

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

Geir Evensen

Norsk Hydro Research Centre, Bergen, Norway

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

$$\begin{aligned} \mathbf{A} &= \bar{\mathbf{A}} + \mathbf{A}' \mathbf{S}^T \mathbf{C}^{-1} (\bar{\mathbf{D}} - \mathbf{H} \bar{\mathbf{A}}) \\ &\quad + \mathbf{A}' + \mathbf{A}' \mathbf{S}^T \mathbf{C}^{-1} (\mathbf{E} - \mathbf{S}) \end{aligned}$$

- Square root analysis based on

$$\begin{aligned} \mathbf{A}^{\text{a}'} \mathbf{A}^{\text{a}'T} &= \mathbf{A}' (\mathbf{I} - \mathbf{S}^T \mathbf{C}^{-1} \mathbf{S}) \mathbf{A}'^T \\ &= \mathbf{A}' \mathbf{W} \end{aligned}$$

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

Rank issues ($m \geq N$)

- Define $\mathbf{S} \in \mathfrak{R}^{m \times N}$ of rank $N - 1$, (defines subspace \mathcal{S}).
- Define $\mathbf{E} \in \mathfrak{R}^{m \times N}$ of rank $N - 1$.
- Define $\mathbf{Y} = (\mathbf{S}, \mathbf{E}) \in \mathfrak{R}^{m \times 2N}$ of rank p .
- Then:
$$\min(m, N - 1) \leq p \leq \min(m, 2N - 2).$$
- Thus, $\mathbf{C} = \mathbf{Y}\mathbf{Y}^T$ may be singular when $m \geq N$.

A pseudo inverse

- A pseudo inversion C^+ may be used.

$$C = Z\Lambda Z^T \Rightarrow C^+ = Z\Lambda^+ Z^T$$

with

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

However...

- Remember the analysis equation

$$\begin{aligned} \mathbf{A}^a \mathbf{A}^{a'T} &= \mathbf{A}' (\mathbf{I} - \mathbf{S}^T \mathbf{C}^+ \mathbf{S}) \mathbf{A}'^T \\ &= \mathbf{A}' \mathbf{W} \mathbf{A}'^T \end{aligned}$$

- Define the SVD

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

and pseudo inverse

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

- Thus

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

Then...

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

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

Thus...

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

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

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

Further...

- Construct the SVD of S :

$$U_0 \Sigma_0 V_0^T = S$$

- From the analysis equation

$$\begin{aligned} A^{a'} A^{a'T} &= A' (I - S^T C^{-1} S) A'^T \\ &= A' (I - V_0 \Sigma_0^T U_0^T C^{-1} U_0 \Sigma_0 V_0^T) \end{aligned}$$

all components of C in S^\perp are rejected.

- Thus, there is no need to use $q > N$ or even a full rank R .
- Better to sample E properly within 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

$$C = SS^T + EE^T,$$

- with

$$U_0 \Sigma_0 V_0^T = S.$$

- Then

$$C = U_0 \Sigma_0 \Sigma_0^T U_0^T + EE^T$$

- and

Low rank approximation (2)

$$\begin{aligned}C &= U_0 \Sigma_0 \Sigma_0^T U_0^T + \mathbf{E} \mathbf{E}^T \\&= U_0 (\Sigma_0 \Sigma_0^T + U_0^T \mathbf{E} \mathbf{E}^T U_0) U_0^T \\&\approx U_0 \Sigma_0 (I + \Sigma_0^+ U_0^T \mathbf{E} \mathbf{E}^T U_0 \Sigma_0^{+T}) \Sigma_0^T U_0^T \\&\left(= U_0 \Sigma_0 \Sigma_0^T U_0^T + (U_0 \Sigma_0 \Sigma_0^+ U_0^T) \mathbf{E} \mathbf{E}^T (U_0 \Sigma_0^{+T} \Sigma_0^T U_0^T) \right) \\&\left(= \mathbf{S} \mathbf{S}^T + (\mathbf{S} \mathbf{S}^+) \mathbf{E} \mathbf{E}^T (\mathbf{S} \mathbf{S}^+) \right)\end{aligned}$$

- $\Sigma_0 \Sigma_0^+ = I_{N-1} \in \Re^{N \times N}$.
- $\mathbf{S} \mathbf{S}^+ = U_0 I_{N-1} U_0^T$ is a orthogonal projection onto \mathcal{S} .

