

Analysis of the Ensemble Kalman Filter for Inverse Problems

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The Role of Inverse Problems and Optimisation
in Uncertainty Quantification

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Outline

- 1 Motivation
- 2 EnKF for Inverse Problems
- 3 Continuous Time Limit
- 4 Long-time Behaviour (Linear Case)
- 5 Numerical Experiments (Linear Case)
- 6 Towards the Nonlinear Case
- 7 Summary

Groundwater Flow Problem

We consider steady groundwater flow in a 2d confined aquifer governed by

$$-\nabla \cdot \kappa \nabla h = f$$

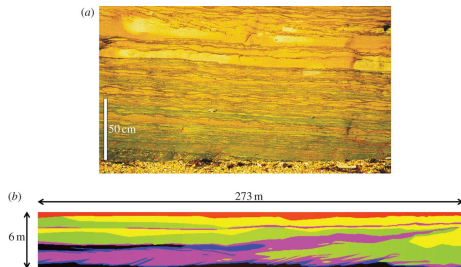
with piezometric head h , source f and hydraulic conductivity κ .

Uncertainty in the hydraulic conductivity κ

- Typical Models: log-normal prior or multipoint prior

Measurements

- Measurements $h(x_j)$ for some set of points $\{x_j\}_{j=1}^K$ in the physical domain



Source: Muggeridge et al.

Inverse Problem

Physical Model

$$\mathcal{G}(u) \rightarrow y$$

- u parameter vector / parameter function
- \mathcal{G} forward response operator
- y result / observations
- Evaluation of \mathcal{G} expensive

Forward Problem

Find the output y for given parameters u

→ **well-posed**

Inverse Problem

Physical Model

$$\mathcal{G}(u) \rightarrow y$$

- u parameter vector / parameter function
- \mathcal{G} forward response operator
- y result / observations
- Evaluation of \mathcal{G} expensive

Forward Problem

Find the output y for given parameters u

→ **well-posed**

Inverse Problem

Find the parameters u from (noisy) observations y

→ **ill-posed**

Inverse Problem

Find the **unknown data** $u \in X$ from noisy observations

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

Deterministic optimization problem

$$\min_u \frac{1}{2} \|y - \mathcal{G}(u)\|^2 + R(u)$$

- $\|y - \mathcal{G}(u)\|$ potential / data misfit
- R regularization term

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Deterministic optimization problem

$$\min_u \frac{1}{2} \|y - \mathcal{G}(u)\|^2 + R(u)$$

- **Large-scale, deterministic optimization problem**
- **No quantification of the uncertainty in the unknown u**
- **Proper choice of the regularization term R**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayesian inverse problem

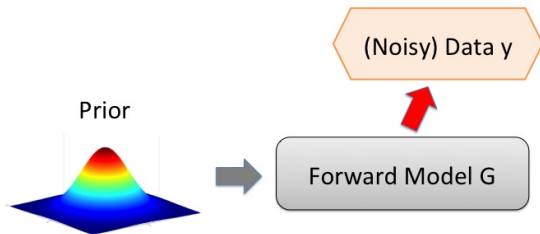
- u, η, y random variables / fields
- Prior μ_0 , posterior μ^y
- Goal of computation: moments of system quantities under the posterior w.r. to noisy data

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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Bayesian inverse problem

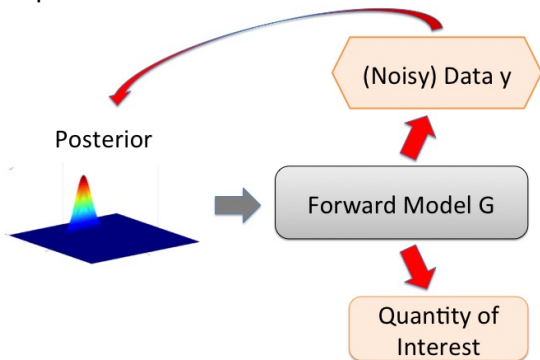


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Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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Bayesian inverse problem

- **Quantification of uncertainty in u and system quantities**
- **Well-posedness of the inverse problem**
- **Incorporation of prior knowledge on the uncertain data u**
- **Need for efficient approximations of the posterior**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayesian inverse problem

Algorithms

- **MCMC**
 - ▶ Dimension robust versions, multilevel strategies, improvements by local approximations, ...
- **Approximations of the forward problem / posterior**
- **Ad hoc methods**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayesian inverse problem

Algorithms

- **MCMC**
- **Approximations of the forward problem / posterior**
 - ▶ Structure exploiting approximations, best Gaussian approximations, transport maps, ...
- **Ad hoc methods**

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayesian inverse problem

Algorithms

- **MCMC**
- **Approximations of the forward problem / posterior**
- **Ad hoc methods**
 - ▶ Ensemble Kalman filter, randomized maximum likelihood, approximate Bayesian computation, ...

Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayesian inverse problem

Algorithms

- **MCMC**
- **Approximations of the forward problem / posterior**
- **Ad hoc methods**
 - ▶ **Ensemble Kalman filter**, randomized maximum likelihood, approximate Bayesian computation, ...

