Analysis of the Ensemble Kalman Filter for Inverse Problems

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11th International EnKF Workshop

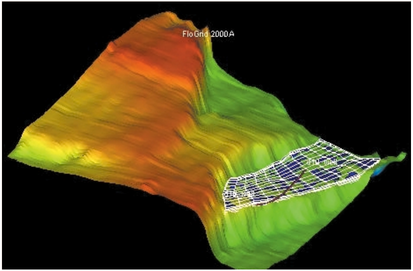
research supported by the Engineering and Physical Sciences Research Council

Outline

Reservoir Modeling

Teal South

- Reservoir in the Gulf of Mexico
- Monthly production rates of oil, water and gas avalaible



Source: Christie et al.

Model

- Five geological layers with uniform properties
- 9 unknown parameters (porosity, horizontal permeability multipliers for each layer, vertical to horizontal permeability ratio, rock compressibility, aquifer strength)
- Matching to the field oil production rate
- Eclipse used to simulate the flow in porous media

Reservoir Modeling

Results (100 forward simulations)

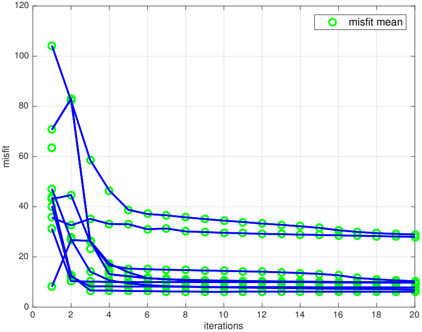


Figure: Misfit of the mean to the (noisy) observational data, J=5, 20 iterations.

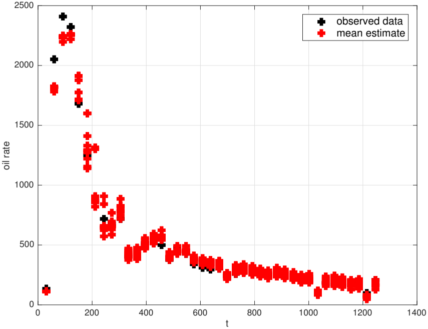


Figure: Prediction of the mean compared to the (noisy) observational data, J=5, 20 iterations.

Inverse Problem

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

$$y = \mathcal{G}(u) + \eta \qquad \text{with } \eta \sim \mathcal{N}(0, \Gamma)$$

- $u \in X$ parameter vector / parameter function
- $\mathcal{G} : X \to Y$ forward response operator; X, Y separable Hilbert spaces
- y result / observations
- Evaluation of $\mathcal{G}$ expensive

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Deterministic optimisation problem

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

- R regularisation term

Bayesian inverse problem

- u, η, y random variables / fields
- Prior μ_0, posterior μ^y

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^y 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

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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

Optimisation viewpoint

Study of the properties of the EnKF as a regularisation technique for minimisation of the least-squares misfit functional

Continuous time limit

Analysis of the properties of the differential equations

EnKF for Inverse Problems

Sequence of Interpolating Measures

For $N \in \mathbb{N}, h := 1/N$, we define a sequence of measures $\mu_n \ll \mu_0$, $n = 1, \ldots, N$, 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 $\mathrm{L_n}$ and approximation of μ_n by a J-particle Dirac measure leads to the EnKF method.

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EnKF for Inverse Problems

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

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

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

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 e.g. [Iglesias, Law, Stuart 2013]

- 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 $\mathrm{span}\{u_0^{(1)}, \ldots, u_0^{(J)}\}$.
- In the linear case, the EnKF estimate converges in the limit $J \to \infty$ to the solution of the regularised least-squares problem.

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Continuous Time Limit

Update of the Iterates

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

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

Limiting SDE

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

$$\mathrm{d}u^{(j)} = C^{up}\Gamma^{-1}(y^\dagger - \mathcal{G}(u^{(j)}))\,\mathrm{d}t + C^{up}\Gamma^{-\frac{1}{2}}\,\mathrm{d}W^{(j)}\,,$$

where $W^{(1)}, \ldots, W^{(J)}$ 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 $C(u_n) = \frac{1}{J}\sum_{j=1}^{J}(u_n^{(j)} - \overline{u}_n) \otimes (u_n^{(j)} - \overline{u}_n)$ and $\overline{u}_n = \frac{1}{J}\sum_{j=1}^{J} u_n^{(j)}$.

Limiting SDE

$$\mathrm{d}u^{(j)} = C(u)A^*\Gamma^{-1}A(u^\dagger + \eta - u^{(j)})\,\mathrm{d}t + C(u)A^*\Gamma^{-\frac{1}{2}}\,\mathrm{d}W^{(j)}\,,$$

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Noise-free Case

Limiting ODE

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Noise-free Case

Limiting ODE

$$\mathrm{d}u^{(j)} = C(u)A^*\Gamma^{-1}A(u^\dagger - u^{(j)})\,\mathrm{d}t\,,$$

or equivalently,

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

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

Long-time Behaviour (Linear Case)

(a) Global Existence of Solutions

(b) Ensemble Collapse

(c) Convergence of Residuals

Long-time Behaviour (Linear Case)

(a) Global Existence of Solutions

Assume that y is the image of a truth $u^\dagger \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \dots, J$ and define $\mathcal{X}_0$ to be the linear span of the $\{u^{(j)}(0)\}_{j=1}^J$.

