POLITECNICO
DI MILANO
Master in Mathematical
Engineering

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE
Master in Computational
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Ensemble Kalman filter for multiscale inverse problems

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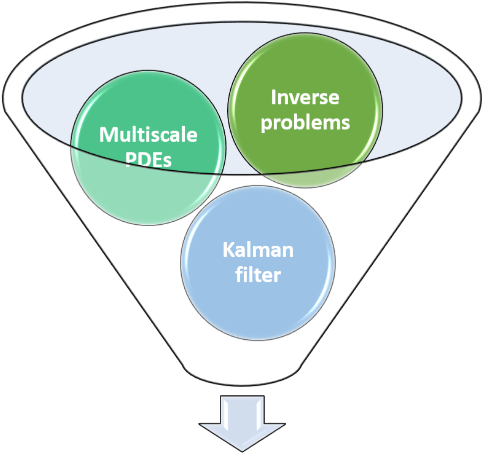
Main ingredients



ENSEMBLE KALMAN FILTER FOR MULTISCALE INVERSE PROBLEMS

Outline

1. Inverse problems
2. Ensemble Kalman method
3. Multiscale inverse problems
4. Numerical experiments

Inverse problem

$$\text{Find} \quad u \in X \quad \text{given} \quad y = \mathcal{G}(u) + \quad \eta \quad \in Y$$

Inverse problem

$$\text{Find } \underbrace{u \in X}_{\text{unknown}} \text{ given } \underbrace{y = \mathcal{G}(u) + \overbrace{\eta}^{\text{noise}}}_{\text{observation}} \in Y$$

- X, Y Hilbert spaces
- $\eta \sim \mathcal{N}(0, \Gamma)$

Inverse problem

$$\text{Find } \underbrace{u \in X}_{\text{unknown}} \text{ given } \underbrace{y = \mathcal{G}(u) + \overbrace{\eta}^{\text{noise}}}_{\text{observation}} \in Y$$

- X, Y Hilbert spaces
- $\eta \sim \mathcal{N}(0, \Gamma)$

- $\mathcal{G}\colon X \to Y$ **forward operator**, $\mathcal{G} = \mathcal{O} \circ \mathcal{S}$
  - $\mathcal{O}\colon H^1(\Omega) \to Y$ observation operator
  - $\mathcal{S}\colon X \to H^1(\Omega)$ solution operator of PDE

$$\begin{cases} -\nabla \cdot (A_u \nabla p) = f & \text{in } \Omega \\ p = g & \text{on } \partial\Omega \end{cases}$$

Overview of different techniques

Given a prior μ_0, consider two families of techniques

- Tikhonov methods $\longrightarrow$ solution is a **point**

$$u^* = \operatorname*{argmin}_{u \in X} \Big(\underbrace{\Psi(u; y)}_{\text{misfit functional}} + \underbrace{\mathcal{R}(u; \mu_0)}_{\text{regularization term}} \Big)$$

Example

Least squares with Tikhonov–Phillips regularization ($\mu_0 = \mathcal{N}(\bar{u}, C)$)

$$u^* = u_{\mathrm{TP}} = \operatorname*{argmin}_{u \in X} \left(\|y - \mathcal{G}(u)\|_\Gamma^2 + \|u - \bar{u}\|_C^2 \right)$$

Overview of different techniques

Given a prior μ_0, consider two families of techniques

- Bayesian methods $\longrightarrow$ solution is a **distribution**

$$\frac{d\mu^y}{d\mu_0}(u) \propto \exp\Big(-\underbrace{\Phi(u;y)}_{\text{potential}}\Big)$$

Example

Gaussian noise and prior measure ($\eta \sim \mathcal{N}(0,\Gamma)$, $\mu_0 = \mathcal{N}(\bar{u}, C)$)

$$\mu^y(u) \propto \exp\left\{-\frac{1}{2}\left(\|y-\mathcal{G}(u)\|_\Gamma^2 + \|u-\bar{u}\|_C^2\right)\right\}$$