Bayesian Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

- X, Y, \mathcal{X} separable Hilbert spaces
- $\mathcal{G} : X \mapsto Y$ forward response operator, $\mathcal{G} = \mathcal{O} \circ G$
- $G : X \mapsto \mathcal{X}$ the forward map modelling the physical process
- $\mathcal{O} : \mathcal{X} \mapsto Y$ bounded, linear observation operator with $Y = \mathbb{R}^K$, $K \in \mathbb{N}$
- $\eta \in Y$ the observational noise, $\eta \sim \mathcal{N}(0, \Gamma)$
- $y \in Y$ observed data
- μ_0 prior probability measure

Bayesian Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Bayes' Theorem (A. M. Stuart 2010)

Assuming $\mathcal{G} \in C(X, Y)$ and $\mu_0(X) = 1$, then the posterior measure μ on $u|y$ is absolutely continuous w.r. to the prior on u and

$$\mu^y(du) = \frac{1}{Z} \exp(-\Phi(u)) \mu_0(du)$$

with $\Phi : X \mapsto \mathbb{R}$, $\Phi(u) = \frac{1}{2}|y - \mathcal{G}(u)|_{\Gamma}^2$ and $Z = \int \exp(-\Phi(u)) \mu_0(du)$.

Bayesian Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Ensemble Kalman Filter

- Fully Bayesian inversion is often too expensive.
- EnKF is widely used.
- Currently, very little analysis of the EnKF is available.

Aim: Build analysis of properties of EnKF for fixed ensemble size.

Bayesian Inverse Problem

Find the unknown data $u \in X$ from noisy observations

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

Ensemble Kalman Filter

Optimization viewpoint

Study of the properties of the EnKF as a regularization technique for minimization of the least-squares misfit functional

Continuous time limit

Analysis of the properties of the differential equations

EnKF for Inverse Problems (M. A. Iglesias, K. J. H. Law, A. M. Stuart 2013)

Sequence of Interpolating Measures

For $N \in \mathbb{N}$, $h := 1/N$, we define a sequence of measures $\mu_n \ll \mu_0$, $n = 1, \dots, N$, which evolve the prior μ_0 into the posterior distribution $\mu_N = \mu^y$, by

$$\mu_{n+1}(du) = \frac{Z_n}{Z_{n+1}} \exp(-h\Phi(u)) \mu_n(du) \Leftrightarrow \mu_{n+1} = L_n \mu_n$$

with **nonlinear operator** L_n corresponding to application of Bayes' theorem and normalisation constant $Z_n = \int \exp(-nh\Phi(u)) \mu_0(du)$ with $\Phi(u) = \frac{1}{2} |y - \mathcal{G}(u)|_{\Gamma}^2$.

Ensemble of Interacting Particles

Initial ensemble $\{u_0^{(j)}\}_{j=1}^J$ constructed by prior knowledge, $u^{(j)} \sim \mu_0$ iid for $J < \infty$.

Linearisation of L_n and approximation of μ_n by a J -particle Dirac measure leads to the EnKF method.

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Update of the EnKF for Inverse Problems

$$\mathbf{u}_{n+1}^{(j)} = \mathbf{u}_n^{(j)} + \mathbf{C}_{n+1}^{up} (\mathbf{C}_{n+1}^{pp} + \frac{1}{h} \Gamma)^{-1} (\mathbf{y}_{n+1}^{(j)} - \mathcal{G}(\mathbf{u}_n^{(j)}))$$

with empirical covariances

$$\mathbf{C}_{n+1}^{up} = \frac{1}{J} \sum_{j=1}^J \mathbf{u}_n^{(j)} \otimes \mathcal{G}(\mathbf{u}_n^{(j)}) - \bar{\mathbf{u}}_n \otimes \bar{\mathcal{G}}(\mathbf{u}_n)$$

$$\mathbf{C}_{n+1}^{pp} = \frac{1}{J} \sum_{j=1}^J \mathcal{G}(\mathbf{u}_n^{(j)}) \otimes \mathcal{G}(\mathbf{u}_n^{(j)}) - \bar{\mathcal{G}}(\mathbf{u}_n) \otimes \bar{\mathcal{G}}(\mathbf{u}_n),$$

$$\text{mean } \bar{\mathbf{u}}_n = \frac{1}{J} \sum_{j=1}^J \mathbf{u}_n^{(j)}, \quad \bar{\mathcal{G}}(\mathbf{u}_n) = \frac{1}{J} \sum_{j=1}^J \mathcal{G}(\mathbf{u}_n^{(j)})$$

and observations $\mathbf{y}_{n+1}^{(j)} = \mathbf{y} + \boldsymbol{\eta}_{n+1}^{(j)}, \boldsymbol{\eta}_{n+1}^{(j)} \sim N(\mathbf{0}, \frac{1}{h} \Gamma)$.

Properties of the EnKF for Inverse Problems

- The ensemble parameter estimate lies in the linear span of the initial ensemble.
- This linear span property implies that the accuracy of the EnKF estimate is bounded from below by the best approximation in $\text{span}\{\mathbf{u}_0^{(1)}, \dots, \mathbf{u}_0^{(J)}\}$.
- In the linear case, the EnKF estimate converges in the limit $J \rightarrow \infty$ to the solution of the regularised least-squares problem.

