

Iterative Regularizing Ensemble Kalman Methods for Inverse Problems

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Nonlinear ill-posed inverse problems

The forward map

Let $G : X \rightarrow Y$ be the forward (parameter-to-observations) map that arises from PDE-constrained problem where u is an unknown parameter (or property)

$$u \longrightarrow G(u)$$

(G nonlinear, compact, sequentially weakly closed operator between separable Hilbert spaces X and Y .)

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Example: steady Darcy flow

$$\begin{aligned} -\nabla \cdot e^u \nabla p &= f && \text{in } D, \\ -e^u \nabla p \cdot n &= B_N && \text{in } \Gamma_N, \\ \rho &= B_D && \text{in } \Gamma_D \end{aligned}$$

where $\partial D = \Gamma_N \cup \Gamma_D$.

$$u = \log(K) \in L^\infty(D) \longrightarrow G(u) = \{p(x_i)\}_{i=1}^N \in \mathbb{R}^M$$

Nonlinear ill-posed inverse problems

The data and the noise level

Let u^\dagger be the “truth”, i.e. $G(u^\dagger)$ are the exact (noise-free) observations.
Assume that we are given *data*

$$y = G(u^\dagger) + \xi^\dagger$$

where ξ^\dagger is noise and we are given a noise level η such that

$$\|y - G(u^\dagger)\| \leq \eta$$

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Given y and η find approximate solutions u to $G(u^\dagger) = G(u)$.

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Ill-posedness (Hadamard)

- Existence
- Uniqueness
- Continuity with respect to the data y

Nonlinear ill-posed inverse problems

Lack of continuity (lack of stability) with respect to the data

We can construct a sequence $u_n \in X$ such that

$$u_n \not\rightarrow u \quad \text{but} \quad G(u_n) \rightarrow G(u)$$

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If we want to compute with standard optimization

$$u = \arg \min_{u \in X} \|y - G(u)\|^2 \rightarrow \min$$

we may observe semiconvergence behavior [*Kirsch, 1996*]

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Regularization

Construct an approximation u^η that is stable, i.e. such that

$$u^\eta \rightarrow u \quad \text{as} \quad \eta \rightarrow 0$$

where

$$G(u) = G(u^\dagger)$$

Regularization Approaches (for nonlinear operators)

- Regularize-then-compute (e.g. Tikhonov, TSVD)
- Compute while regularizing (**Iterative Regularization**)
[Kaltenbacher, 2010]
 - ▶ *regularizing Levenberg-Marquardt*
 - ▶ *Landweber iteration*
 - ▶ *truncated Newton-CG*
 - ▶ *iterative regularized Gauss-Newton method*

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Aim of this work:

Apply ideas from **Iterative Regularization** to develop ensemble Kalman methods as *derivative-free* tools for solving nonlinear ill-posed inverse problem in a general abstract framework.

PDE-constrained Inverse Problems

The Classical (deterministic) Inverse Problem

Given data $y \in Y$ find

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PDE-constrained Inverse Problems

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Given data $y \in Y$ find

$$u = \arg \min_{u \in X} \|y - G(u)\|^2 \rightarrow \min$$

Consider $\mu_0(u) = \mathbb{P}(u)$ the prior on u and

$$y = G(u) + \xi, \quad \xi \sim \mathcal{N}(0, \Gamma)$$

The Bayesian Inverse Problem

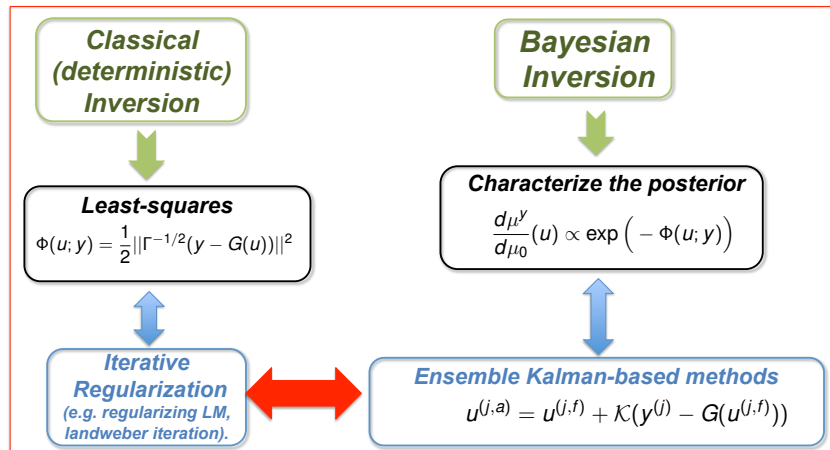
Characterize the posterior $\mu^y(u) = \mathbb{P}(u|y)$:

$$\frac{d\mu^y}{d\mu_0}(u) \propto \exp\left(-\Phi(u; y)\right)$$

where

$$\Phi(u; y) = \frac{1}{2} \|\Gamma^{-1/2}(y - G(u))\|^2$$

Overview of this work



Reference

Iterative Regularization for Data Assimilation in Petroleum Reservoirs

Multiscale Inverse Problems Workshop, Warwick University, June 17-19, 2013.

<http://www2.warwick.ac.uk/fac/sci/math/research/events/2012-2013/nonsymp/mip/schedule/>



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Iterative regularization for ensemble data assimilation in reservoir models

Marco A. Iglesias

(Submitted on 21 Jan 2014)

We propose the application of iterative regularization for the development of ensemble methods for solving Bayesian inverse problems. In concrete, we construct (i) a variational iterative regularizing ensemble Levenberg–Marquardt method (IR–enLM) and (ii) a derivative–free iterative ensemble Kalman smoother (IR–ES). The aim of these methods is to provide a robust ensemble approximation of the Bayesian posterior. The proposed methods are based on fundamental ideas from iterative regularization methods that have been widely used for the solution of deterministic inverse problems [21]. In this work we are interested in the application of the proposed ensemble methods for the solution of Bayesian inverse problems that arise in reservoir modeling applications. The proposed ensemble methods use key aspects of the regularizing Levenberg–Marquardt scheme developed by Hanke [16] and that we recently applied for history matching in [18].

