Rank consideration in the EnKF analysis: A new efficient analysis scheme

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Based on Evensen 2004, submitted to Ocean Dynamics

Background

- EnKF/EnKS is an error subspace method.
- Analysis is a combination of forecast ensemble.
- Inversion may be singular when $m \geq N$.
- Is it possible to work entirely in the ensemble sub space?

EnKF analysis equations

- Standard analysis may be written

$$
\begin{aligned}
\boldsymbol{A} = \overline{\boldsymbol{A}} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}(\overline{\boldsymbol{D}} - \boldsymbol{H}\overline{\boldsymbol{A}}) \\
+ \boldsymbol{A}' + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}(\boldsymbol{E} - \boldsymbol{S})
\end{aligned}
$$

- Square root analysis based on

$$
\begin{aligned}
\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\boldsymbol{W}
\end{aligned}
$$

- with $\boldsymbol{C} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}$, and $\boldsymbol{S} = \boldsymbol{H}\boldsymbol{A}'$.

Rank issues $(m \geq N)$

- Define $\boldsymbol{S} \in \Re^{m \times N}$ of rank $N-1$, (defines subspace $\mathcal{S}$).
- Define $\boldsymbol{E} \in \Re^{m \times N}$ of rank $N-1$.
- Define $\boldsymbol{Y} = (\boldsymbol{S}, \boldsymbol{E}) \in \Re^{m \times 2N}$ of rank p.
- Then:

$$\min(m, N-1) \leq p \leq \min(m, 2N-2).$$

- Thus, $\boldsymbol{C} = \boldsymbol{Y}\boldsymbol{Y}^{\mathrm{T}}$ may be singular when $m \geq N$.

A pseudo inverse

- A pseudo inversion $\boldsymbol{C}^{+}$ may be used.

$$\boldsymbol{C} = \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}} \Rightarrow \boldsymbol{C}^{+} = \boldsymbol{Z}\boldsymbol{\Lambda}^{+}\boldsymbol{Z}^{\mathrm{T}}$$

with

$$\text{diag}(\boldsymbol{\Lambda}^{+}) = (\lambda_1^{-1}, \ldots, \lambda_p^{-1}, 0, \ldots, 0).$$

However. . .

- Remember the analysis equation

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

$$= \boldsymbol{A}'\boldsymbol{W}\boldsymbol{A}'^{\mathrm{T}}$$

- Define the SVD

$$\boldsymbol{Y} = (\boldsymbol{S}, \boldsymbol{E}) = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}$$

and pseudo inverse

$$\boldsymbol{Y}^{+} = \boldsymbol{V}\boldsymbol{\Sigma}^{+}\boldsymbol{U}^{\mathrm{T}}$$

- Thus

$$\boldsymbol{C}^{+} = (\boldsymbol{Y}\boldsymbol{Y}^{\mathrm{T}})^{+} = \boldsymbol{Y}^{+\mathrm{T}}\boldsymbol{Y}^{+}$$

Then. . .

- with $\boldsymbol{E} \in \Re^{m \times q}$ and $q \geq N$
- and $\boldsymbol{S} = (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{Y}^{\mathrm{T}}$, we get

$$\begin{aligned}
\boldsymbol{W} &= \boldsymbol{I}_N - (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{Y}^{\mathrm{T}}(\boldsymbol{Y}\boldsymbol{Y}^{\mathrm{T}})^{+}\boldsymbol{Y}(\boldsymbol{I}_N, \boldsymbol{0})^{\mathrm{T}} \\
&= \boldsymbol{I}_N - (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{V}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{U}\boldsymbol{\Sigma}^{+\mathrm{T}}\boldsymbol{V}^{\mathrm{T}}\boldsymbol{V}\boldsymbol{\Sigma}^{+}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}(\boldsymbol{I}_N, \boldsymbol{0})^{\mathrm{T}} \\
&= \boldsymbol{I}_N - (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{V}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{\Sigma}^{+\mathrm{T}}\boldsymbol{\Sigma}^{+}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}(\boldsymbol{I}_N, \boldsymbol{0})^{\mathrm{T}} \\
&= (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{V}\left\{\boldsymbol{I}_{N+q} - \begin{pmatrix} \boldsymbol{I}_p & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}_{N+q}\right\}\boldsymbol{V}^{\mathrm{T}}(\boldsymbol{I}_N, \boldsymbol{0})^{\mathrm{T}} \\
&= (\boldsymbol{I}_N, \boldsymbol{0})\boldsymbol{V}\begin{pmatrix} \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I}_{N+q-p} \end{pmatrix}_{N+q}\boldsymbol{V}^{\mathrm{T}}(\boldsymbol{I}_N, \boldsymbol{0})^{\mathrm{T}}.
\end{aligned}$$

Thus. . .

