The Error-subspace Transform Kalman Filter

Lars Nerger, Wolfgang Hiller, and Jens Schröter

Alfred Wegener Institute for Polar and Marine Research, Bremerhaven, Germany
Contact: Lars.Nerger@awi.de · http://www.awi.de

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.

Comparison of Filters

The equations for the ETKF, ESTKF and SEIK filter algorithms are displayed on the right hand side. The equations have only subtle differences.

Error space representation

The ETKF uses the ensemble perturbation matrix $\mathbf{Z}$ to represent the estimated error space. In contrast, ESTKF and SEIK use a basis of the error space, which has one column less than $\mathbf{Z}$.

State analysis update

The correction of the state estimate (ensemble mean) is identical in all three filters.

Ensemble transformation

The ensemble transformation is computed in different representations. Matrix $\mathbf{A}$ of the ESTKF is smaller than $\tilde{\mathbf{A}}$ of the ETKF by one row and one column. When both filters use the same definition of matrix square root, they provide identical ensemble transformations.

The smaller transformation matrix $\mathbf{A}$ of the ESTKF slightly reduces the computational cost compared to the ETKF. The cost can be further reduced by using the Cholesky decomposition instead of the singular value decomposition. However, the ensemble quality deteriorates with a Cholesky decomposition.

Computing times

(Ensemble size 20; Lorenz96 model; 50000 steps)

ETKF	ESTKF	SEIK-Cholesky
46.0s	44.7s	26.7s

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 ESTKF provides ensemble transformations that are analytically identical to those of the ETKF. In a numerical application, small differences can occur due to the finite numerical precision.
- 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].

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

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

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

SEIK

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

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

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 Ω and $\mathbf{T}$.

Ensemble Transformations

ETKF	ESTKF	SEIK
Analysis covariance matrix		
$\tilde{\mathbf{P}}^a = \mathbf{Z}^f\tilde{\mathbf{A}}(\mathbf{Z}^f)^T$	$\mathbf{P}^a = \mathbf{S}^f\mathbf{A}(\mathbf{S}^f)^T$	$\hat{\mathbf{P}}^a = \mathbf{L}^f\hat{\mathbf{A}}(\mathbf{L}^f)^T$
with transformation matrix		
$\tilde{\mathbf{A}} \in \mathbb{R}^{N\times N}$	$\mathbf{A} \in \mathbb{R}^{(N-1)\times(N-1)}$	$\hat{\mathbf{A}} \in \mathbb{R}^{(N-1)\times(N-1)}$
$\tilde{\mathbf{A}}^{-1} = (N-1)\mathbf{I} + (\mathbf{HZ}^f)^T\mathbf{R}^{-1}\mathbf{HZ}^f$	$\mathbf{A}^{-1} = (N-1)\mathbf{I} + (\mathbf{HS}^f)^T\mathbf{R}^{-1}\mathbf{HS}^f$	$\hat{\mathbf{A}}^{-1} = (N-1)\mathbf{T}^T\mathbf{T} + (\mathbf{HL}^f)^T\mathbf{R}^{-1}\mathbf{HL}^f$
Ensemble transformation		
$\tilde{\mathbf{X}}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{Z}^f\tilde{\mathbf{C}}$	$\mathbf{X}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{S}^f\mathbf{C}\Omega^T$	$\hat{\mathbf{X}}^a = \overline{\mathbf{X}^a} + \sqrt{N-1}\mathbf{L}^f\hat{\mathbf{C}}\Omega^T$
with square-root		
$\tilde{\mathbf{C}}\tilde{\mathbf{C}}^T = \tilde{\mathbf{A}}$	$\mathbf{C}\mathbf{C}^T = \mathbf{A}$	$\hat{\mathbf{C}}\hat{\mathbf{C}}^T = \mathbf{U}$

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.

The filters compute square roots of different matrices ($\tilde{\mathbf{A}}$, $\mathbf{A}$, $\hat{\mathbf{A}}$). The ensemble transformations in ETKF and ESTKF are identical if the symmetric square root is used. For SEIK, the transformation deviates slightly. In addition, it varies with the order of the ensemble members in the ensemble matrix.

Assimilation Experiments

Twin experiments were conducted using the nonlinear Lorenz96 model [4] implemented in PDAF [5]. 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 decompostion were used. The global formulations of the filters were used. Localization is not required for the small Lorenz96 model if the ensemble size is large enough.

