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On the form of the transformation matrix in Ensemble Square Root Filters

Abstract

We argue that the one-sided solution for the ensemble transformation matrix (ETM) in the ensemble transform Kalman filter (ETKF), $\mathbf{T}=\mathbf{C}(\Gamma+\mathbf{I})^{-1/2}$, and similar expressions in related ensemble square root Kalman filters (EnSKF) should not be used in practice; and should always be replaced by the symmetric solution, $\mathbf{T}=\mathbf{C}(\Gamma+\mathbf{I})^{-1/2}\mathbf{C}$, or by corresponding expressions in other flavours of EnSKF.

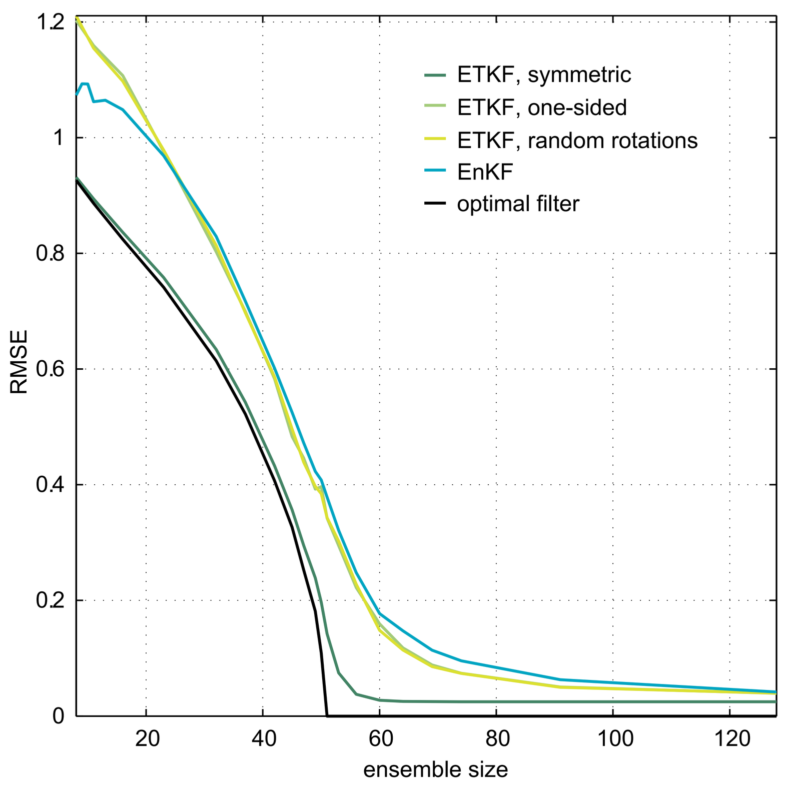


Figure 1 RMSE of different filters for the *LA model* (no inflation factor is used for ETKF).

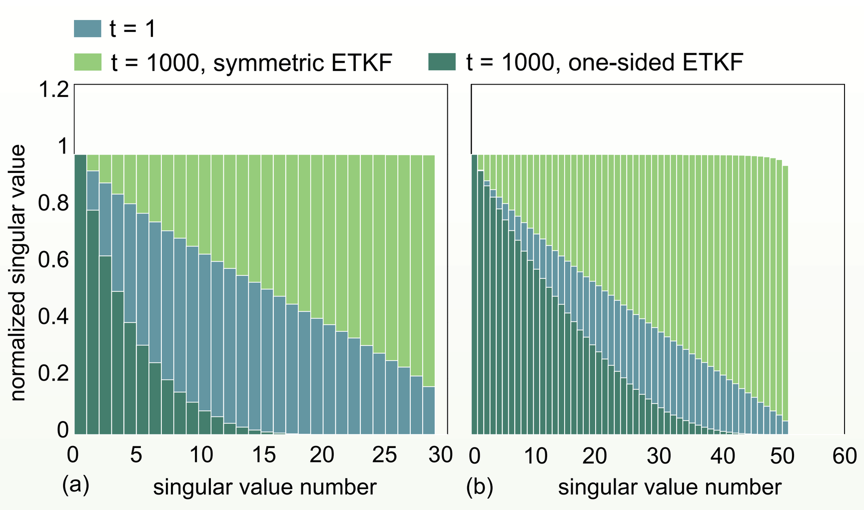


Figure 2 Normalised singular-value spectrum for **X** from for the *LA model* for (a) n=30 and (b) n=60. The number of degrees of freedom in the *LA model* is 51.

Background

The success of ensemble data assimilation depends on the properties of the ensemble, from which background error covariances are approximated. Two commonly used approaches are the classic Ensemble Kalman Filter with perturbed observations (EnKF)[1]; and EnSKFs[2], where ensemble perturbations are transformed to be consistent with Kalman filter theory. Square root filters have the advantage of being deterministic; and therefore less prone to sampling error.