- Thus for $\boldsymbol{W}$ to have rank $\geq N-1$ we must have

$$p = \text{rank}\left(\boldsymbol{S}^{m\times N}, \boldsymbol{E}^{m\times q}\right) \leq q+1$$

- Thus, at least $N-3$ of the dimensions spanned by $\boldsymbol{E}$ must be fully contained in $\mathcal{S}$.
- Kepert pointed out problem with $q=N$ and $p=2N-2$ where loss of ensemble rank occured when $m \geq N$.

Further....

- Construct the SVD of $\boldsymbol{S}$:

$$\boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{V}_0^{\mathrm{T}} = \boldsymbol{S}$$

- From the analysis equation

$$\begin{aligned}\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\ &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{V}_0\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{V}_0^{\mathrm{T}}\right)\end{aligned}$$

  all components of $\boldsymbol{C}$ in $\mathcal{S}^{\perp}$ are rejected.
- Thus, there is no need to use $q > N$ or even a full rank $\boldsymbol{R}$.
- Better to sample $\boldsymbol{E}$ properly within $\mathcal{S}$.

Low rank approximation (1)

- Why invert an $m \times m$ matrix when we are computing the analysis in an N-dimensional ensemble space?
- Use

$$\boldsymbol{C} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}},$$

- with

$$\boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{V}_0^{\mathrm{T}} = \boldsymbol{S}.$$

- Then

$$\boldsymbol{C} = \boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}$$

- and

Low rank approximation (2)

$$
\begin{aligned}
\boldsymbol{C} &= \boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}} \\
&= \boldsymbol{U}_0(\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{\mathrm{T}} + \boldsymbol{U}_0^{\mathrm{T}}\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\boldsymbol{U}_0)\boldsymbol{U}_0^{\mathrm{T}} \\
&\approx \boldsymbol{U}_0\boldsymbol{\Sigma}_0(\boldsymbol{I} + \boldsymbol{\Sigma}_0^{+}\boldsymbol{U}_0^{\mathrm{T}}\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\boldsymbol{U}_0\boldsymbol{\Sigma}_0^{+\mathrm{T}})\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}} \\
&\left(= \boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}} + (\boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{+}\boldsymbol{U}_0^{\mathrm{T}})\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}(\boldsymbol{U}_0\boldsymbol{\Sigma}_0^{+\mathrm{T}}\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}})\right) \\
&\left(= \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + (\boldsymbol{S}\boldsymbol{S}^{+})\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}(\boldsymbol{S}\boldsymbol{S}^{+})\right)
\end{aligned}
$$

- $\boldsymbol{\Sigma}_0\boldsymbol{\Sigma}_0^{+} = \boldsymbol{I}_{N-1} \in \Re^{N\times N}$.
- $\boldsymbol{S}\boldsymbol{S}^{+} = \boldsymbol{U}_0\boldsymbol{I}_{N-1}\boldsymbol{U}_0^{\mathrm{T}}$ is a orthogonal projection onto $\mathcal{S}$.

Low rank approximation (3)

$$C \approx U_0\Sigma_0(I + \Sigma_0^{+}(U_0^{T}E)(E^{T}U_0\Sigma_0^{+T}))\Sigma_0^{T}U_0^{T}$$
$$= U_0\Sigma_0(I + X_0X_0^{T})\Sigma_0^{T}U_0^{T}$$

- where we defined

$$U_1\Sigma_1V_1^{T} = X_0 = \Sigma_0^{+}U_0^{T}E$$

Low rank approximation (4)

- We then get

$$\boldsymbol{C} = \boldsymbol{U}_0\boldsymbol{\Sigma}_0(\boldsymbol{I} + \boldsymbol{U}_1\boldsymbol{\Sigma}_1^2\boldsymbol{U}_1^{\mathrm{T}})\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}}$$
$$= \boldsymbol{U}_0\boldsymbol{\Sigma}_0\boldsymbol{U}_1(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)\boldsymbol{U}_1^{\mathrm{T}}\boldsymbol{\Sigma}_0^{\mathrm{T}}\boldsymbol{U}_0^{\mathrm{T}}$$