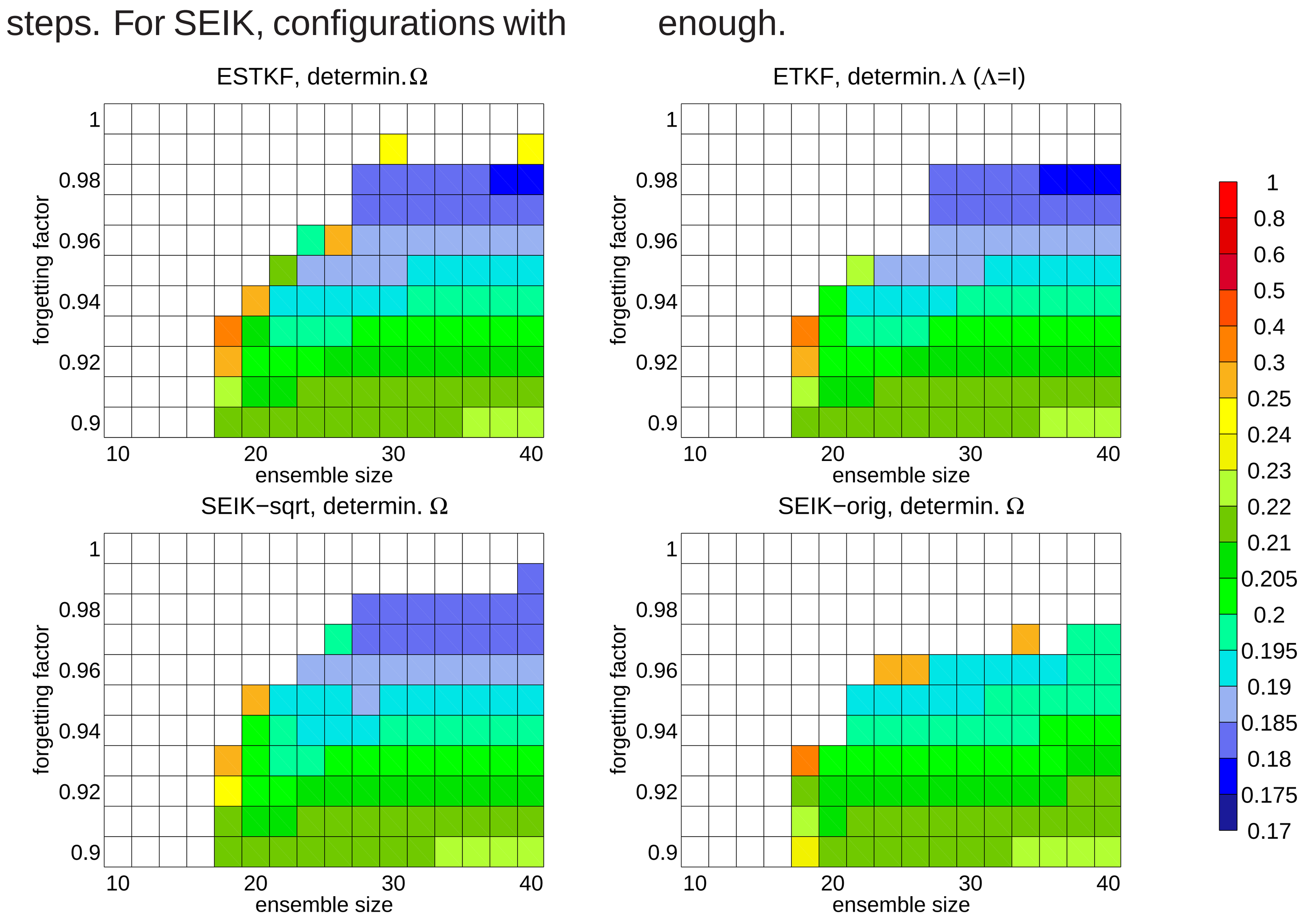

Figure 1: Mean RMS errors over 10 experiments are shown as functions of the ensemble size and forgetting factor (covariance inflation). The results from ESTKF and ETKF are almost identical. Analytically, both filters are equivalent. Thus, the differences are only caused by the finite precision of the numerical computations. The SEIK filter with symmetric square root also provides very similar results. Errors from the SEIK filter using a Cholesky decomposition of the transformation matrix $\hat{\mathbf{A}}$ are larger. This is caused by an inferior ensemble quality in which a small number of ensemble members carry most of the variance.

References

[1] CH Bishop et al.. (2001). Adaptive Sampling with the Ensemble Transform Kalman Filter. Part I: Theoretical Aspects. *Mon. Wea. Rev.* 129: 420–436

[2] L Nerger et al. (2012) A Unification of Ensemble Square Root Kalman Filters. Mon. Wea. Rev., In press

[3] DT Pham et al. (1998). Singular evolutive Kalman filters for data assimilation in oceanography. *C. R. Acad. Sci.* Series II 326: 255–260

[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*