Inverse Problems Without Adjoints: Ensemble Approaches

Andrew Stuart

Computing and Mathematical Sciences
California Institute of Technology

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Overview

Ensemble Kalman Methods For Inverse Problems

- Reich [38] (Assimilation step in data assimilation)
- Chen & Oliver [11] (Randomized maximum likelihood)
- Emerick and Reynolds [14] (Iterative ensemble smoother)
- Ernst, Sprungk and Starkloff [15] (Limitation in non-Gaussian setting)
- Iglesias, Law and S [25] (Ensemble Kalman inversion – EKI)
- Iglesias [24] (Stopping rules for EKI)
- Evensen [16] (Iterative ensemble smoothers)
- Blömker, Schillings and Wacker [8], [9] (Numerical analysis perspective)
- Schneider, S and Wu [44] (Learning SDEs w/EKI)
- Schneider, S and Wu [43] (Sparsity w/EKI)

Inverse Problem

Problem Statement

Find u from y where $\mathrm{G} : \mathcal{U} \mapsto \mathcal{Y}$, $\eta \sim N(0, \Gamma)$ is noise and

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

Main Approaches

Optimization $\quad \Phi(u) = \frac{1}{2}|y - G(u)|_{\Gamma}^{2} + \frac{1}{2}|u|_{\Sigma}^{2};$

Probability $\quad \mathbb{P}(u|y) \propto \exp\big(-\Phi(u)\big).$

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Here $\langle \cdot, \cdot \rangle_A = \langle \cdot, A^{-1} \cdot \rangle$ and $|\cdot|_A = |A^{-\frac{1}{2}} \cdot |$.

Inverse Problem

Filtering Dynamical Systems

$$\begin{aligned}
\text{Dynamics Model:} \quad & v_{n+1} = \Psi(v_n) + N(0,\Sigma), \quad n \in \mathbb{Z}^+ \\
\text{Data Model:} \quad & y_{n+1} = Hv_{n+1} + N(0,\Gamma), \quad n \in \mathbb{Z}^+ \\
\text{State Estimation:} \quad & v_n | \{y_\ell\}_{\ell=1}^n .
\end{aligned}$$

Inverse Problem: Dynamical Formulation

$$\begin{aligned}
\text{Dynamics Model:} \quad & u_{n+1} = u_n, \quad n \in \{0,\cdots,M-1\} \\
\text{Dynamics Model:} \quad & w_{n+1} = \mathsf{G}(u_n), \quad n \in \{0,\cdots,M-1\} \\
\text{Data Model:} \quad & y_{n+1} = w_{n+1} + N(0,M\Gamma), \quad n \in \{0,\cdots,M-1\} \\
\text{Parameter Estimation:} \quad & u_n | \{y_\ell = y\}_{\ell=1}^n
\end{aligned}$$

Discrete Time: Ensemble Kalman Inversion

Covariances

$$C_n^{ww} = \frac{1}{J}\sum_{j=1}^{J}\big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big)\otimes\big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big), \quad \overline{w}_n = \frac{1}{J}\sum_{j=1}^{J}\mathsf{G}(u_n^{(j)}),$$

$$C_n^{uw} = \frac{1}{J}\sum_{j=1}^{J}\big(u_n^{(j)} - \overline{u}_n\big)\otimes\big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big), \quad \overline{u}_n = \frac{1}{J}\sum_{j=1}^{J}u_n^{(j)}.$$

Iteration $n \mapsto n+1$

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

Continuous Time: Ensemble Kalman Inversion

Means

$$\overline{u}(t) = \frac{1}{J}\sum_{j=1}^{J} u^{(j)}(t),$$

$$\overline{G}(t) = \frac{1}{J}\sum_{j=1}^{J} G\big(u^{(j)}(t)\big).$$

Continuous Time Limit

$$u_n^{(j)} \approx u^{(j)}(t)|_{t=n/M}$$

$$\dot{u}^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}\Big\langle \mathrm{G}(u^{(k)}) - \bar{\mathrm{G}}, \mathrm{G}(u^{(j)}) - y\Big\rangle_{\Gamma}\Big(u^{(k)} - \bar{u}\Big)$$

