A Regularizing Ensemble Kalman Method for PDE-constrained Inverse Problems

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Outline

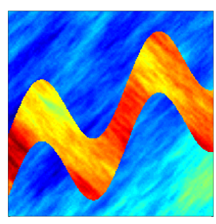
Outline

1. Introduction
2. Numerical Investigation of the Scheme
3. Applications

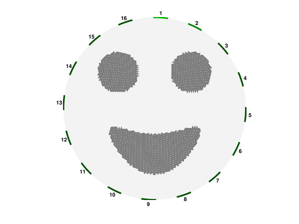
Inferring/estimating functions which are inputs for a PDE model, given measurements/observations form the output.

PDE-constrained applications

Porous media flow



Electrical Impedance Tomography



M. A.Iglesias
A regularizing ensemble Kalman method for PDE-constrained inverse problems.
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Computational Geosciences, (2015) 19:177-212

Let $\mathcal{G} : X \to \mathbb{R}^J$.

Forward Model

Given $u \in X$ compute

$$y = \mathcal{G}(u).$$

Let $\eta \in \mathbb{R}^J$ be a realization of an observational noise.

Inverse Problem

Given $y \in \mathbb{R}^J$ find $u \in X$:

$$y = \mathcal{G}(u) + \eta.$$

Forward groundwater flow model:

Forward Problem: Darcy flow

$$\begin{aligned} -\nabla\cdot\kappa\nabla p &= f \quad \text{in } D, \\ -\kappa\nabla p\cdot n &= B_N \quad \text{in } \Gamma_N. \\ p &= B_D \quad \text{in } \Gamma_D \end{aligned}$$

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

$$u = \log(\kappa(x)) \in X \equiv L^{\infty}(D) \longrightarrow \mathcal{G}(u) = \{p(x_i)\}_{i=1}^{J} \in \mathbb{R}^J$$

Inverse Problem

Given $y \in \mathbb{R}^J$ find $u \in X$:

$$y = \mathcal{G}(u) + \eta.$$

Bayesian Inversion

Prior

Probabilistic information about u *before* data is collected:

$$\mu_0(u) = \mathbb{P}(u)$$

Likelihood

Since $y = \mathcal{G}(u) + \eta$, if $\eta \sim N(0, \Gamma)$, then $\mathbb{P}(y|u) = N(\mathcal{G}(u), \Gamma)$. Then ($\Gamma-$weighted) model-data misfit Φ is the negative log-likelihood:

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

Posterior

Probabilistic information about u *after* data is collected:

$$\mu^y(u) = \mathbb{P}(u|y).$$

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

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Posterior

Probabilistic information about u *after* data is collected:

$$\mu^y(u) = \mathbb{P}(u|y).$$

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

Challenge

To explore the probability measure μ^y.

- $\mathcal{G}$ is highly nonlinear; μ^y cannot be characterized with a few parameters.
- The problem is high dimensional (X is discretized with 10^6-10^9 cells).
- Standard sampling methods for Bayesian inference do not work.
- Infinite-dimensional Bayesian framework [Stuart, 2010]; MCMC method for functions (pcn-MCMC) [Cotter, et-al, 2013].
- Well-known for continuous $\mathcal{G}$.

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The Classical (deterministic) formulation of the Inverse Problem

Given data $y \in Y$ find

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

For most PDE-constrained applications $\mathcal{G} : X \to \mathbb{R}^M$ is compact (unless X is finite dimensional)

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

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

$$u_n \nrightarrow u \qquad \text{but} \qquad \mathcal{G}(u_n) \to \mathcal{G}(u)$$

If we want to compute the minimizer above with standard optimization we may observe semiconvergence behavior *[Kirsch, 1996]*

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*

Introduce noise level

$$||\Gamma^{-1/2}(y - \mathcal{G}(u^{\dagger}))|| \leq \eta$$

Regularization

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

$$u^{\eta} \to u \qquad \text{as} \qquad \eta \to 0$$

where

$$\mathcal{G}(u) = \mathcal{G}(u^{\dagger})$$

Merging the Bayesian and the Classical approach

Consider $\mu_0(u) = \mathbb{P}(u) = \mathcal{N}(0, C)$ the prior on u and

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

The Bayesian Inverse Problem

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

$$\frac{\mu^y(u)}{\mu_0(u)} \propto \exp\Big(-\frac{1}{2}||\Gamma^{-1/2}(y - \mathcal{G}(u))||^2\Big) \quad y^{(j)} = y + \eta^{(j)} \sim N(0, \Gamma)$$