In the case where the forward operator is linear and the prior is Gaussian, we show that the proposed IR–enLM and IR–ES coincide with standard randomized maximum likelihood (RML) and the ensemble smoother (ES) respectively. For the general nonlinear case, we develop a numerical framework to assess the performance of the proposed ensemble methods at capturing

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Iterative ensemble Kalman “Smoother”

Assume that the data $y = G(u^\dagger) + \xi$ with $\xi \sim N(0, \Gamma)$.

Consider an initial ensemble $u_0^{(1)}, \dots, u_0^{(N_e)}$.

Prediction $u_n^{(j)} \rightarrow G(u_n^{(j)})$

$$\begin{aligned}\bar{u}_n &= \frac{1}{N_e} \sum_{j=1}^{N_e} u_n^{(j)}, & \bar{w}_n &= \frac{1}{N_e} \sum_{j=1}^{N_e} G(u_n^{(j)}) \\ C^{ww} &= \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (G(u_n^{(j)}) - \bar{w}_n)(G(u_n^{(j)}) - \bar{w}_n)^T, \\ C^{uw} &= \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (u_n^{(j)} - \bar{u}_n)(G(u_n^{(j)}) - \bar{w}_n)^T\end{aligned}$$

Analysis $u_n^{(j)} \rightarrow u_{n+1}^{(j)}$

$$u_{n+1}^{(j)} = u_n^{(j)} + C^{uw}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_n^{(j)})), \quad y^{(j)} = y + \eta^{(j)}$$

Ensemble Kalman Methods for Inverse Problems

Augmented analysis

$$\begin{aligned}u_{n+1}^{(j)} &= u_n^{(j)} + C^{uw}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_n^{(j)})) \\w_{n+1}^{(j)} &= G(u_n^{(j)}) + C^{ww}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_n^{(j)}))\end{aligned}$$

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$$z_{n+1}^{(j)} = z_n^{(j)} + C^f H^T (H C^f H^T + \Gamma)^{-1} (y^{(j)} - H z_n^{(j)})$$

where

$$z = (u, w)^T \in Z \equiv X \times Y \quad H = (0, I) \quad C^f = \begin{pmatrix} C^{uu} & C^{uw} \\ (C^{uw})^T & C^{ww} \end{pmatrix}$$

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Kalman as a Tikhonov-regularized linear inverse problems

$$\bar{z}_{n+1} = \frac{1}{N_e} \sum_{j=1}^{N_e} z_{n+1}^{(j)} = \operatorname{argmin}_z \left(\|\Gamma^{-\frac{1}{2}}(y - Hz)\|^2 + \|(C^f)^{-\frac{1}{2}}(z - \bar{z}_n)\|_Z^2 \right)$$

where $\bar{z}_n \equiv \frac{1}{N_e} \sum_{j=1}^{N_e} z_n^{(j)}$.

Kalman as a Tikhonov-regularized linear inverse problems

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In summary, this iterative method is solving a sequence of linear inverse problems: Given y , find z such that

$$y = Hz$$

Ensemble Kalman Methods for Inverse Problems

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Preliminary work on Kalman methods for inverse problems



M. Iglesias, K. Law and A.M. Stuart,

Ensemble Kalman methods for inverse problems. *Inverse Problems*. 29 (2013) 045001
<http://arxiv.org/abs/1209.2736>

Ensemble Kalman Methods for Inverse Problems

- This algorithm can be formulated in a general abstract framework on Hilbert spaces.
- No localization/inflation/truncation of any type was considered. The main focus was the initial ensemble.
- We consider both initial ensemble sample from the prior but also the first elements of a basis.
- Invariance subspace property $\mathcal{A} = \text{span}\{u_0^{(j)}\}_{j=1}^{N_e}$.

Theorem (Iglesias, Law, Stuart)

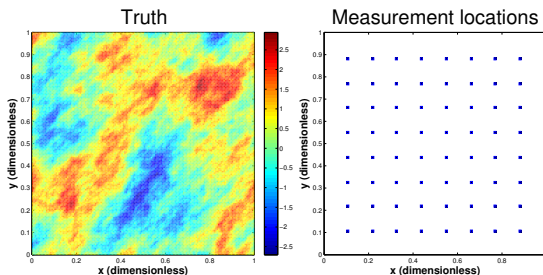
$$\bar{u}_n^{(j)} \in \mathcal{A} \text{ for all } (n, j) \in \mathbb{N} \times \{1, \dots, N_e\}.$$

- Even though the problem is defined on a compact subspace \mathcal{A} , we found that further regularization is needed.

Synthetic experiment with a toy (groundwater) model

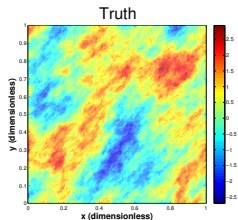
Consider

- Initial ensemble generated from a prior $\mathbb{P}(u) = N(\bar{u}, C)$.
- Let $G(u)$ be the forward operator that arises from a reservoir model.

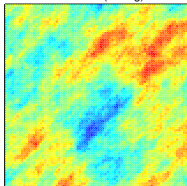


Consider a truth $u^\dagger \sim \mathbb{P}(u)$ from which synthetic data are generated by $y = G(u^\dagger) + \eta$ ($\eta \sim N(0, \Gamma)$ (prescribed Γ covariance of the Gaussian noise)).