Outline

Kalman filter

Kalman filter estimates state $z_n \in Z$ of a linear dynamical system

$$z_{n+1} = G z_n$$

given observations $y_n \in Y$

$$y_n = H z_n + \eta_n$$

where

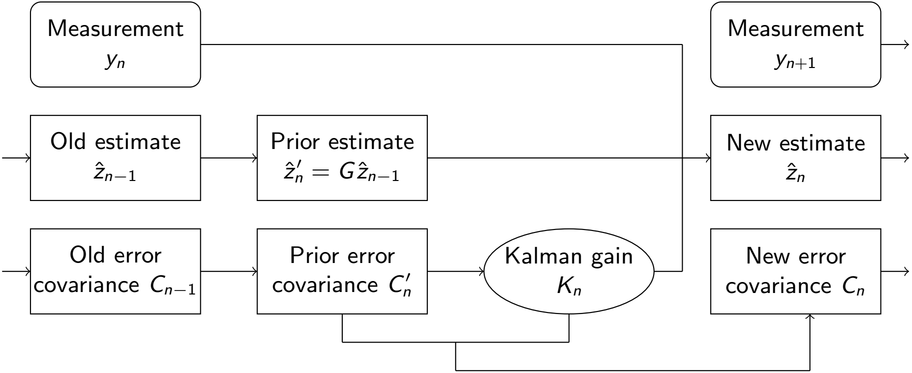
- G transition matrix
- H observation matrix
- $\eta_n \sim \mathcal{N}(0, \Gamma)$ noise

Kalman filter

$$z_{n+1} = Gz_n$$
$$y_n = Hz_n + \eta_n$$

Compute the estimation $\hat{z}_n$ in order to minimize

$$\mathrm{MSE} = \mathbb{E}[(z_n - \hat{z}_n)^T(z_n - \hat{z}_n)]$$



Kalman filter for inverse problems

Idea (see Iglesias et al. (2013))

Apply Kalman filter to solve inverse problems

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Issue

There are no dynamics

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Apply Kalman filter to solve inverse problems

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Introduce artificial dynamics

$$\begin{cases} z_{n+1} = \Xi(z_n) \\ y_n = Hz_n + \eta_n \end{cases}$$

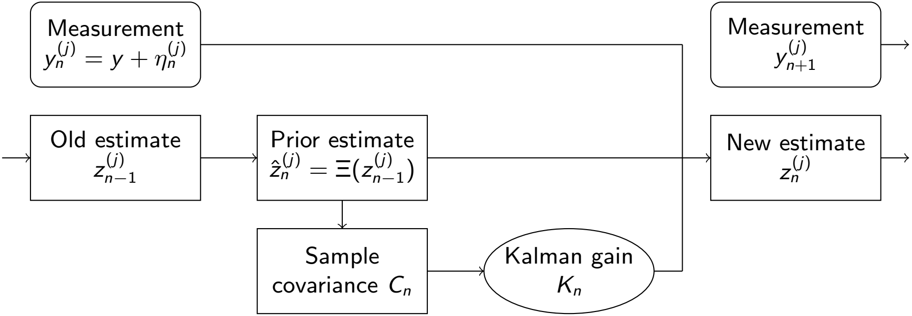
where

- $z_n = \begin{bmatrix} u_n & v_n \end{bmatrix}^T \in Z = X \times Y$
- $\Xi(z_n) = \begin{bmatrix} u_n & \mathcal{G}(u_n) \end{bmatrix}^T$, $H = \begin{bmatrix} 0 & I \end{bmatrix}^T$

Observations are obtained by randomizing y: $y_n = y + \eta_n$

Ensemble Kalman filter

- Initial ensemble z_0 : $z_0^{(j)} = \begin{bmatrix} \psi^{(j)} & \mathcal{G}(\psi^{(j)}) \end{bmatrix}^T$, $\psi^{(j)} \sim \mu_0$, $j = 1, \dots, J$
- Iterate for $n = 1, \dots, N$



- Compute the solution $u_{\mathrm{EnKF}} = \frac{1}{J} \sum_{j=1}^{J} u_N^{(j)}$

