# *Ensemble Kalman filter* for inverse problems

## UQ Reading Group

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# Recap

## State estimation with *Kalman filter*

Dynamical system:

$$x_n = F_n x_{n-1} + G_n u_n + w_n$$
$$y_n = H_n x_n + v_n$$

Prediction step:

$$\hat{x}_{n|n-1} = F_n \hat{x}_{n-1} + G_n u_n$$
$$P_{n|n-1} = F_n P_{n-1} F_n^T + Q_n$$

Update step:

$$K_n = P_{n|n-1} H_n^T (H_n P_{n|n-1} H_n^T + R_n)^{-1}$$
$$\hat{x}_n = \hat{x}_{n|n-1} + K_n (y_n - H_n \hat{x}_{n|n-1})$$
$$P_n = (I - K_n H_n) P_{n|n-1}$$

# Inverse problem

Let $X, Y$ be Hilbert spaces. Find $u \in X$ such that

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

for given observations $y \in Y$, the *forward response operator* $\mathcal{G} : X \to Y$ and $\eta \sim \mathcal{N}(0, \Gamma)$.

We assume that the data $y \in Y$ is given by some $u^* \in X$ and $\eta^* \in Y$, i.e.

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

# Formulation of inverse problems in *EnKF* setting

State space:

$$Z = X \times Y$$

Artificial dynamics:

$$\begin{aligned} z_{n+1} &= \Phi(z_n), \\ y_{n+1} &= Hz_{n+1} + \eta_{n+1}, \end{aligned}$$

where

$$\Phi(z_n) := \begin{pmatrix} u_n \\ \mathcal{G}(u_n) \end{pmatrix} \text{ for } z_n = \begin{pmatrix} u_n \\ p_n \end{pmatrix},$$

the projection operator $H : Z \to Y$ is defined by

$$H = \begin{pmatrix} 0 & I \end{pmatrix},$$

and $\eta_n \overset{\text{iid}}{\sim} \mathcal{N}(0, \Gamma)$.

# The ensemble

Ensemble of interacting particles $\{z_n^{(j)}\}_{j=1}^J$ to capture statistical properties of the state's distribution

Parameter estimate:

$$u_n := \frac{1}{J}\sum_{j=1}^{J} u_n^{(j)} = \frac{1}{J}\sum_{j=1}^{J} H^{\perp} z_n^{(j)}$$

# Regularization

Searching $u$ in $X$ is impossible, since the inversion of $\mathcal{G}$ is ill-posed.

Prior information is assumed available as a probability measure $\mu_0$.

Use approximation space $\mathcal{A}$, a linear subspace generated by the initial ensemble members $\{\psi^{(j)}\}_{j=1}^{J}$ defined as $\psi^{(j)} \overset{\text{iid}}{\sim} \mu_0$, i.e.

$$\mathcal{A} := \text{span}\{\psi^{(j)}\}_{j=1}^{J}.$$

Note that if $\mu_0 = \mathcal{N}(\bar{u}, C)$, then we may additionally consider

$$\psi^{(j)} = \bar{u} + \sqrt{\lambda_j}\phi_j,$$

where $(\lambda_j, \phi_j)$ are the eigenvalue/eigenvector pairs of $C$ (K-L basis).

# The algorithm

1. Initialize $z_0^{(j)} = \psi^{(j)}$ for $j = 1, \ldots, J$.

For $n = 1, \ldots$

2. Prediction step:

$$\hat{z}_{n+1}^{(j)} = \Phi(z_n^{(j)})$$

$$\bar{z}_{n+1} = \frac{1}{J} \sum_{j=1}^{J} \hat{z}_{n+1}^{(j)} \approx x_{n+1|n}$$

$$C_{n+1} = \frac{1}{J} \sum_{j=1}^{J} \hat{z}_{n+1}^{(j)} (\hat{z}_{n+1}^{(j)})^T - \bar{z}_{n+1} (\bar{z}_{n+1})^T \approx P_{n+1|n}$$