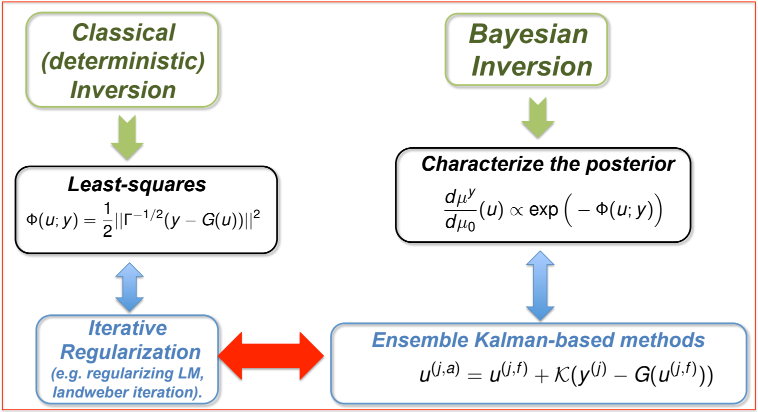
Ensemble Approximating the Bayesian posterior $\mu^y(u) = \mathbb{P}(u|y)$

Randomizing least-squares, e.g.

$$\frac{1}{2}||\Gamma^{-1/2}(y^{(j)} - \mathcal{G}(u))||^2 \to \min \quad y^{(j)} = y + \eta^{(j)} \sim N(0, \Gamma)$$

or, for example, Randomized Maximum Likelihood

$$\frac{1}{2}||\Gamma^{-1/2}(y^{(j)} - \mathcal{G}(u^{(j)}))||^2 + ||C^{-1/2}(u - u^{(j)})||_X^2 \to \min \quad u^{(j)} \sim \mathcal{N}(0, C)$$



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Ensemble Kalman Smoother [Evensen, 2006]

Bayesian Inverse Problem

Given a prior $\mu_0(u)$ of on u and data

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

find $\mu(u) = \mathbb{P}(u|y)$.

$$\mu(u) \propto \mu_0(u) \exp\left\{ -\frac{1}{2}||\Gamma^{-1/2}(y - \mathcal{G}(u))||^2 \right\}$$

Define

$$z = \begin{pmatrix} u \\ \mathcal{G}(u) \end{pmatrix}, \qquad y = Hz + \eta, \qquad H = (0, I)$$

Alternative Bayesian Inverse Problem

Given a prior on z, $\mu_0(z)$ and data y, find $\mu(z) = \mathbb{P}(z|y)$

$$\frac{\mu(z)}{\mu_0(z)} \propto \exp\left\{ -\frac{1}{2}||\Gamma^{-1/2}(y - \mathcal{G}(u))||^2 \right\}$$

Bayesian Inverse Problem

Given a prior on z, $\mu_0(z)$ and data y, find $\mu(z) = \mathbb{P}(z|y)$

$$\mu(u) \propto \mu_0(u) \exp\Big\{ -\frac{1}{2}||\Gamma^{-1/2}(y - \mathcal{G}(u))||^2 \Big\}$$

Construct an initial ensemble

$$z_0^{(j,f)} = \begin{pmatrix} u_0^{(j)} \\ \mathcal{G}(u_0^{(j)}) \end{pmatrix}, \qquad \{u_0^{(j)}\}_{j=1}^{N_e} \sim \mu_0$$

Compute mean and covariance

$$\overline{z}^f = \frac{1}{N_e}\sum_{j=1}^{N_e} z^{(j,f)} \qquad C^f = \frac{1}{(N_e-1)}\sum_{j=1}^{N_e} z^{(j,f)}(z^{(j,f)})^T - \overline{z}^f(\overline{z}^f)^T$$

