# Mean preserving rotations in SQRT schemes

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In a recent manuscript by Pavel Sakov

`www.marine.CSIRO.au/%7Esakov/etm.pdf`

it has shown that some SQRT filter formulations may introduce a shift in the mean of the ensemble perturbations which degrades the results. This is also the case for the EnKF version of the SQRT filter as discussed in *Evensen* (2004, 2006). Thus the EnKF SQRT algorithm has been updated accordingly resulting an improved analysis scheme which have better properties than the previous version which did not preserve the mean of the perturbations.

## 1 Mean preserving rotation

Refering to *Evensen* (2006) the basic equation for the update of the perturbations is Eq. (13.7), i.e.,

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}. \tag{1}$$

The product $\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}$ is one part of the factorization of a symmetric matrix

$$\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S} = \boldsymbol{V}_2\big(\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2\big)\boldsymbol{V}_2^{\mathrm{T}}. \tag{2}$$

Here $\boldsymbol{S} = \boldsymbol{\mathcal{M}A'}$ is the measurements of the ensemble perturbations $\boldsymbol{A'}$, and $\boldsymbol{C} = \boldsymbol{SS}^{\mathrm{T}} + \boldsymbol{C}_{\epsilon\epsilon}$ is the matrix to be inverted in the Kalman filter analysis schemes (see Chapter 9.3 for the notation *Evensen*, 2006).

We should require that the analysis satisfy

$$\boldsymbol{A}^{\mathrm{a}\prime}\mathbf{1}_N = 0, \tag{3}$$

with $\mathbf{1}_N \in \Re^{N\times N}$ being the matrix with all elements equal to $1/N$, and $N$ is the number of ensemble members.

Then, writing the update equation (1) as

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{T} \tag{4}$$

and using that the ensemble mean $\boldsymbol{A}'\mathbf{1}_N = 0$ it is sufficient to require that

$$\boldsymbol{T}\mathbf{1}_N = a\mathbf{1}_N, \tag{5}$$

where $a$ is an arbitrary coefficient (see the paper by Sakov for further explanations). This is not satisfied using $\boldsymbol{T} = \boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}$ as in the Eq. (1).

However, note that if we multiply from the right by $\boldsymbol{V}_2^{\mathrm{T}}$ we obtain

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}\boldsymbol{V}_2^{\mathrm{T}}. \tag{6}$$

This means that we are updating the perturbations using the symmetric square root of (2) rather than the factorization, and it is clear that this does not change the resulting variance of the updated ensemble perturbations (by evaluating $\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}}$). In addition it can be shown that it preserves the mean equal to zero (see manuscript by Sakov).

The EnKF square root schemes have now been updated to use the symmetric square root and now computes the updated perturbations according to (6).

# 2 Random mean preserving rotation

Sakov also gave a procedure for computing a random rotation which preserves the mean. An arbitrary orthonormal matrix may not satisfy the contidion

$$\boldsymbol{\Theta}\mathbf{1}_N = \mathbf{1}_N, \tag{7}$$

and may therefore introduce a norzero mean in the updated perturbations. This new precedure is now also used in the EnKF square root scheme.

From the examples below it is seen that the random rotation does not introduce any artifacts in the linear model, as long as it is mean preserving (as discussed next). In a nonlinear model the additional random rotation may introduce a dynamically less consistent update since it effectively replaces all ensemble members with new members which are linear combinations of the previous ones, and these are not necessarily solutions of the nonlinear equations.

# 3 Using the mean preserving rotation with a single meansurement

As discussed in Chapter 13.1.3 in *Evensen* (2006), the assimilation of a single measurement in a scalar model, led to an updated ensemble of perturbations that were all equal to zero, except for the first element that contained all the variance, (thus a shift in the mean was also introduced). In a scalar model we have $\boldsymbol{S} = \boldsymbol{A}' \in \Re^{1\times N}$ and it was shown in *Evensen* (2006) that the analyzed perturbations in this case became

$$\boldsymbol{S}^{\mathrm{a}} = \left(\sigma\sqrt{1-\sigma^2/\lambda}, 0, \ldots, 0\right). \tag{8}$$

Here $\sigma = \sqrt{\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}}$ is the forecast standard deviation, and the parameter $\lambda = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + (N-1)\boldsymbol{C}_{\epsilon\epsilon}$ is just the $\boldsymbol{C}$-matrix. Note also that $\boldsymbol{v}_1$, i.e., the first column of $\boldsymbol{V}_2$, equals $\boldsymbol{v}_1 = \boldsymbol{S}/\sqrt{\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}}$.