Update of the EnKF for Inverse Problems

$$u_{n+1}^{(j)} = u_n^{(j)} + C_{n+1}^{up} (C_{n+1}^{pp} + \frac{1}{h}\Gamma)^{-1} (y_{n+1}^{(j)} - \mathcal{G}(u_n^{(j)}))$$

with empirical covariances

$$C_{n+1}^{up} = \frac{1}{J} \sum_{j=1}^J u_n^{(j)} \otimes \mathcal{G}(u_n^{(j)}) - \bar{u}_n \otimes \bar{\mathcal{G}}(u_n)$$

$$C_{n+1}^{pp} = \frac{1}{J} \sum_{j=1}^J \mathcal{G}(u_n^{(j)}) \otimes \mathcal{G}(u_n^{(j)}) - \bar{\mathcal{G}}(u_n) \otimes \bar{\mathcal{G}}(u_n),$$

$$\text{mean } \bar{u}_n = \frac{1}{J} \sum_{j=1}^J u_n^{(j)}, \quad \bar{\mathcal{G}}(u_n) = \frac{1}{J} \sum_{j=1}^J \mathcal{G}(u_n^{(j)})$$

and observations $y_{n+1}^{(j)} = y + \eta_{n+1}^{(j)}$, $\eta_{n+1}^{(j)} \sim N(0, \frac{1}{h}\Gamma)$.

Properties of the EnKF for Inverse Problems

- The ensemble parameter estimate lies in the **linear span of the initial ensemble**.
- This linear span property implies that the accuracy of the EnKF estimate is **bounded from below by the best approximation** in $\text{span}\{u_0^{(1)}, \dots, u_0^{(J)}\}$.
- In the **linear case**, the EnKF estimate converges in the limit $J \rightarrow \infty$ to the solution of the **regularised least-squares problem**.

Continuous Time Limit

Update of the Iterates

$$\begin{aligned}u_{n+1}^{(j)} &= u_n^{(j)} + h C_{n+1}^{up} (h C_{n+1}^{pp} + \Gamma)^{-1} (y^\dagger - \mathcal{G}(u_n^{(j)})) \\ &\quad + h^{\frac{1}{2}} C_{n+1}^{up} (h C_{n+1}^{pp} + \Gamma)^{-1} \Gamma^{\frac{1}{2}} \zeta_{n+1}^j\end{aligned}$$

with $\zeta_{n+1} \sim \mathcal{N}(0, id)$.

Limiting SDE

Interpreting the iterate as $u_n^{(j)} \approx u^{(j)}(nh)$ gives

$$du^{(j)} = C^{up} \Gamma^{-1} (y^\dagger - \mathcal{G}(u^{(j)})) dt + C^{up} \Gamma^{-\frac{1}{2}} dW^{(j)},$$

where $W^{(1)}, \dots, W^{(J)}$ are pairwise independent cylindrical Wiener processes and y^\dagger denotes the noisy observational data $\mathcal{G}(u^\dagger) + \eta^\dagger$ with $\eta^\dagger \sim \mathcal{N}(0, \Gamma)$.

Continuous Time Limit (Linear Case)

Assumption: Linear response operator $\mathcal{G}(u) = Au$ with $A \in \mathcal{L}(X, Y)$

$$u_{n+1}^{(j)} = u_n^{(j)} + hC(u_n)A^*\Gamma^{-1}(y_{n+1}^{(j)} - Au_{n+1}^{(j)})$$

with $C(u_n) = \frac{1}{J} \sum_{j=1}^J (u_n^{(j)} - \bar{u}_n) \otimes (u_n^{(j)} - \bar{u}_n)$ and $\bar{u}_n = \frac{1}{J} \sum_{j=1}^J u_n^{(j)}$.

Limiting SDE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^\dagger + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)},$$

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Noise-free Case

Limiting ODE

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Noise-free Case

Limiting ODE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^\dagger - u^{(j)}) dt,$$

or equivalently,

$$\frac{d}{dt}u^{(j)} = -C(u)D_u\Phi(u^{(j)}; y)$$

with potential $\Phi(u; y) = \frac{1}{2}\|\Gamma^{-\frac{1}{2}}(y - Au)\|^2$ and $\Gamma^{-1} = I$.

Continuous Time Limit (Linear Case)

Assumption: Linear response operator $\mathcal{G}(u) = Au$ with $A \in \mathcal{L}(X, Y)$

$$u_{n+1}^{(j)} = u_n^{(j)} + hC(u_n)A^*\Gamma^{-1}(y_{n+1}^{(j)} - Au_{n+1}^{(j)})$$

with $C(u_n) = \frac{1}{J} \sum_{j=1}^J (u_n^{(j)} - \bar{u}_n) \otimes (u_n^{(j)} - \bar{u}_n)$ and $\bar{u}_n = \frac{1}{J} \sum_{j=1}^J u_n^{(j)}$.

Noise-free Case

Limiting ODE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^\dagger - u^{(j)}) dt,$$

or equivalently,

$$\frac{d}{dt}u^{(j)} = \frac{1}{J} \sum_{k=1}^J \langle a^{(k)} - \bar{a}, y^\dagger - a^{(j)} \rangle_\Gamma (u^{(k)} - \bar{u})$$

with $a^{(k)} = Au^{(k)}$ and $\bar{a} = \frac{1}{J} \sum_{j=1}^J a^{(j)}$.