Low rank approximation (3)

$$\begin{aligned} C &\approx U_0 \Sigma_0 (I + \Sigma_0^+ (U_0^T E) (E^T U_0 \Sigma_0^{+T})) \Sigma_0^T U_0^T \\ &= U_0 \Sigma_0 (I + X_0 X_0^T) \Sigma_0^T U_0^T \end{aligned}$$

• where we defined

$$U_1 \Sigma_1 V_1^T = X_0 = \Sigma_0^+ U_0^T E$$

Low rank approximation (4)

- We then get

$$\begin{aligned} C &= U_0 \Sigma_0 (I + U_1 \Sigma_1^2 U_1^T) \Sigma_0^T U_0^T \\ &= U_0 \Sigma_0 U_1 (I + \Sigma_1^2) U_1^T \Sigma_0^T U_0^T \end{aligned}$$

- And the pseudo inverse becomes

$$\begin{aligned} C^+ &= (U_0 \Sigma_0^{+T} U_1) (I + \Sigma_1^2)^{-1} (U_0 \Sigma_0^{+T} U_1)^T \\ &= X_1 (I + \Sigma_1^2)^{-1} X_1^T \end{aligned}$$

with

$$X_1 = U_0 \Sigma_0^{+T} U_1$$

Low rank approximation (5)

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

with

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

Low rank approximation (6)

- We then get as before

$$\begin{aligned} A^{a'} A^{a'T} &= A' (I - [U_2 \Sigma_2 V_2^T]^T [U_2 \Sigma_2 V_2^T]) A'^T \\ &= A' (I - V_2 \Sigma_2^T \Sigma_2 V_2^T) A'^T \\ &= A' V_2 (I - \Sigma_2^T \Sigma_2) V_2^T A'^T \\ &= \left(A' V_2 \sqrt{I - \Sigma_2^T \Sigma_2} \right) \left(A' V_2 \sqrt{I - \Sigma_2^T \Sigma_2} \right)^T. \end{aligned}$$

- The analysis equation becomes

$$A^{a'} = A' V_2 \sqrt{I - \Sigma_2^T \Sigma_2}.$$

Verification experiments

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

Exp 22: Standard EnKF with low rank R_e .

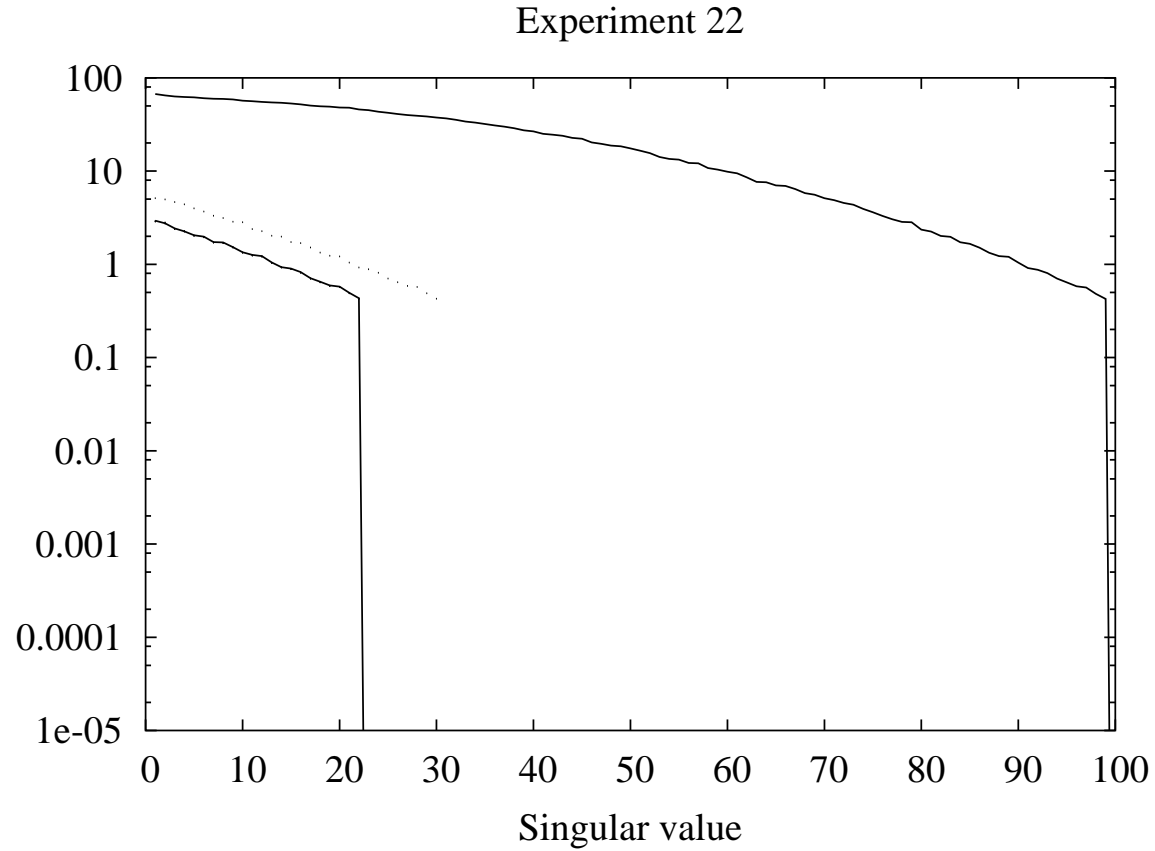
Exp 2: Standard EnKF with full rank R .