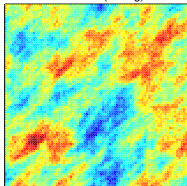
Reconstructing the truth with the mean of an ensemble of $N_e = 75$ (with small noise)



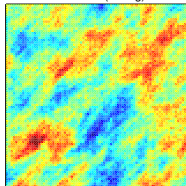
Ensemble mean (no reg). Iter:1



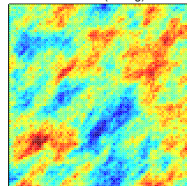
Ensemble mean (no reg). Iter:2



Ensemble mean (no reg). Iter:3



Ensemble mean (no reg). Iter:12



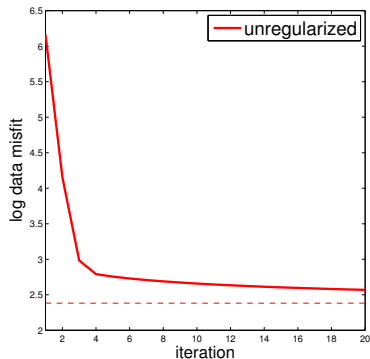
Performance

$$\bar{u}_n \equiv \frac{1}{N} \sum_{j=1}^N u_n^{(j)}$$

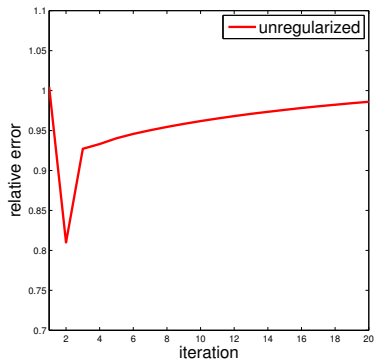
$$\|\Gamma^{-1/2}(y - \bar{u}_n)\|_{l_2}$$

$$\|\bar{u}_n - u^\dagger\|_{L^2(D)}$$

Data misfit



Error w.r.t truth



Recall the standard update formula yields a mean defined by

$$\bar{z}_{n+1} = \operatorname{argmin}_z \left(\|\Gamma^{-\frac{1}{2}}(\mathbf{y} - H\mathbf{z})\|^2 + \|(\mathbf{C}^f)^{-\frac{1}{2}}(\mathbf{z} - \bar{z}_n)\|_Z^2 \right)$$

Recall the standard update formula yields a mean defined by

$$\bar{z}_{n+1} = \operatorname{argmin}_z \left(\|\Gamma^{-\frac{1}{2}}(y - Hz)\|^2 + \|(C^f)^{-\frac{1}{2}}(z - \bar{z}_n)\|_Z^2 \right)$$

We propose in



M. A. Iglesias

Iterative regularization for ensemble-based data assimilation in reservoir models.

In review (<http://arxiv.org/abs/1401.5375>). 2014 (Submitted to Computational Geosciences)

to modify the ensemble method

$$z_{n+1}^{(j)} = z_n^{(j)} + C^f H^T \left(HC^f H^T + \alpha \Gamma \right)^{-1} (y^{(j)} - Hz_n^{(j)})$$

so that the mean is given by

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i.e. **Regularizing Kalman as in Levenberg-Marquardt!!** where a selection of α guided by **Iterative Regularization** methods.

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i.e. **Regularizing Kalman as in Levenberg-Marquardt!!** where a selection of α guided by **Iterative Regularization** methods. More precisely, we propose

$$\rho \|\Gamma^{-1/2}(y - H\bar{z}_n)\| \leq \|\Gamma^{-1/2}(y - H\bar{z}_{n+1}(\alpha))\| \leq \|\Gamma^{-1/2}(y - H\bar{z}_n)\|$$

where ρ is a tunable parameter in $(0, 1)$.

Proposition [Iglesias 2014]

$$\alpha \rightarrow \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_{n+1}(\alpha))\|$$

is continuous and monotone nondecreasing. Moreover,

- $\lim_{\alpha \rightarrow 0} \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_{n+1}(\alpha))\| = \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_n)\|$
- $\lim_{\alpha \rightarrow \infty} \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_{n+1}(\alpha))\| = 0$

Thus, there exists α such that

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$$\rho \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_n)\| \leq \|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_{n+1}(\alpha))\|$$

Stopping criteria: *Discrepancy Principle*

We terminate the algorithm whenever

$$\|\Gamma^{-1/2}(\mathbf{y} - H\bar{\mathbf{z}}_n)\| \leq \tau \eta \|\Gamma^{-1/2}\|$$

for a prescribed value $\tau > 1/\rho$ where $\eta = \|\mathbf{y} - G(\mathbf{u}^\dagger)\|$ is the noise level.

Then we can show that the selection of α is consistent with the **discrepancy principle** to the linear inverse problem corresponding to the analysis step.

An iterative regularizing ensemble Kalman method

Let $\rho < 1$ and $\tau > 1/\rho$. Generate an initial ensemble $u_0^{(j)} \sim \mu_0$

A regularizing Kalman method

- (1) Prediction Step:** Evaluate $w_m^{(j,f)} = G(u_m^{(j)})$ define \bar{w}_m^f
- (2) Stopping criteria.** If

$$\|\Gamma^{-1/2}(y - \bar{w}_m^f)\| \leq \tau\eta$$

Stop. Otherwise: define C_m^{uw} , \bar{u}_m , C_m^{ww} and

- (3) Analysis step:** Compute the updated ensembles

$$u_{m+1}^{(j)} = u_m^{(j)} + C_m^{uw}(C_m^{ww} + \alpha_m\Gamma)^{-1}(y^{(j)} - w_m^{(j,f)})$$

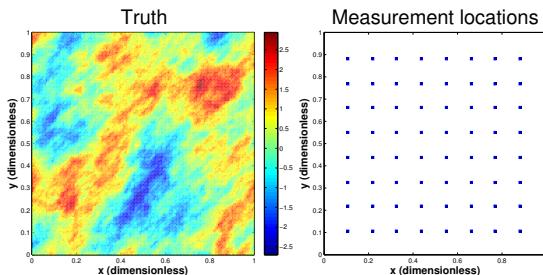
for α_m such that

$$\alpha_m \|\Gamma^{1/2}(C_m^{ww} + \alpha_m\Gamma)^{-1}(y^\eta - \bar{w}_m^f)\| \leq \rho \|\Gamma^{-1/2}(y^\eta - \bar{w}_m^f)\|$$

