

# Implementation of IES in ERT and validation

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<https://www.nonlin-processes-geophys-discuss.net/npg-2019-10/>

# Some definitions

Prior ensemble and perturbed measurements

$$\mathbf{X} = \left( \mathbf{x}_1^f, \mathbf{x}_2^f, \dots, \mathbf{x}_N^f \right) \quad \text{and} \quad \mathbf{D} = \left( \mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_N \right)$$

Ensemble means

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_{j=1}^N \mathbf{x}_j \quad \text{and} \quad \bar{\mathbf{d}} = \frac{1}{N} \sum_{j=1}^N \mathbf{d}_j$$

Ensemble anomaly matrices and covariances

$$\mathbf{A} = \mathbf{X} \left( \mathbf{I}_N - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) / \sqrt{N-1} \quad \rightarrow \quad \overline{\mathbf{C}}_{xx} = \mathbf{A} \mathbf{A}^T$$

$$\mathbf{E} = \mathbf{D} \left( \mathbf{I}_N - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) / \sqrt{N-1} \quad \rightarrow \quad \overline{\mathbf{C}}_{dd} = \mathbf{E} \mathbf{E}^T$$

# IES: Ensemble subspace version

Original cost functions

$$\mathcal{J}(\mathbf{x}_j) = (\mathbf{x}_j - \mathbf{x}_j^f)^T \mathbf{C}_{xx}^{-1} (\mathbf{x}_j - \mathbf{x}_j^f) + (\mathbf{g}(\mathbf{x}_j) - \mathbf{d}_j)^T \mathbf{C}_{dd}^{-1} (\mathbf{g}(\mathbf{x}_j) - \mathbf{d}_j).$$

**Solution is contained in the ensemble subspace**, thus

$$\mathbf{x}_j^a = \mathbf{x}_j^f + \mathbf{A}\mathbf{w}_j,$$

and,

$$\mathcal{J}(\mathbf{w}_j) = \mathbf{w}_j^T \mathbf{w}_j + \left( \mathbf{g}(\mathbf{x}_j^f + \mathbf{A}\mathbf{w}_j) - \mathbf{d}_j \right)^T \mathbf{C}_{dd}^{-1} \left( \mathbf{g}(\mathbf{x}_j^f + \mathbf{A}\mathbf{w}_j) - \mathbf{d}_j \right)$$

**Reduces dimension of problem from state size to ensemble size.**

$$\mathbf{w}_j^{i+1} = \mathbf{w}_j^i - \gamma \nabla \mathcal{J}_j^i$$

# Gradient and Hessian of cost function

Gradient

$$\nabla \mathcal{J}(\boldsymbol{w}_j) = 2\boldsymbol{w}_j + 2(\mathbf{G}_j \mathbf{A})^T \mathbf{C}_{dd}^{-1} (\mathbf{g}(\mathbf{x}_j^f + \mathbf{A}\boldsymbol{w}_j) - \mathbf{d}_j),$$

Hessian (approximate)

$$\nabla \nabla \mathcal{J}(\boldsymbol{w}_j) \approx 2\mathbf{I} + 2(\mathbf{G}_j \mathbf{A})^T \mathbf{C}_{dd}^{-1} (\mathbf{G}_j \mathbf{A})$$

# Gauss-Newton iterations

$$\mathbf{w}_j^{i+1} = \mathbf{w}_j^i - \gamma \Delta \mathbf{w}_j^i$$

$$\begin{aligned}\Delta \mathbf{w}_j^i &= \left\{ \mathbf{w}_j^i - (\mathbf{G}_j^i \mathbf{A})^T \left( (\mathbf{G}_j^i \mathbf{A})(\mathbf{G}_j^i \mathbf{A})^T + \mathbf{C}_{dd} \right)^{-1} \right. \\ &\quad \times \left. \left( (\mathbf{G}_j^i \mathbf{A}) \mathbf{w}_j^i + \mathbf{d}_j - \mathbf{g}(\mathbf{x}_j^f + \mathbf{A} \mathbf{w}_j^i) \right) \right\}.\end{aligned}$$

with

$$\mathbf{G}_j^i = (\nabla \mathbf{g} |_{\mathbf{x}_j^f + \mathbf{A} \mathbf{w}_j^i})^T.$$

$G_j^i A$ 

Define the linear regression

$$C_{yx}^i = G_i C_{xx}^i \quad \text{or} \quad G_i = C_{yx}^i (C_{xx}^i)^{-1}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

$$\mathbf{C}_{yx}^i = \mathbf{G}_i \mathbf{C}_{xx}^i \quad \text{or} \quad \mathbf{G}_i = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1}$$

and write

$$\mathbf{G}_j^i \mathbf{A} \triangleq \mathbf{G}_i \mathbf{A} = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1} \mathbf{A} \quad \text{Average sensitivity}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

$$\mathbf{C}_{yx}^i = \mathbf{G}_i \mathbf{C}_{xx}^i \quad \text{or} \quad \mathbf{G}_i = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1}$$

and write

$$\begin{aligned} \mathbf{G}_j^i \mathbf{A} &\triangleq \mathbf{G}_i \mathbf{A} = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1} \mathbf{A} && \text{Average sensitivity} \\ &\approx \overline{\mathbf{G}}_i \mathbf{A} = \mathbf{Y}_i \mathbf{A}_i^T (\mathbf{A}_i \mathbf{A}_i^T)^+ \mathbf{A} && \text{Ensemble repr.} \end{aligned}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

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$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

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$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

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and write

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 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A} && (\mathbf{A}_i = \mathbf{A} \boldsymbol{\Omega}_i) \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A}_i \boldsymbol{\Omega}_i^{-1} && \mathbf{A}_i^+ \mathbf{A}_i = \Pi_{A^T} = \left( \mathbf{I} - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right)
 \end{aligned}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