Mathematical Structure

Gradient Flow In Parameter Space

- Ensemble Filtering Continuous Time: Bergemann & Reich (2010a, 2010b, 2012) [4, 5, 6]
- Ensemble Filtering Continuous Time: Reich (2011) [38]
- Connection to Foais/Prodi: Titi and coworkers [21, 2]
- 3DVAR Filtering Continuous Time: Blömker, Law, S & Zygalakis (2013) [7]
- Ensemble Filtering Continuous Time: Kelly, Law & S (2015) [28]
- Ensemble Inversion Continuous Time: Schillings & S (2017) [42]
- Text: Reich & Cotter (2015) [39]
- Text: Law, S & Zygalakis (2015) [31]
- Ensemble Filtering Continuous Time: Lange & Stannat [30]
- Ensemble Square Root Filtering Continuous Time: Lange & Stannat [29]
- Tikhonov Regularization: Chada, S & Tong [10]

Gradient Flow In Space Of Probability Measures

- Jordan, Kinderlehrer & Otto 1998 [26]
- Otto 2001 [34]
- Benamou & Brenier 2000 [3]
- Ambrosio, Gigli & Savare 2008 [1]
- Villani 2008 [45]
- Reich & Cotter 2013 [40]
- Garbuno-Inigo, Hoffmann, Li & Stuart 2020 [17]
- Garbuno-Inigo, Nüsken & Reich [18]

Ensemble Kalman Sampling (EKS)

Continuous Time Formulation: Put EKI in a heat bath

$$\dot{u}^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}\Big\langle \mathsf{G}(u^{(k)}) - \bar{\mathsf{G}}, \mathsf{G}(u^{(j)}) - y \Big\rangle_\Gamma \left(u^{(k)} - \bar{u}\right) - C(u)\Sigma^{-1}u^{(j)} + \sqrt{2C(u)}\,\dot{W}^{(j)}.$$

EKS Is Self-Preconditioned Langevin Equation (Linear G)

$$\dot{u}^{(j)} = -C(u)\nabla\Phi(u^{(j)}) + \sqrt{2C(u)}\,\dot{W}^{(j)}, \quad \Phi(u) = \frac{1}{2}|y - G(u)|_\Gamma^2 + \frac{1}{2}|u|_\Sigma^2,$$

$$\bar{u} = \frac{1}{J}\sum_{k=1}^{J} u^{(k)}, \quad C(u) = \frac{1}{J}\sum_{k=1}^{J}\left(u^{(k)} - \bar{u}\right)\otimes\left(u^{(k)} - \bar{u}\right).$$

Self-Preconditioned Langevin Equation [17]

Mean Field Limit: Nonlinear Nonlocal Fokker-Planck Eq.

$$\dot{u} = -\mathcal{C}(\rho)\nabla\Phi(u) + \sqrt{2\mathcal{C}(\rho)}\dot{W},$$

$$\mathcal{C}(\rho) = \int (u-\bar{u}) \otimes (u-\bar{u})\rho(u,t)du, \quad \bar{u} = \int u\rho(u,t)du,$$

$$\partial_t \rho = \nabla \cdot \big(\rho\,\mathcal{C}(\rho)\,\nabla\Phi\big) + \mathcal{C}(\rho) : D^2\rho, \quad \rho(0) = \rho_0.$$

Theorem [26],[17]

The nonlinear nonlocal Fokker-Planck equation may be written as

$$\partial_t \rho = \nabla \cdot \left(\rho\,\mathcal{C}(\rho)\nabla\frac{\delta\mathcal{E}}{\delta\rho}\right) \;, \mathcal{E}(\rho) = \int (\Phi + \ln\rho)\,\rho\,\mathrm{d}u.$$

- $\rho_\infty(u) := \exp\big(-\Phi(u)\big)$ is a steady-state of the Fokker-Planck equation.