Then, the limiting ODE has a unique solution $u^{(j)}(\cdot) \in C([0, \infty); \mathcal{X}_0)$ for $j = 1, \dots, J$.

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Sketch of Proof

Quantities

$$e^{(j)} = u^{(j)} - \overline{u}\,, \qquad r^{(j)} = u^{(j)} - u^\dagger\,,$$

$$E_{lj} = \langle Ae^{(l)}, Ae^{(j)}\rangle_\Gamma\,, \qquad R_{lj} = \langle Ar^{(l)}, Ar^{(j)}\rangle_\Gamma\,, \qquad F_{lj} = \langle Ar^{(l)}, Ae^{(j)}\rangle_\Gamma\,.$$

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Sketch of Proof

$$\frac{\mathrm{d}}{\mathrm{d}t} e^{(j)} = -\frac{1}{J} \sum_{k=1}^J E_{jk} d^{(k)}, \quad \frac{\mathrm{d}}{\mathrm{d}t} r^{(j)} = -\frac{1}{J} \sum_{k=1}^J F_{jk} r^{(k)}, \qquad j = 1, \dots, J$$

$$\frac{\mathrm{d}}{\mathrm{d}t} E = -\frac{2}{J} E^2, \qquad \frac{\mathrm{d}}{\mathrm{d}t} R = -\frac{2}{J} F F^\top, \qquad \frac{\mathrm{d}}{\mathrm{d}t} F = -\frac{2}{J} F E$$

Global existence of $\mathbf{E}$, $\mathbf{R}$ and $\mathbf{F}$ $\Rightarrow$ global existence of $\mathbf{r}$ and $\mathbf{e}$

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(b) Ensemble Collapse

Assume that y is the image of a truth $u^\dagger \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \dots, J$.

The solution of

$$\frac{\mathrm{d}}{\mathrm{d}t} E = -\frac{2}{J} E^2$$

with initial cond. $E(0) = X \Lambda_0 X^*$, $\Lambda_0 = \text{diag}\{\lambda_0^{(1)}, \dots, \lambda_0^{(J)}\}$, $X \in \mathbb{R}^{J \times J}$ orthogonal, is given by $E(t) = X \Lambda(t) X^*$.

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

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

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

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

Long-time Behaviour (Linear Case)

(c) Convergence of Residuals

Assume that y is the image of a truth $u^\dagger \in \mathcal{X}$ under A.Let $Y^\parallel$ denote the linear span of the $\{Ae^{(j)}(0)\}_{j=1}^J$ and let $Y^\perp$ denote the orthogonal complement of $Y^\parallel$ in $\mathcal{Y}$ with respect to the inner product $\langle \cdot, \cdot \rangle_\Gamma$ and assume that the initial ensemble members are chosen so that $Y^\parallel$ has the maximal dimension $\min\{J-1, \dim(\mathcal{Y})\}$.

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 $Ar_\parallel^{(j)}(t) \to 0$ as $t \to \infty$ 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.

Long-time Behaviour (Linear Case)

Idea of Proof

Subspace property

$$Ae^{(j)}(t) = \sum_{k=1}^{J} \ell_{jk}(t) Ae^{(k)}(0)$$

where the matrix $L = \{\ell_{jk}\}$ is invertible.

Decomposition of the residual

$$Ar^{(j)}(t) = \sum_{k=1}^{J} \alpha_k Ae^{(k)}(t) + Ar_{\perp}^{(1)}$$

Convergence of the residuals

Boundedness of the coefficient vector

$$|\alpha(t)|^2 \leq \frac{\lambda_0^{(J)}}{\lambda_0^{\min}} |\alpha(0)|^2$$

gives convergence of the residuals.

Long-time Behaviour for Noisy Data (Linear Case)

Find the parameters u from (noisy) observations $y^\dagger$

$$y^\dagger = Au^\dagger + \eta^\dagger$$

Global Existence of Solutions ✓

Ensemble Collapse ✓

Convergence of Residuals $\rightarrow$ **convergence of the misfit**

Variants on EnKF

Variance Inflation

$$\frac{\mathrm{d}u^{(j)}}{\mathrm{d}t} = -\big(\alpha C_0 + C(u)\big) D_u \Phi(u^{(j)}; y), \quad j = 1, \ldots, J\,,$$

where C_0 is a self-adjoint, strictly positive operator.