Gaussian Approximation: $\mu_0(z) = N(\overline{z}^f, C^f)$,

Ensemble Kalman Smoother

Since $\mu_0(z) = N(\overline{z}^f, C^f)$, then

$$\mu(u) \propto \mu_0(u) \exp\left\{ -\frac{1}{2}||\Gamma^{-1/2}(y - \mathcal{G}(u))||^2 \right\} = N(\overline{z}^a, C^a)$$

where

$$\overline{z}^{(a)} = \overline{z}^{(f)} + \underbrace{C^f H^T \left(HC^f H^T + \Gamma\right)^{-1}}_{K}(y - H\overline{z}^{(f)})$$

$$C^a = (I - K)C^f$$

Updated each ensemble according to

$$z^{(j,a)} = z^{(j,f)} + C^f H^T \left(HC^f H^T + \Gamma\right)^{-1}(y^{(j)} - Hz^{(j,f)})$$

with

$$y^{(j)} = y + \eta^{(j)}, \qquad \eta^{(j)} \sim N(0, \Gamma)$$

Ensemble Kalman Smoother

Updated each ensemble according to

$$z^{(j,a)} = z^{(j,f)} + C^f H^T \left(H C^f H^T + \Gamma \right)^{-1} (y^{(j)} - H z^{(j,f)})$$

Claim 1: $\{z^{(j,a)}\}_{j=1}^{N_e} \approx \mathbb{P}(z|y)$.

Recall that $z = \begin{pmatrix} u \\ \mathcal{G}(u) \end{pmatrix}$. Then,

$$u^{(j)} = u_0^{(j)} + C^{uw}(C^{ww} + \Gamma)^{-1}(y^{(j)} - G(u_0^{(j)})$$

$$C^{uw} = \frac{1}{(N_e - 1)} \sum_{j=1}^{N_e} (u_0^{(j)} - \overline{u}_0)(\mathcal{G}(u_0^{(j)}) - \mathcal{G}(\overline{u}_0))^T$$

$$C^{ww} = \frac{1}{(N_e - 1)} \sum_{j=1}^{N_e} (\mathcal{G}(u_0^{(j)}) - \mathcal{G}(\overline{u}_0))(\mathcal{G}(u_0^{(j)}) - \mathcal{G}(\overline{u}_0))^T$$

Claim 2: $\{u^{(j)}\}_{j=1}^{N_e} \approx \mathbb{P}(u|y)$.

Observation: $\{u^{(j)}\}_{j=1}^{N_e} = \mathbb{P}(u|y)$ if $\mathcal{G}$ is linear and μ_0 is Gaussian.

It kind of works....sometimes.

$$u^{(j)} = u_0^{(j)} + C^{uw}(C^{ww} + \Gamma)^{-1}(y^{(j)} - \mathcal{G}(u_0^{(j)})$$

Underestimates the uncertainty

Iterative smoothers

$$u_n^{(j)} = u_{n-1}^{(j)} + C_{n-1}^{uw}(C_{n-1}^{ww} + \Gamma)^{-1}(y^{(j)} - \mathcal{G}(u_{n-1}^{(j)})$$

Overestimates the uncertainty

Ad-hoc fixes of Iterative smoothers

$$u_n^{(j)} = u_{n-1}^{(j)} + \rho \circ C_{n-1}^{uw}(C_{n-1}^{ww} + \alpha\Gamma)^{-1}(y^{(j)} - \mathcal{G}(u_{n-1}^{(j)})$$

ρ is a localization matrix and α is an inflation parameter

Understanding the iterative ensemble smoother with iterative regularization

Suppose we are interested in solving

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

where X has norm $||C^{-1/2}\cdot||$

Levenberg-Marquardt

u_{n+1} iteration level is given by

$$u_{n+1} = u_n + \arg\min_{v\in X} ||\Gamma^{-1/2}(y - \mathcal{G}(u_n) - D\mathcal{G}(u_n)v)||^2 + \alpha||C^{-1/2}v||_X^2$$

After some computations

$$u_{n+1} = u_n + C\, D\mathcal{G}^*(u_n)(D\mathcal{G}(u_n)\, C\, D\mathcal{G}^*(u_n) + \alpha\Gamma)^{-1}(y - \mathcal{G}(u_n))$$

Regularizing LM scheme [Hanke,1997]

Hanke proposed a way to select α and a stoping criteria (δ= noise level):

$$||\Gamma^{-1/2}(y - \mathcal{G}(u_n))|| \approx \delta$$

so that

$$u_{n+1} = u_n + C\,D\mathcal{G}^*(u_n)(D\mathcal{G}(u_n)\,C\,D\mathcal{G}^*(u_n) + \alpha\Gamma)^{-1}(y - \mathcal{G}(u_n))$$

generates a stable approximation to the solution of the classical inverse problem.