An additional multiplication from the right with $\boldsymbol{V}^{\mathrm{T}}$ gives

$$\begin{aligned}
\boldsymbol{S}^{\mathrm{a}} &= \sigma\sqrt{1-\sigma^2/\lambda}\,\boldsymbol{v}_1 && (9)\\
&= \sigma\sqrt{1-\sigma^2/\lambda}\,\boldsymbol{S}/\sqrt{\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}} && (10)\\
&= \sqrt{1-\sigma^2/\lambda}\,\boldsymbol{S} && (11)\\
&= \sqrt{1-\frac{\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}}{\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}+(N-1)\boldsymbol{C}_{\epsilon\epsilon}}}\,\boldsymbol{S}, && (12)
\end{aligned}$$

which again results in the correct variance of the update. It is also clear that the mean of $\boldsymbol{S}^{\mathrm{a}}$ is identical to zero, since the analysis scales all perturbations equally, and the mean of $\boldsymbol{S}$ is equal to zero per definition.

For a state vector which is a function of space the arguments above will still be valid for the measurement location. However, on other spatial locations the rows in $\boldsymbol{A}'$ will not be parallel to $\boldsymbol{v}_1$ and thus orthogonal to $(\boldsymbol{v}_2, \ldots, \boldsymbol{v}_N)$, and there will be contributions to all ensemble perturbations. Obviously these contributions will be very small for grid points close to the measurement location when smooth model states are used.

Based on this discussion it is not clear if an additional random rotation is needed. Afterall, the variance reduction is equally spread out among all the ensemble members.

# 4 Example

The plots below compares results using the old scheme (X) and the new scheme with mean preserving rotations (Y), for the experiments *Exps. F* and *G* and also *Exps. 6–10* from *Evensen* (2006). It is clear from Fig. 1 that the residuals are reduced in all experiments, when the new mean preserving rotations are used. Further, the RMS residuals also indicate an improvement in both *Exps. F* and *G* in Fig. 2. In particular we also note that the use of improved sampling has an important effect as well, when it comes to reducing the residuals and to reproducing the correct error statistics.

Additional experiments (Z) were also run where the mean preserving rotation was used but the mean preserving random rotation from the (Y) cases were excluded. In *Exps. F* and *G* this did not impact the average of the residuals but seemed to increase the spread slighly. Thus, this is an indication that the random mean preserving rotation should be retained.

The singular spectra in Fig. 3 show an important improvement. In the old scheme the random rotation introduced a rank reduction in the ensemble as was explained in *Evensen* (2006). However, in the new scheme this is entirely avoided, and the spectra show no trace of the random rotation at all. Similar conclusions can be drawn from the *Exps. 6–10.* In particular note that it appears to be better to use a low rank approximation of the error covariance matrix for the measurement errors, rather than specifying a full rank matrix in the cases where the number of measurements are larger than the number of ensemble members.