# The algorithm (*cont.*)

3. Update step:

$$K_{n+1} = C_{n+1} H^T (H C_{n+1} H^T + \Gamma)^{-1}$$

$$\begin{aligned} z_{n+1}^{(j)} &= \hat{z}_{n+1}^{(j)} + K_{n+1}(y_{n+1}^{(j)} - H \hat{z}_{n+1}^{(j)}) \\ &= (I - K_{n+1} H) \hat{z}_{n+1}^{(j)} + K_{n+1} y_{n+1}^{(j)} \end{aligned}$$

$$u_{n+1} = \frac{1}{J} \sum_{j=1}^{J} u_{n+1}^{(j)} = \frac{1}{J} \sum_{j=1}^{J} H^{\perp} z_{n+1}^{(j)}$$

# The algorithm (*cont.*)

4. Check for convergence: For some fixed $\tau > 1$, terminate if

$$\|y - \mathcal{G}(u_{n+1})\|_\Gamma \leq \tau \|\eta^*\|_\Gamma. \quad \text{(Discrepancy principle)}$$

End for-loop $n$

# Property

## Entire ensemble stays in $\mathcal{A}$ for every step

Recall that

$$\mathcal{A} := \text{span}\{\psi^{(j)}\}_{j=1}^{J}.$$

### Theorem

*For every $n \in \mathbb{N}_0$ and $j \in \{1, \ldots, J\}$, it holds*

$$u_n^{(j)} \in \mathcal{A},$$

*and hence*

$$u_n \in \mathcal{A}.$$

# Property (*cont.*)

For the proof, we need some identities:

$$\hat{z}_{n+1}^{(j)} = \begin{pmatrix} \hat{u}_{n+1}^{(j)} \\ \hat{p}_{n+1}^{(j)} \end{pmatrix} = \begin{pmatrix} u_n^{(j)} \\ \mathcal{G}(u_n^{(j)}) \end{pmatrix}, \quad z_n^{(j)} = \begin{pmatrix} u_n^{(j)} \\ p_n^{(j)} \end{pmatrix}, \quad \bar{z}_n = \begin{pmatrix} \bar{u}_n \\ \bar{p}_n \end{pmatrix}$$

$$\bar{u}_n = \frac{1}{J}\sum_{j=1}^{J} \hat{u}_n^{(j)} = \frac{1}{J}\sum_{j=1}^{J} u_{n-1}^{(j)}, \quad \bar{p}_n = \frac{1}{J}\sum_{j=1}^{J} \hat{p}_n^{(j)} = \frac{1}{J}\sum_{j=1}^{J} \mathcal{G}(u_{n-1}^{(j)})$$

$$C_n = \begin{pmatrix} C_n^{uu} & C_n^{up} \\ (C_n^{up})^T & C_n^{pp} \end{pmatrix}, \quad C_n^{uu} = \frac{1}{J}\sum_{j=1}^{J} \hat{u}_n^{(j)} (\hat{u}_n^{(j)})^T - \bar{u}_n \bar{u}_n^T$$

$$C_n^{up} = \frac{1}{J}\sum_{j=1}^{J} \hat{u}_n^{(j)} (\hat{p}_n^{(j)})^T - \bar{u}_n \bar{p}_n^T, \quad C_n^{pp} = \frac{1}{J}\sum_{j=1}^{J} \hat{p}_n^{(j)} (\hat{p}_n^{(j)})^T - \bar{p}_n \bar{p}_n^T$$

**Proof.**

Induction over $n \rightarrow$ **Blackboard** □

# Lower bound for approximation error in $\mathcal{A}$

## Corollary

*The error between $u_n$ and the solution $u^*$ satisfies*

$$\|u_n - u^*\| \geq \inf_{v \in \mathcal{A}} \|v - u^*\|.$$

# Connection between *regularized LS* and *EnKF* for inverse problems

Consider $\mathcal{G}(u) := Gu$ for some linear operator $G : X \to Y$.

*Tikhonov-Phillips* regularized functional:

$$I(u) := \|y - Gu\|_\Gamma^2 + \|u - \bar{u}\|_C^2$$

Under some assumptions, a regularized LS solution exists:

$$u_{\mathrm{TP}} := \underset{u \in D(C^{-1/2})}{\arg\min}\ I(u) = \bar{u} + CG^*(GCG^* + \Gamma)^{-1}(y - G\bar{u})$$

# Connection between *regularized LS* and *EnKF* for inverse problems (*cont.*)

Consider $\psi^{(j)} \sim \mu_0 := \mathcal{N}(\bar{u}, C)$ and set $n = 0$ in the algorithm above.

