A note on the use of square root analysis schemes for the EnKF

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This note points out a problem with the SQRT analysis scheme when only one single measurement is assimilated or when the matrix $\boldsymbol{C}$ is diagonal. It will motivate the use of an additional random rotation in the square root analysis schemes.

1 Analysis of the SQRT analysis

We will now look at the special case where a single measurement ($m = 1$) it used with a scalar state ($n = 1$). The SQRT analysis scheme can then be derived as follows

$$\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} = \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \tag{1}$$

$$= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}}\right)\boldsymbol{A}'^{\mathrm{T}} \tag{2}$$

$$= \boldsymbol{A}'\boldsymbol{Z}\left(\boldsymbol{I} - \boldsymbol{\Lambda}\right)\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{A}'^{\mathrm{T}} \tag{3}$$

$$= \boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I} - \boldsymbol{\Lambda}}\left(\boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I} - \boldsymbol{\Lambda}}\right)^{\mathrm{T}}. \tag{4}$$

Thus we define the update equation for the ensemble perturbations as:

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I} - \boldsymbol{\Lambda}}. \tag{5}$$

In this particular example the following is clear:

1. If a direct measurement operator is used, then the measurment operator, $\boldsymbol{H} \in \Re^{1\times 1}$, is $\boldsymbol{H} = 1$ and $\boldsymbol{S} = \boldsymbol{A}'$.
2. Further, since only the first eigenvalue in $\boldsymbol{\Lambda}$ is nonzero, then the first eigenvector in $\boldsymbol{Z}$ must be identically proportional to $\boldsymbol{S}^{\mathrm{T}}$ (note that we have $\boldsymbol{S} \in \Re^{1\times N}$ in the case with one measurement). This is seen from the equality between Eqs (1) and (2).
3. However, all the remaining $N - 1$ eigenvectors are orthogonal to the first eigenvector, and thus also orthogonal to $\boldsymbol{S}^{\mathrm{T}}$.

Thus, the update equation (5) will lead to an ensemble of updated perturbations where the first member will be equal to $\boldsymbol{S}(\boldsymbol{S}^{\mathrm{T}}/||\boldsymbol{S}||)\sqrt{1-\lambda_1}$ and all the $N - 1$ remaining perturbations will be identical to zero.

Note that the resulting ensemble still has the correct variance, but it is all determined by the first ensemble member.

This example can clearly be extended to cases with larger state spaces. E.g., if $n > 1$ there will still be a problem at the measurement locations. In fact the rank of the ensemble is reduced to one at the measurement location.

With more than one measurement the situation changes sligthly but the same problem will occur if $\boldsymbol{C}^{-1}$ is diagonal. Then each of the m columns in $\boldsymbol{S}^{\mathrm{T}}$ will be proportional to one of the first m eigenvectors in $\boldsymbol{Z}$. Thus, the first m ensemble perturbations will represent the analysis variance while the remainder will be zero.

This problem is easily avoided by the insertion of a random orthogonal matrix product $\boldsymbol{I} = \boldsymbol{V}^{\mathrm{T}}\boldsymbol{V}$ in (4), i.e.,

$$\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} = \boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I}-\boldsymbol{\Lambda}}\boldsymbol{V}^{\mathrm{T}}\boldsymbol{V}\left(\boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I}-\boldsymbol{\Lambda}}\right)^{\mathrm{T}} \tag{6}$$

which leads to the following update equation

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{Z}\sqrt{\boldsymbol{I}-\boldsymbol{\Lambda}}\boldsymbol{V}^{\mathrm{T}}. \tag{7}$$

This is equivalent to a random rotation of the eigenvectors in $\boldsymbol{Z}$, which has the effect of randomly distributing the variance reduction among all the ensemble members.

The random orthogonal matrix $\boldsymbol{V}^{\mathrm{T}}$ is easily constructed from a singlular value decomposition of a random matrix $\boldsymbol{B} \in \Re^{N\times N}$, i.e. $\boldsymbol{B} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}$. The following is an extract of the Fortran 90 code used to generate the random orthogonal matrix, $\boldsymbol{V}^{\mathrm{T}}$.

```
allocate( U0(nrens,nrens), B0(nrens,nrens), sig0(nrens), V0(nrens,nrens) )
call random_number(B0)
call dgesvd('N', 'A', nrens, nrens, B0, nrens, sig0, U0, nrens, V0, nrens, work, lwork, ierr)
if (ierr /= 0) print *, 'ierr',ierr
X=matmul(X,V0)
deallocate(B0, sig0, U0, V0)
```