- And the pseudo inverse becomes

$$\boldsymbol{C}^{+} = (\boldsymbol{U}_0\boldsymbol{\Sigma}_0^{+\mathrm{T}}\boldsymbol{U}_1)(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-1}(\boldsymbol{U}_0\boldsymbol{\Sigma}_0^{+\mathrm{T}}\boldsymbol{U}_1)^{\mathrm{T}}$$
$$= \boldsymbol{X}_1(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-1}\boldsymbol{X}_1^{\mathrm{T}}$$

with

$$\boldsymbol{X}_1 = \boldsymbol{U}_0\boldsymbol{\Sigma}_0^{+\mathrm{T}}\boldsymbol{U}_1$$

Low rank approximation (5)

$$\begin{aligned}
\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{+}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{X}_1(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-1}\boldsymbol{X}_1^{\mathrm{T}}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - [(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-\frac{1}{2}}\boldsymbol{X}_1^{\mathrm{T}}\boldsymbol{S}]^{\mathrm{T}}[(\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-\frac{1}{2}}\boldsymbol{X}_1^{\mathrm{T}}\boldsymbol{S}]\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{X}_2^{\mathrm{T}}\boldsymbol{X}_2\right)\boldsymbol{A}'^{\mathrm{T}},
\end{aligned}$$

with

$$\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}} = \boldsymbol{X}_2 = (\boldsymbol{I} + \boldsymbol{\Sigma}_1^2)^{-\frac{1}{2}}\boldsymbol{X}_1^{\mathrm{T}}\boldsymbol{S}$$

Low rank approximation (6)

- We then get as before

$$\begin{aligned}
\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - [\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}]^{\mathrm{T}}[\boldsymbol{U}_2\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}]\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{V}_2\boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2\boldsymbol{V}_2^{\mathrm{T}}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\boldsymbol{V}_2\left(\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2\right)\boldsymbol{V}_2^{\mathrm{T}}\boldsymbol{A}'^{\mathrm{T}} \\
&= \left(\boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}\right)\left(\boldsymbol{A}'\boldsymbol{V}_2\sqrt{\boldsymbol{I} - \boldsymbol{\Sigma}_2^{\mathrm{T}}\boldsymbol{\Sigma}_2}\right)^{\mathrm{T}}.
\end{aligned}$$

- The analysis equation becomes

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

Verification experiments

- 500 measurements and 100 ensemble members
- 5 updates with measurement error variance of 0.5.

Exp 22: Standard EnKF with low rank $\boldsymbol{R}_{\mathrm{e}}$.

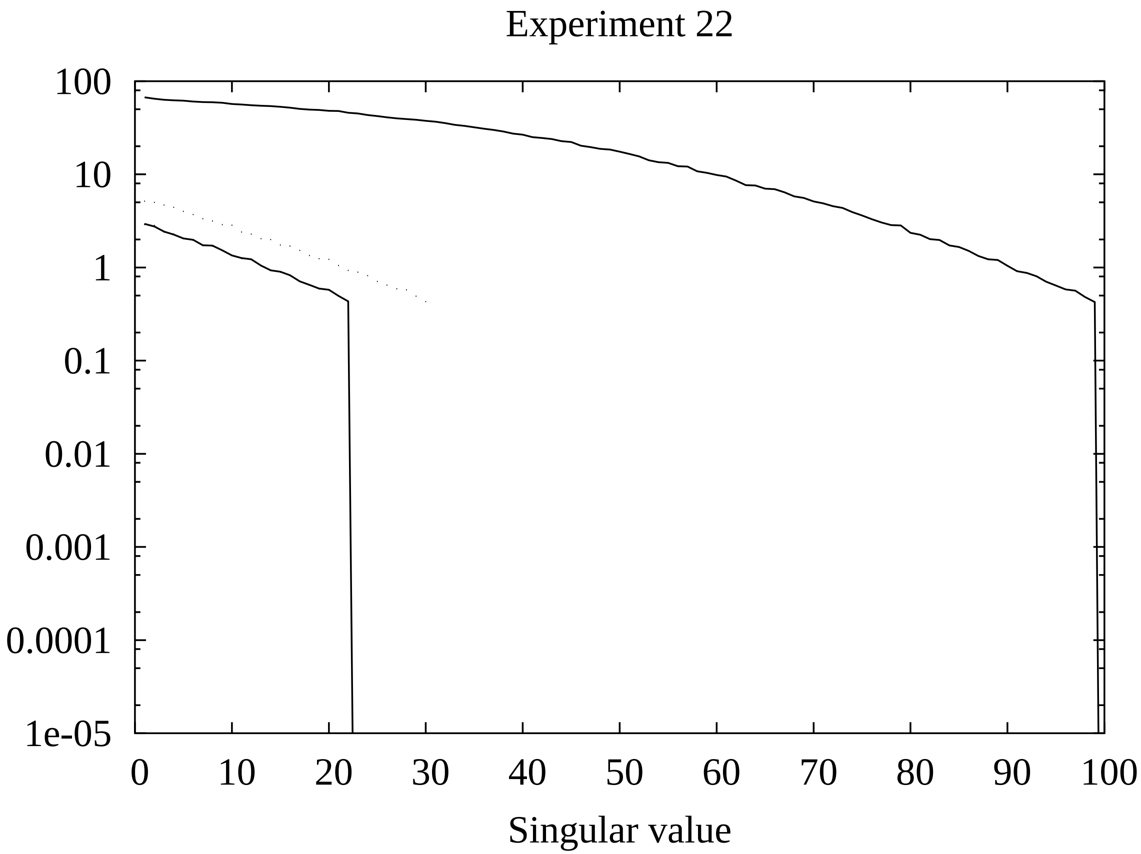
Exp 2: Standard EnKF with full rank $\boldsymbol{R}$.