Define

$$m_J := \frac{1}{J}\sum_{j=1}^{J} u_0^{(j)} \xrightarrow{J\to\infty} \bar{u}, \quad C_J := \frac{1}{J-1}\sum_{j=1}^{J}(u_1^{(j)} - m_J)(u_1^{(j)} - m_J)^T \xrightarrow{J\to\infty} C.$$

Compute

$$C_1^{up} = \ldots = \frac{1}{J}\sum_{j=1}^{J}(u_0^{(j} - m_J)(u_0^{(j)} - m_J)^T = \left(\frac{J-1}{J}\right) C_J G^*,$$

$$C_1^{pp} = \ldots = \left(\frac{J-1}{J}\right) G C_J G^*.$$

→ **Blackboard**

# Application I

## Elliptic equation

Consider the one-dimensional elliptic equation

$$\begin{cases} -\frac{d^2 p}{dx^2} + p = u \\ p(0) = p(\pi) = 0. \end{cases}$$

We have $G = A^{-1}$, where $A = (-\frac{d^2}{dx^2} + 1)$ and $D(A) = H^2(I) \cap H_0^1(I)$ with $I = (0, \pi)$.

**Inverse problem**: Recover $u$ from noisy observations of $p$, that is

$$y = p + \eta = A^{-1} u + \eta,$$

where $\eta \sim \mathcal{N}(0, \gamma^2 I)$.

# Application I (*cont.*)

## Elliptic equation

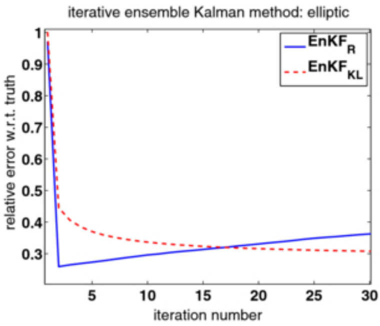
Choose $C = \beta(A - I)^{-1}$ in Tikhonov regularization of the form $\|u\|_C^2$.

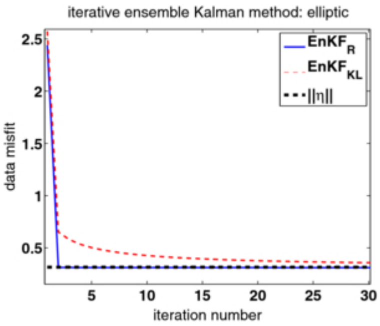
Set $\beta = 10$ and $\gamma = 0.01$.

Recall that $\mathcal{A} := \mathrm{span}\{\psi^{(j)}\}_{j=1}^J$. Let $EnKF_R$ and $EnKF_{KL}$ denote the two scenarios for randomly ($R$) generated $\mathcal{A}$ and $\mathcal{A}$ generated with a truncated K-L basis ($KL$).

# Application I (*cont.*)

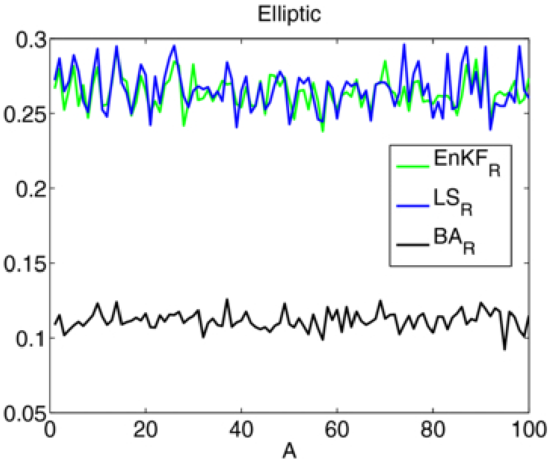
## Elliptic equation



# Application I (*cont.*)

## Elliptic equation



# Application II

## Groundwater flow

Consider the equation for flow in $\Omega := [0,6]^2$

$$-\nabla \cdot \exp(u) \nabla h = f,$$

where $u := \log K$ and $f$ is defined by

$$f(x_1, x_2) := \begin{cases} 0 & \text{if } 0 < x_2 \leq 4, \\ 137 & \text{if } 4 < x_2 < 5, \\ 274 & \text{if } 5 \leq x_2 \leq 6. \end{cases}$$