Theorem [17]

- G linear then $\|\rho(\cdot,t) - \rho_\infty\|_{L^1} \leq C\exp(-t)$ (independent of G)

Guiding Examples

- Learn dynamical systems from time-averaged data [12]
- Simplified GCM [35, 22]
- Unscented Kalman Filtering [27]
- Unscented Kalman Inversion [23]

Data From Dynamics

Time-Averaged Data

$$\frac{dv}{dt} = F(v; u), \quad v(0) = v_0,$$
$$y = G_T(u; v_0) = \frac{1}{T}\int_0^T \varphi\big(v(t)\big)\,dt.$$

Central Limit Theorem

$$G_T(u; v_0) = G(u) + \frac{1}{\sqrt{T}} N(0, \Sigma),$$
$$y = G(u) + \frac{1}{\sqrt{T}} N(0, \Sigma).$$

Example 1 – 3D NS With Hydrostatic Assumption

Governing Dynamics

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathrm{v}) + \frac{\partial \rho \omega}{\partial z} = 0 \\
&\frac{D\mathrm{v}}{\partial t} + \Omega k \times \mathrm{v} + \frac{\nabla p}{\rho} + \nabla \Phi = F \\
&\frac{DT}{\partial t} - \frac{RT\omega}{C_p p} = Q \\
&\frac{\partial p}{\partial z} = -\rho g \\
&p = \rho R T
\end{aligned}
$$

ρ : fluid density; v, ω : horizontal and vertical velocities;
T : temperature; p : pressure, Φ : geopotential; k unit vertical.
D/Dt represents the derivative following a fluid parcel.
Q : radiation, to be learned.

Closure Model (Radiation Model)

$$Q = -k_T(\phi,\sigma)(T - T_{eq}(\phi,p))$$

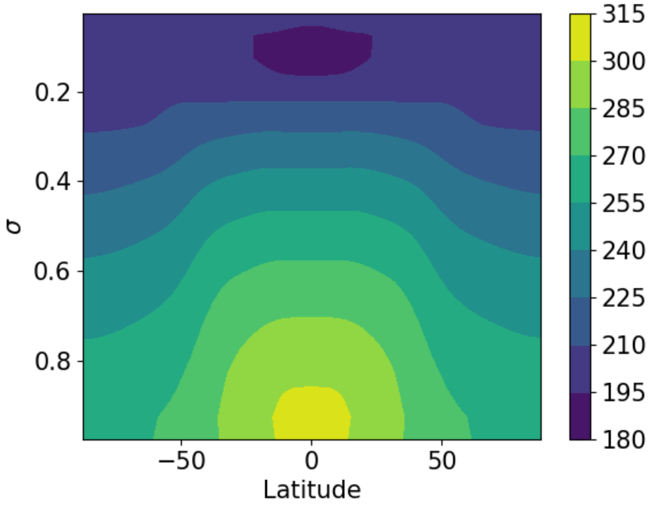
$$k_T = k_a + (k_s - k_a)\max\left(0, \frac{\sigma-\sigma_b}{1-\sigma_b}\right)\cos^4\phi$$

$$T_{eq} = \max\left\{200K, [315K - \Delta T_y \sin^2\phi - \Delta\theta_z \log(\frac{p}{p_0})\cos^2\phi](\frac{p}{p_0})^\kappa\right\}$$

$$k_a = 1/40 \ \mathrm{day}^{-1} \quad k_s = 1/4 \ \mathrm{day}^{-1} \quad \Delta T_y = 60 \ K \quad \Delta\theta_z = 10 \ K$$