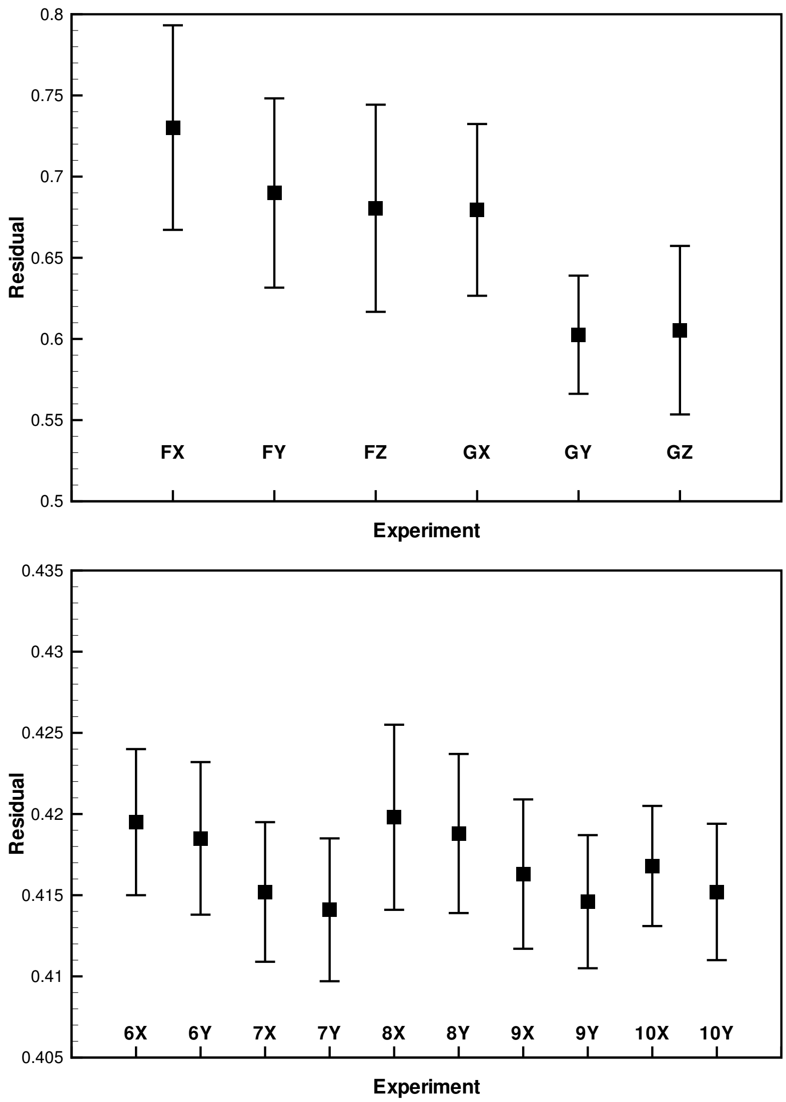


Figure 1: Mean residual and std dev for the experiments.