Boundary conditions are given by

$$h(x,0) = 100, \;\; \frac{\partial h}{\partial x}(6,y) = 0, \;\; -exp(u)\frac{\partial h}{\partial x}(0,y) = 500, \;\; \frac{\partial h}{\partial x}(x,6) = 0.$$

# Application II (*cont.*)

## Groundwater flow

**Goal**: Find *hydraulic conductivity* $K$ (or its logarithm $u$) of an aquifer from hydraulic head measurements.

**Setup**:

$$\mathcal{G}(u) := \{h(x_k)\}_{k\in\mathbb{K}}, \;\; \mu_0 \sim \mathcal{N}(\bar{u}, \beta L^{-\alpha}) \;\text{ with }\; L := -\Delta,$$

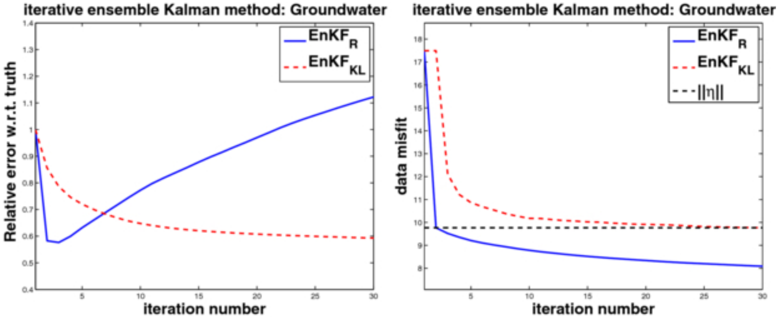
$$\text{simulated data } y = \mathcal{G}(u^*) + \eta^*, \text{where } \eta^* \sim \mathcal{N}(0,\Gamma)$$

Set

$$\Gamma = \gamma^2 I, \;\; \alpha = 1.3, \;\; \beta = 0.5, \;\; \bar{u} = 4, \;\; \gamma = 7.$$

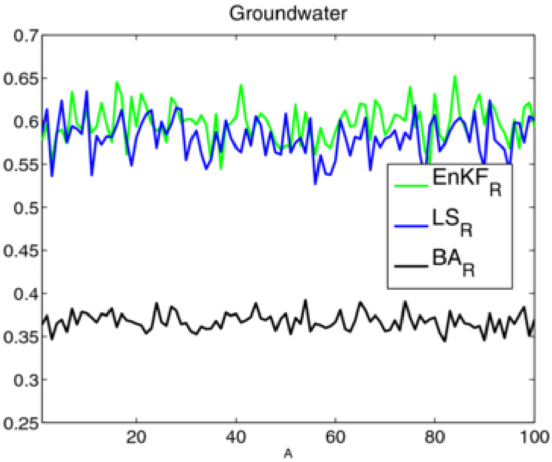
# Application II (*cont.*)

## Groundwater flow



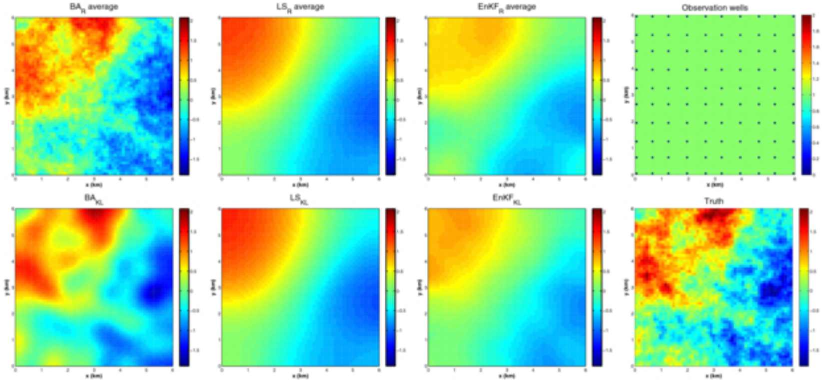
# Application II (*cont.*)

## Groundwater flow



# Application II (*cont.*)

## Groundwater flow



# Application III

## Navier-Stokes equation

Consider 2D Navier-Stokes equation on $\mathbb{T}^2 := [-1,1)^2$ with periodic boundary conditions:

$$\begin{cases} \partial_t \mathbf{v} - \nu \Delta \mathbf{v} + \mathbf{v} \nabla \cdot \mathbf{v} + \nabla p = f & \text{for all } (x,t) \in \mathbb{T}^2 \times (0,\infty) \\ \nabla \cdot \mathbf{v} = 0 & \text{for all } (x,t) \in \mathbb{T}^2 \times (0,\infty) \\ \mathbf{v} = \mathbf{u} & \text{for all } (x,t) \in \mathbb{T}^2 \times \{0\} \end{cases}$$

Data $y$ are *velocity* measurements here.