Synthetic experiment with a toy (groundwater) model

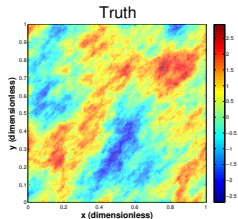
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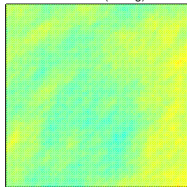


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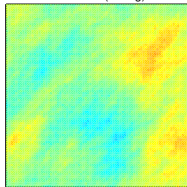
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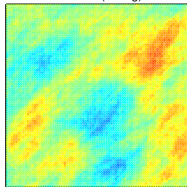
Ensemble mean (no reg). Iter:5



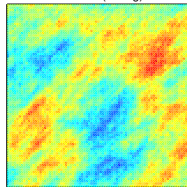
Ensemble mean (no reg). Iter:9



Ensemble mean (no reg). Iter:13



Ensemble mean (no reg). Iter:17



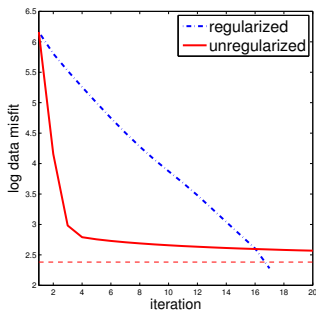
Performance

$$\bar{u}_n \equiv \frac{1}{N} \sum_{j=1}^N u_n^{(j)}$$

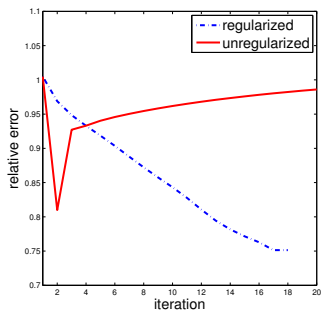
$$\|\Gamma^{-1/2}(y - \bar{u}_n)\|_{\ell^2}$$

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Data misfit

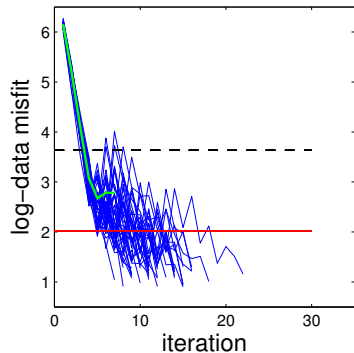


Error w.r.t truth

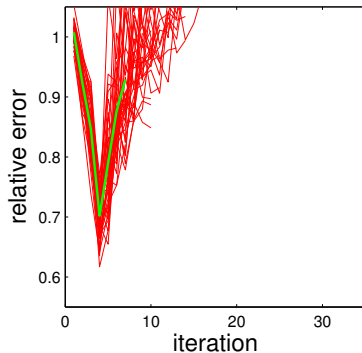


Regularizing properties as a function of ρ

$N_e=100, \rho=0.2$

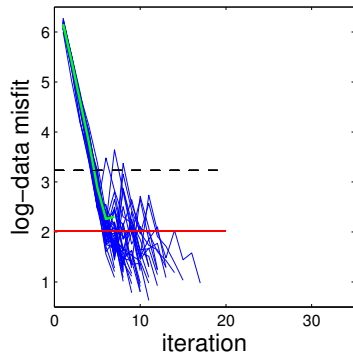


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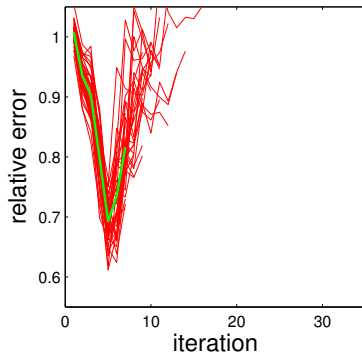