Exp 4: Square root EnKF with full rank R_e .

Exp 5a: Low rank square root EnKF with full rank R_e .

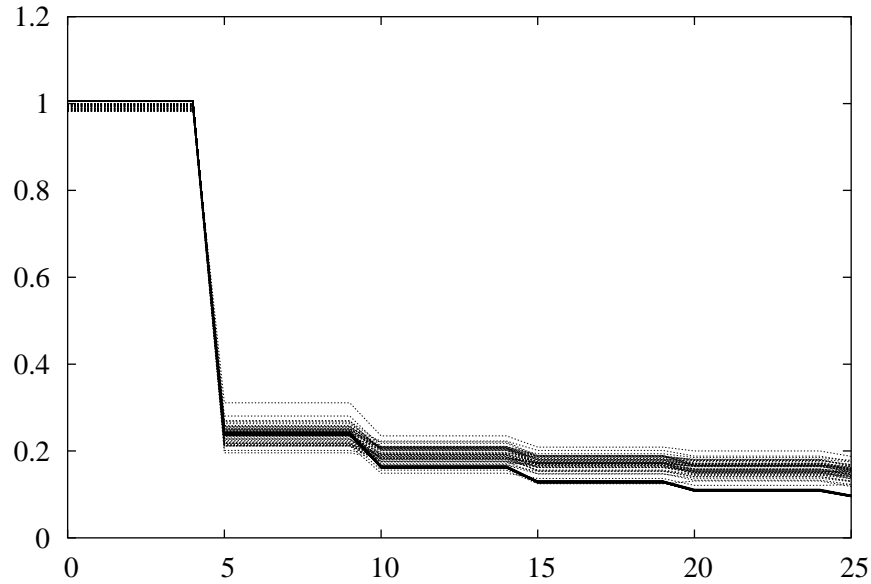
Exp 6: Low rank square root EnKF using E .

