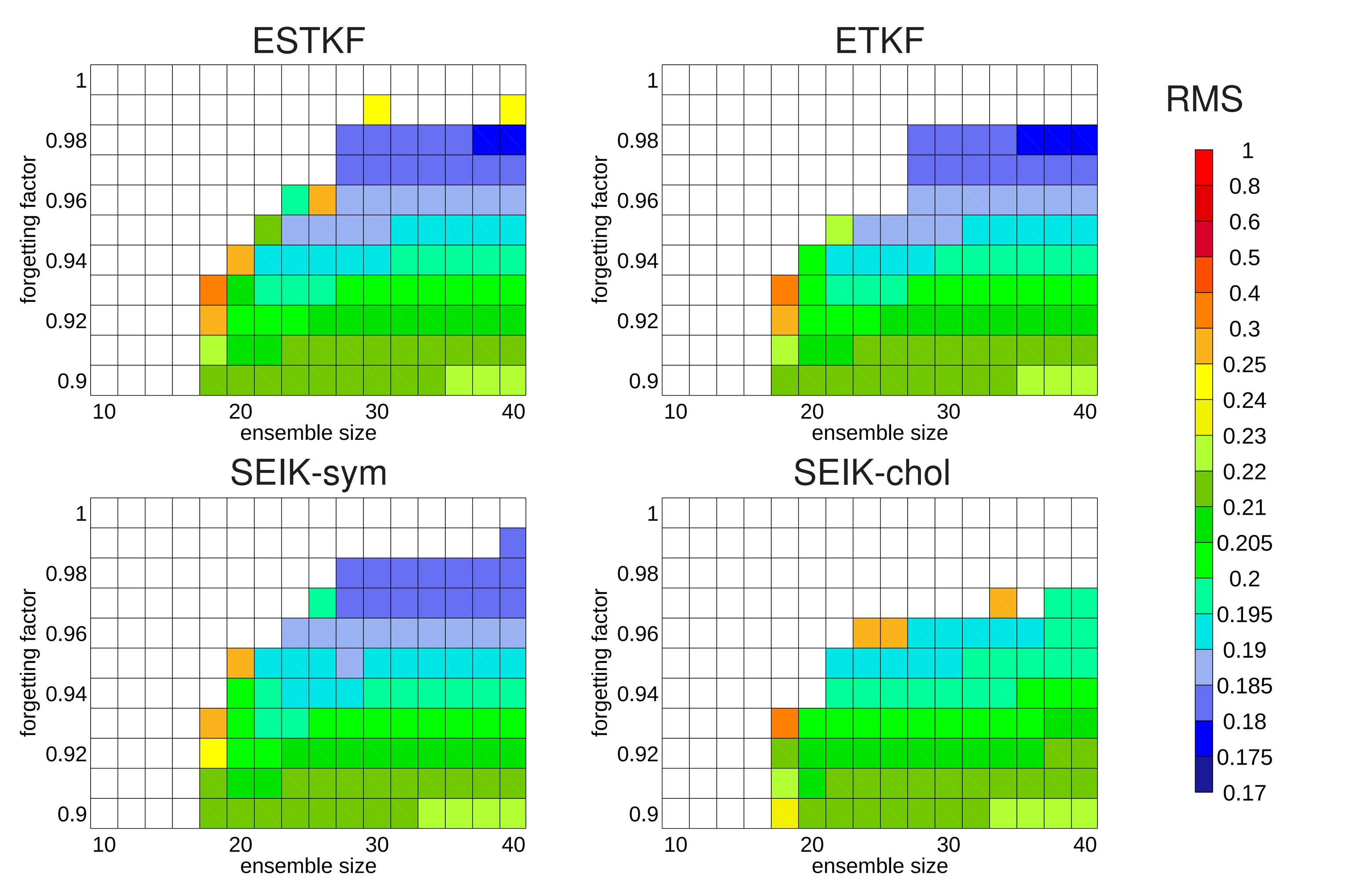
Ensemble weight matrices

The figure below shows a comparison of the weight matrices used for the ensemble transformation for a single analysis step. All matrices are projected to be of size $N \times N$, e.g. for ESTKF $\mathbf{W} = \mathbf{T}\mathbf{C}\mathbf{T}^\mathbf{T}$ and for ETKF $\tilde{\mathbf{W}} = \tilde{\mathbf{T}}\tilde{\mathbf{C}}$. ETKF's $\mathbf{W}$ is closest to the Identity, the transformation of the ESTKF is identical up to numerical precision. SEIK's $\mathbf{W}$ differs more from the identity in case of a Cholesky square-root (*SEIK-chol*). With the symmetric square-root (*SEIK-sym*), the transformation in SEIK is minimally different from that of the ETKF and ESTKF, but depends on the ensemble ordering.



Assimilation Experiments

Twin experiments were conducted using the nonlinear Lorenz96 model [4] implemented in PDAF [5, 6]. Synthetic observations of the full state were generated from a model run. Observations were assimilated at each time step over 50000 time steps. For SEIK, configurations with either symmetric square root or with a square-root based on Cholesky decomposition were used. The global formulations of the filters were used.



The figure shows mean RMS errors as functions of the ensemble size and forgetting factor (covariance inflation). As expected, the results from ESTKF and ETKF are almost identical. The differences are only caused by the finite precision of the numerical computations.

The SEIK filter with symmetric square root provides very similar results. Errors from the SEIK filter using a Cholesky square root of $\hat{\mathbf{A}}$ are larger. This is caused by an inferior ensemble quality in which a small number of ensemble members carry most of the variance.

References

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[4] EN Lorenz. (1996). Predictability - a problem partly solved. *Proceedings Seminar on Predictability*, ECMWF, Reading, UK, 1–18.

[5] Parallel Data Assimilation Framework (PDAF) – an open source framework for ensemble data assimilation. *http://pdaf.awi.de*

[6] Nerger, L. and W. Hiller (2013). Software for Ensemble-based Data Assimilation Systems – Implementation Strategies and Scalability. *Computers & Geosciences.* 55: 110–118