Regularizing properties as a function of ρ

$N_e=100, \rho=0.3$

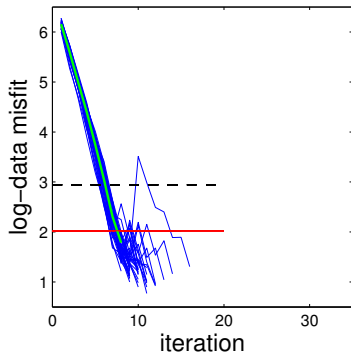


$N_e=100, \rho=0.3$

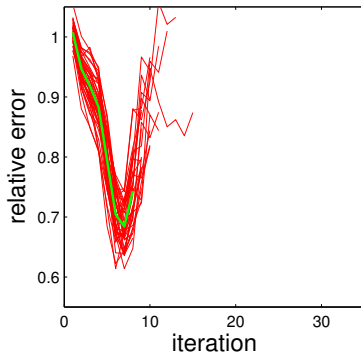


Regularizing properties as a function of ρ

$N_e=100, \rho=0.4$

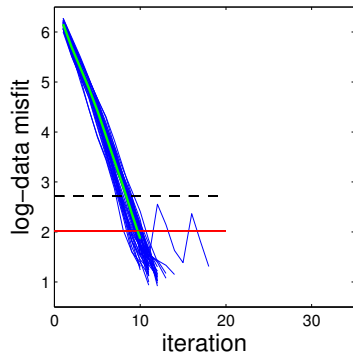


$N_e=100, \rho=0.4$

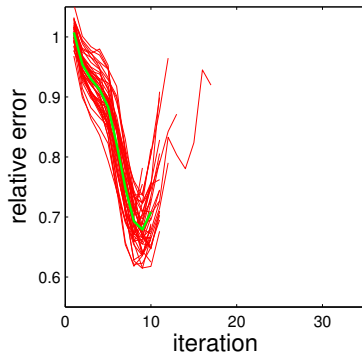


Regularizing properties as a function of ρ

$N_e=100, \rho=0.5$

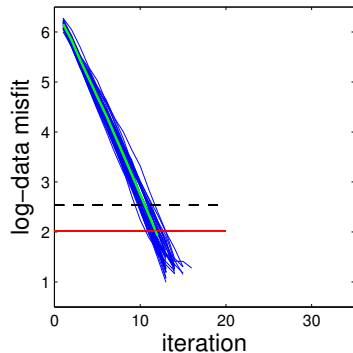


$N_e=100, \rho=0.5$

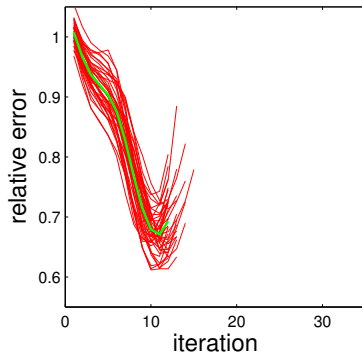


Regularizing properties as a function of ρ

$N_e=100, \rho=0.6$

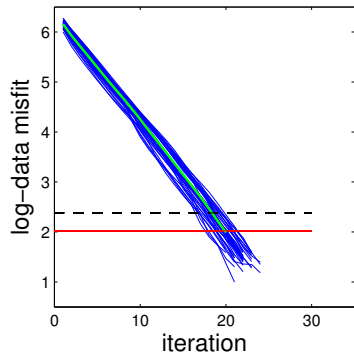


$N_e=100, \rho=0.6$

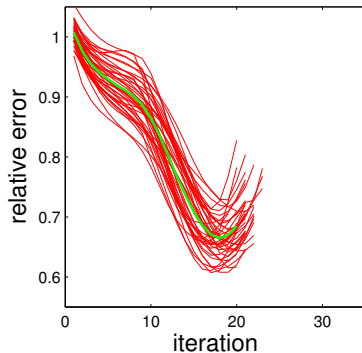


Regularizing properties as a function of ρ

$N_e=100, \rho=0.7$

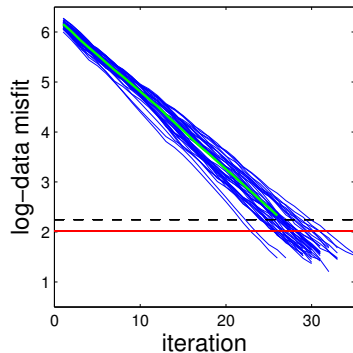


$N_e=100, \rho=0.7$

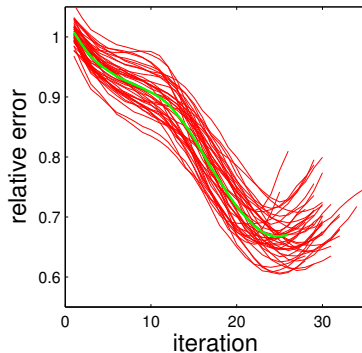


Regularizing properties as a function of ρ

$N_e=100, \rho=0.8$

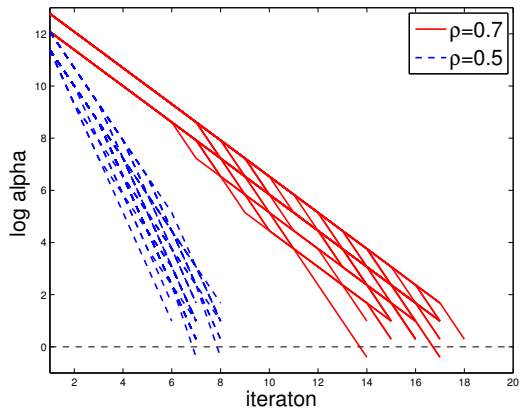


$N_e=100, \rho=0.8$

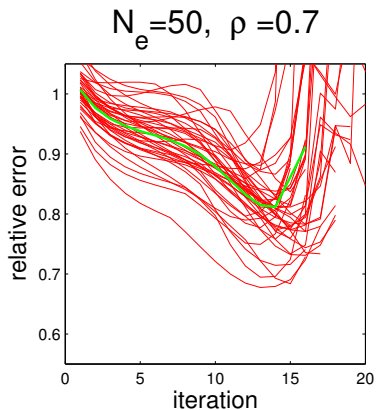
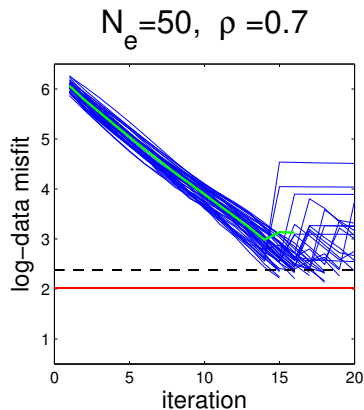


Regularization parameter α

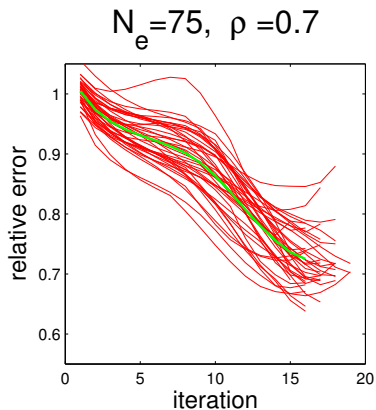
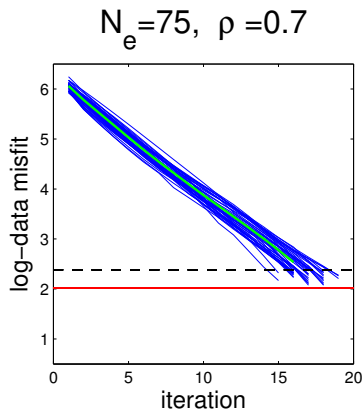
Plot of $\log \alpha$