Global Existence of Solutions (Linear Case)

Theorem

The following differential inequalities for the quantities $d^{(j)} = u^{(j)} - \bar{u}$ and $r^{(j)} = u^{(j)} - u^\dagger$ hold

$$\frac{1}{2} \frac{d}{dt} |Ad^{(j)}|_\Gamma^2 \leq 0, \quad \frac{1}{2} \frac{d}{dt} |Ar^{(j)}|_\Gamma^2 \leq 0$$

implying **global existence** of r and d .

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Sketch of Proof

Quantities

$$\begin{aligned} d^{(j)} &= u^{(j)} - \bar{u}, & r^{(j)} &= u^{(j)} - u^\dagger, \\ D_{lj} &= \langle Ad^{(l)}, Ad^{(j)} \rangle_\Gamma, & R_{lj} &= \langle Ar^{(l)}, Ar^{(j)} \rangle_\Gamma, & F_{lj} &= \langle Ar^{(l)}, Ad^{(j)} \rangle_\Gamma. \end{aligned}$$

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implying global existence of r and d .

Sketch of Proof

$$\frac{d}{dt} d^{(j)} = -\frac{1}{J} \sum_{k=1}^J D_{jk} d^{(k)}, \quad \frac{d}{dt} r^{(j)} = -\frac{1}{J} \sum_{k=1}^J F_{jk} r^{(k)}, \quad j = 1, \dots, J$$

$$\frac{d}{dt} D = -\frac{2}{J} D^2, \quad \frac{d}{dt} R = -\frac{2}{J} FF^\top, \quad \frac{d}{dt} F = -\frac{2}{J} FD$$

Global existence of D , R and $F \Rightarrow$ global existence of r and d

Ensemble Collapse (Linear Case)

Theorem

The solution of

$$\frac{d}{dt}D = -\frac{2}{J}D^2$$

with initial condition $D(0) = D_0 = X\Lambda_0X^*$, $\Lambda_0 = \text{diag}\{\lambda_0^{(1)}, \dots, \lambda_0^{(J)}\}$ and $X \in \mathbb{R}^{J \times J}$ orthogonal, is given by

$$D(t) = X\Lambda(t)X^* .$$

$\Lambda(t)$ satisfies the following decoupled ODE

$$\frac{d\lambda^{(j)}}{dt} = -\frac{2}{J}(\lambda^{(j)})^2$$

with solution $\lambda^{(j)}(t) = \left(\frac{2}{J}t + \frac{1}{\lambda_0^{(j)}}\right)^{-1}$, if $\lambda_0^{(j)} \neq 0$, otherwise $\lambda^{(j)}(t) = 0$.

Ensemble Collapse (Linear Case)

Theorem

The solution of

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with solution $\lambda^{(j)}(t) = \left(\frac{2}{J}t + \frac{1}{\lambda_0^{(j)}}\right)^{-1}$, if $\lambda_0^{(j)} \neq 0$, otherwise $\lambda^{(j)}(t) = 0$.

The rate of convergence of D and F is algebraic with a constant growing with larger ensemble size J .

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

$$-\frac{d^2 p}{dx^2} + p = u \quad \text{in } D := (0, \pi), \quad p = 0 \quad \text{in } \partial D,$$

where

$A = \mathcal{O} \circ L^{-1}$ with $L = -\frac{d^2}{dx^2} + id$ and $D(L) = H^2(D) \cap H_0^1(D)$

$\mathcal{O} : X \mapsto \mathbb{R}^K$, equispaced observation points in D with spacing $\tau_N^{\mathcal{O}} = 2^{-N_K}$ at $x_k = \frac{k}{2^{N_K}}$, $k = 1, \dots, 2^{N_K} - 1$, $o_k(\cdot) = \delta(\cdot - x_k)$ with $K = 2^{N_K} - 1$.

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

$$-\frac{d^2p}{dx^2} + p = u \quad \text{in } D := (0, \pi), \quad p = 0 \quad \text{in } \partial D .$$

The goal of computation is to recover the unknown data u^\dagger from observations

$$y = \mathcal{O}L^{-1}u^\dagger = Au^\dagger .$$

Numerical Experiments (Linear Case)

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Computational Setting

- Noise-free case, $\Gamma = I$.
- $u \sim \mathcal{N}(0, C)$ with $C = \beta(A - id)^{-1}$ and with $\beta = 10$.
- Finite element method using continuous, piecewise linear ansatz functions on a uniform mesh with meshwidth $h = 2^{-8}$ (the spatial discretization leads to a discretization of u , ie. $u \in \mathbb{R}^{2^8-1}$).
- The space $\mathcal{A} = \text{span}\{u_0^{(j)}\}_{j=1}^J$ is chosen based on the KL expansion of $C = \beta(A - id)^{-1}$.

