

# ANALYSIS OF ENSEMBLE FILTERS FOR DATA ASSIMILATION AND INVERSE PROBLEMS

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Supported by EPSRC, ERC and ONR

March 24th 2013, KAUST

# Outline

- 1 **REFERENCES**
- 2 ENSEMBLE KALMAN FILTER
- 3 THEORETICAL PROPERTIES OF ENSEMBLE KALMAN FILTER
- 4 ENSEMBLE FILTERS FOR INVERSE PROBLEMS
- 5 NUMERICAL RESULTS
- 6 CONTINUOUS TIME LIMIT: INVERSE PROBLEMS
- 7 CONCLUSIONS

## References

- 1 “Ensemble Kalman methods for inverse problems”  
MA Iglesias KJH Law and AM Stuart  
Inverse Problems **29**(2013), 045001  
`arxiv.1209.2736`
- 2 “Well-posedness of ensemble Kalman filters”  
DB Kelly and AM Stuart  
In preparation.

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## The Filtering Problem

### Partially Observed Dynamics

Discrete-time dynamical system

$$z_{n+1} = \Xi(z_n). \quad (1)$$

with linear noisy observations

$$y_{n+1} = Hz_{n+1} + \eta_{n+1} \quad \text{where } \eta_n \sim N(0, \Gamma).$$

### State Estimation

Try to estimate  $z_n$  given  $\{y_j\}_{j=1}^n$ .

## Approximate Gaussian Filters

### Prediction Step

$$\hat{z}_{n+1} = \Xi(z_n).$$

### Analysis Step

$$z_{n+1} = \operatorname{argmin}_z \left( \|C_{n+1}^{-\frac{1}{2}}(z - \hat{z}_{n+1})\|^2 + \|\Gamma^{-1/2}(y_{n+1} - Hz)\|^2 \right)$$

### Design Parameter

The operators  $C_{n+1}$  characterize model uncertainty and are design parameters.

# The Ensemble Kalman Filter

## Prediction Step

$$\hat{z}_{n+1}^j = \Xi(z_n^j), \quad j \in \{1, \dots, J\}.$$

Estimate model uncertainty:

$$\begin{aligned} \bar{z}_{n+1} &= \frac{1}{J} \sum_{j=1}^J \hat{z}_{n+1}^j \\ C_{n+1} &= \frac{1}{J} \sum_{j=1}^J \hat{z}_{n+1}^j (\hat{z}_{n+1}^j)^T - \bar{z}_{n+1} \bar{z}_{n+1}^T \end{aligned}$$

## Analysis Step

$$\begin{aligned} S_{n+1} &= HC_{n+1}H^T + \Gamma, & K_{n+1} &= C_{n+1}H^T S_{n+1}^{-1} \\ z_{n+1}^j &= (I - K_{n+1}H)\hat{z}_{n+1}^j + K_{n+1}y_{n+1}^j, & j &\in \{1, \dots, J\}. \end{aligned}$$

## Perturbed Observations Data

$$y_n^j = y_n + \eta_n^j, \quad \eta_n^j \sim N(0, \Gamma)$$

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## The Setting

We work in a setting that includes Lorenz '63, Lorenz '96 and Navier-Stokes on a 2D torus.

## The Model

$$\frac{dz}{dt} + Az + B(z, z) = f$$

### Assumptions 1

For all  $w \in V$

$$\langle Aw, w \rangle \geq \lambda \|w\|^2, \quad \langle B(w, w), w \rangle = 0.$$

### Assumptions 2

For all  $w_i \in V$

$$\langle B(w_1, w_2), w_2 \rangle \leq K \|w_1\| \|w_2\| \|w_2\|, \quad \langle B(w_1, w_2), w_3 \rangle \leq K \|w_1\| \|w_2\| \|w_3\|.$$