Ensemble Kalman filter

Properties

- $u_{\mathrm{EnKF}} \in \mathrm{span}\,\left(\{\psi^{(j)}\}_{j=1}^{J}\right)$
- If $\mathcal{G}$ **linear** then $u_{\mathrm{EnKF}}(N = 1) \to u_{\mathrm{TP}}$ as $J \to \infty$
- Easily parallelizable

Ensemble Kalman filter

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Warning

$J \cdot N$ evaluations of the forward operator $\mathcal{G}$ required

Outline

Multiscale inverse problems

$$\text{Find } u \in X \text{ given } y = \mathcal{G}^\varepsilon(u) + \eta \in Y$$

where

$$\mathcal{G}^\varepsilon = \mathcal{O} \circ \mathcal{S}^\varepsilon$$

and $\mathcal{S}^\varepsilon$ is the solution operator of a multiscale PDE

$$\begin{cases} -\nabla \cdot (A_u^\varepsilon \nabla p^\varepsilon) = f & \text{in } \Omega \\ p^\varepsilon = g & \text{on } \partial\Omega \end{cases} \qquad A_u^\varepsilon(x) = A\left(u(x), \frac{x}{\varepsilon}\right)$$

Multiscale inverse problems

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Issue

Evaluation of $\mathcal{G}^\varepsilon$ computationally very expensive if $\varepsilon \ll 1$

Homogenization

Theorem

There exist A_u^0 and p^0 such that

$$p^\varepsilon \rightharpoonup p^0 \text{ in } H^1(\Omega)$$

where p^0 is the solution of

$$\begin{cases} -\nabla \cdot (A_u^0 \nabla p^0) = f & \text{in } \Omega \\ p^0 = g & \text{on } \partial\Omega \end{cases}$$

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Idea (see Nolen et al. (2012))

Replace $\mathcal{G}^\varepsilon$ with $\mathcal{G}_h^0 = \mathcal{O} \circ \mathcal{S}_h^0$, where $\mathcal{S}_h^0$ is the solution operator corresponding to the FEM discretizazion of the homogenized problem

A one-dimensional example

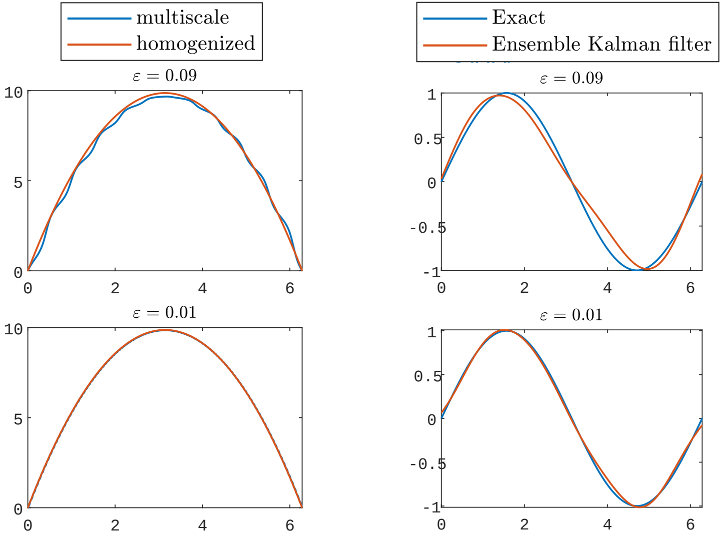

Figure : Left: solution of the PDE. Right: unknown of the inverse problem.