Numerical Experiments (Linear Case)

Underdetermined case, $\mathbf{K} = 2^4 - 1$, EnKF ensemble $\mathbf{J} = 2$

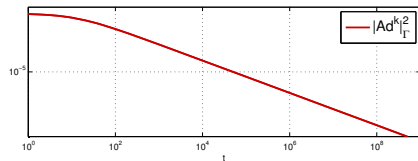
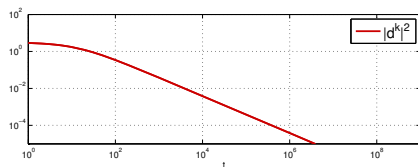


Figure: Quantities $|d^{(k)}|^2$ (above), $|Ad^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

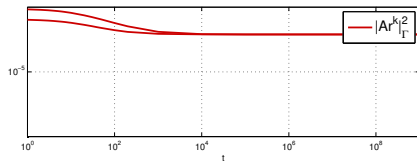
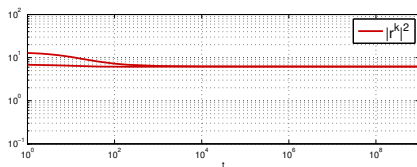


Figure: Quantities $|r^{(k)}|^2$ (above), $|Ar^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

Numerical Experiments (Linear Case)

Underdetermined case, $K = 2^4 - 1$, EnKF ensemble $J = 2$

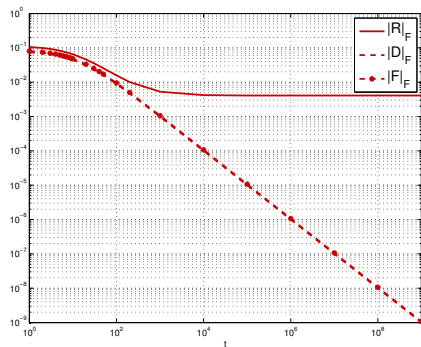


Figure: $\|D\|_F$, $\|F\|_F$, $\|R\|_F$ w.r. to time t .

Numerical Experiments (Linear Case)

Underdetermined case, $K = 2^4 - 1$, EnKF ensemble $J=128$

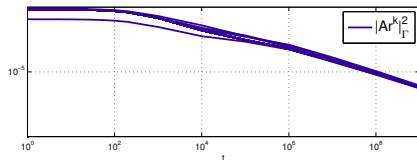
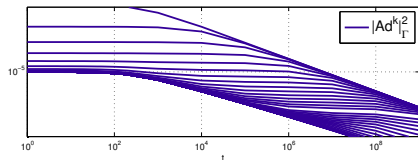
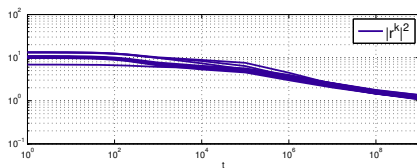
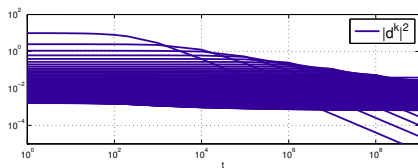


Figure: Quantities $|d^{(k)}|^2$ (above), $|Ad^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

Figure: Quantities $|r^{(k)}|^2$ (above), $|Ar^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

Numerical Experiments (Linear Case)

Underdetermined case, $K = 2^4 - 1$, EnKF ensemble $J=128$

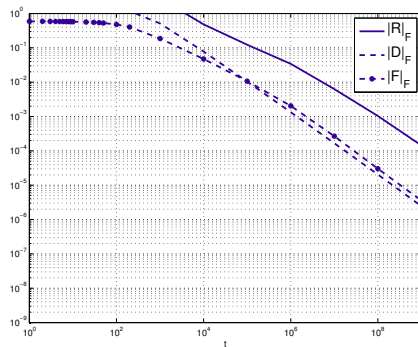


Figure: $\|D\|_F$, $\|F\|_F$, $\|R\|_F$ w.r. to time t .

Convergence of Residuals (Linear Case)

Theorem

Assume that y is the image of a truth $u^\dagger \in X$ under A and the forward operator A is one-to-one. Let Y^\parallel denote the linear span of the $\{Ad^{(j)}(0)\}_{j=1}^J$ and let Y^\perp denote the orthogonal complement of Y^\parallel in Y and assume that the initial ensemble members are chosen so that Y^\parallel has the maximal dimension $\min\{J - 1, \dim(Y)\}$.

Then $Ar^{(j)}(t)$ may be decomposed uniquely as

$$Ar_{\parallel}^{(j)}(t) + Ar_{\perp}^{(j)}(t) \quad \text{with } Ar_{\parallel}^{(j)} \in Y^\parallel \text{ and } Ar_{\perp}^{(j)} \in Y^\perp.$$

Furthermore $Ar_{\parallel}^{(j)}(t) \rightarrow 0$ as $t \rightarrow \infty$ and $Ar_{\perp}^{(j)}(t) = Ar_{\perp}^{(j)}(0) = Ar_{\perp}^{(1)}$.

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Adaptive choice of the initial ensemble to ensure convergence of the residuals.