In the EnSKFs the ensemble mean is updated using the standard Kalman Filter equations, while the ensemble perturbations **X** around this mean are updated using:

$$\mathbf{X}^a=\mathbf{X}^f\mathbf{T}, \quad (1)$$

where **T** is the ETM; and superscripts **a** and **f** refer to analysis and forecast. **T** is defined so that the analysis error covariance of the ensemble match the theoretical value from Kalman Filter theory. The particular form of the solution for the ETM depends on the flavour of EnSKF. In ETKF[3]

$$\mathbf{T}=[\mathbf{I}+(\mathbf{HX}^f)^T\mathbf{R}^{-1}\mathbf{HX}^f/(m-1)]^{-1/2}, \quad (2)$$

where **m** is the ensemble size. Given the eigenvalue decomposition of $[\mathbf{I}+(\mathbf{HX}^f)^T\mathbf{R}^{-1}\mathbf{HX}^f/(m-1)]=\mathbf{C}\Gamma\mathbf{C}^T$; where **C** is orthonormal and Γ is a diagonal matrix of eigenvalues; the solution for **T** is

$$\mathbf{T}=\mathbf{C}\Gamma^{-1/2}\mathbf{U}, \quad (3)$$

where **U** is an arbitrary orthonormal matrix. The importance of the particular form of **T** has previously been underestimated. The three different solutions used in the literature are the one-sided solution[3,2]:

$$\mathbf{T}=\mathbf{C}\Gamma^{-1/2}; \quad (4)$$

the symmetric solution[4,5]:

$$\mathbf{T}=\mathbf{C}\Gamma^{-1/2}\mathbf{C}\mathbf{T}; \quad (5)$$

and the solution with random rotations[6,7] given by (3) if **U** is assumed to be a random orthonormal matrix.

In early works on the ETKF[3,2] the one-sided solution was used. It was subsequently realised that the symmetric solution has some advantages[5]. However, these advantages were reported as only giving a "small improvement". The solution with random rotations has also been recommended[6,7] as an improvement over the one-sided solution.

We compare the performance of the EnSKF with each formulation for **T** (3-5) and the EnKF. As a test bed we perform twin experiments using two small 1D models: a *Linear Advection (LA) model*, where a 1D field is advected over a periodic domain at constant speed[6]; and the highly non-linear *Lorenz-40 model* [8].

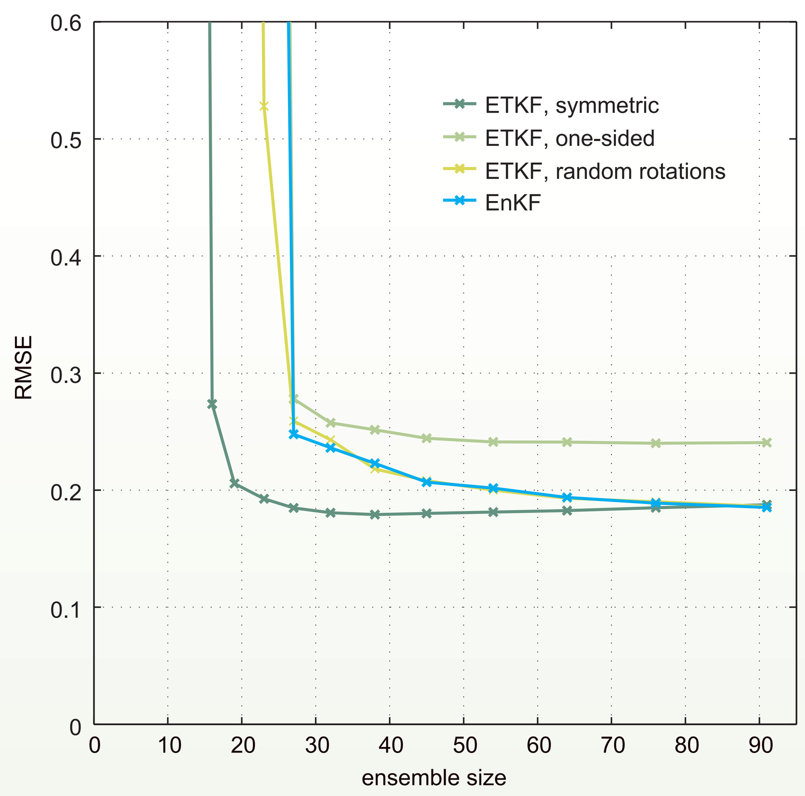


Figure 4 The best RMSE from Figure 3 for a given ensemble size of all inflation factors.