Theorem [Hanke 1997]

The LM scheme terminates after a finite number of iterations $n^\star$ and

$$u_{n^\star} \to u \qquad \text{as} \qquad \eta \to 0 \qquad (\text{where } \mathcal{G}(u) = \mathcal{G}(u^\dagger))$$

$u^\dagger$ is the truth

Consider an initial ensemble $\{u_0^{(j)}\}_{j=1}^{N_e} \subseteq X$

Linearize around the ensemble mean $\overline{u}_n \equiv \frac{1}{N_e}\sum_{j=1}^{N_e} u_n^{(j)}$

$$w_n^{(j)} \equiv \mathcal{G}(u_n^{(j)}) \approx \mathcal{G}(\overline{u}_n) + D\mathcal{G}(\overline{u}_n)(u_n^{(j)} - \overline{u}_n)$$

$$C_n^{uu} D\mathcal{G}^*(\overline{u}_n)v \approx C_n^{uw} v \qquad D\mathcal{G}(\overline{u}_n)C_n^{uu} D\mathcal{G}(\overline{u}_n)^* v \approx C_n^{ww} v$$

Recall the update formula for the regularizing LM scheme

$$u_{n+1} = u_n + C\, D\mathcal{G}^*(u_n)(D\mathcal{G}(u_n)\, C\, D\mathcal{G}^*(u_n) + \alpha\Gamma)^{-1}(y - \mathcal{G}(u_n))$$

Replace

$$\begin{aligned} u_n &\Longrightarrow \overline{u}_n, \\ C\, D\mathcal{G}^*(u_n) &\Longrightarrow C_n^{uu} D\mathcal{G}^*(\overline{u}_n) \approx C_n^{uw} \\ D\mathcal{G}(u_n)\, C\, D\mathcal{G}^*(u_n) &\Longrightarrow D\mathcal{G}(\overline{u}_n) C_n^{uu} D\mathcal{G}^*(\overline{u}_n) \approx C_n^{ww} \end{aligned}$$

Update formula for the mean of the ensemble

$$\overline{u}_{n+1} = \overline{u}_n + C_n^{uw}(C_n^{ww} + \alpha\Gamma)^{-1}(y - \overline{w}_n)$$

where $\overline{w}_n \equiv \frac{1}{N_e}\sum_{j=1}^{N_e} \mathcal{G}(u_n^{(j)})$.
We propose to update each ensemble in a consistent fashion

$$u_{n+1}^{(j)} = u_n^{(j)} + C_n^{uw}(C_n^{ww} + \alpha\Gamma)^{-1}(y^{(j)} - \mathcal{G}(u_n^{(j)}))$$

Selection of α:

$$\rho||\Gamma^{-1/2}(y - \overline{w}_n))||_Y \leq \alpha||\Gamma^{1/2}(C_n^{ww} + \alpha\Gamma)^{-1}(y - \overline{w}_n)||_Y$$

Stopping criteria

$$||\Gamma^{-1/2}(y - \overline{w}_n)||_Y \approx \delta$$

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 $w_m^{(j,f)} = \mathcal{G}(u_m^{(j)})$ define $\overline{w}_m^f$

(2) Stopping criteria. If

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

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

(3) Analysis step: Compute the updated ensembles

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

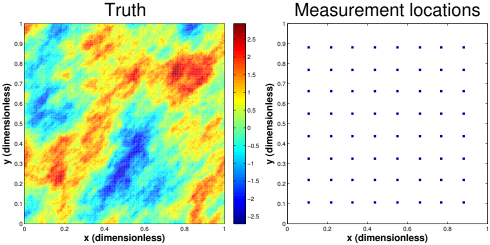
for α_m such that

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

Outline

Initial ensemble generated from a prior $\mathbb{P}(u) = N(\overline{u}, C)$.

$\mathcal{G}(u)$ be the forward operator that arises from Darcy flow.