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 &\approx \overline{\mathbf{G}}_i \mathbf{A} = \mathbf{Y}_i \mathbf{A}_i^T (\mathbf{A}_i \mathbf{A}_i^T)^+ \mathbf{A} && \text{Ensemble repr.} \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A} && (\mathbf{A}_i = \mathbf{A} \boldsymbol{\Omega}_i) \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A}_i \boldsymbol{\Omega}_i^{-1} && \mathbf{A}_i^+ \mathbf{A}_i = \Pi_{A^T} = \left( \mathbf{I} - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) \\
 &= \mathbf{S}_i = \begin{cases} \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1} & \text{linear case} \end{cases}
 \end{aligned}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

$$\mathbf{C}_{yx}^i = \mathbf{G}_i \mathbf{C}_{xx}^i \quad \text{or} \quad \mathbf{G}_i = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1}$$

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 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A} && (\mathbf{A}_i = \mathbf{A} \boldsymbol{\Omega}_i) \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A}_i \boldsymbol{\Omega}_i^{-1} && \mathbf{A}_i^+ \mathbf{A}_i = \Pi_{A^T} = \left( \mathbf{I} - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) \\
 &= \mathbf{S}_i = \begin{cases} \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1} & \text{linear case} \\ \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1} & n \geq N - 1, \end{cases}
 \end{aligned}$$

$$\mathbf{G}_j^i \mathbf{A}$$

Define the linear regression

$$\mathbf{C}_{yx}^i = \mathbf{G}_i \mathbf{C}_{xx}^i \quad \text{or} \quad \mathbf{G}_i = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1}$$

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 \mathbf{G}_j^i \mathbf{A} &\triangleq \mathbf{G}_i \mathbf{A} = \mathbf{C}_{yx}^i (\mathbf{C}_{xx}^i)^{-1} \mathbf{A} && \text{Average sensitivity} \\
 &\approx \overline{\mathbf{G}}_i \mathbf{A} = \mathbf{Y}_i \mathbf{A}_i^T (\mathbf{A}_i \mathbf{A}_i^T)^+ \mathbf{A} && \text{Ensemble repr.} \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A} && (\mathbf{A}_i = \mathbf{A} \boldsymbol{\Omega}_i) \\
 &= \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A}_i \boldsymbol{\Omega}_i^{-1} && \mathbf{A}_i^+ \mathbf{A}_i = \Pi_{A^T} = \left( \mathbf{I} - \frac{1}{N} \mathbf{1} \mathbf{1}^T \right) \\
 &= \mathbf{S}_i = \begin{cases} \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1} & \text{linear case} \\ \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1} & n \geq N-1, \\ \mathbf{Y}_i \mathbf{A}_i^+ \mathbf{A}_i \boldsymbol{\Omega}_i^{-1} & n < N-1, \end{cases}
 \end{aligned}$$

# Equation for $\mathbf{W}$

Matrix form with  $\mathbf{S}_i = \mathbf{Y}_i \boldsymbol{\Omega}_i^{-1}$

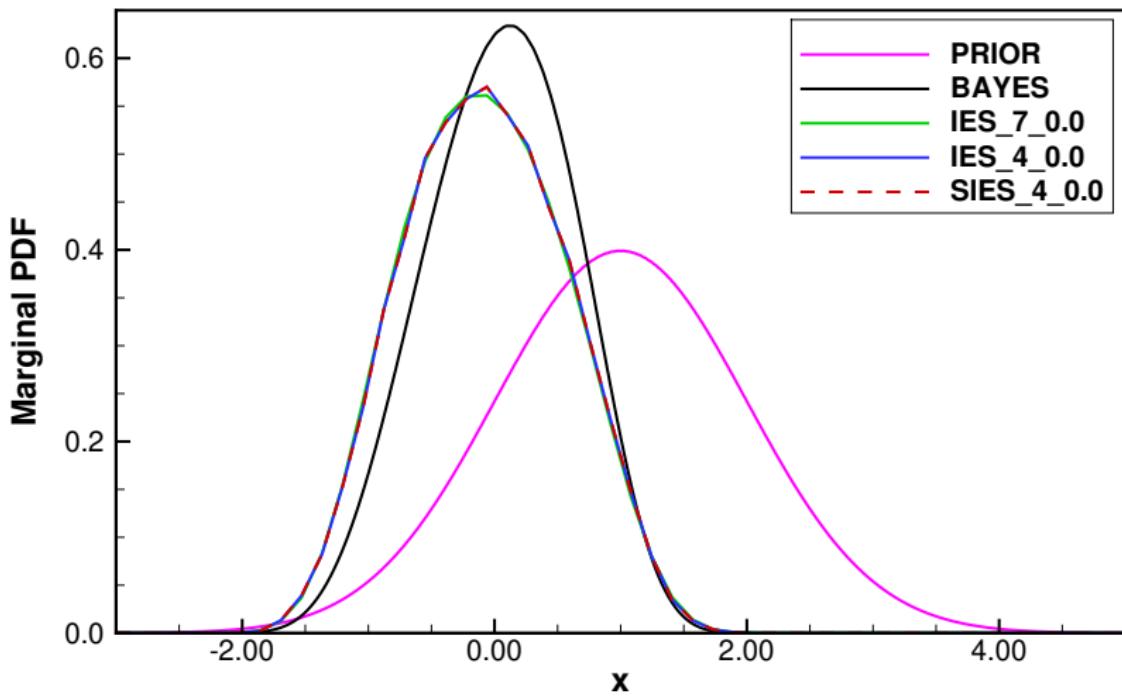
$$\mathbf{W}_{i+1} = \mathbf{W}_i - \gamma \left( \mathbf{W}_i - \mathbf{S}_i^T (\mathbf{S}_i \mathbf{S}_i^T + \mathbf{C}_{dd})^{-1} (\mathbf{S}_i \mathbf{W}_i - \mathbf{D} + \mathbf{g}(\mathbf{X}_i)) \right)$$