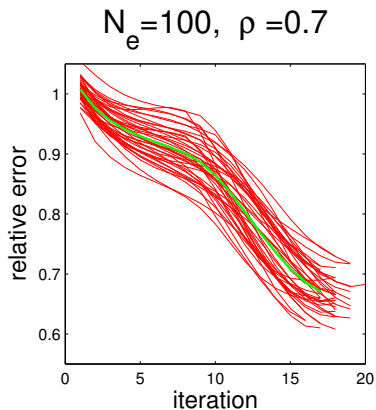
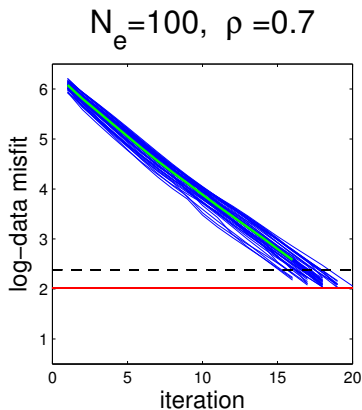
Regularizing properties as a function of the ensemble size



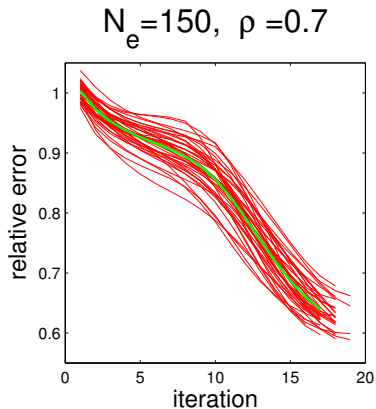
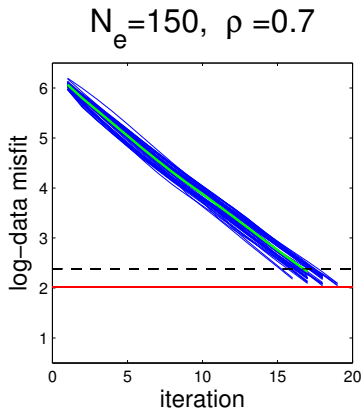
Regularizing properties as a function of the ensemble size



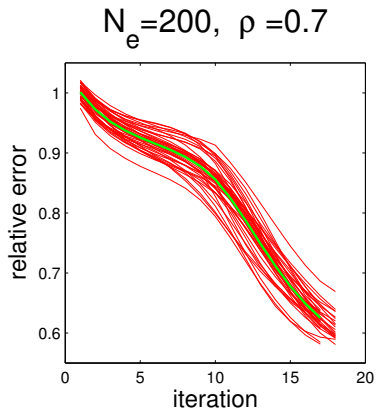
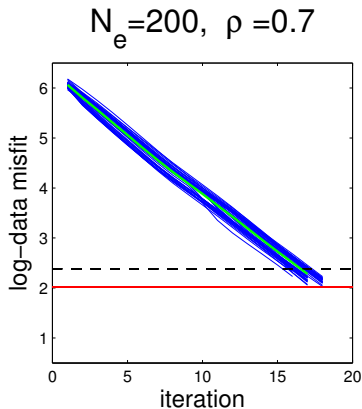
Regularizing properties as a function of the ensemble size



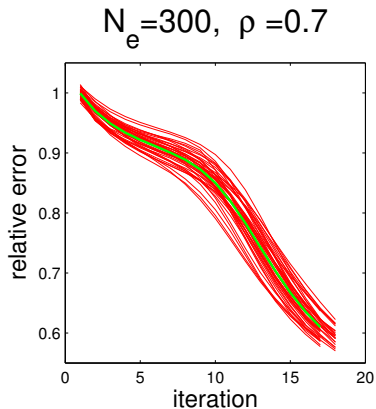
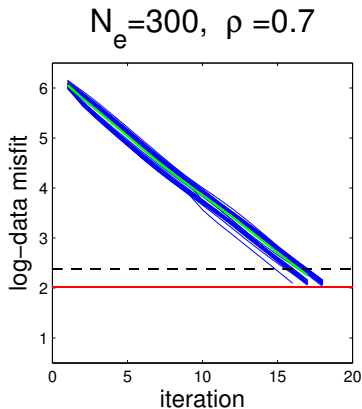
Regularizing properties as a function of the ensemble size



Regularizing properties as a function of the ensemble size



Regularizing properties as a function of the ensemble size

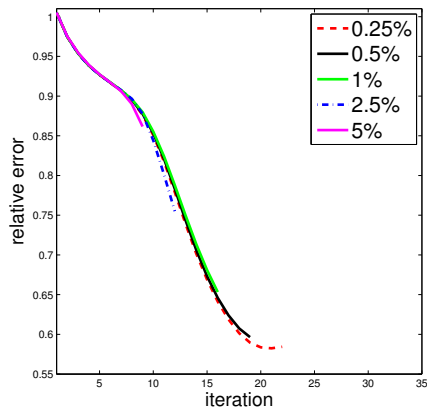
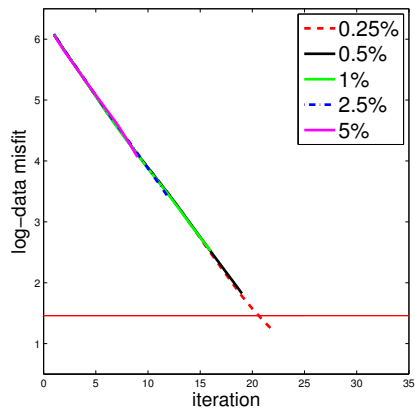


Convergence as the noise level decreases

$$\bar{u}_n \equiv \frac{1}{N} \sum_{j=1}^N u_n^{(j)}$$

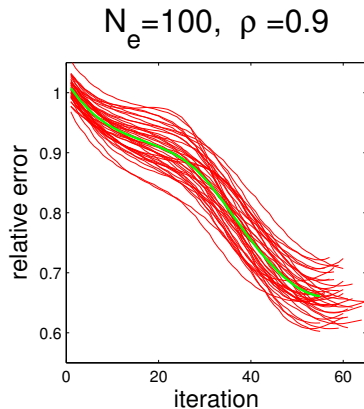
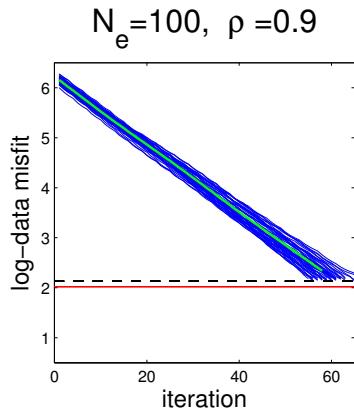
$$\|\Gamma^{-1/2}(y - \bar{u}_n)\|_{\ell^2}$$

$$\|\bar{u}_n - u^\dagger\|_{L^2(D)}$$



Computational cost

Cost approx 6000!!!