Exp 4: Square root EnKF with full rank $\boldsymbol{R}_{\mathrm{e}}$.

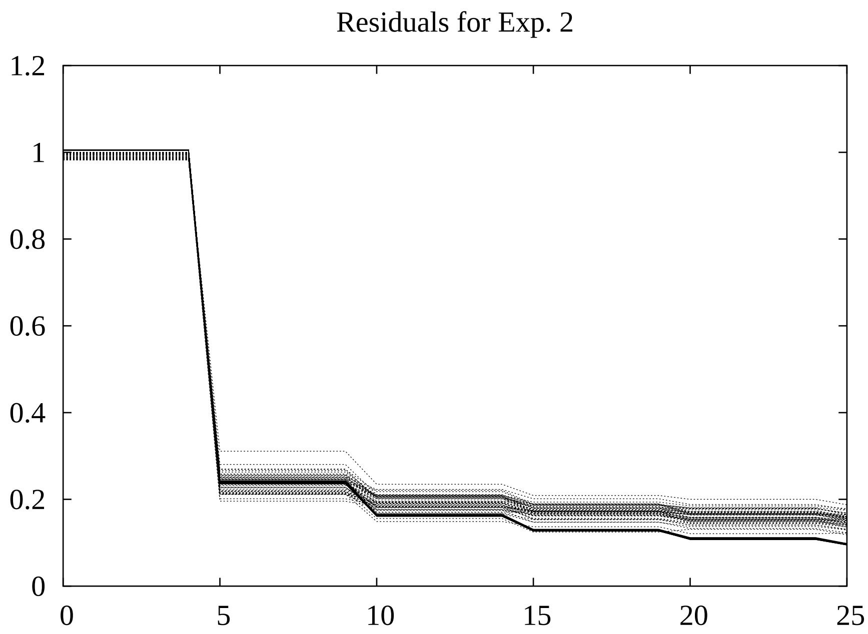
Exp 5a: Low rank square root EnKF with full rank $\boldsymbol{R}_{\mathrm{e}}$.