# IES ensemble subspace algorithm

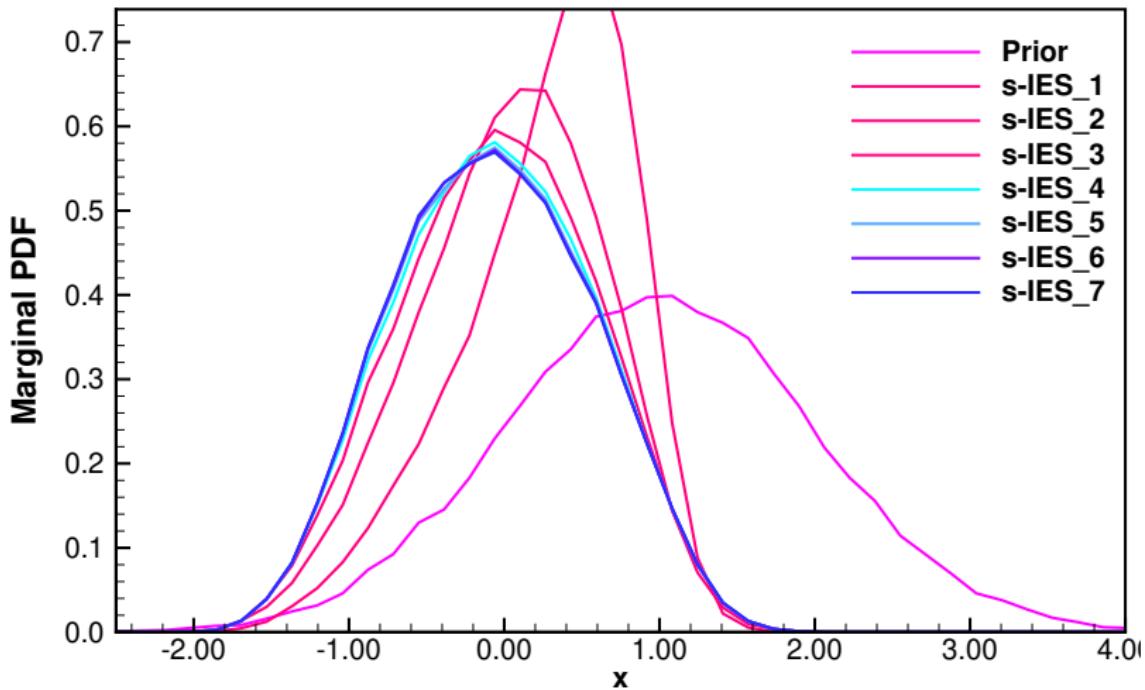
- 1: Inputs:  $\mathbf{X}$ ,  $\mathbf{D}$ , (and  $\mathbf{C}_{dd}$ )
- 2:  $\mathbf{W}_1 = 0$
- 3: **for**  $i = 1$ , Convergence **do**
- 4:    $\mathbf{Y}_i = \mathbf{g}(\mathbf{X}_i)(\mathbf{I} - \frac{1}{N}\mathbf{1}\mathbf{1}^T)/\sqrt{N-1}$
- 5:    $\Omega_i = \mathbf{I} + \mathbf{W}_i(\mathbf{I} - \frac{1}{N}\mathbf{1}\mathbf{1}^T)/\sqrt{N-1}$
- 6:    $\Omega_i^T \mathbf{S}_i^T = \mathbf{Y}_i^T$   $\mathcal{O}(mN^2)$
- 7:    $\mathbf{H}_i = \mathbf{S}_i \mathbf{W}_i + \mathbf{D} - \mathbf{g}(\mathbf{X}_i)$   $\mathcal{O}(mN^2)$
- 8:    $\mathbf{W}_{i+1} = \mathbf{W}_i - \gamma \left( \mathbf{W}_i - \mathbf{S}_i^T (\mathbf{S}_i \mathbf{S}_i^T + \mathbf{C}_{dd})^{-1} \mathbf{H}_i \right)$   $\mathcal{O}(mN^2)$
- 9:    $\mathbf{X}_{i+1} = \mathbf{X}(\mathbf{I} + \mathbf{W}_{i+1}/\sqrt{N-1})$   $\mathcal{O}(nN^2)$
- 10: **end for**

- ▶ Order  $\mathcal{O}(mN^2)$  and  $\mathcal{O}(nN^2)$
- ▶ No pseudo inversions of large matrices.

## Example nonlinear model



## Iterations nonlinear model



## Equation for $\mathbf{W}$

Standard form ( $\mathcal{O}(m^3)$ )

$$\mathbf{W}_{i+1} = \mathbf{W}_i - \gamma \left( \mathbf{W}_i - \mathbf{S}_i^T (\mathbf{S}_i \mathbf{S}_i^T + \mathbf{C}_{dd})^{-1} \mathbf{H}_i \right)$$

From Woodbury, rewrite as

$$\mathbf{W}_{i+1} = \mathbf{W}_i - \gamma \left\{ \mathbf{W}_i - (\mathbf{S}_i^T \mathbf{C}_{dd}^{-1} \mathbf{S}_i + \mathbf{I}_N)^{-1} \mathbf{S}_i^T \mathbf{C}_{dd}^{-1} \mathbf{H} \right\}$$

For  $\mathbf{C}_{dd} = \mathbf{I}_m$  we have ( $\mathcal{O}(mN^2)$ )

$$\mathbf{W}_{i+1} = \mathbf{W}_i - \gamma \left\{ \mathbf{W}_i - (\mathbf{S}_i^T \mathbf{S}_i + \mathbf{I}_N)^{-1} \mathbf{S}_i^T \mathbf{H} \right\}$$

## Subspace inversion (*Evensen, 2004*)

- ▶ Why invert  $m$ -dimensional matrix when solving for  $N$  coefficients?