## Discrete Time Filter: Well-Posedness

### Assumptions

$$\Gamma = \gamma^2 I, H = I.$$

### Theorem (Kelly, AMS)

There is constant  $\beta$  independent of  $n$  such that

$$\mathbb{E}|z_n^j - z_n|^2 \leq \exp(2\beta n) \mathbb{E}|z_0^j - z_0|^2 + K(J) \left( \frac{\exp(2\beta n) - 1}{\exp(2\beta) - 1} \right) \gamma^2.$$

## Continuous Time Limit

### Scalings

$$\Gamma = \frac{1}{h}\Gamma_0, \quad z_n = z(nh), \quad z_n^j = z^j(nh), \quad h \ll 1.$$

### Limiting SPDEs

$$\frac{dz^j}{dt} + Az^j + B(z^j, z^j) = f + CH^*\Gamma_0^{-1} \left( \Gamma_0^{\frac{1}{2}} \frac{dW^j}{dt} - Hz \right).$$

### Coupling

Coupled through the empirical covariance  $C$

## Continuous Time Limit: Well-Posedness

### Assumptions

$$\Gamma_0 = \gamma^2 I, H = I.$$

### Theorem (Kelly, AMS)

There is constant  $\beta$  independent of  $t$  such that

$$\mathbb{E}|z^j(t) - z(t)|^2 \leq \exp(2\beta t) \mathbb{E}|z^j(0) - z(0)|^2 + K(J) \left( \frac{\exp(2\beta t) - 1}{\exp(2\beta) - 1} \right) \gamma^2.$$

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## The Inverse Problem

$X, Y$  Banach spaces and  $G : X \rightarrow Y$ .

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

Prior knowledge of subsurface properties, for example:

$$u \sim \mu_0.$$

Model/Data mismatch:

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

## Example 1. Porous Media Flow: Forward Problem

### State Variable

$h$ : pore pressure (head)

### Parameter

$e^u = K$ : permeability (hydraulic conductivity)

### Single-phase Darcy Flow

$$\begin{aligned} -\nabla \cdot e^u \nabla h &= f, & x \in D \\ -e^u \nabla h \cdot \mathbf{n} &= 0, & x \in \partial D \end{aligned}$$

## Example 1. Porous Media Flow: Inverse Problem

Pressure at well locations  $x^\ell$ :

$$G^\ell(u) = h(x^\ell), \quad \ell \in \{1, \dots, L\},$$

Measurement operator:

$$G(u) = \left( G^1(u), \dots, G^L(u) \right)$$

### Unknown

$e^u = K$ : permeability.  $u = \log(K) \in X := L^\infty(D)$ .

### Data

$$y = G(u) + \eta \in Y := \mathbb{R}^L.$$



## Example 1. Porous Media Flow: Applications

### Estimation of subsurface properties

- Hydrology
- Fossil fuel extraction: oil, shale gas
- Carbon sequestration
- Compressed air storage
- Nuclear waste burial

## Example 2. Navier Stokes Equation: Forward Problem

### State Variable

$v$ : fluid velocity

### Parameter

$u$  =: initial fluid velocity

**Navier-Stokes Equation as an ODE in  $L^2_{\text{div}}(\mathbb{T}^2)$**

$$\frac{dv}{dt} + \nu Av + B(v, v) = f, \quad v(0) = u$$

## Example 2. Navier Stokes Equation: Inverse Problem

Fluid velocity at a finite set of points in space-time:

$$G^{j,k}(u) = v(x_j, t_k), \quad (j, k) \in \{1, \dots, J\} \times \{1, \dots, K\}.$$