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

For the numerical investigation with respect to the approximation properties of the Bayesian posterior see

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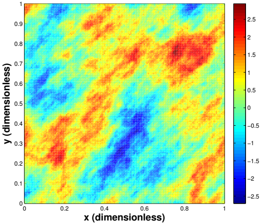
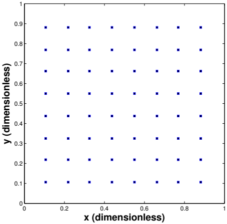
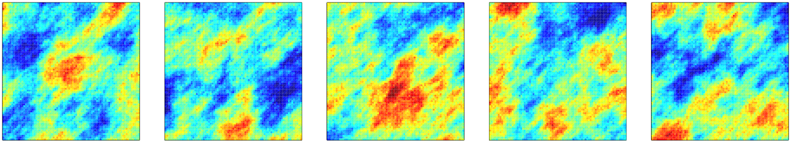
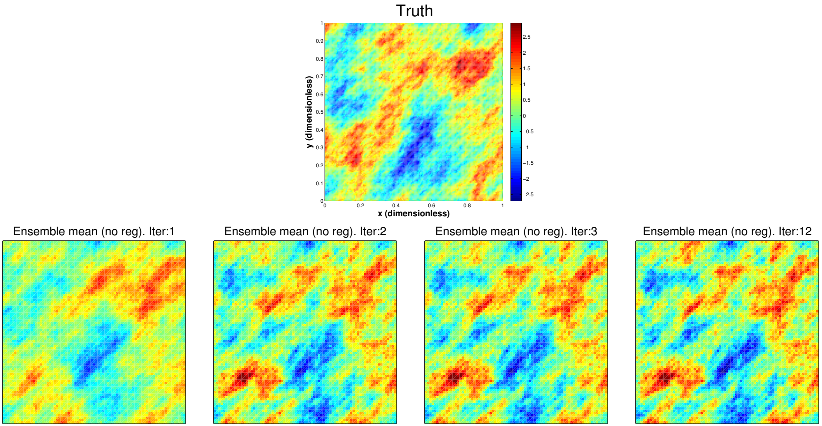




Some elements from the initial ensemble



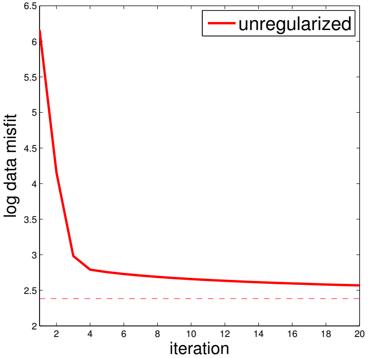
Reconstructing the truth with the mean of an ensemble of $N_e = 75$ (with small noise)



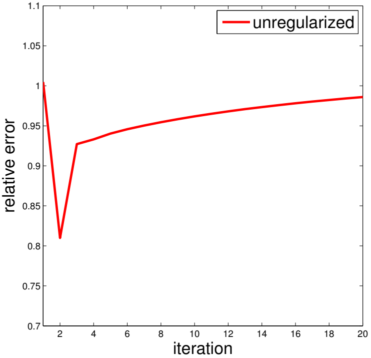
$$\overline{u}_n \equiv \frac{1}{N_e}\sum_{j=1}^{N_e} u_n^{(j)}$$

$$||\Gamma^{-1/2}(y - \mathcal{G}(\overline{u}_n))||_{l^2} \qquad ||\overline{u}_n - u^{\dagger}||_{L^2(D)}$$

Data misfit



Error w.r.t truth



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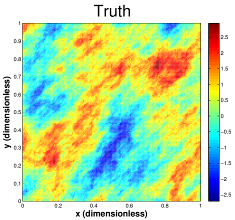
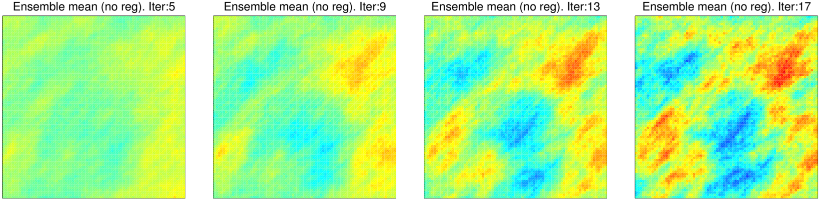
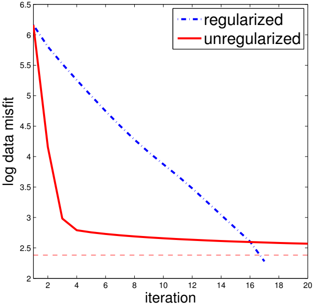




$$\overline{u}_n \equiv \frac{1}{N}\sum_{j=1}^{N} u_n^{(j)}$$

$$||\Gamma^{-1/2}(y - \mathcal{G}(\overline{u}_n))||_{l^2} \qquad\qquad ||\overline{u}_n - u^{\dagger}||_{L^2(D)}$$