$$\begin{aligned} & (\mathbf{S}\mathbf{S}^T + \mathbf{C}_{dd}) \\ &= (\mathbf{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T\mathbf{U}^T + \mathbf{C}_{dd}) \\ &\approx \mathbf{U}\boldsymbol{\Sigma}(\mathbf{I}_N + \boldsymbol{\Sigma}^+\mathbf{U}^T\mathbf{C}_{dd}\mathbf{U}(\boldsymbol{\Sigma}^+)^T)\boldsymbol{\Sigma}^T\mathbf{U}^T \\ &\quad = \mathbf{S}\mathbf{S}^T + (\mathbf{S}\mathbf{S}^+)^T\mathbf{C}_{dd}(\mathbf{S}\mathbf{S}^+)^T \\ &= \mathbf{U}\boldsymbol{\Sigma}(\mathbf{I}_N + \mathbf{Z}\boldsymbol{\Lambda}\mathbf{Z}^T)\boldsymbol{\Sigma}^T\mathbf{U}^T \\ &= \mathbf{U}\boldsymbol{\Sigma}\mathbf{Z}(\mathbf{I}_N + \boldsymbol{\Lambda})\mathbf{Z}^T\boldsymbol{\Sigma}^T\mathbf{U}^T \end{aligned}$$

$$(\mathbf{S}\mathbf{S}^T + \mathbf{C}_{dd})^{-1} \approx \mathbf{U}(\boldsymbol{\Sigma}^+)^T\mathbf{Z}(\mathbf{I}_N + \boldsymbol{\Lambda})^{-1}(\mathbf{U}(\boldsymbol{\Sigma}^+)^T\mathbf{Z})^T$$

- ▶ Cost is  $\mathcal{O}(m^2N)$ .

# Subspace inversion with $C_{dd} \approx \mathbf{E}\mathbf{E}^T$ .

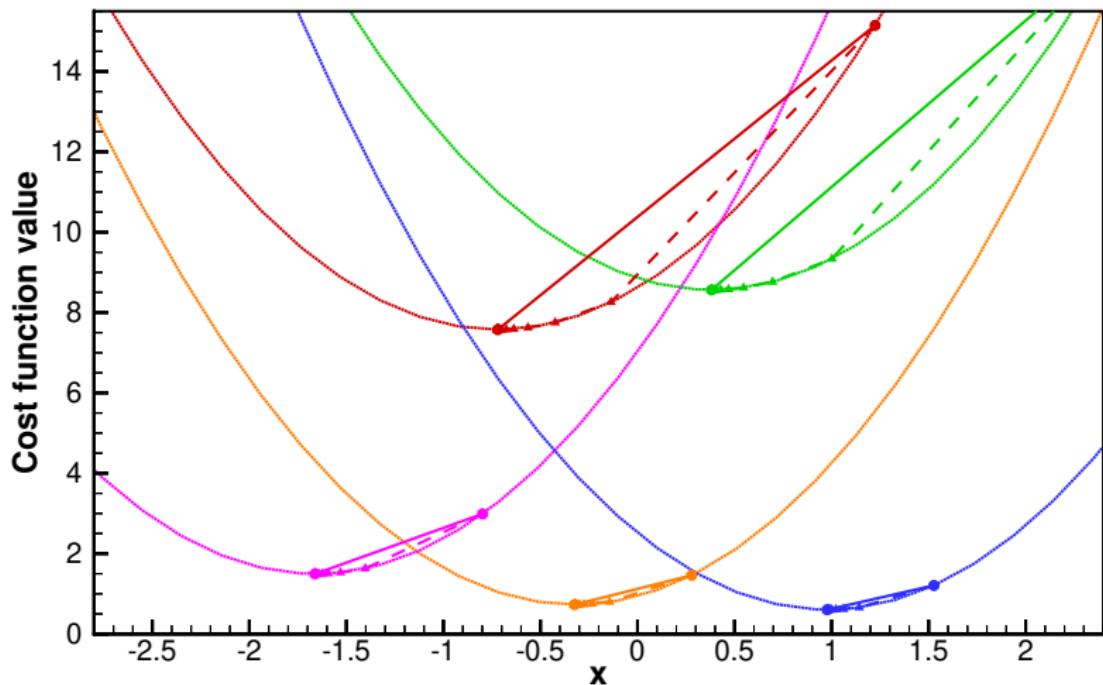
- Do not form  $C_{dd}$  but work directly with  $\mathbf{E}$ .

$$\begin{aligned}
 & (\mathbf{S}\mathbf{S}^T + \mathbf{E}\mathbf{E}^T) \\
 &= (\mathbf{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T\mathbf{U}^T + \mathbf{E}\mathbf{E}^T) \\
 &\approx \mathbf{U}\boldsymbol{\Sigma}(\mathbf{I}_N + \boldsymbol{\Sigma}^+\mathbf{U}^T\mathbf{E}\mathbf{E}^T\mathbf{U}(\boldsymbol{\Sigma}^+)^T)\boldsymbol{\Sigma}^T\mathbf{U}^T \\
 &= \mathbf{S}\mathbf{S}^T + (\mathbf{S}\mathbf{S}^+)\mathbf{E}\mathbf{E}^T(\mathbf{S}\mathbf{S}^+)^T \\
 &= \mathbf{U}\boldsymbol{\Sigma}(\mathbf{I}_N + \mathbf{Z}\boldsymbol{\Lambda}\mathbf{Z}^T)\boldsymbol{\Sigma}^T\mathbf{U}^T \\
 &= \mathbf{U}\boldsymbol{\Sigma}\mathbf{Z}(\mathbf{I}_N + \boldsymbol{\Lambda})\mathbf{Z}^T\boldsymbol{\Sigma}^T\mathbf{U}^T
 \end{aligned}$$