Convergence analysis

- $u_N^\varepsilon = \{u_N^{\varepsilon(j)}\}_{j=1}^J$ ensemble generated by EnKF with $\mathcal{G}^\varepsilon$
- $u_{N,h}^0 = \{u_{N,h}^{0(j)}\}_{j=1}^J$ ensemble generated by EnKF with $\mathcal{G}_h^0$
- norm of the ensemble defined by

$$\|u\| := \frac{1}{J}\sum_{j=1}^{J}\|u^{(j)}\|_X$$

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Main assumptions

- $\mathcal{O}$ Lipschitz from L^2 to Y
- A elliptic and Lipschitz from X to L^∞
- Algorithm stable

Convergence analysis

Theorem

Under the previous assumptions

$$\mathbb{E}\left[\|u_N^{\varepsilon} - u_{N,h}^{0}\|\right] \leq C(\varepsilon + h^{s+1})$$

where $s = \min\{r, q\}$, $p^0 \in H^{q+1}(\Omega)$ *and* r *degree of the FEM basis*

Convergence analysis

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where $s = \min\{r, q\}$, $p^0 \in H^{q+1}(\Omega)$ *and* r *degree of the FEM basis*

Idea of the proof

- Let $u_N^0 = \{u_N^{0(j)}\}_{j=1}^J$ be the ensemble generated by EnKF with $\mathcal{G}^0$
- By triangle inequality

$$\mathbb{E}\left[\|u_N^{\varepsilon} - u_{N,h}^0\|\right] \leq \underbrace{\mathbb{E}\left[\|u_N^{\varepsilon} - u_N^0\|\right]}_{\substack{\text{multiscale} \\ \text{convergence} \\ \varepsilon \to 0 \\ \Downarrow \\ \leq C_1 \varepsilon}} + \underbrace{\mathbb{E}\left[\|u_N^0 - u_{N,h}^0\|\right]}_{\substack{\text{FEM} \\ \text{convergence} \\ h \to 0 \\ \Downarrow \\ \leq C_2 h^{s+1}}}$$

Bayesian interpretation of the ensemble Kalman filter

Posterior distribution approximated by sum of Dirac masses (see Schillings and Stuart (2017))

$$\mu_N = \frac{1}{J} \sum_{j=1}^{J} \delta_{u_N^{(j)}}$$

- $\mu_N^\varepsilon = \frac{1}{J} \sum_{j=1}^{J} \delta_{u_N^{\varepsilon(j)}}$ posterior generated by EnKF with $\mathcal{G}^\varepsilon$
- $\mu_{N,h}^0 = \frac{1}{J} \sum_{j=1}^{J} \delta_{u_{N,h}^{0(j)}}$ posterior generated by EnKF with $\mathcal{G}_h^0$

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- $\mu_{N,h}^{0} = \frac{1}{J}\sum_{j=1}^{J}\delta_{u_{N,h}^{0(j)}}$ posterior generated by EnKF with $\mathcal{G}_h^{0}$

Warning

The posterior distributions are random probability measures

Convergence of the posterior distributions

Theorem

Under the same assumptions of the convergence result

$$\mu_N^\varepsilon - \mu_{N,h}^0 \xrightarrow{L^1} 0 \qquad as \qquad \varepsilon, h \to 0$$

which means

$$\mathbb{E}\left[\left|\int f \,\mathrm{d}\mu_N^\varepsilon - \int f \,\mathrm{d}\mu_{N,h}^0\right|\right] \to 0$$

for all bounded and continuous functions $f \in C_B^0$

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for all bounded and continuous functions $f \in C_B^0$

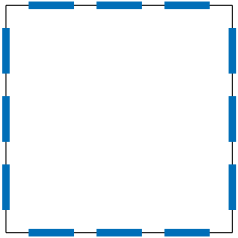
Idea of the proof

- Exploit properties of Wasserstein distance to quantify distance between discrete measures
- Apply convergence result presented before

Outline

Observations and exact solution

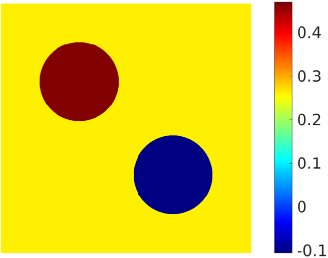
Setting from Abdulle and Di Blasio (2018)