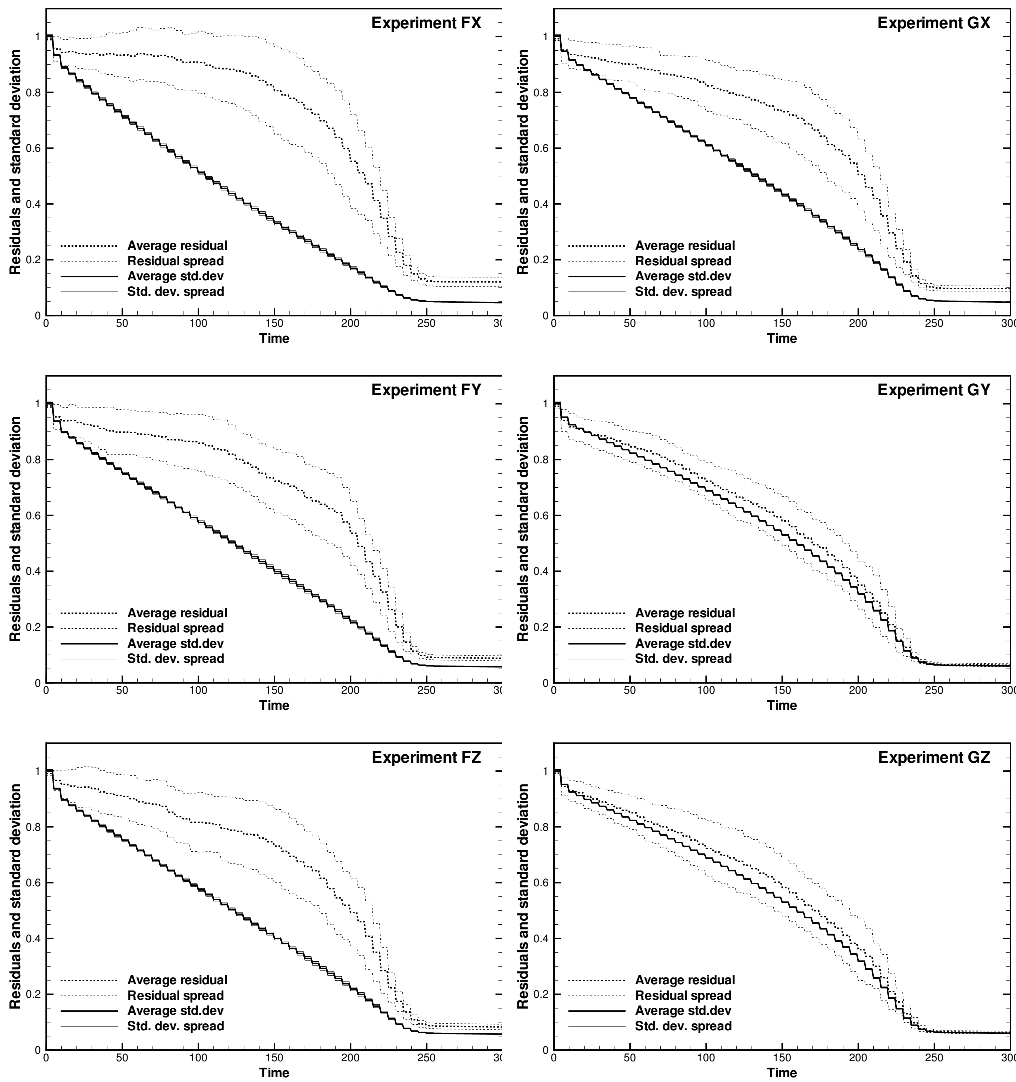


Figure 2: RMS residuals and ensemble singular value spectra for some of the experiments, without (upper) and with (middle) mean preserving rotations. The lower plots are with mean preserving rotation, but without mean preserving random rotation.

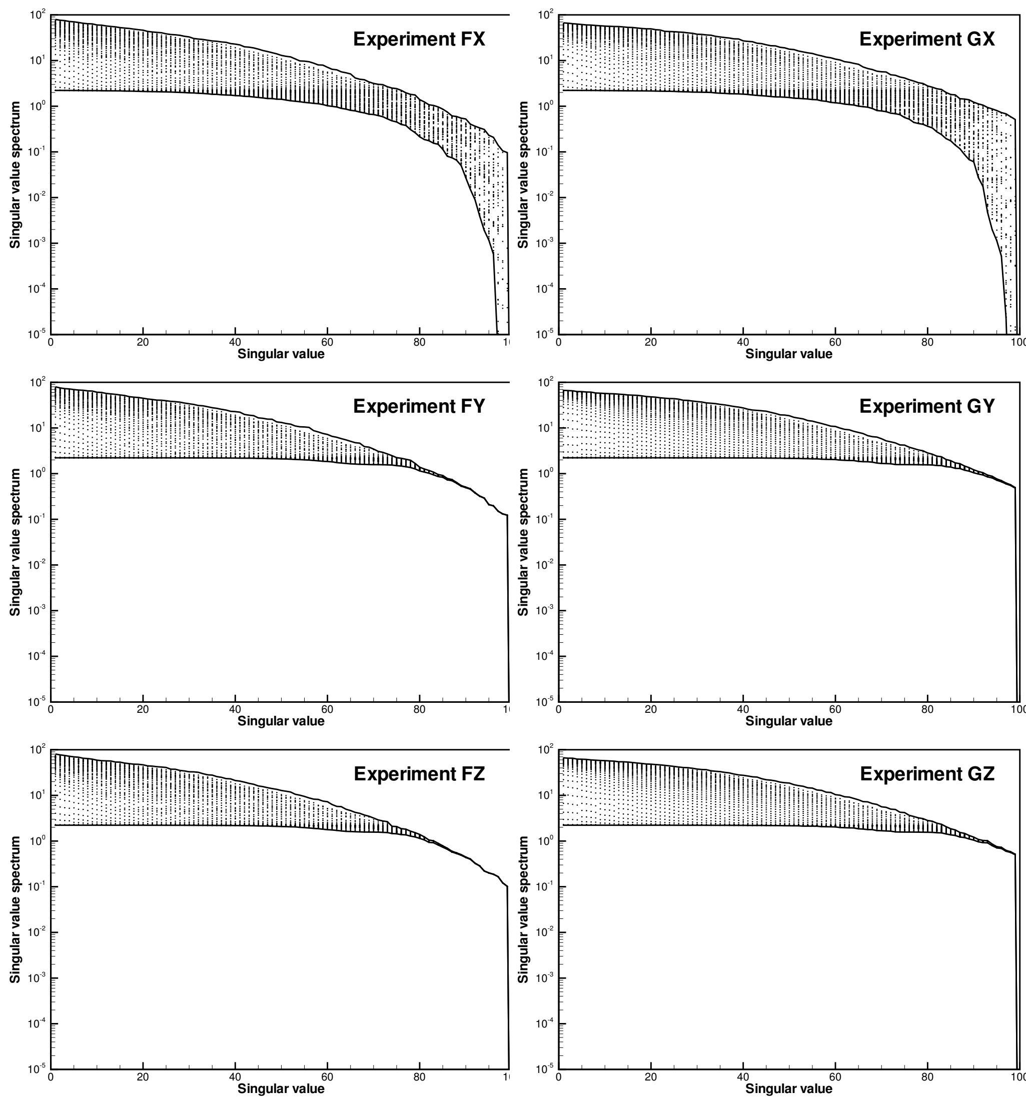


Figure 3: Singular value spectra of the ensemble perturbations for the same experiments as in 2.