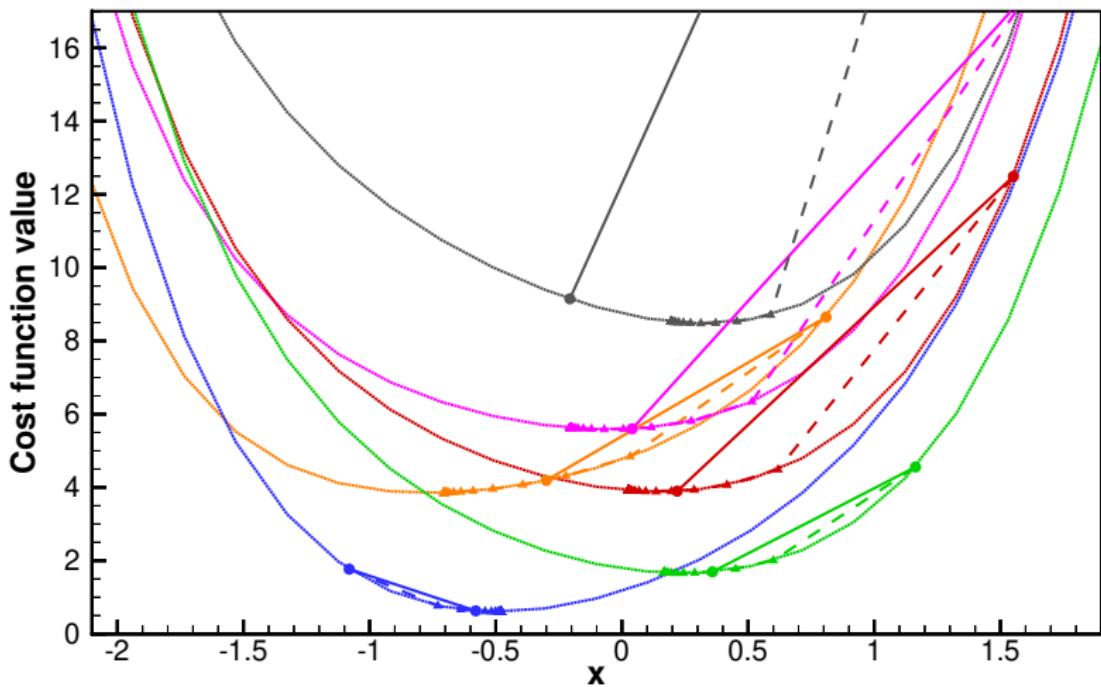
$$(\mathbf{S}\mathbf{S}^T + \mathbf{E}\mathbf{E}^T)^{-1} \approx \mathbf{U}(\boldsymbol{\Sigma}^+)^T\mathbf{Z}(\mathbf{I}_N + \boldsymbol{\Lambda})^{-1}(\mathbf{U}(\boldsymbol{\Sigma}^+)^T\mathbf{Z})^T$$

- Cost is  $\mathcal{O}(mN^2)$ .

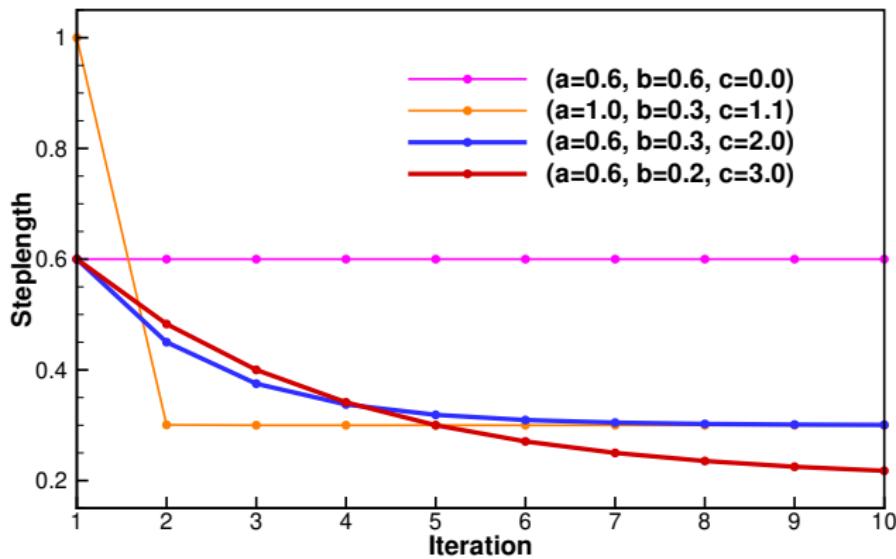
## IES costfunctions: Linear case



## IES costfunctions: Nonlinear case



# Steplength scheme



$$\gamma_i = b + (a - b)2^{(-(i-1)/(c-1))}$$

ERT: <https://github.com/equinor/ert>

ERT

File View Help

Configure Create Plot Export Data Run Workflow Manage Cases Plugins Run Analysis Load results manually Help

Simulation mode: Iterated Ensemble Smoother

Current case: ES\_NORMAL

Runpath: poly\_out/real\_%d/iter\_%d

Number of realizations: 100

Number of iterations: 10

Target case format: ES\_NORMAL\_%d

Analysis Module: IES\_ENKF

Active realizations 0-99

Configuration Summary

FORWARD MODEL  
poly\_eval

PARAMETERS  
COEFFS

OBSERVATIONS  
POLY\_OBS

ERT: <https://github.com/equinor/ert>

ERT

File View Help

Edit variables

Gauss Newton Maximum Steplength

Gauss Newton Minimum Steplength

Gauss Newton Steplength Decline

*A good start is max steplength of 0.6, min steplength of 0.3, and decline of 2.5*

*A steplength of 1.0 and one iteration results in ES update*

Inversion algorithm

*0: Exact inversion with diagonal R=I  
1: Subspace inversion with exact R  
2: Subspace inversion using R=EE'  
3: Subspace inversion using E*