Standard EnKF with low rank R_e

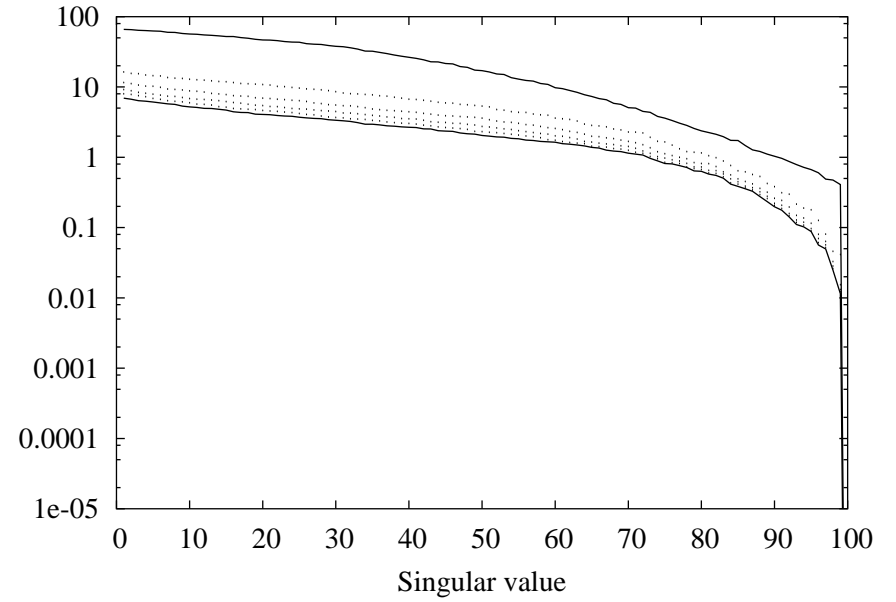


Standard EnKF with full rank R

Residuals for Exp. 2

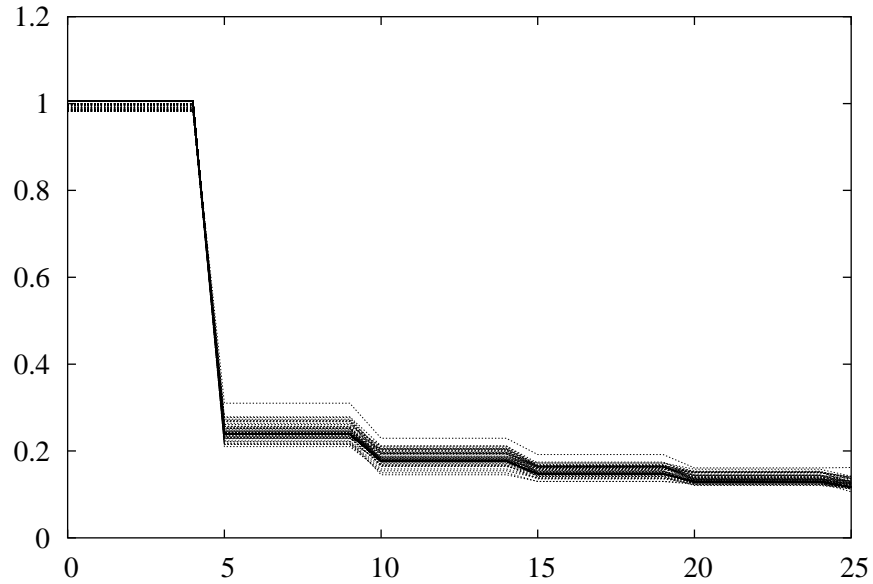


Experiment 2

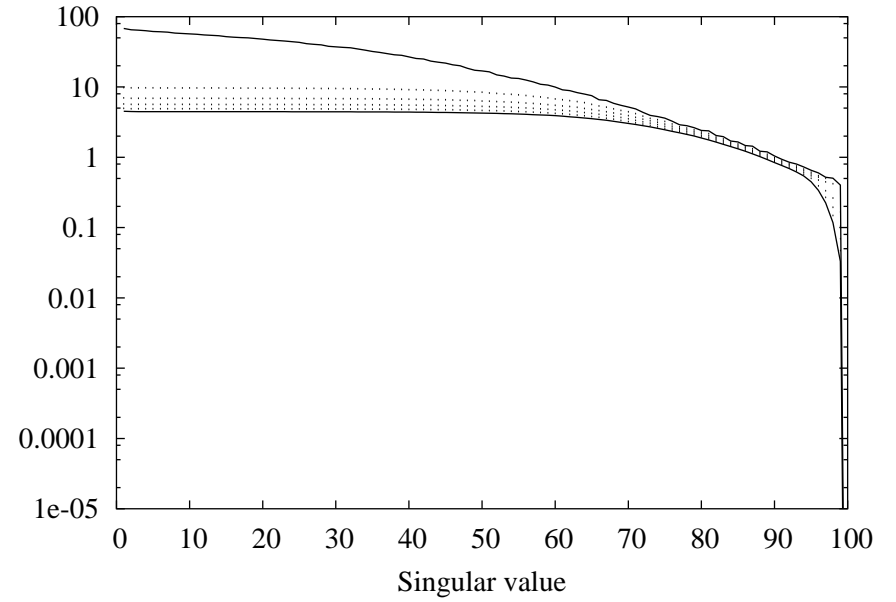


$\sqrt{\text{EnKF}}$ with full rank R

Residuals for Exp. 4

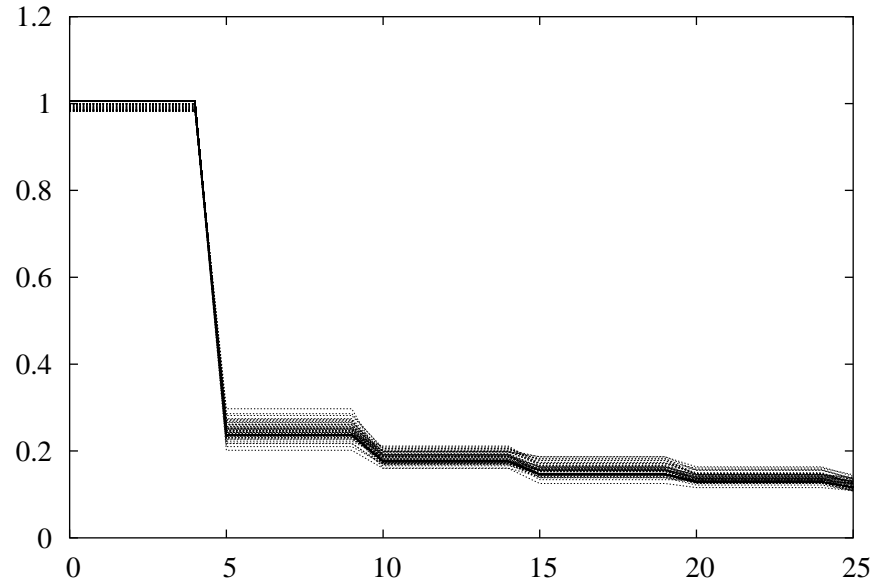