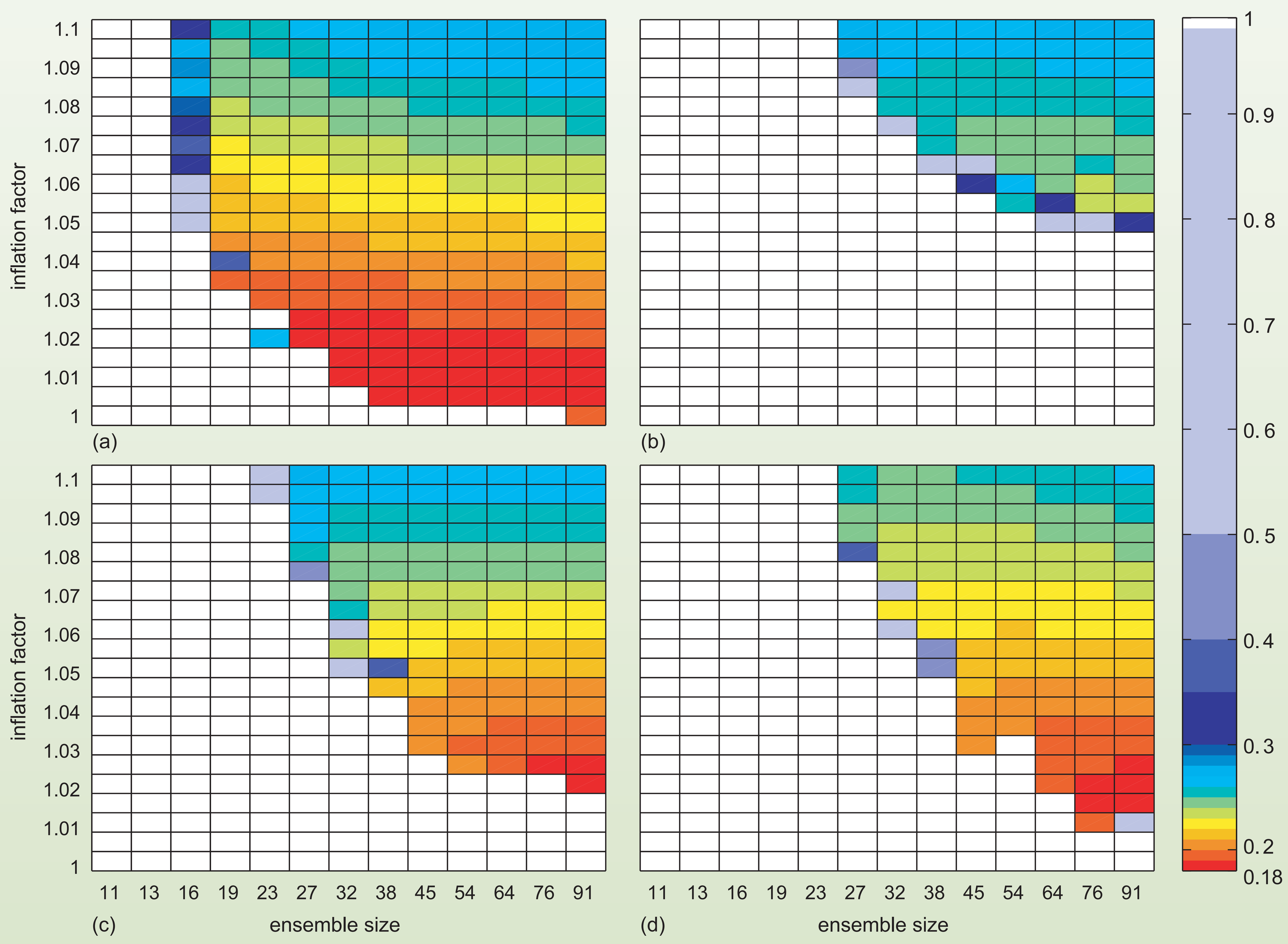


Figure 3 RMSE for the *Lorenz-40* model averaged over a long run for the ETKF with the (a) symmetric, (b) one-sided and (c) random rotations formulation for **T**; and (d) the EnKF with perturbed observations. The fractal dimension of the *Lorenz-40 model* is 27.

Results

The root mean-squared error (RMSE) for experiments using the *LA model* are plotted for each filter as a function of ensemble size in **Figure 1**. The superior performance of the symmetric ETM is clear. An explanation for this is partially given in **Figure 2**, where the normalized singular value spectrum of **X** is shown. This shows that the symmetric form in (5) orthogonalises **X**, thereby increasing the quality of the ensemble as an orthogonal basis.

The RMSE for the *Lorenz-40* model is shown as a function of ensemble size and inflation factor in **Figure 3**. Because the performance of each filter depends on the inflation factor, we present the RMSE versus ensemble size for the best inflation factor for each ensemble size in **Figure 4**. Again, the superior performance of the symmetric formulation is clearly evident; and again the symmetric filter acts to orthogonalise **X** (**Figure 5**).