Print extensive log for IES

IES Log File

Singular value truncation

Number of singular values

Include AA projection

*Any benefit of using the projection is unclear*

Close

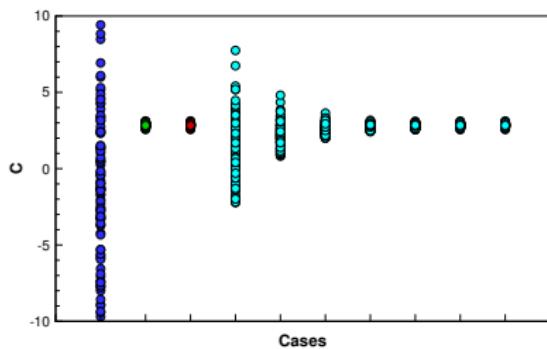
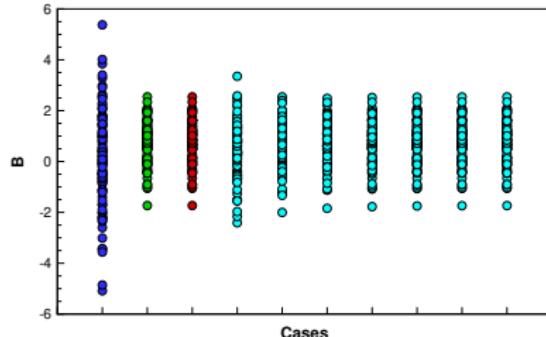
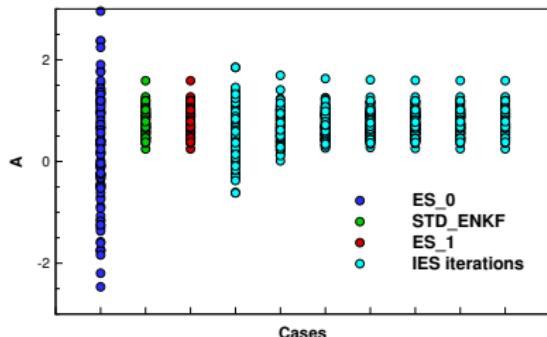
## Poly case

Several simple tests are run using a “linear” model

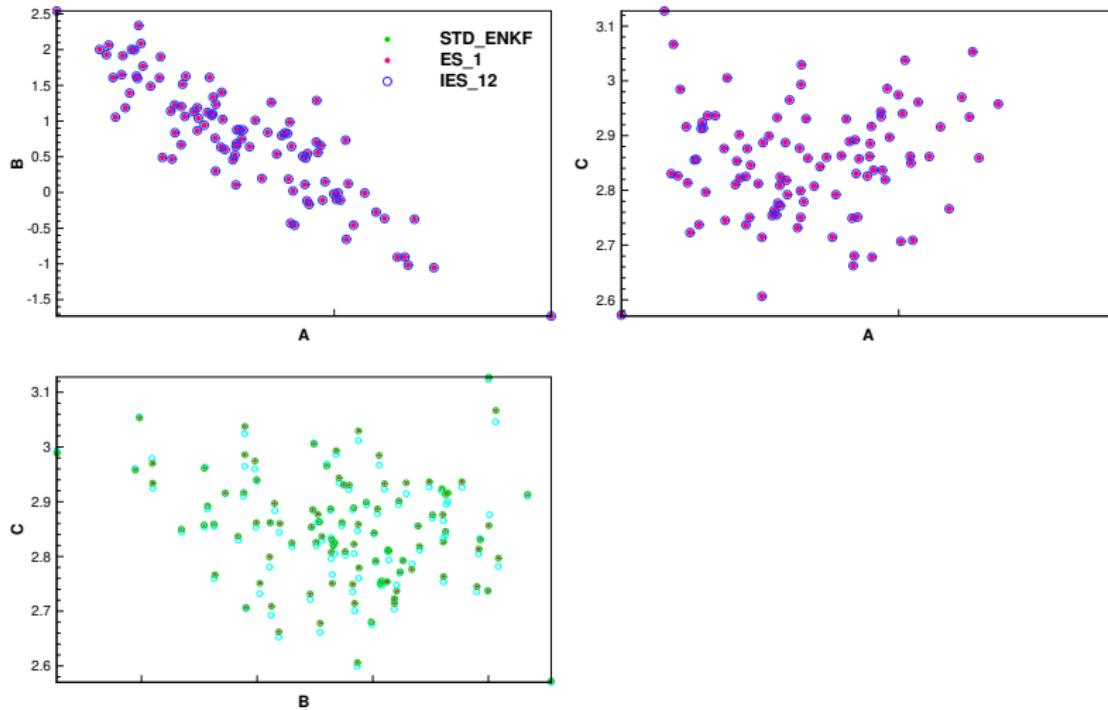
$$y(x) = ax^2 + bx + c \quad (1)$$

- ▶ Coefficients  $a$ ,  $b$ , and  $c$  are random Gaussian variables.
- ▶ Measurements  $(d_1, \dots, d_5)$  at  $x = (0, 2, 4, 6, 8)$ .
- ▶ Polynomial curve fitting to the 5 data points.
- ▶ Gauss-linear problem solved exactly by the ES.

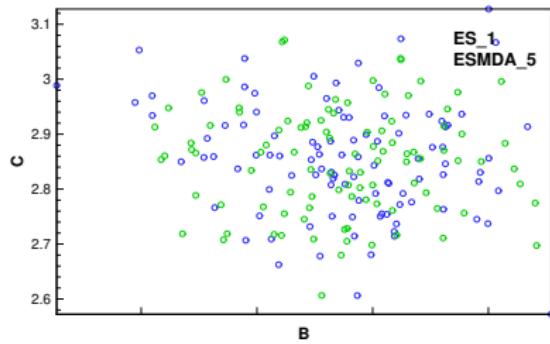
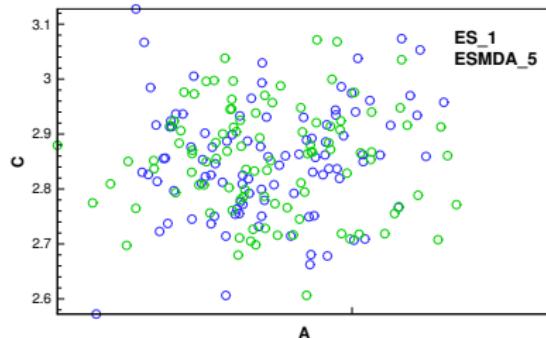
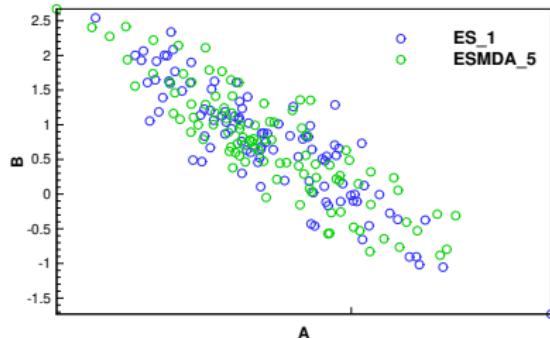
# Subspace IES verification