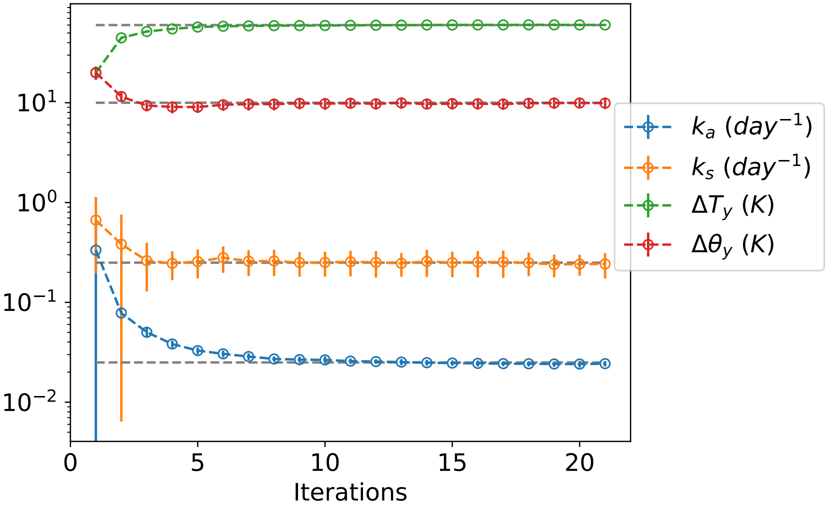
Here σ is the vertical coordinate, ϕ is the latitude, $p_0 = 10^5 Pa$ is the reference sea-level pressure, and $\kappa = \dfrac{R}{C_p}$.

Zonally/Temporally Averaged Temperature



Data used for training

Convergence History



Behaviour of UKI

Rough Forward Models

- Affine invariance and ensemble samplers: Goodman and Weare [19]
- Other ensemble samplers: Leimkuhler, Matthews and Weare [32]
- Ensemble GP samplers: Reich and co-workers [33, 41]
- Multiscale analysis: Duncan, S & Wolfram [13]
- Related analysis for MCMC: Plechac and Simpson [37]

Inverse Problem

Problem Statement

Find u from y where $\mathrm{G}: \mathcal{U} \mapsto \mathcal{Y}$, $\eta \sim N(0, \Gamma)$ is noise and

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

Main Approaches

$$\textit{Optimization} \quad \Phi(u) = \frac{1}{2}|y - G(u)|_\Gamma^2 + \frac{1}{2}|u|_\Sigma^2;$$

$$\textit{Probability} \quad \mathbb{P}(u|y) \propto \exp\big(-\Phi(u)\big).$$

Here $\langle \cdot, \cdot \rangle_A = \langle \cdot, A^{-1} \cdot \rangle$ and $|\cdot|_A = |A^{-\frac{1}{2}} \cdot |$.

EKS

Sample Path

$$\dot{u} = F(u, \rho; G) + \sqrt{2\mathcal{C}(\rho)}\,\dot{W},$$

Fokker-Planck

$$\partial_t \rho = \nabla \cdot \Big(\nabla \cdot \big(\mathcal{C}(\rho)\rho\big) - F(u, \rho; G)\rho\Big).$$

EKS

Assumption

The forward model $G = G_\epsilon$ where

$$G_\epsilon(u) = G_0(u) + G_1(u/\epsilon),$$

$$G_0 \in C^1(\mathbb{R}^d, \mathbb{R}^K), \; G_1 \in C^1(\mathbb{T}^d, \mathbb{R}^K) \text{ and } \int_{\mathbb{T}^d} G_1(y)\, dy = 0.$$

Multiscale Expansion Result

In limit $\epsilon \to 0$

$$\rho(u, t; G_\epsilon) \to \rho(u, t; G_0).$$

Self-Preconditioned Langevin Equation

Sample Path

$$\dot{u} = -\mathcal{C}(\rho)\nabla\Phi(u) + \sqrt{2\mathcal{C}(\rho)}\dot{W}$$

Fokker-Planck

$$\partial_t \rho = \nabla \cdot \big(\mathcal{C}(\rho)\,(\nabla V \rho + \nabla \rho)\big).$$