Accelerating EnKF

Recall the augmented analysis

$$\begin{aligned}u_{n+1}^{(j)} &= u_n^{(j)} + C^{uw}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_n^{(j)})) \\w_{n+1}^{(j)} &= G(u_n^{(j)}) + C^{ww}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_n^{(j)}))\end{aligned}$$

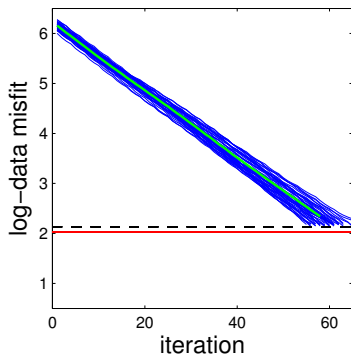
Use the second equation to do some linear iterations when ρ is large (and so is α). **adhoc!!**

Computational cost

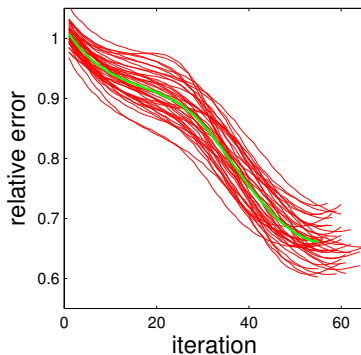
1 nonlinear iteration every iteration

Cost approx 6000!!!

$N_e=100, \rho=0.9$



$N_e=100, \rho=0.9$

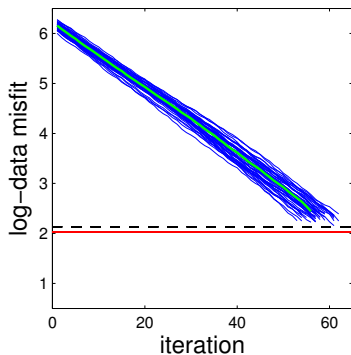


Computational cost

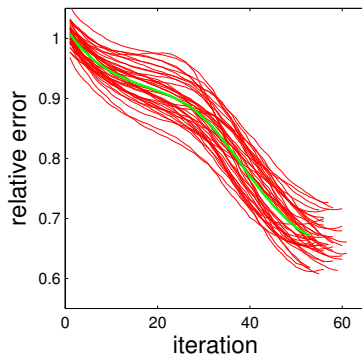
1 nonlinear iteration every 5

Cost approx 1200!!!

$N_e=100, \rho=0.9$



$N_e=100, \rho=0.9$

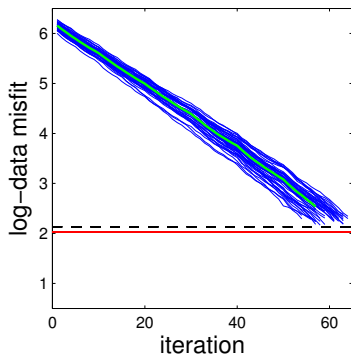


Computational cost

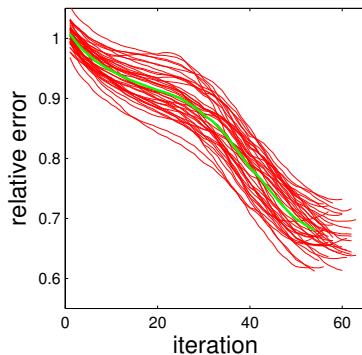
1 nonlinear iteration every 10

Cost approx 600!!!

$N_e=100, \rho=0.9$



$N_e=100, \rho=0.9$

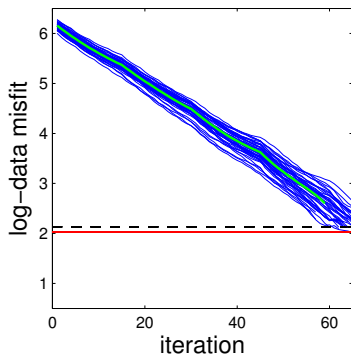


Computational cost

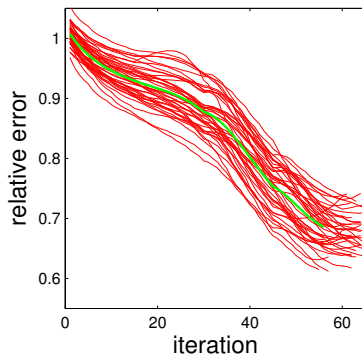
1 nonlinear iteration every 15

Cost approx 400!!!

$N_e=100, \rho=0.9$



$N_e=100, \rho=0.9$

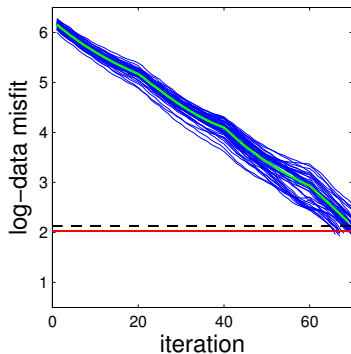


Computational cost

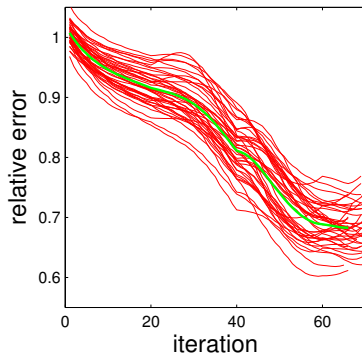
1 nonlinear iteration every 20

Cost approx 300!!!