# Application III (*cont.*)

## Navier-Stokes equation

Similar setting as in examples before.

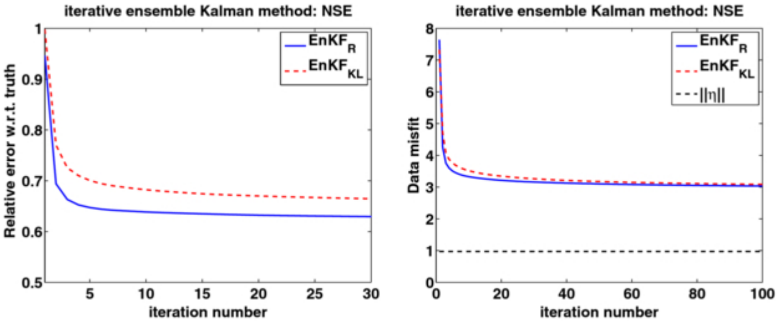
The prior $\mu_0$ is an *empirical measure*:

> *"The prior $\mu_0$ is defined to be the empirical measure supported on the attractor, i.e. it is defined by samples of a trajectory of the forward model after convergence to statistical equilibrium. We use 104 time-steps to construct this empirical measure."*

$\mathcal{A}$ is again generated by $J$ samples of $\mu_0$ or by the K-L basis with the empirical mean and empirical covariance.

# Application III (*cont.*)

## Navier-Stokes equation

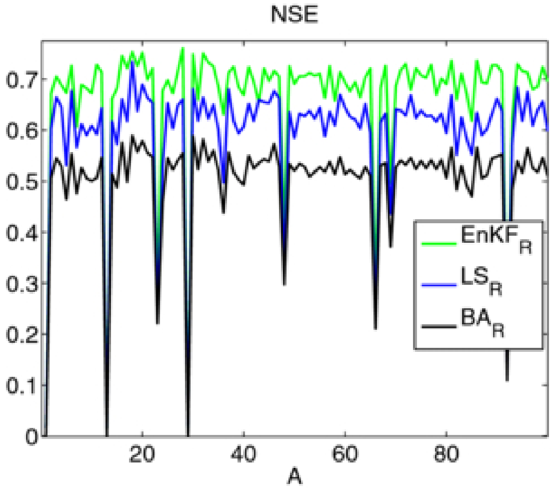



Different behavior compared to previous examples:

- **NOT** because of non-Gaussian prior
- $\rightarrow$ Mild ill-posedness due to small viscosity $\nu = 0.01$

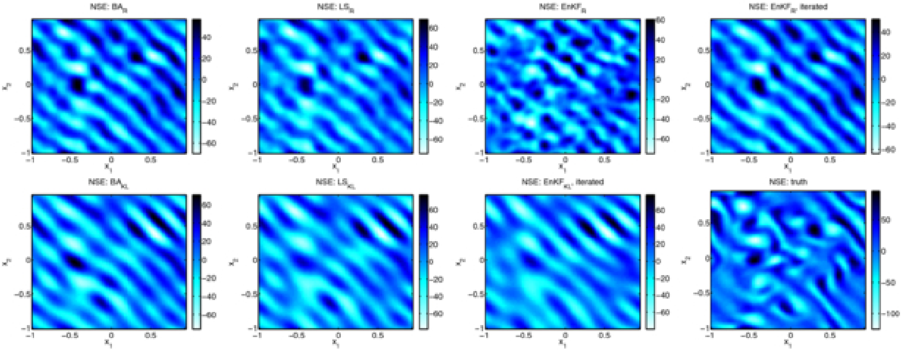
# Application III (*cont.*)

## Navier-Stokes equation



# Application III (*cont.*)

## Navier-Stokes equation



# THE END

Thank you!