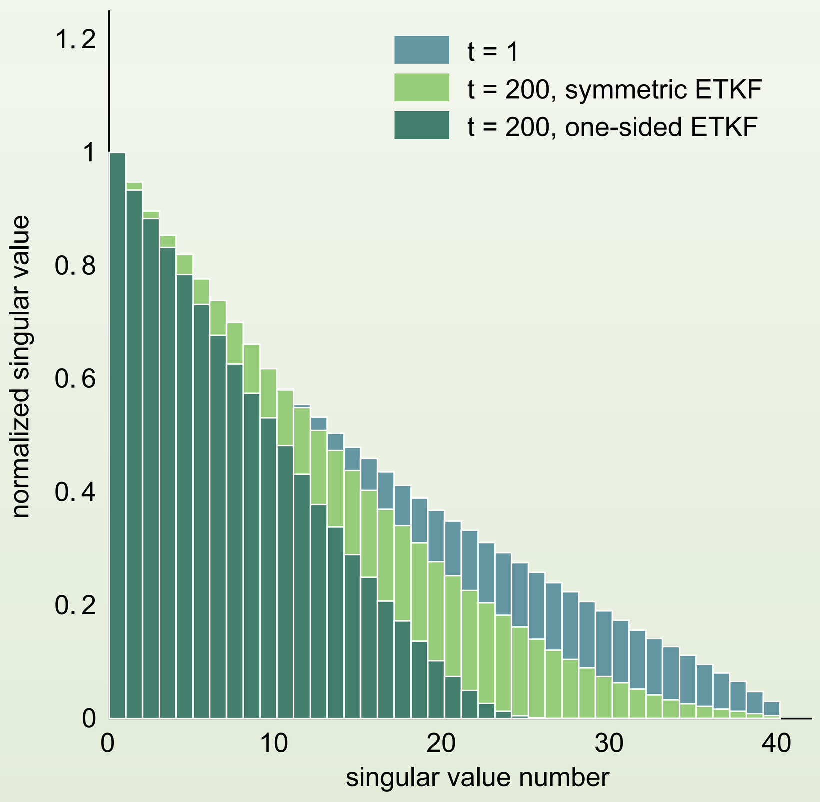


Figure 5 Normalised singular-value spectrum of **X** for the *Lorenz-40* model.

Discussion

We argue that the EnSKF with the symmetric form for **T** outperforms other filters because it has the following properties:

(a) *Centered Analysis:* the correct ensemble mean is preserved[3];

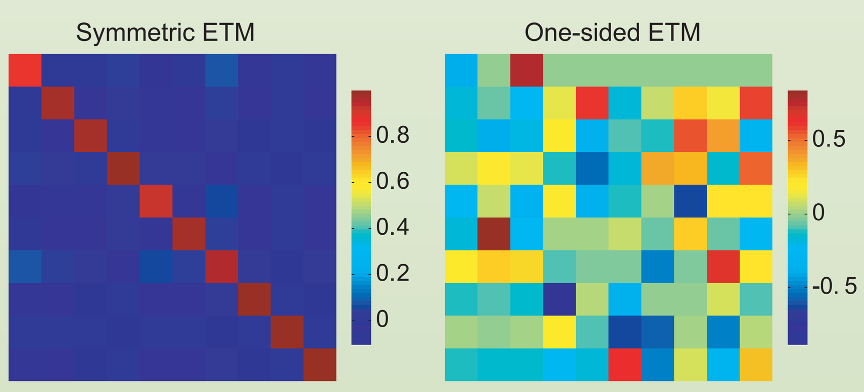
(b) *Continuity:* If $\mathbf{I}+(\mathbf{HX}^f)^T\mathbf{R}^{-1}\mathbf{HX}^f/(m-1)\rightarrow\mathbf{I}$, then $\mathbf{T}\rightarrow\mathbf{I}$. In practice, typically $\mathbf{T}\approx\mathbf{I}$ (**Figure 6**); thus updates to **X** are small; and the problem of initialisation is diminished;

(c) *Minimal length solution:* the distance between $\mathbf{X}^f$ and $\mathbf{X}^a$ is minimised[4];

(d) *Symmetry:* yields the only symmetric positive definite solution to (2).

Conclusions

Based on a series of experiments with two small models, we have demonstrated that the symmetric ETM in the ETKF yields a significantly better performance than that of other forms. We attribute this superior performance to a number of attractive properties of the ETM and argue that only the symmetric form should be used in practice.



> **Figure 6** Examples of **T** produced using the symmetric (left) and one-sided (right) solution. Here, **T** is calculated using an ensemble of 10 members of length 40; each state element is normally distributed around zero with the variance of 1, and there are two observations with error variance of 1.

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