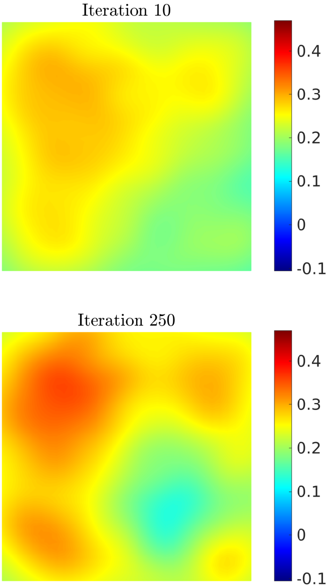
Measurements ($i = 1, \ldots, 12$)

$$y_i = \int_{\Gamma_i} A^{\varepsilon} \nabla p_k^{\varepsilon} \cdot \nu \phi_i ds + \eta_i$$

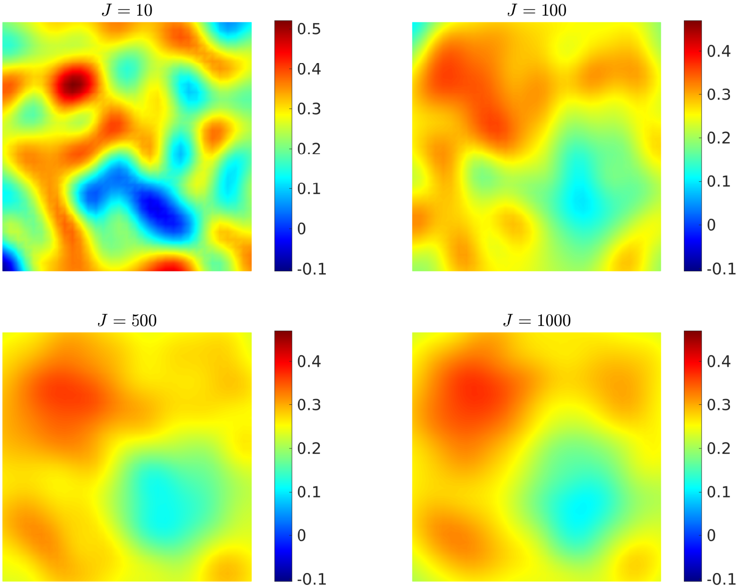
Exact unknown



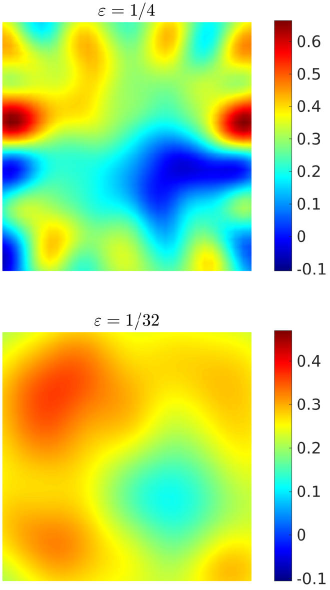
Sensitivity w.r.t. N



Sensitivity w.r.t. J



Sensitivity w.r.t. ε



Modelling error

Idea (see Kaipio and Somersalo (2005))

The observation can be seen as data generated by the discrete homogenized operator affected by two sources of error

$$y = \mathcal{G}_h^0(u^*) + \underbrace{[\mathcal{G}^\varepsilon(u^*) - \mathcal{G}_h^0(u^*)]}_{=\ \mathcal{E}} + \eta$$

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$$y = \mathcal{G}_h^0(u^*) + \underbrace{[\mathcal{G}^\varepsilon(u^*) - \mathcal{G}_h^0(u^*)]}_{=\ \mathcal{E}} + \eta$$

Assume that

$$\mathcal{E} \sim \mathcal{N}(m, \Sigma)$$

then $\mathcal{E} = m + \zeta$ with $\zeta \sim \mathcal{N}(0, \Sigma)$ and

$$\underbrace{y - m}_{=\ \tilde{y}} = \mathcal{G}_h^0(u^*) + \underbrace{\zeta + \eta}_{=\ \tilde{\eta}}$$