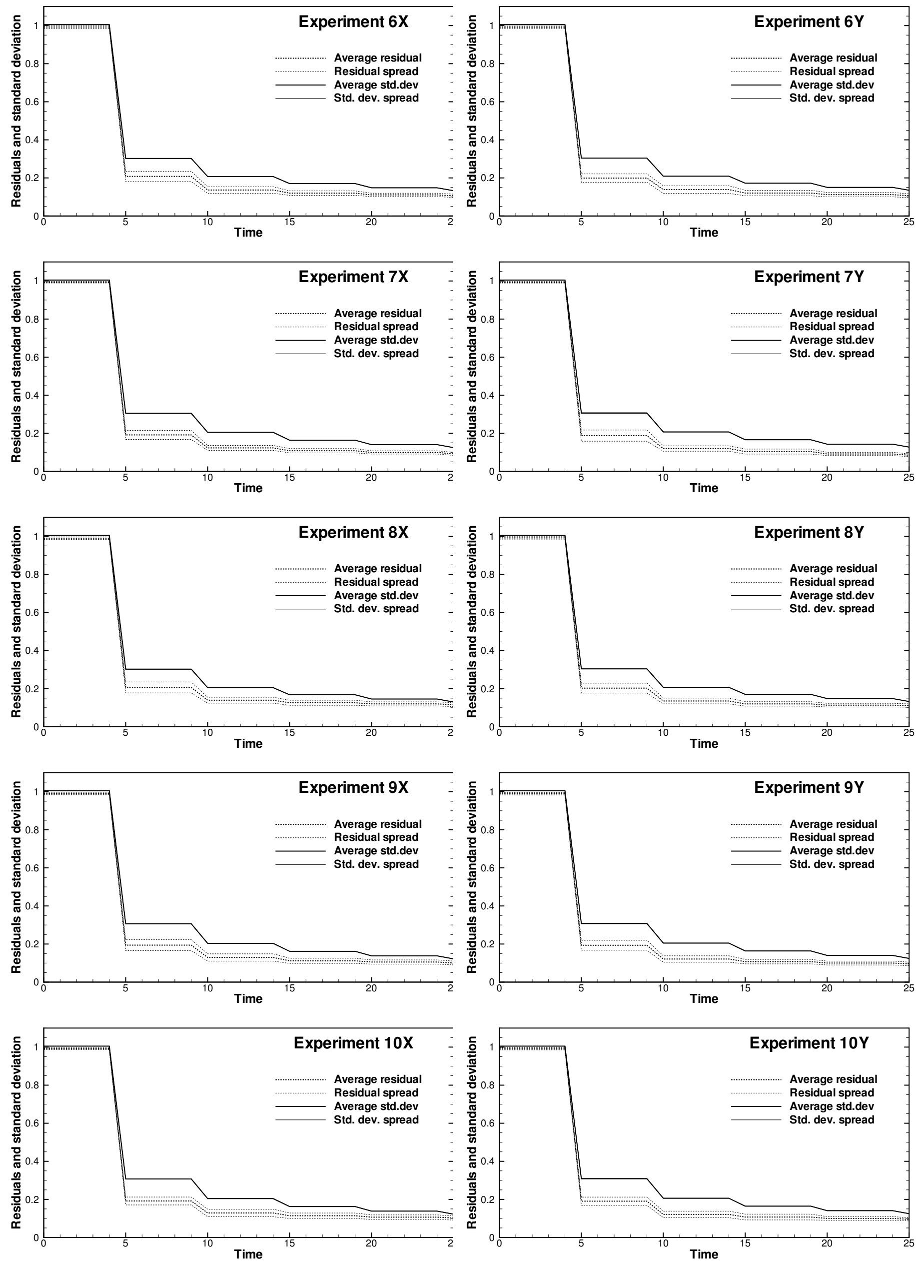


Figure 4: RMS residuals and ensemble singular value spectra for some of the experiments, without (left) and with (right) mean preserving rotations.