Measurement operator:

$$G(u) = (G^{1,1}(u), \dots, G^{J,K}(u)),$$

### Unknown

$$u \in X := \dot{L}_{\text{div}}^2(\mathbb{T}^2).$$

### Data

$$y = G(u) + \eta \in Y := \mathbb{R}^{JK}.$$

## Example 2. Navier Stokes Equation: Applications

### Determination of Initial Fluid Velocity Field

- Weather Forecasting
- Oceanography
- Atmospheric Chemistry

## Filtering and Inverse Problems

### Artificial Dynamics

Define

$$z = \begin{pmatrix} u \\ p \end{pmatrix}, \quad \Xi(z) = \begin{pmatrix} u \\ G(u) \end{pmatrix}, \quad z_{n+1} = \Xi(z_n).$$

and then data is, for  $H = (0, I)$ ,

$$y_n = Hz_n + \eta_n \quad \text{where } \eta_n \sim N(0, \Gamma).$$

### We Are In General Setting Above

We can estimate  $z_n$  given  $\{y_j\}_{j=1}^n$  and, in this particular inverse problems setting,  $u_n$  given  $\{y_j\}_{j=1}^n$ .

### For Ensemble Methods

$$y_n^j = y + \eta_n^j, \quad \eta_n^j \sim N(0, \Gamma)$$

## Key Theoretical Result

### Linear Span of Initial Ensemble

$$\mathcal{A} = \text{span}\{u_0^j\}_{j=1}^J.$$

### Theorem (Iglesias, Law, AMS)

$$u_n^j \in \mathcal{A} \text{ for all } (n, j) \in \mathbb{N} \times \{1, \dots, J\}.$$

### Implications

- Compare EnKF with Best Approximation (BA) in  $\mathcal{A}$ .
- Compare EnKF with Least Squares (LSQ) in  $\mathcal{A}$ .
- Study Effect of choice of  $\mathcal{A}$ .

### Specific Case of Invariant Subspace Property

G. Li and A. Reynolds. *An iterative ensemble Kalman filter for data assimilation*. SPE Annual Technical Conference, 2007.

## Sketch Proof

$$z_0^j = \begin{pmatrix} u_0^j \\ \rho_0 \end{pmatrix}.$$

## Prediction Step

$$\begin{pmatrix} \hat{u}_{n+1}^j \\ \hat{\rho}_{n+1}^j \end{pmatrix} = \begin{pmatrix} u_n^j \\ G(u_n^j) \end{pmatrix}$$

Compute empirical covariance to estimate model uncertainty:

$$C_{n+1} = \begin{pmatrix} C_{n+1}^{uu} & C_{n+1}^{up} \\ (C_{n+1}^{up})^T & C_{n+1}^{pp} \end{pmatrix}$$

## Analysis Step

$$\begin{aligned} u_{n+1}^j &= u_n^j + C_{n+1}^{up} (C_{n+1}^{pp} + \Gamma)^{-1} (y_{n+1}^j - G(u_n^j)) \\ \rho_{n+1}^j &= G(u_n^j) + C_{n+1}^{pp} (C_{n+1}^{pp} + \Gamma)^{-1} (y_{n+1}^j - G(u_n^j)) \end{aligned}$$

## Sketch Proof (Continued)

Define

$$\begin{aligned}\tilde{p}_n^j &= \hat{p}_n^j - \frac{1}{J} \sum_{k=1}^J \hat{p}_n^k \\ d_{n+1}^j &\equiv (C_{n+1}^{pp} + \Gamma)^{-1} (y_{n+1}^j - G(u_n^j))\end{aligned}$$

EnKF updates can be written as

$$u_{n+1}^j = u_n^j + \frac{1}{J} \sum_{k=1}^J \langle \tilde{p}_{n+1}^k, d_{n+1}^j \rangle u_n^k$$

**EnKF mean (parameter) at the final time**

$$\bar{u} = \sum_{k=1}^J \alpha_j u_0^k \in \mathcal{A} \equiv \text{span}\{u_0^1, \dots, u_0^J\}.$$



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## Best Approximation (BA)