Self-Preconditioned Langevin Equation

Assumption

The forward model $G = G_\epsilon$ where

$$G_\epsilon(u) = G_0(u) + G_1(u/\epsilon),$$

$$G_0 \in C^1(\mathbb{R}^d, \mathbb{R}^K),\ G_1 \in C^1(\mathbb{T}^d, \mathbb{R}^K) \text{ and } \int_{\mathbb{T}^d} G_1(y)\, dy = 0.$$

Multiscale Expansion Result

In limit $\epsilon \to 0$

$$\rho(u, t; \Phi_\epsilon, \mathcal{C}) \to \rho(u, t; \Phi_*, \mathcal{D}).$$

Here $\Phi_* \neq \Phi_0$ and $\mathcal{C} \succeq \mathcal{D}$.

Example 2 – Linear + Periodic

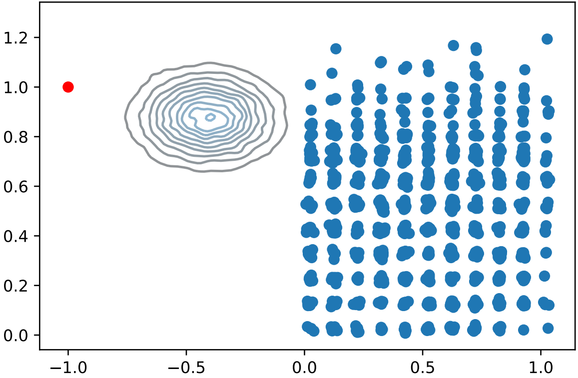
Available Forward Model $G_\epsilon(\cdot)$

$$G_\epsilon(u) = Au + \left[\sin\left(\frac{2\pi u_1}{\epsilon}\right), \sin\left(\frac{2\pi u_2}{\epsilon}\right)\right]^\top \text{ with } A = \begin{pmatrix} -1 & 0 \\ 0 & 2 \end{pmatrix}.$$

Desired Forward Model $G_0(\cdot)$

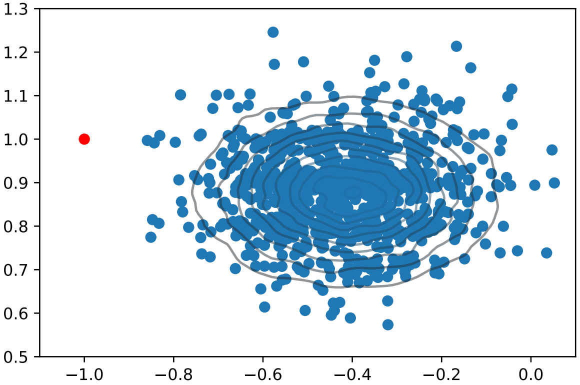
$$G_0(u) = Au \text{ with } A = \begin{pmatrix} -1 & 0 \\ 0 & 2 \end{pmatrix}.$$

Noisy Misfit



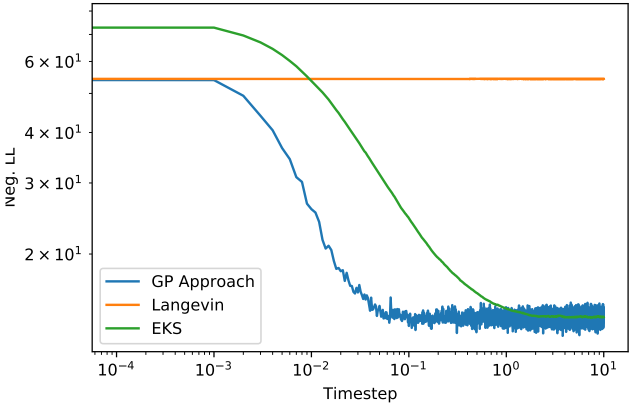
Linear + Periodic – Ensemble Langevin sampler