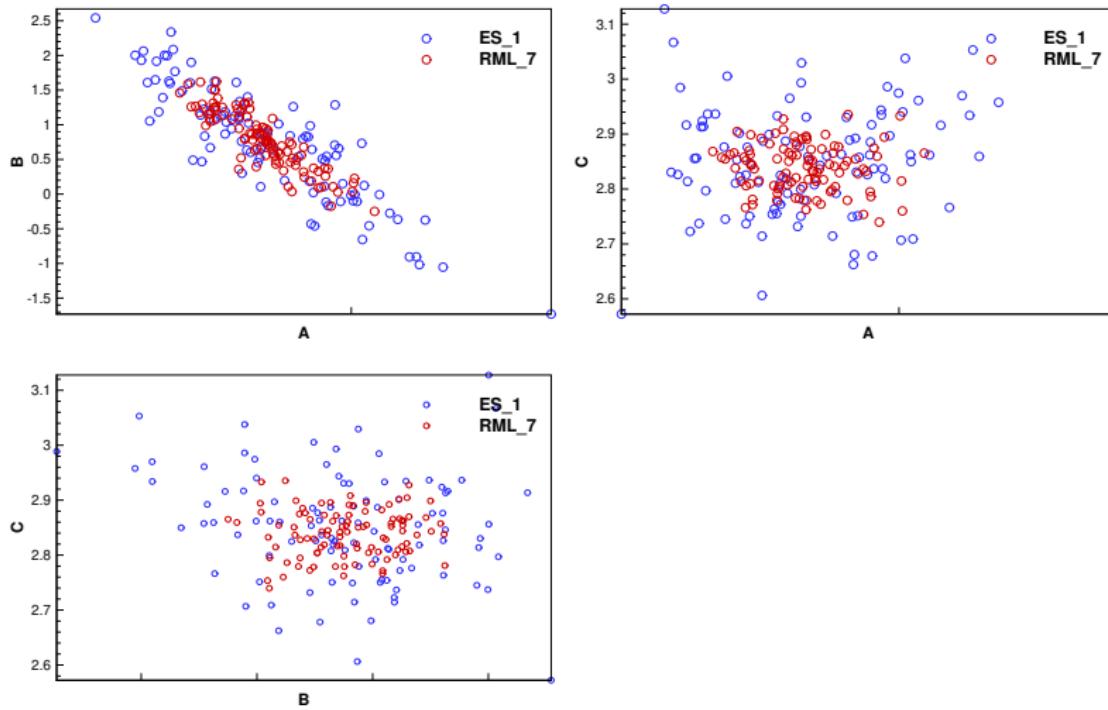
# Subspace IES verification



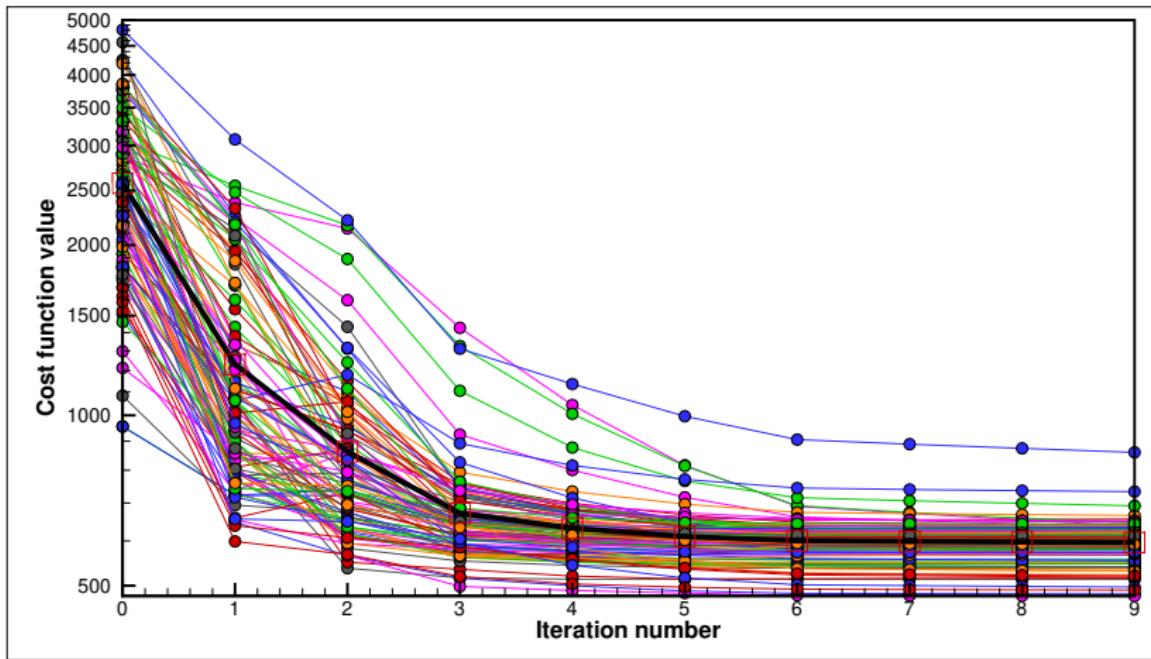
# Subspace IES vs. ESMDA



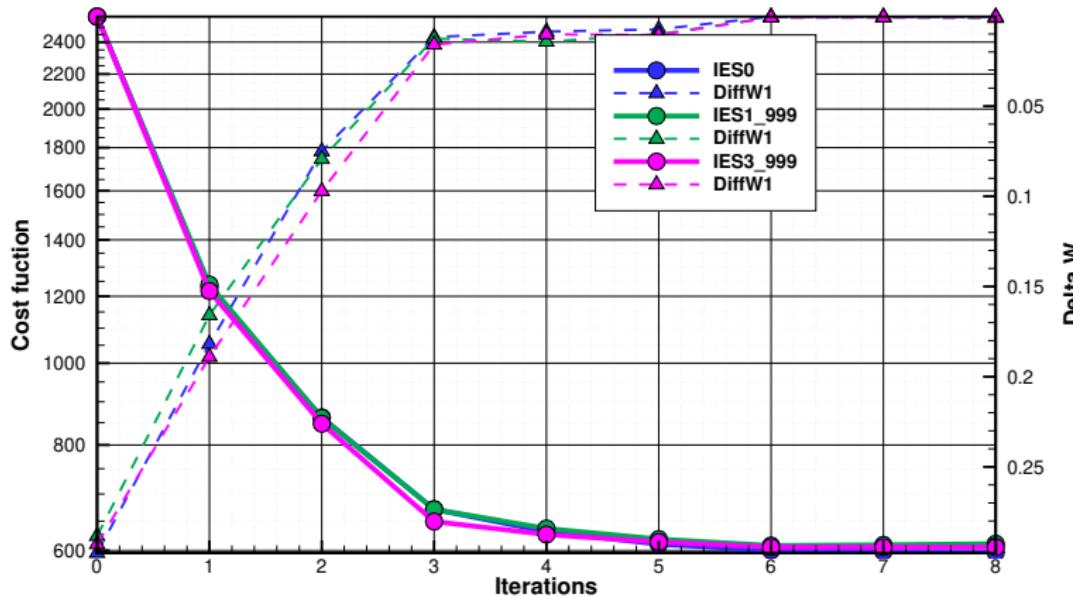
# Subspace IES vs. EnRML implementation



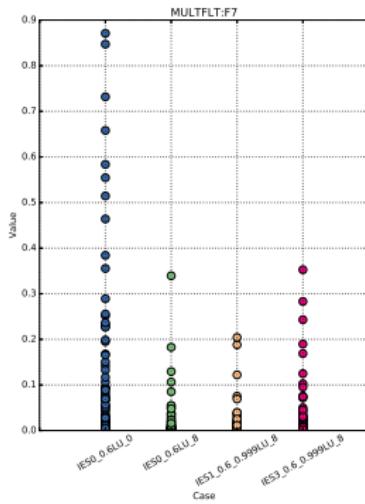
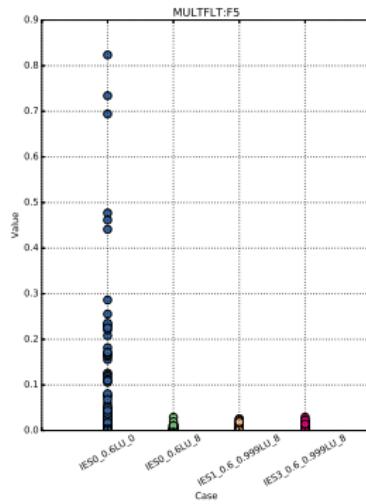
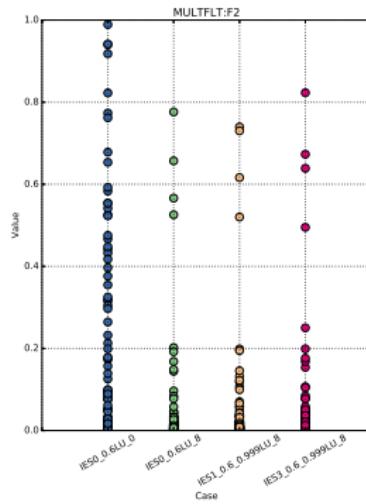
# Reek case: Ensemble of cost functions



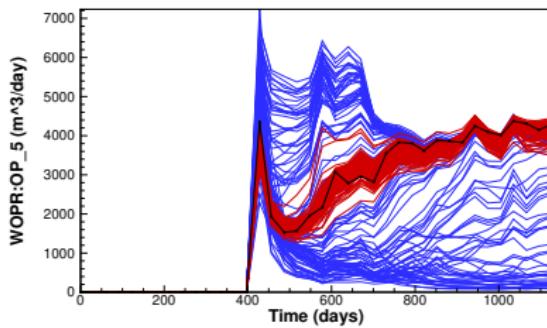
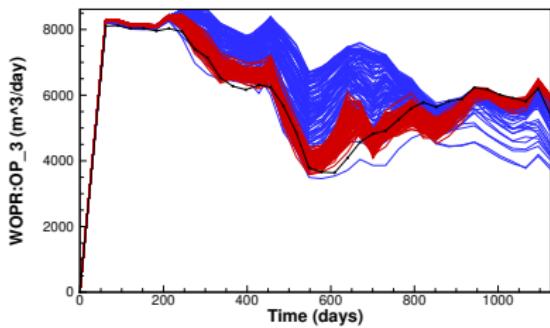
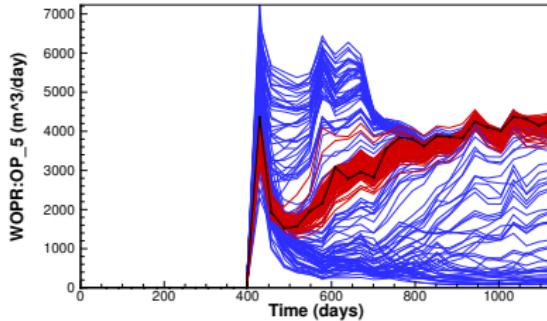
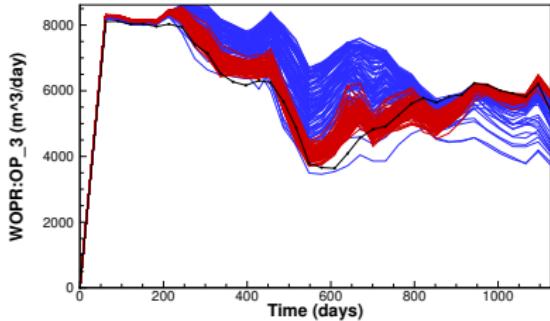
# Reek case: Averaged cost function



# Reek case: Fault multiplier



# Reek case: Oil production



## Summary

- ▶ Robust implementation of a robust IES formulation in ERT.
- ▶ IES algorithm formulated for big data and big models.
- ▶ Convergence properties meet requirements for operational use.
- ▶ Pointed out the value of test-based code development.
- ▶ ERT is a flexible tool for reservoir HM.

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