### Best Approximation in a Compact Set

$u^\dagger =$  truth

$\mathcal{A} =$  compact subset of  $\mathcal{X}$

$u_{\text{BA}} = \operatorname{argmin}_{u \in \mathcal{A}} (\|u - u^\dagger\|)$

## Regularized Least Squares (LSQ)

### Minimization Over a Compact Set

$$\begin{aligned}\mathcal{A} &= \text{compact subset of } X \\ u_{\text{LSQ}} &= \operatorname{argmin}_{u \in \mathcal{A}} \left( \Phi(u; y) \right)\end{aligned}$$

### Truncated Iteration

$$\begin{aligned}\Phi(u_{k+1}; y) &\leq \Phi(u_k; y) \\ u_{\text{LSQ}} &= u_K\end{aligned}$$

## Recap of Algorithms

### EnKF

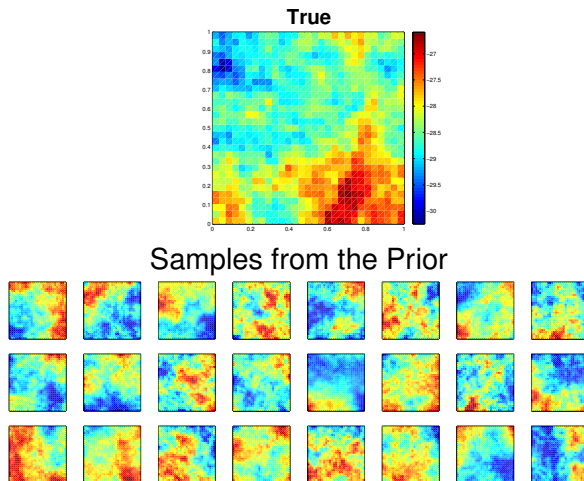
$$\bar{u} = \sum_{j=1}^J \alpha_j u_0^j \in \mathcal{A} \equiv \text{span}\{u_0^1, \dots, u_0^J\}.$$

### BA

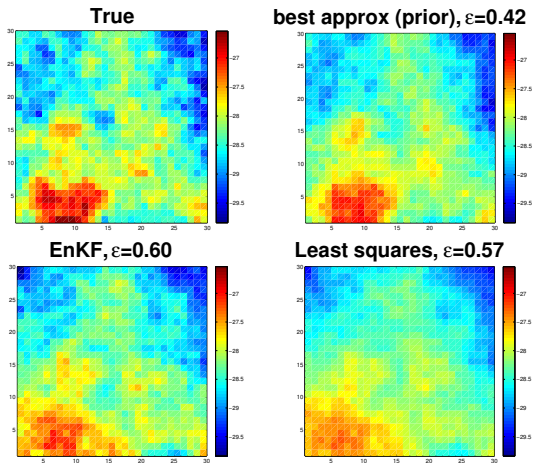
$$u_{\text{BA}} = \underset{\alpha \in \mathbb{R}^J}{\text{argmin}} \left\| u^\dagger - \sum_{j=1}^J \alpha_j u_0^j \right\|^2, \quad u^\dagger = \text{truth}$$

### LSQ Variants On

$$u_{\text{LSQ}} = \underset{\alpha \in \mathbb{R}^J}{\text{argmin}} \quad \Phi \left( \sum_{j=1}^J \alpha_j u_0^j; y^\dagger \right), \quad y = \text{data}$$

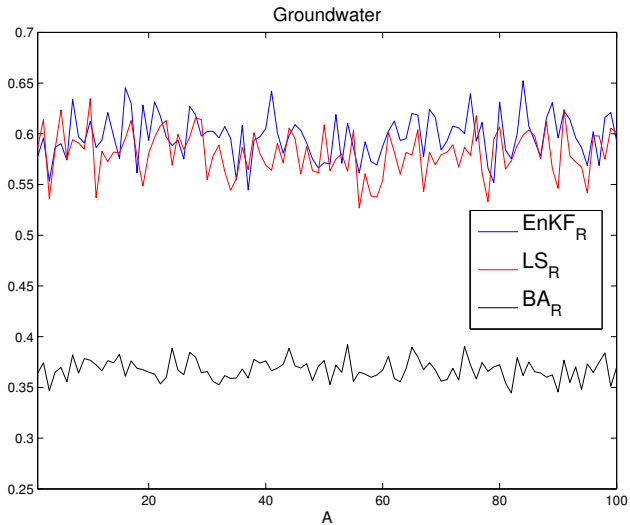


## EnKF (Elliptic)



Cost EnKF=  $1 \times 10^2$  forward models.  
 Cost LS=  $3.6 \times 10^3$  forward models