Noisy Misfit



Linear + Periodic – Ensemble Kalman sampler

Noisy Misfit



Linear + Periodic – Misfit along iteration

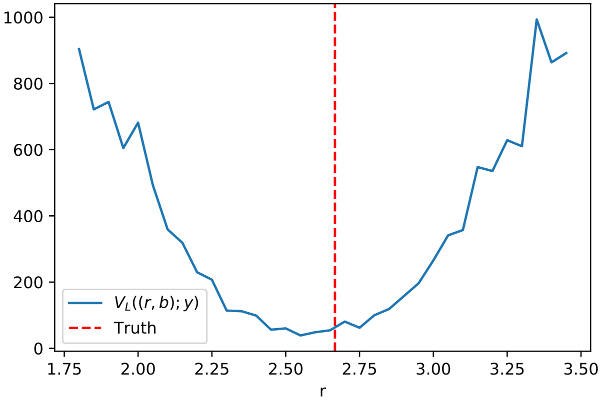
Example 3 – Lorenz '63

Governing Dynamics

$$
\begin{aligned}
\dot{x} &= 10\,(y - x) \\
\dot{y} &= r\,x - y - x\,z \\
\dot{z} &= x\,y - b\,z
\end{aligned}
$$

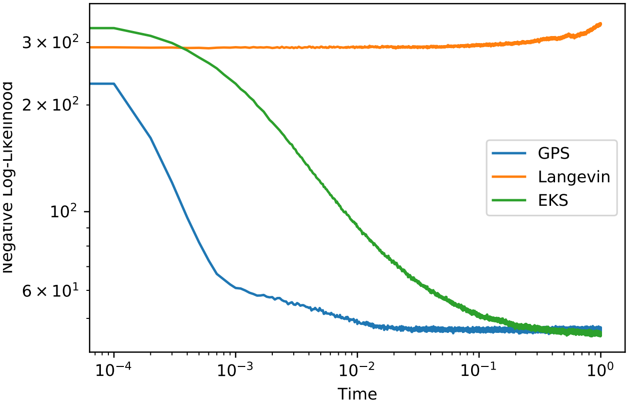
- 2-dimensional unknown: $u = [r, b]^\top$
- Forward map G only available to us approximately via G_T.
- Noise η only available to us approximately via G_T.

Noisy Misfit



Lorenz '63 – Misfit versus parameter

Noisy Misfit



Lorenz '63 – Misfit along iteration

Refineable Ensemble Methods

- Random particles: Haber, Lucka and Ruthotto (2018) [20]
- Multiscale particles: Pavliotis, S & Vaes (2021) [36]

Multiscale-EKS

Sample Path

$$
\begin{aligned}
\dot{u} = -\frac{1}{J\sigma^2}\sum_{j=1}^{J}\langle G(u^{(j)}) - G(u), G(u) - y\rangle_\Gamma \,(u^{(j)} - u) \\
- C(\Xi)\Sigma^{-1}u + \nu\sqrt{2C(\Xi)}\,\dot{w},
\end{aligned}
$$

$$
u^{(j)} = u + \sigma\,\xi^{(j)}, \qquad j = 1, \dots, J,
$$

$$
\dot{\xi}^{(j)} = -\frac{1}{\delta^2}\,\xi^{(j)} + \sqrt{\frac{2}{\delta^2}}\,\dot{w}^{(j)}, \qquad \xi^{(j)}(0) \sim \mathcal{N}(0, I_d), \qquad j = 1, \dots, J,
$$

Covariance

$$
C(\Xi) = \frac{1}{J}\sum_{j=1}^{J}(\xi^{(j)} \otimes \xi^{(j)}).
$$

Multiscale-EKS

Sample Path

$$\dot{\mathfrak{u}}_t = -\nabla\Phi_R(\mathfrak{u}_t) + \nu\sqrt{2}\,\dot{w}_t.$$

Define the exponent β is defined as follows:

$$\beta = \begin{cases} 1 & \text{if } G \in C^2(\mathbb{T}^d, \mathbb{R}^K), \\ 2 & \text{if } G \in C^3(\mathbb{T}^d, \mathbb{R}^K). \end{cases}$$

Theorem [36]