Numerical Experiments (Linear Case)

Underdetermined case, $\mathbf{K} = 2^4 - 1$, $\mathbf{J} = 5$

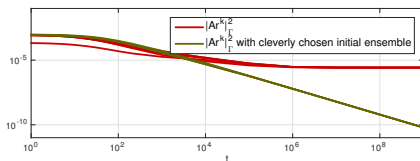
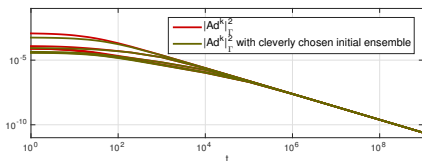
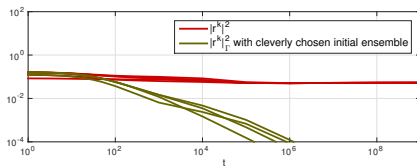
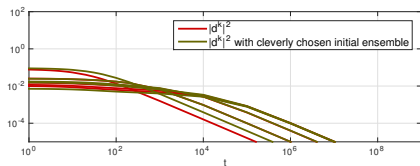


Figure: Quantities $|d^{(k)}|^2$ (above), $|Ad^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

Figure: Quantities $|r^{(k)}|^2$ (above), $|Ar^{(k)}|_{\Gamma}^2$ (below) w.r. to time t .

Numerical Experiments (Linear Case)

Underdetermined case, $\mathbf{K} = 2^4 - \mathbf{1}$, $\mathbf{J} = \mathbf{5}$

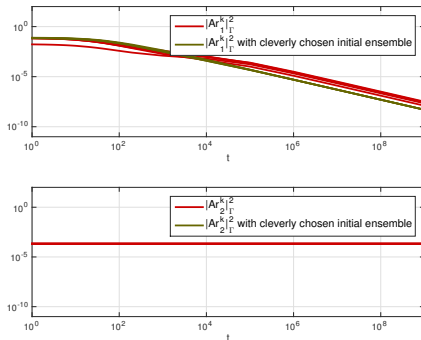


Figure: Quantities $|Ar_{\parallel}^{(j)}|^2_{\Gamma}$, $|Ar_{\perp}^{(j)}|^2_{\Gamma}$ with respect to time t .

Towards the Nonlinear Case

2-dimensional elliptic equation

$$-\operatorname{div}(e^u \nabla p) = f \quad \text{in } D := (-1, 1)^2, \quad p = 0 \quad \text{in } \partial D,$$

where

$f(x) = 100$ the right hand side,

$\mathcal{O} : X \mapsto \mathbb{R}^K$, equispaced observation points in D with spacing $\tau_N^{\mathcal{O}} = 2^{-N_K}$ at $x_k = \frac{k}{2^{N_K}}$, $k = 1, \dots, 2^{N_K} - 1$, $o_k(\cdot) = \delta(\cdot - x_k)$ with $K = 2^{N_K} - 1$.

Towards the Nonlinear Case

2-dimensional elliptic equation

$$-\operatorname{div}(e^u \nabla p) = f \quad \text{in } D := (-1, 1)^2, \quad p = 0 \quad \text{in } \partial D.$$

The goal of computation is to recover the unknown data u^\dagger from observations

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

Towards the Nonlinear Case

2-dimensional elliptic equation

$$-\operatorname{div}(e^u \nabla p) = f \quad \text{in } D := (-1, 1)^2, \quad p = 0 \quad \text{in } \partial D.$$

The goal of computation is to recover the unknown data u^\dagger from observations

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

Computational Setting

- Noise-free case, $\Gamma = I$.
- $u \sim \mathcal{N}(0, C)$ with $C = \beta(-\Delta)^{-2}$ and with $\beta = 1$.
- Finite element method using continuous, piecewise linear ansatz functions on a uniform mesh with meshwidth $h = 2^{-4}$ (the spatial discretization leads to a discretization of u , ie. $u \in \mathbb{R}^{2^4-1^2}$).
- The space $\mathcal{A} = \operatorname{span}\{u_0^{(j)}\}_{j=1}^J$ is chosen based on the KL expansion of $C = \beta(A)^{-1}$.

Towards the Nonlinear Case

Underdetermined case, $K = 49$, $J = 75$

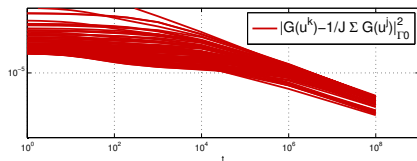
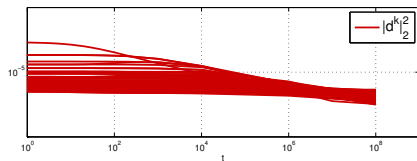


Figure: Quantities $|d^{(k)}|_2^2$ (above), $|\mathcal{G}(u^{(k)}) - \frac{1}{J} \sum_{j=1}^J \mathcal{G}(u^{(j)})|_{\Gamma}^2$ (below) w.r. to time t .

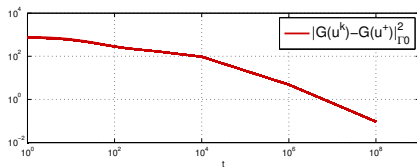
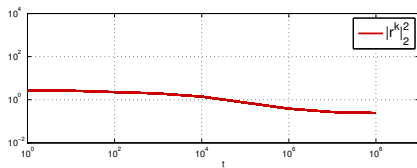


Figure: Quantities $|r^{(k)}|_2^2$ (above), $|\mathcal{G}(u^{(k)}) - \mathcal{G}(u^{\dagger})|_{\Gamma}^2$ (below) w.r. to time t .