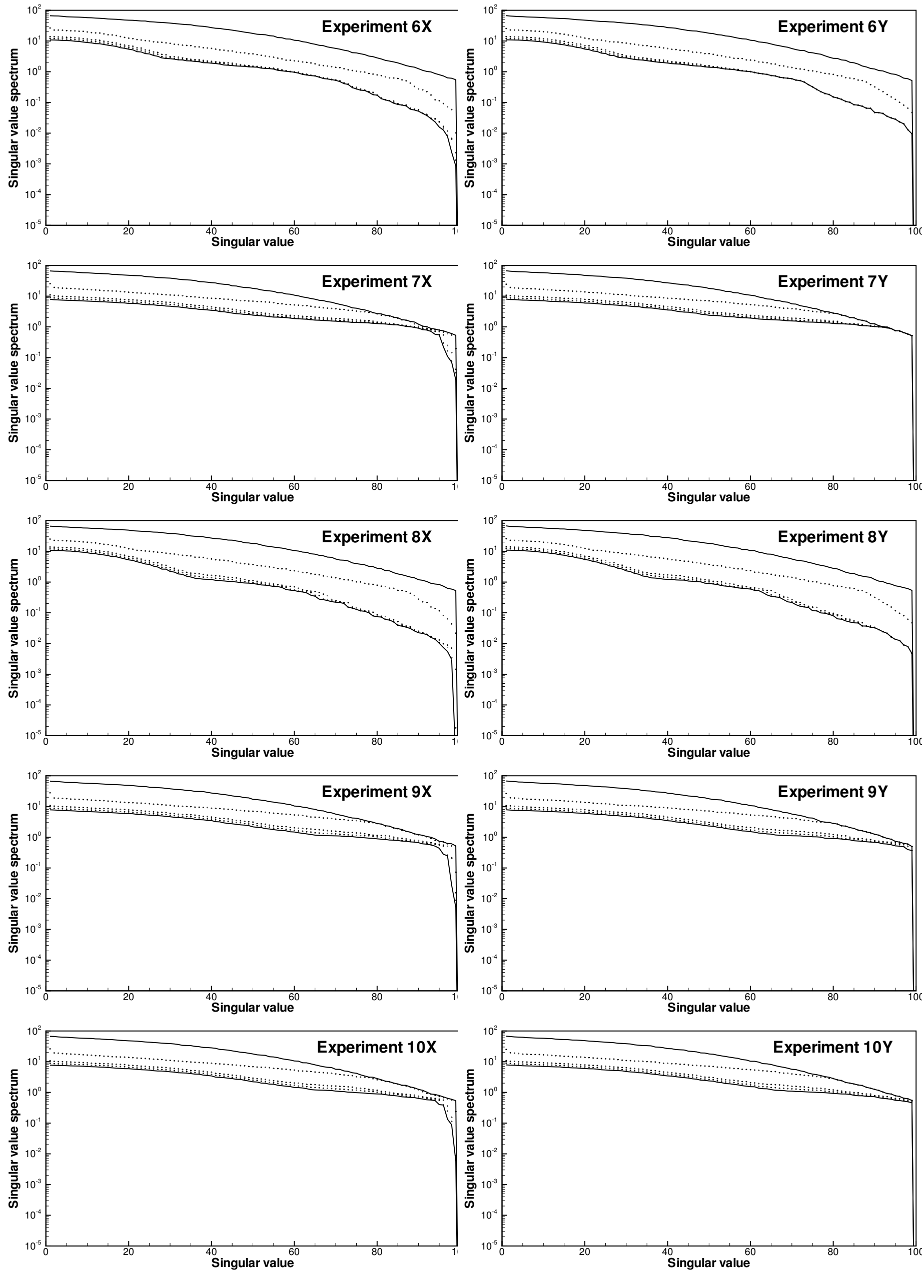


Figure 5: Singular value spectra of the ensemble perturbations

# References

Evensen, G., Sampling strategies and square root analysis schemes for the EnKF, *Ocean Dynamics*, *54*, 539–560, 2004.

Evensen, G., The combined parameter and state estimation problem, *Computational Geosciences*, 2006, submitted 2005.