Let $p > 1$. Then

$$\mathbb{E}\left(\sup_{0\le t\le T} \|u(t) - \mathfrak{u}(t)\|^p\right) \le C(\delta^p + \sigma^{\beta p}).$$

Example 3: Darcy Flow

Problem Setting

- Forward: Find pressure $p(\cdot)$ from permeability $a(\cdot)$:

$$\begin{aligned} -\nabla \cdot (a(x)\nabla p(x)) &= f(x), \quad x \in D \\ p(x) &= 0, \qquad x \in \partial D. \end{aligned}$$

- Inverse: Find a from linear functionals $\{\ell_j\}$ of p.
- Prior on a: $\mathcal{C} = (-\Delta + \tau^2\mathcal{I})^{-\alpha}$, $\mathcal{C}\varphi_j = \lambda_j\varphi_j$, $\log a \sim N(0, \mathcal{C})$:

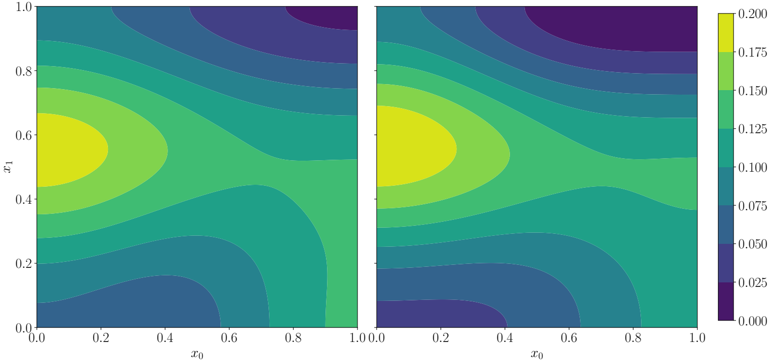
$$\log a(x) = \sum_{j \in \mathbb{Z}_+^2} u_j \sqrt{\lambda_j}\, \varphi_j(x), \quad u_j \sim N(0,1) \text{ i.i.d.}\,.$$

- Likelihood $y|u \sim N(\mathrm{G}(u), \gamma^2 I)$,

$$\mathrm{G}_j(u) = \ell_j\big(p(\cdot; u)\big), \quad j = 1, \cdots, 50.$$

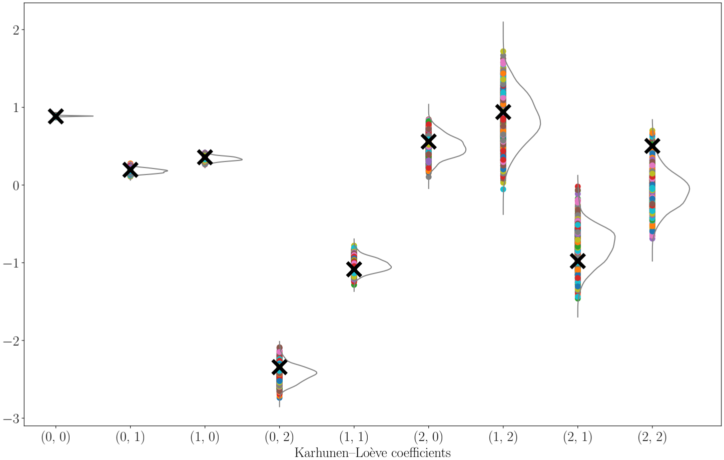
- Posterior $u|y$.

Posterior Mean



True permeability (left); Posterior mode permeability (right)

Posterior Variability



Posterior in Karhunen-Loeve coefficients u

Closing

Conclusions

1. Inverse problems of increasing importance.
   - Often forward model is expensive.
   - Often forward model adjoints impossible/expensive.
   - Sometimes only rough forward model available.
2. Ensemble methods attractive in this setting.
   - Gradient flow structure: parameter space;
   - Gradient flow structure: probability space.
   - Multiscale analysis of rough forward models.
   - Multiscale approach to refineable approximations.
3. Many open mathematical questions.

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