Towards the Nonlinear Case

Underdetermined case, $K = 49$, $J = 75$

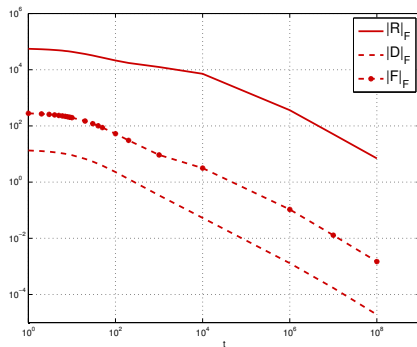


Figure: $\|D\|_F$, $\|F\|_F$, $\|R\|_F$ w.r. to time t .

Towards the Nonlinear Case

Underdetermined case, $K = 49$, $J = 75$

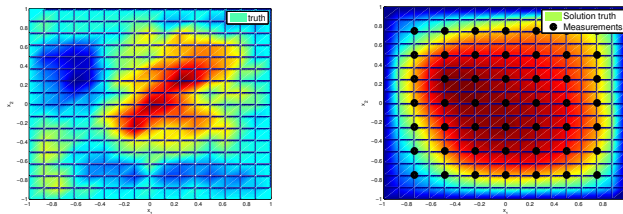


Figure: Comparison of the truth and the ensemble members w.r. to x over time (left) and comparison of the forward solution $G(u^\dagger)$ and the estimated solutions of the forward problem (right).







Conclusions and Outlook

- Deriving the continuous time limit allows to determine the asymptotic behaviour of important quantities of the algorithm.
- The continuous approach offers the possibility to improve the performance of the approach by choosing appropriate numerical discretisation schemes based on the properties of the solution.
- This approach is not limited to the linear case and may give also some insights for the nonlinear case.

Conclusions and Outlook

- Analysis of the SDE for the linear and nonlinear case.
- Improving the performance of the algorithm by controlling the approximation quality of the subspace spanned by the ensemble.
- Analysis of EnKF variants
 - ▶ Variance inflation
 - ▶ Localization
 - ▶ Iterative regularization
 - ▶ Markov mixing
- Use the EnKF as iterative solver for linear equations.
- Apply the ideas to large-scale forward models using industrial solvers.

References

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<http://arxiv.org/abs/1401.5375>.
-  M A Iglesias, K J H Law and A M Stuart 2013 Ensemble Kalman methods for inverse problems *Inverse Problems* **29** 045001.
-  F Le Gland, V Monbet and V-D Tran 2011 Large sample asymptotics for the ensemble Kalman filter *Dan Crisan, Boris Rozovskii. The Oxford Handbook of Nonlinear Filtering, Oxford University Press*, 598-631.
-  D T B Kelly, K J H Law and A M Stuart 2014 Well-posedness and accuracy of the ensemble Kalman filter in discrete and continuous time *Nonlinearity* **27** 2579-2603.
-  C Schillings and A M Stuart 2015 Analysis of the Ensemble Kalman Filter for Inverse Problems (*in preparation*).

Long-time Behaviour (Linear Case)

In the Presence of Noise

Quantities

$$d^{(j)} = u^{(j)} - \bar{u}, \quad r^{(j)} = u^{(j)} - u^\dagger,$$

Asymptotic Behaviour of Solutions

Applying Itô's formula yields

$$\mathbb{E} \frac{1}{J} d \sum_{j=1}^J |Ad^{(j)}|_{\Gamma}^2 = \frac{1}{J} \sum_{j=1}^J \mathbb{E} \left(-\frac{2}{J} |Ad^{(j)}|_{\Gamma}^4 \right) dt$$

and

$$\mathbb{E} \frac{1}{J} d \sum_{j=1}^J |Ar^{(j)}|_{\Gamma}^2 = \frac{1}{J} \sum_{j=1}^J \sum_{k=1}^J \mathbb{E} \left(-\frac{2}{J} F_{jk}^2 \right) dt$$

Numerical Experiments (Linear Case)

Underdetermined case, $\mathbf{K} = 2^4 - \mathbf{1}$, $\mathbf{J} = 5$, $\Gamma = 0.01I$

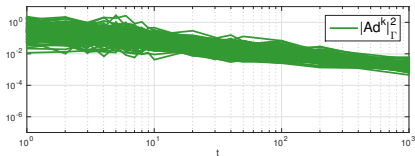
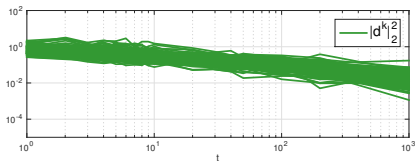


Figure: Quantities $|d_k|_2^2$, $|Ad_k|_\Gamma^2$ with respect to time t .