## Porous Media Flow



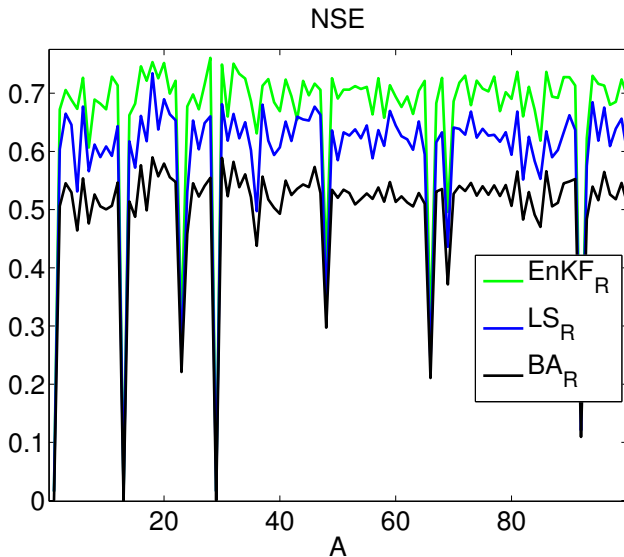
# Navier-Stokes

## Choice of Initial Ensemble

- For Porous media flow used draws from Gaussian prior.
- For Porous media flow also used Karhunen-Loeve (KL) basis.
- For NSE use draws from the attractor.
- For NSE also use draws from KL basis of empirical Gaussian.



## Navier-Stokes



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## Scaling Limit

If we scale the noise covariance  $\Gamma \rightarrow h^{-1}\Gamma_0$  and consider the limit  $h \rightarrow 0$  then we obtain the following system of SDEs:

$$\frac{du^j}{dt} = \frac{1}{J} \sum_{k=1}^J \left\langle G(u^k) - \bar{G}, \Gamma_0^{-1} \left( \frac{dz^j}{dt} - G(u^j) \right) \right\rangle$$

$$\frac{dz^j}{dt} = y + \sqrt{\Gamma_0} \frac{dW^j}{dt}$$

$$\bar{G} = \frac{1}{J} \sum_{k=1}^J G(u^k).$$

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## Summary

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- The error incurred by **EnKF** is similar to that of derivative-based **LSQ** optimization techniques in  $\mathcal{A}$ .
- Both **EnKF** and **LSQ** produce errors of the same magnitude as **BA**.
- The choice of the initial ensemble  $\mathcal{A}$  can have considerable impact on accuracy of **EnKF**.

<http://homepages.warwick.ac.uk/~masdr>

In addition to the two papers highlighted at the start, upon which the talk is based, the following papers are also of background interest:

- **Elliptic Inverse Problem:** M.Dashti and A.M. Stuart, "Uncertainty quantification and weak approximation of an elliptic inverse problem." *SIAM J. Numerical Analysis* 49(2011), 2524–2542.
- **Navier-Stokes Inverse Problem:** S.L. Cotter, M. Dashti and A.M.Stuart. "Bayesian inverse problems for functions and applications to fluid mechanics". *Inverse Problems* 25 (2009) 115008.
- **Invariant Subspace Property:** G. Li and A. Reynolds. *An iterative ensemble Kalman filter for data assimilation*. In SPE Annual Technical Conference and Exhibition, 2007.