Experiment 4

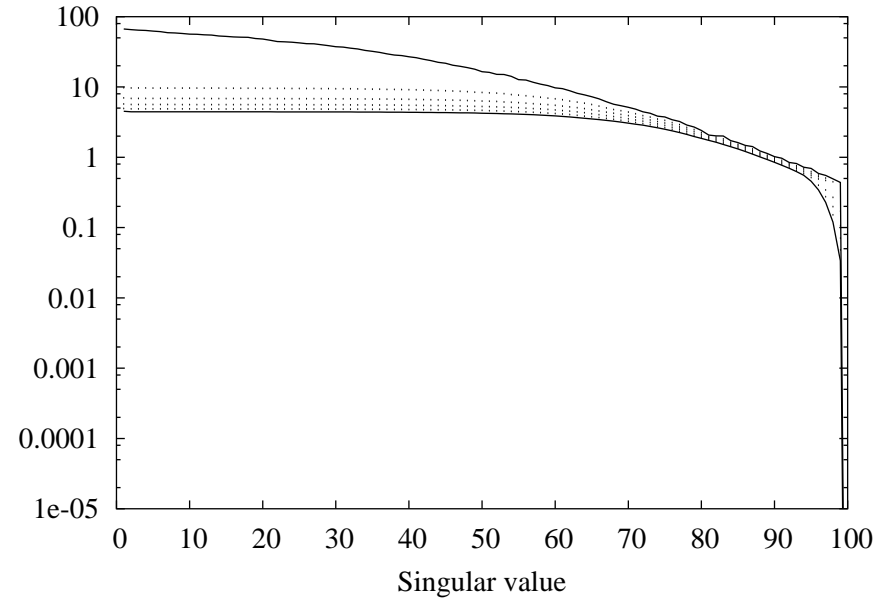


Low rank $\sqrt{\mathbf{E}n\mathbf{K}\mathbf{F}}$ with full rank R

Residuals for Exp. 5a

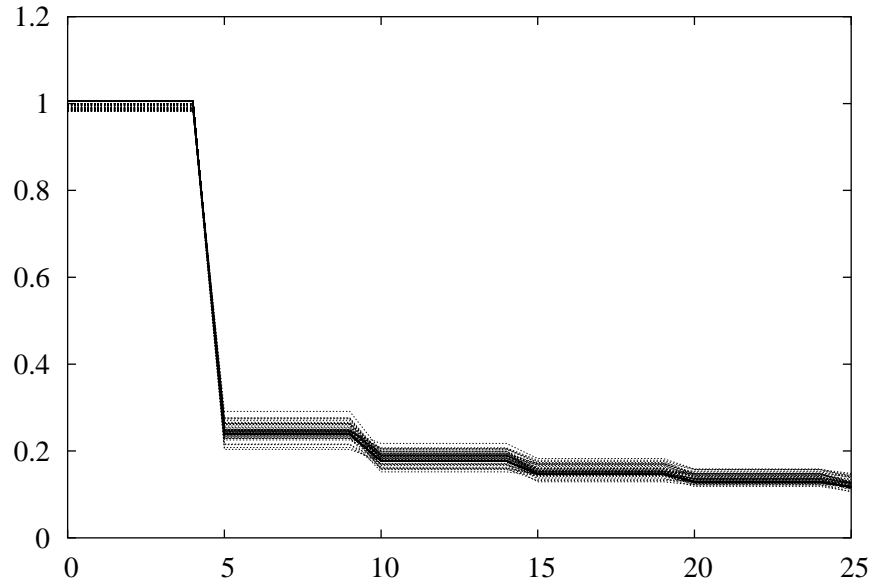


Experiment 5a

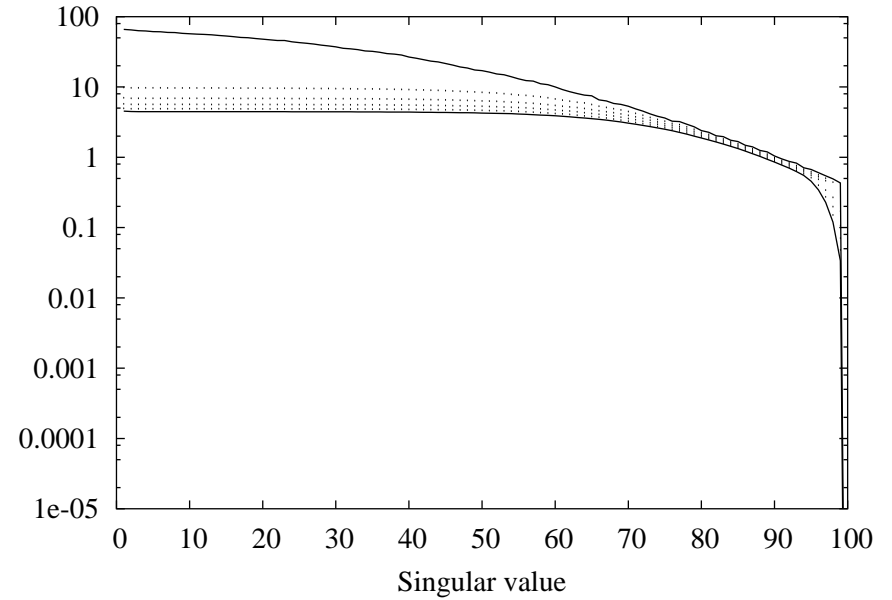


Low rank \sqrt{EnKF} using E for R

Residuals for Exp. 6



Experiment 6



Summary

- No benefit from using a full rank R .
- Computationally efficient low rank SQR analysis scheme derived.
- Eliminates all $\mathcal{O}(m^2)$ operations.
- Solves full problem (no additional approximations).
- $E \in \mathfrak{R}^{m \times N}$ 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>