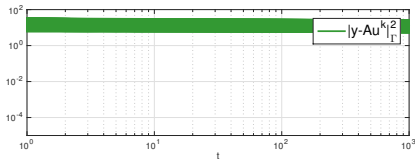
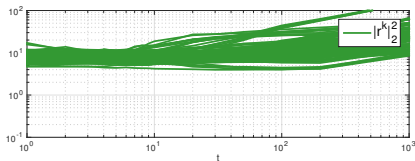


Figure: Quantities $|r^k|_2^2$, $|Ar^k|_\Gamma^2$ with respect to time t .

Numerical Experiments (Linear Case)

Underdetermined case, $\mathbf{K} = 2^4 - \mathbf{1}$, $\mathbf{J} = 5$, $\Gamma = 0.01\mathbf{I}$

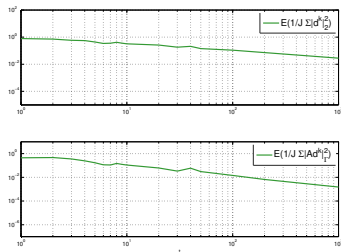


Figure: Mean of the quantities $|d_k|_2^2$, $|Ad_k|_\Gamma^2$ with respect to time t , 25 realisations of the noise in the iterations and of the noise in the observations.

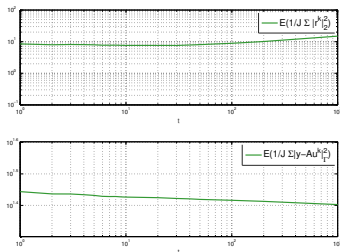


Figure: Mean of the quantities $|r^k|_2^2$, $|Ar^k|_\Gamma^2$ with respect to time t , 25 realisations of the noise in the iterations and of the noise in the observations.

Solving linear equations with the EnKF

We consider the one dimensional elliptic equation

$$-\operatorname{div}(u\nabla p) = f \quad \text{in } D := (0, \pi), \quad p = 0 \quad \text{in } \partial D,$$

with $u(x) = 1 + 0.1 \sin(\pi x) + 0.05 \sin(2\pi x)$, $f(x) = \frac{1}{10}x$.

The goal of computation is the solution p .

- $\Gamma = I$.
- Finite element method using continuous, piecewise linear ansatz functions on a uniform mesh with meshwidth $h = 2^{-8}$ (the spatial discretization leads to a discretization of p , i.e. $p \in \mathbb{R}^{2^8-1}$).
- The space $\mathcal{A} = \operatorname{span}\{u_0^{(j)}\}_{j=1}^J$ is chosen based on the eigenfunctions of the Laplace operator, i.e. $\sin(jx)$, $j = 1, \dots, J$.
- Variation of the cardinality of the linear space \mathcal{A} , i.e. $\#\mathcal{A} = \{10, 256\}$.

Numerical Results

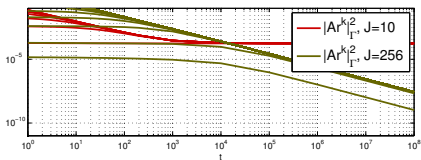
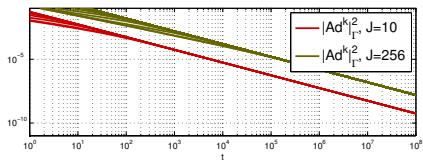
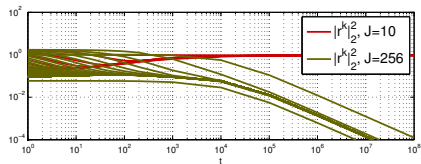
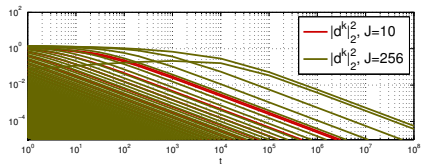


Figure: Quantities $|d_k^k|_2^2$, $|Ad_k^k|_\Gamma^2$ with respect to time t .

Figure: Quantities $|r^k|_2^2$, $|Ar^k|_\Gamma^2$ with respect to time t .

Numerical Results

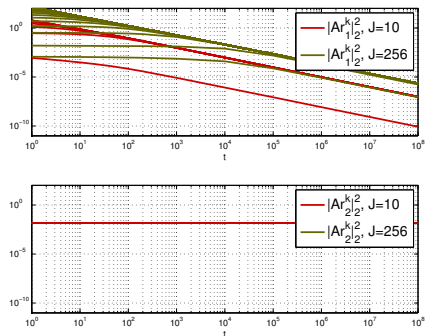


Figure: Quantities $|Ar_{\parallel}^{(j)}|_{\Gamma}^2$, $|Ar_{\perp}^{(j)}|_{\Gamma}^2$ with respect to time t .

Numerical Results

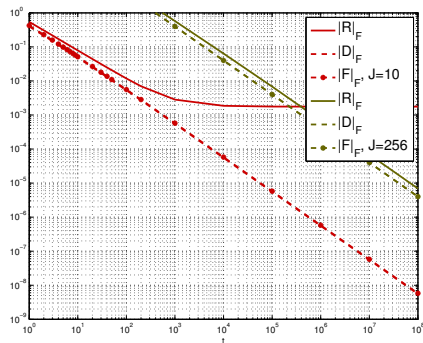


Figure: Quantities $\|D\|_F$, $\|F\|_F$, $\|R\|_F$ with respect to time t .