Estimation of the sample mean m and covariance Σ

Two approaches can be followed

1. **offline:**
    - sample $\{u_i\}_{i=1}^{N_\mathcal{E}}$ from the prior distribution μ_0
    - compute $\mathcal{E}_i = \mathcal{G}^\varepsilon(u_i) - \mathcal{G}_h^0(u_i)$
    - $m = \frac{1}{N_\mathcal{E}} \sum_{i=1}^{N_\mathcal{E}} \mathcal{E}_i$ and $\Sigma = \frac{1}{N_\mathcal{E}} \sum_{i=1}^{N_\mathcal{E}} (\mathcal{E}_i - m)(\mathcal{E}_i - m)^T$

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2. **online:** subdivide the EnKF in $\mathcal{L}$ levels, each one with N^ℓ iterations
   - sample $\{u_i^\ell\}_{i=1}^{N_\mathcal{E}^\ell}$ from the distribution μ_0^ℓ $(\mu_0^{\ell+1} = \mu_{N^\ell}^\ell)$
   - compute $\mathcal{E}_i^\ell = \mathcal{G}^\varepsilon(u_i^\ell) - \mathcal{G}_h^0(u_i^\ell)$
   - $m^\ell = \frac{1}{N_\mathcal{E}^\ell} \sum_{i=1}^{N_\mathcal{E}^\ell} \mathcal{E}_i^\ell$ and $\Sigma^\ell = \frac{1}{N_\mathcal{E}^\ell} \sum_{i=1}^{N_\mathcal{E}^\ell} (\mathcal{E}_i^\ell - m^\ell)(\mathcal{E}_i^\ell - m^\ell)^T$

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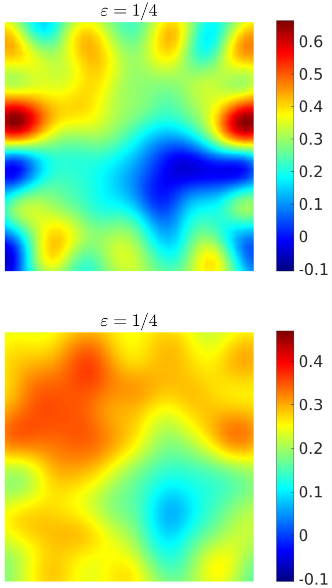
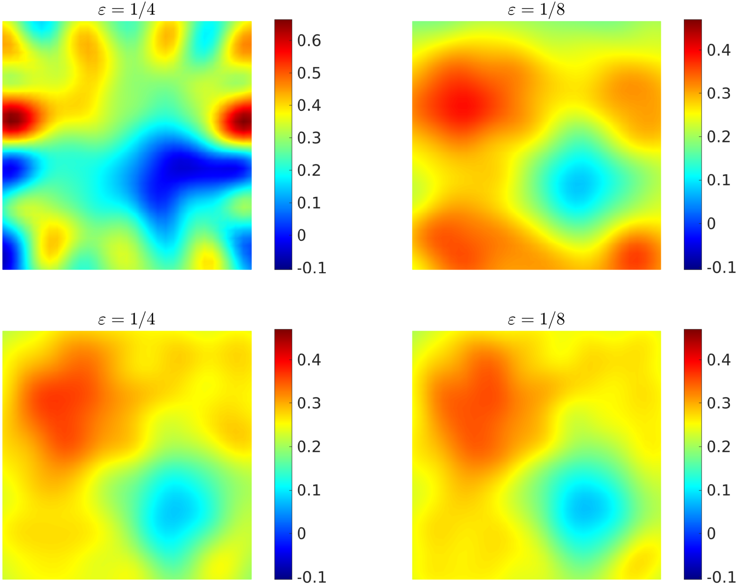
Warning

Online approximation is better, but computationally more expensive

Offline modelling error estimation



Online modelling error estimation



Conclusions

- The ensemble Kalman filter can be used for multiscale inverse problems
- The multiscale forward operator can be replaced by the homogenized one, taking into account the modelling error when ε is big
- The ensemble Kalman filter is easily parallelizable to reduce the computational time

References

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