Data misfit



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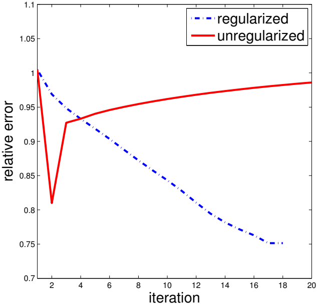
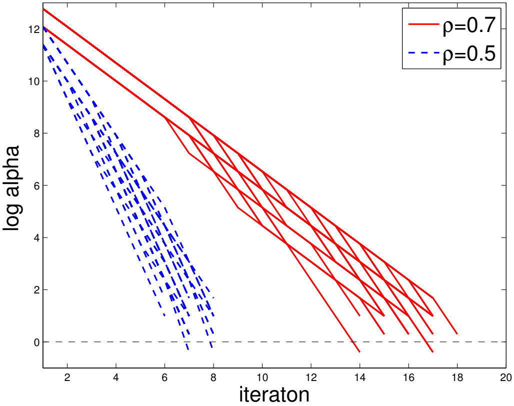
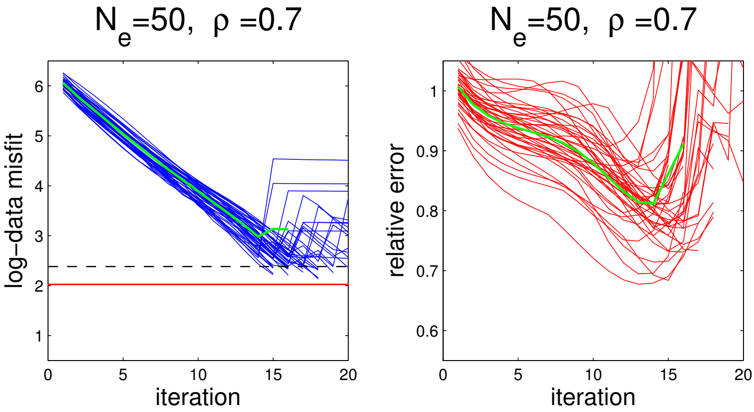


Regularization parameter α

Plot of $\log \alpha$



Regularizing properties as a function of the ensemble size



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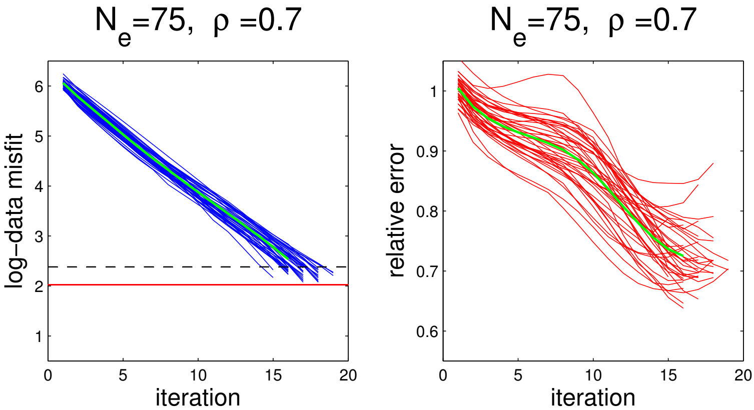
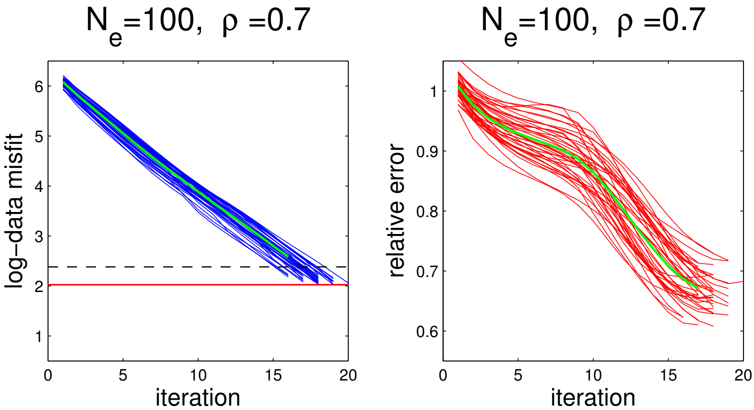