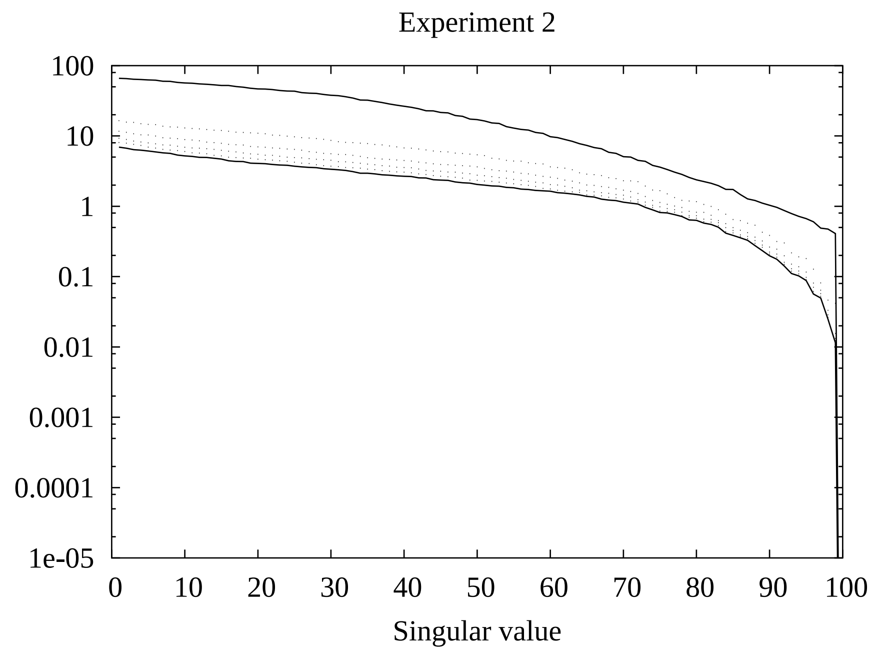
Exp 6: Low rank square root EnKF using $\boldsymbol{E}$.