$N_e=100, \rho=0.9$



$N_e=100, \rho=0.9$



Connections with variational Iterative Regularization

Assume that at a given iteration level

$$G(u_m^{(j)}) \approx G(\bar{u}_m) + DG(\bar{u}_m)(u_m^{(j)} - \bar{u}_m)$$

The update formula becomes

$$\bar{u}_{m+1} = \bar{u}_m + C_m^{uu} DG(\bar{u}_m)^* (DG(\bar{u}_m) C_m^{uu} DG(\bar{u}_m)^* + \alpha_m \Gamma)^{-1} (y - G(\bar{u}_m))$$

where

$$C_m^{uu} = \frac{1}{N_e - 1} \sum_{j=1}^{N_e} (u_m^{(j,f)} - \bar{u}_m^f)(u_m^{(j,f)} - \bar{u}_m^f)^T$$

Connections with variational Iterative Regularization

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If we replace C_m^{uu} by the prior error covariance C , then

$$\bar{u}_{m+1} = \bar{u}_m + CDG(\bar{u}_m)^* (DG(\bar{u}_m) CDG(\bar{u}_m)^* + \alpha_m \Gamma)^{-1} (y - G(\bar{u}_m))$$

This is Levenberg-Marquardt applied for the minimization

$$u = \arg \min_{u \in X} \|\Gamma^{-1/2} (y - G(u))\|^2 \rightarrow \min$$

in X with norm $\|C^{-1/2} \cdot\|_X$. (No regularization term!!!!)

The regularizing LM

Selecting α_m and the stopping criteria according to the discrepancy principle yields the **regularizing Levenberg-Marquardt** of [Hanke, 1997]:

Theorem [Hanke 1997]

\bar{u}_m converges after a finite number of iterations and

$$\bar{u}_m \rightarrow u \quad \text{as} \quad \eta \rightarrow 0 \quad (\text{where } G(u) = G(u^\dagger))$$

The regularizing LM scheme for reservoir modeling applications



M. A. Iglesias

Iterative regularization for ensemble-based data assimilation in reservoir models. *In review* (<http://arxiv.org/abs/1401.5375>). 2014

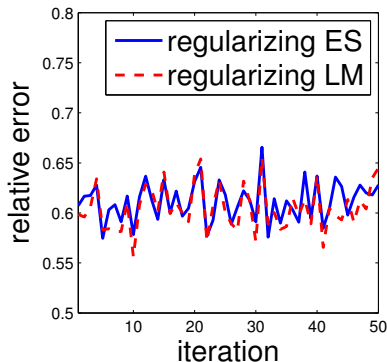
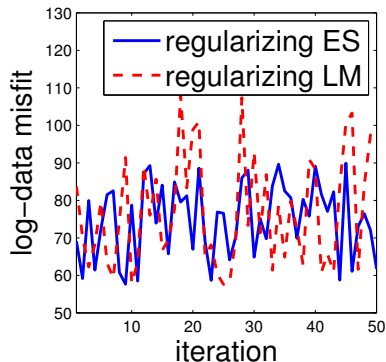


M. A. Iglesias and C. Dawson

The regularizing Levenberg-Marquardt scheme for history matching of petroleum reservoirs, *Computational Geosciences*, (2013) 17:1033-1053

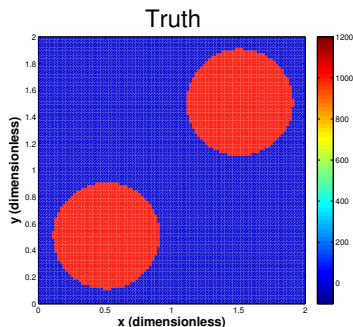
The proposed ES as an approximate regularizing LM scheme

Comparing ES with the regularizing LM scheme (on the same subspace)



Ensemble Kalman method for geometric inverse problems

Suppose we are interested in recovering something like:



We parametrize the permeability in terms of a level set function u . i.e.

$$K(u) = K_i \mathbb{1}_{u < 0} + K_e \mathbb{1}_{u \geq 0}$$

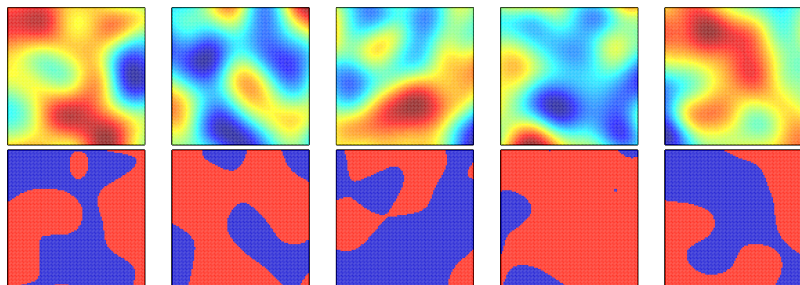
$p = G(u)$ is, as before, the solution to $-\nabla \cdot K(u) \nabla p = f$ evaluated at some locations. **We invert noisy measurements: $y = G(u) + \xi$**

Ensemble Kalman method for geometric inverse problems

Let us consider an artificial prior (for the initial ensemble)

$$\mu_0 = N(0, C)$$

with some covariance that reflects the regularity of the shape.



$$K(u) = K_i \mathbb{1}_{u < 0} + K_e \mathbb{1}_{u \geq 0}$$

Ensemble Kalman method for geometric inverse problems

Summary

- Iterative regularization provides strategies for regularizing Kalman based methods.
- Regularization has strong effect in the robustness and accuracy of ensemble methods for solving both classical and Bayesian inverse problems.
- Further investigations are required to establish the mathematical properties of these approximations.

References



M. A. Iglesias

Iterative regularization for ensemble-based data assimilation in reservoir models. *In review* (<http://arxiv.org/abs/1401.5375>). 2014



M. Iglesias, K. Law and A.M. Stuart,

Ensemble Kalman methods for inverse problems. *Inverse Problems*. 29 (2013) 045001
<http://arxiv.org/abs/1209.2736>



M. A. Iglesias and C. Dawson

The regularizing Levenberg-Marquardt scheme for history matching of petroleum reservoirs, *Computational Geosciences*, (2013) 17:1033-1053