Regularizing properties as a function of the ensemble size



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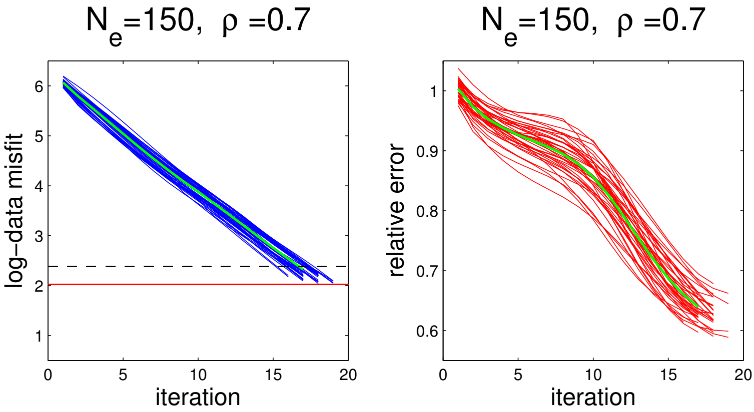

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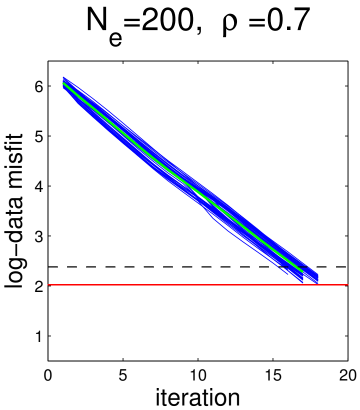

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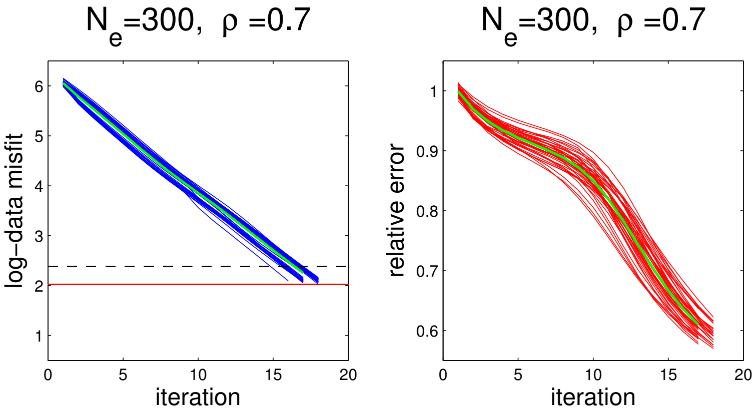
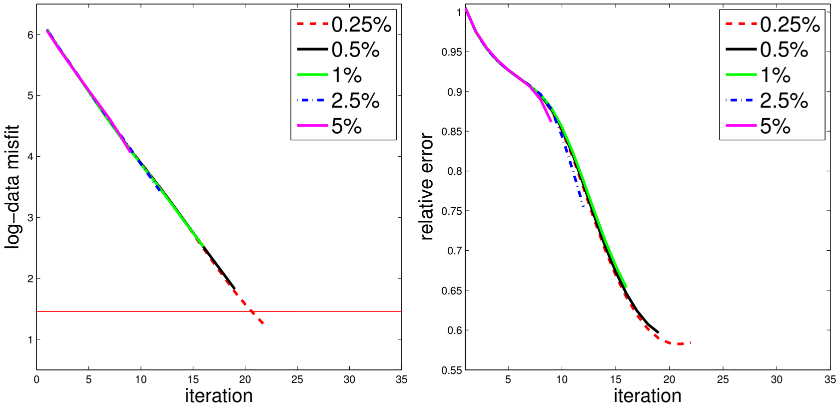