Standard EnKF with low rank R_e

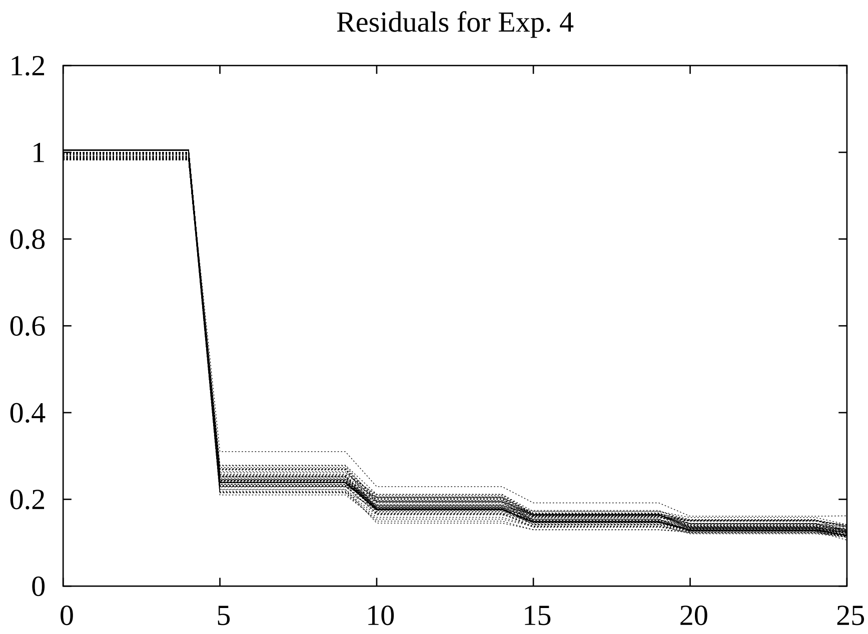


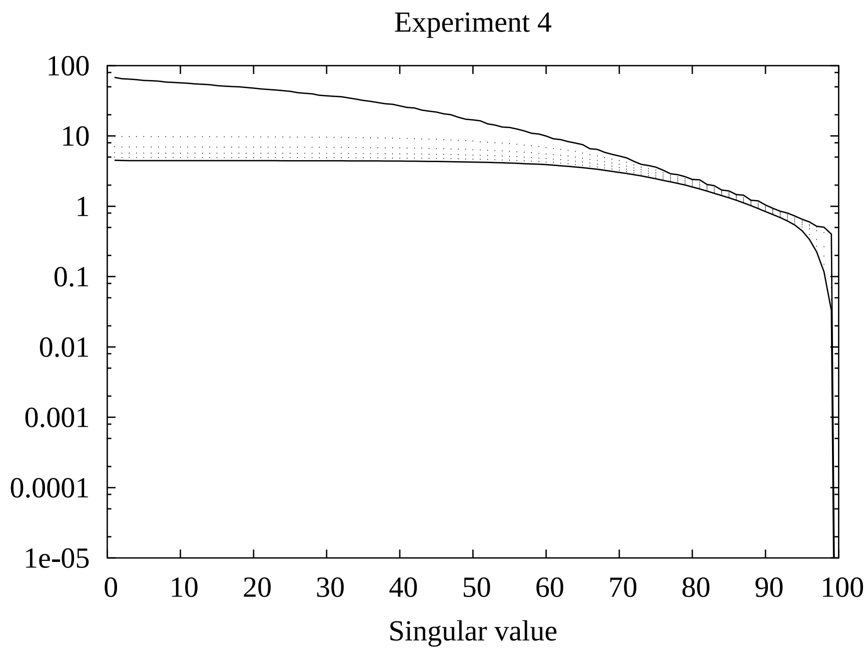
Standard EnKF with full rank R



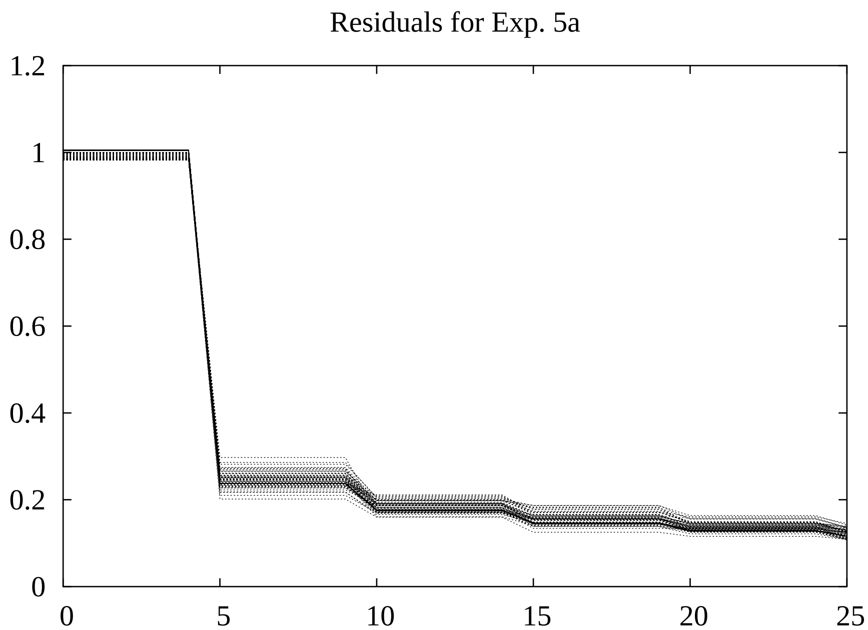


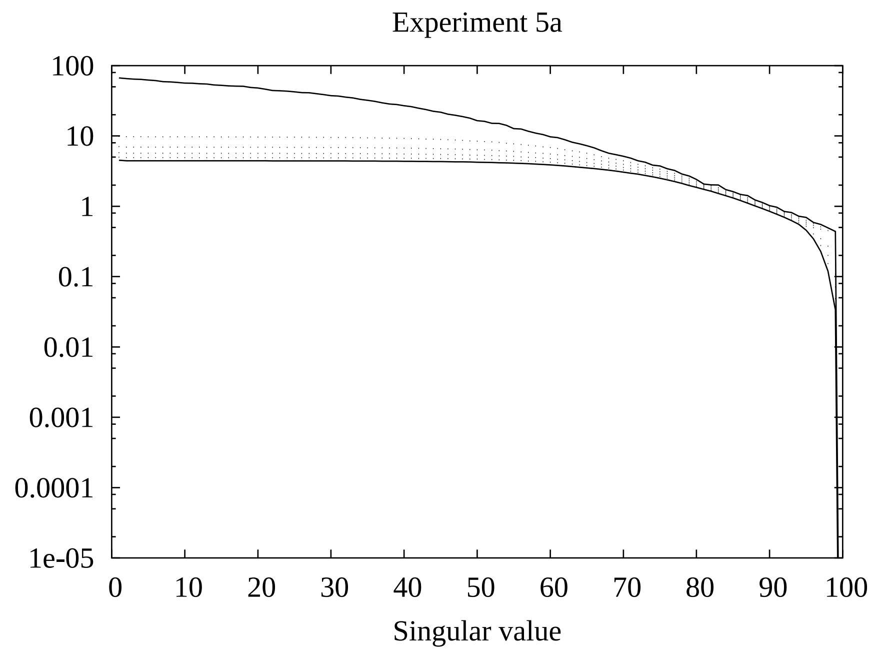
$\sqrt{\text{EnKF}}$ with full rank R



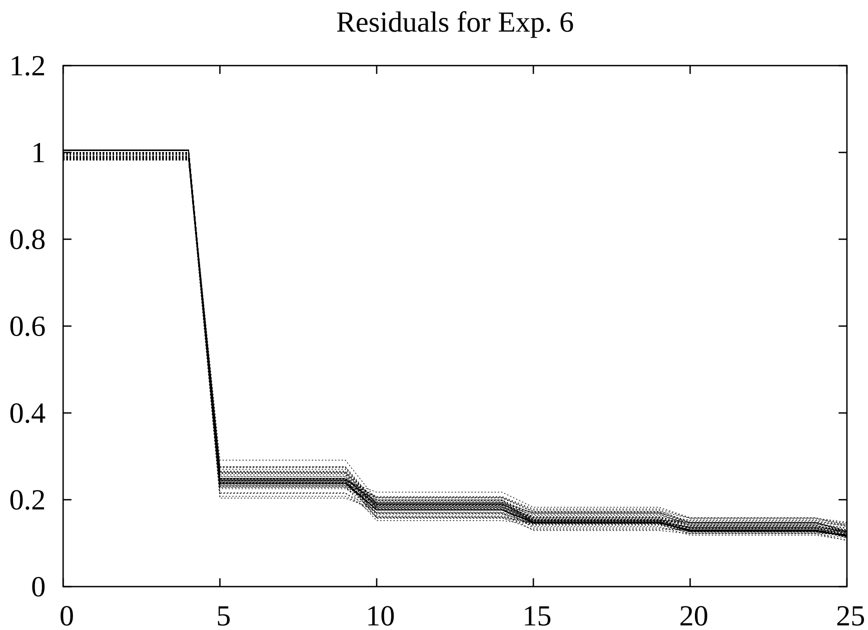


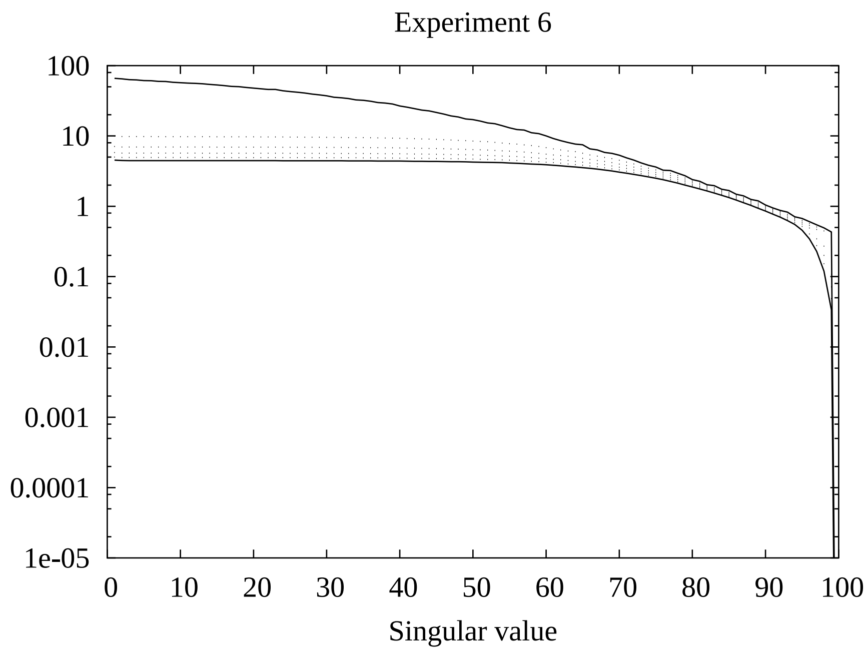
Low rank $\sqrt{\text{EnKF}}$ with full rank R





Low rank $\sqrt{\text{EnKF}}$ using E for R





Summary

- No benefit from using a full rank $\boldsymbol{R}$.
- Computationally efficient low rank SQRT analysis scheme derived.
- Eliminates all $\mathcal{O}(m^2)$ operations.
- Solves full problem (no additional approximations).
- $\boldsymbol{E} \in \Re^{m \times N}$ must be contained in $\mathcal{S}$.
- Details in Evensen 2004, Ocean Dynamics.
- F90 code for new routines available from http://www.nersc.no/~geir/EnKF