Localisation

Randomised Search

Variants on EnKF

Variance Inflation

Localisation

$$\rho : D \times D \to \mathbb{R} , \qquad \rho(x,y) = \exp(-|x-y|^r) ,$$

where $D \subset \mathbb{R}^d$ denotes the physical domain and $|\cdot|$ is a suitable norm in D, $r \in \mathbb{N}$.

$$\frac{\mathrm{d}u^{(j)}}{\mathrm{d}t} = -C^{\mathrm{loc}}(u) D_u \Phi(u^{(j)}; y), \quad j = 1, \dots, J ,$$

where $C^{\mathrm{loc}}(u)\phi(x) = \int_D \phi(y) k(x,y) \rho(x,y) \,\mathrm{d}y$ with k being the kernel of $C(u)$, $\phi \in \mathcal{X}$.

Randomised Search

Variants on EnKF

Variance Inflation

Localisation

Randomised Search

$$\mu_{n+1} = L_n P_n \mu_n \ .$$

where P_n is any Markov kernel which preserves μ_n.

$$\frac{\mathrm{d}u^{(j)}}{\mathrm{d}t} = \frac{1}{J}\sum_{k=1}^{J}\big\langle \mathcal{G}(u^{(k)}) - \overline{\mathcal{G}}, y - \mathcal{G}(u^{(j)})\big\rangle_{\Gamma}\big(u^{(k)} - \overline{u}\big)$$

$$-u^{(j)} - tC_0 D_u \Phi(u^{(j)}; y) + \sqrt{2C_0}\frac{\mathrm{d}W^{(j)}}{\mathrm{d}t} \ .$$

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

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

where

$A = \mathcal{O} \circ L^{-1}$ with $L = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + id$ 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
$x_k = \frac{k}{2^{N_K}},\ k = 1, \ldots, 2^{N_K} - 1$, $o_k(\cdot) = \delta(\cdot - x_k)$ with $K = 2^{N_K} - 1$.

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

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

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Computational Setting

- Noisy 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 discretisation leads to a discretisation of u, i.e. $u \in \mathbb{R}^{2^8-1}$).
- The space $\mathcal{A} = \mathrm{span}\{u_0^{(j)}\}_{j=1}^{J}$ is chosen based on the KL expansion of $C = \beta(A - id)^{-1}$ (in red and green) and in an adaptive way minimising $Ar_\perp^{(j)}(t)$ (in blue) .

Numerical Experiments (Linear Case)

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

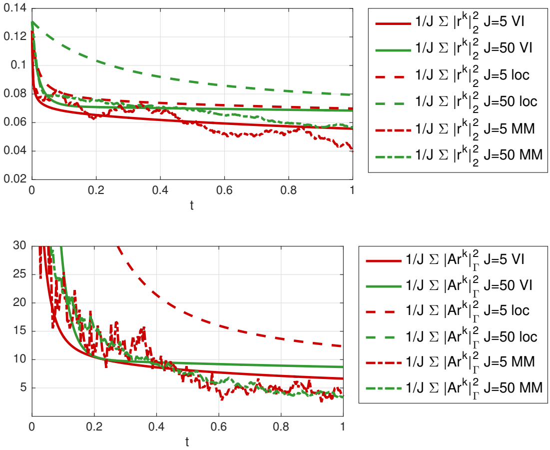

Figure: Quantities $|r|_2^2$, $|Ar|_\Gamma^2$ w.r. to time t, $J = 5$ (red) and $J = 50$ (green) for the discussed variants, $\beta = 10$, $\beta = 10$, $K = 2^4 - 1$, initial ensemble chosen based on KL expansion of $C = \beta(A - id)^{-1}$.

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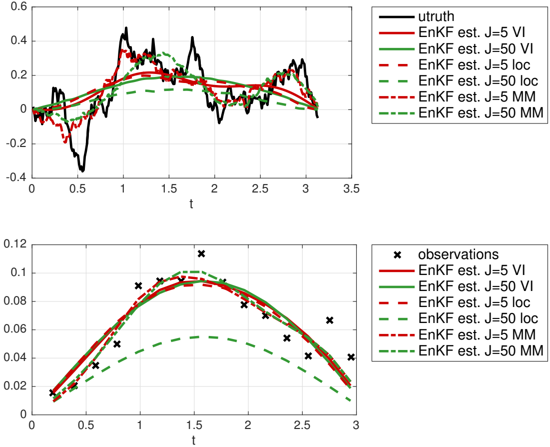

Figure: Comparison of the EnKF estimate with the truth and the observations, $J = 5$ (red) and $J = 50$ (green) for the discussed variants, $\beta = 10$, $K = 2^4 - 1$, initial ensemble chosen based on KL expansion of $C = \beta(A - id)^{-1}$.

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 method by choosing appropriate numerical discretisation schemes based on the properties of the solution.
- Generalisation of the results to noisy observational data, i.e. $Au^\dagger + \eta^\dagger$.
- Improving the performance of the algorithm by controlling the approximation quality of the subspace spanned by the ensemble.
- Analysis of EnKF variants
  - Variance inflation
  - Localisation
  - Iterative regularisation
  - Markov mixing

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