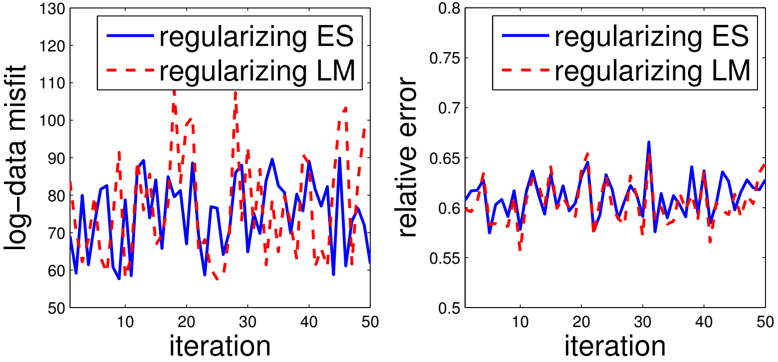
Convergence as the noise level decreases

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

$||\Gamma^{-1/2}(y - \mathcal{G}(\overline{u}_n))||_{l^2}$ $\qquad$ $||\overline{u}_n - u^{\dagger}||_{L^2(D)}$



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



Outline

In Collaboration with Michael Tretyakov (UoN, maths) and Minho Park (UoN, maths), Mikhail Matveev (UoN, engineering)

Forward map: Resin Transfer Molding

$$\begin{aligned} -\nabla\cdot e^{u}\nabla p &= f && \text{in } D(t)\\ p &= p_{in} && \text{on } \Gamma_{in}\\ p &= p_f && \text{on } \Gamma_s(t)\\ -e^{u}\nabla p\cdot n &= 0 && \text{on } \Gamma_N \end{aligned}$$

Moving boundary

$$\frac{d\Gamma_s(t)}{dt} = -e^{u}\nabla p$$

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

The Inverse Problem

Find $u \in X$ given

$$y = G(u) + \eta \qquad \eta \sim N(0,\Gamma)$$

.

The Forward model

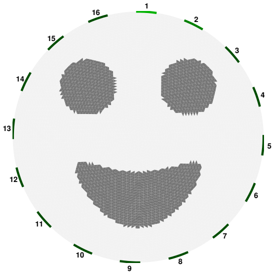
Complete Electrode Model: Forward and Inverse Problem

Given κ, $\{z_m\}_{m=1}^{n_e}$ and $I = \{I_m\}_{m=1}^{n_e}$ compute v and $V = \{V_m\}_{m=1}^{n_e}$

$$
\begin{aligned}
\nabla \cdot \kappa \nabla v &= 0 \quad \text{in } D, \\
v + z_m \kappa \nabla v \cdot \nu &= V_m \quad \text{on } e_m, \quad m = 1, \ldots, n_e, \\
\nabla v \cdot \nu &= 0 \quad \text{on } \partial D \setminus \cup_{m=1}^{n_e} e_m, \\
\int_{e_m} \kappa \nabla v \cdot \nu \, ds &= I_m \quad m = 1, \ldots, n_e,
\end{aligned}
$$

Inverse Problem:

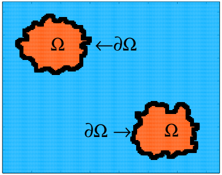
Given $I^{(1)}, \ldots, I^{(N)}$ and the observations of voltages $V^{(1)}, \ldots, V^{(N)}$ find κ and z_m



Permeability κ defined through level set function u:

$$\kappa(x) = \kappa_1 \, \chi_{\{u<0\}}(x) + \kappa_2 \, \chi_{\{u\geq 0\}}(x).$$

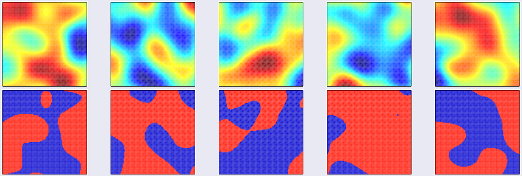
$u \mapsto \kappa$ is discontinuous

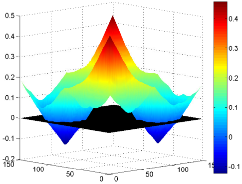


Forward Map and initial ensemble

$$u \longrightarrow \kappa \longrightarrow \mathcal{G}(u) = \{p(x_i)\}_{i=1}^{N} \in \mathbb{R}^M$$

Gaussian prior $\mu_0 = N(0, C_0)$ on the level-set function.
Covariance C_0 reflects the regularity of the shape.





M. A. Iglesias, Y. Lu and A. M . Stuart
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Submitted, 2015. http://arxiv.org/abs/1504.00313

Solving EIT

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.
- The stabilization of the proposed method is suitable for solving level-set based geometric inverse problems.
- Further investigations are required to establish the mathematical properties of these approximations.

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