ANALYSIS OF THE ENSEMBLE KALMAN FILTER FOR INVERSE PROBLEMS

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ABSTRACT. Notes for a 90-minute presentation on the Ensemble Kalman Filter for the Uncertainty Quantification seminar at Freie Universität Berlin, held on Tuesday, the 8th of June, 2016. Based on the eponymous article (`http://arxiv.org/abs/1602.02020`) by Schillings and Stuart.

Ensemble Kalman Filter (EnKF): methodology for

- state estimation in partial, noisily observed dynamical systems
- parameter estimation in inverse problems

EnKF is:

- not well understood; theory often deals with large ensemble limit
- robust, considered effective in situations far from large ensemble limit

More precisely: EnKF is a Monte Carlo approximation of linear Kalman filter, in which ensemble of $E \in \mathbb{N}$ state estimates is used to estimate the covariance operator (computational savings can be important in high-dimensional scenarios) (see [2, Section 7.4]).

1. Introduction

Summary

- Derive continuous-time limit of EnKF for inverse problems
- Analyse long-time behaviour of resulting dynamical system
- For linear inverse problems, continuous-time limit corresponds to gradient flows for data misfit in each ensemble member; empirical covariance matrix of ensemble serves as pre-conditioner

Let $\mathcal{G} : \mathcal{X} \to \mathcal{Y}$ be a map between separable Hilbert spaces.

Inverse problem (IP):recover unknown u from observation y, where

$$y = \mathcal{G}(u) + \eta, \tag{0a}$$

where

- η - observational noise,
- $\mathcal{G}$ - compact operator
- inversion is ill-posed on $\mathcal{Y}$.

Assume $\mathcal{Y} = \mathbb{R}^K$ for $K \in \mathbb{N}$ (finite-dimensional setting).

In such inverse problems, least squares functional ("model-data misfit")

$$\Phi(u; y) = \frac{1}{2} \left\| \Gamma^{-1/2}(y - \mathcal{G}(u)) \right\|_{\mathcal{Y}}^2 \tag{0b}$$

where the covariance operator $\Gamma : \mathcal{Y} \to \mathcal{Y}$ satisfies $\Gamma > 0$.

If inverse problem ill-posed, need to regularise the problem of minimising the model-data misfit Φ. One approach is Bayesian regularisation: if (u, y) as a joint random variable in $\mathcal{X} \times \mathcal{Y}$, $\eta \sim N(0, \Gamma)$ independent of $u \sim \mu_0$, then solution of IP given by $\mathcal{X}$-valued RV $u|y$, where

$$u|y \sim \mu(du) = \frac{1}{Z} \exp\left(-\Phi(u; y)\right) \mu_0(du) \tag{1}$$

for Z normalisation constant. μ - "posterior", μ_0 - "prior", $Z^{-1} \exp\left(-\Phi(u; y)\right)$ - "likelihood of u given observation y"

Here: view EnKF as derivative-free optimisation technique, with ensemble used as proxy for derivative information (i.e. EnKF regularises the problem of minimising least-squares data misfit functional Φ).

Goal: understand in what sense that the continuous-time limit of EnKF corresponds to set of preconditioned gradient flows for data misfit in each ensemble member.

EnKF algorithm nonlinear even for linear inverse problems, because empirical covariance matrix of ensemble couples ensemble members together.

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2. EnKF for Inverse Problems

Main point: Iterative EnKF as approximation of Sequential Monte Carlo (SMC) method for IPs. Let

- $N \in \mathbb{N}$ denote final discrete time,
- $h = N^{-1}$ denote time step,
- $1 \leq n \leq N$ denote discrete time.

For posterior distribution μ in (1), define probability measure at time n by

$$\mu_n(du) \propto \exp\left(-nh\Phi(u;y)\right)\mu_0(du),$$

so terminal measure $\mu_N = \mu$ equals desired posterior. Then

$$\mu_{n+1}(du) = \frac{1}{Z_n}\exp\left(-h\Phi(u;y)\right)\mu_n(du), \tag{2}$$

for normalisation constant

$$Z_n = \int \exp\left(-h\Phi(u)\right)\mu_n(du).$$

Let L be the nonlinear operator corresponding to Bayes' theorem that satisfies

$$\mu_{n+1} = L_n \mu_n. \tag{3}$$

2.1. Sequential Monte Carlo.

Sequential Monte Carlo. Idea: approximate μ_n by weighted sum of Dirac masses. Fix ensemble of J particles $(u_n^{(j)})_{j=1}^J \in \mathcal{X}$ and corresponding weights $(w_n^{(j)})_{j=1}^J$ (nonnegative, sum to one)

$$\mu_n \approx \sum_{j=1}^J w_n^{(j)} \delta_{u_n^{(j)}} \tag{3a}$$

All SMC methods consist of a way to evolve the particles and weights at time n forward in time. SMC used for Bayesian inverse problems; convergence proven for $J \to \infty$.

SMC can perform poorly when weights degenerate (one weight ≈ 1 and all others ≈ 0). EnKF tries to prevent degeneracy of weights by setting $w_n^{(j)} = J^{-1}$ for all $1 \leq n \leq N$, i.e. by equally weighting all the particles. This way, we only need to evolve the particles forward in time, since weights remain the same. Let $u_n = (u_n^{(j)})_{j=1}^J$.

Notation: for $u = (u^{(j)})_{j=1}^J \in \mathcal{X}^J$ be arbitrary, define sample means

$$\overline{u} = \frac{1}{J}\sum_{j=1}^J u^{(j)}, \quad \overline{\mathcal{G}} = \frac{1}{J}\sum_{j=1}^J \mathcal{G}(u^{(j)}). \tag{3a}$$

Return to SMC: how to evolve particles forward in time. Under substitution $\Gamma \mapsto h^{-1}\Gamma$ in (0b), the mapping takes the form of the "update step"

$$u_{n+1}^{(j)} = u_n^{(j)} + C^{up}(u_n)\left(C^{pp}(u_n) + h^{-1}\Gamma\right)^{-1}\left(y_{n+1}^{(j)} - \mathcal{G}(u_n^{(j)})\right), \quad j = 1, \dots, J. \tag{4}$$

where perturbed observation $y_{n+1}^{(j)}$ satisfies

$$y_{n+1}^{(j)} = y + \xi_{n+1}^{(j)}. \tag{4a}$$

where

$$\xi_{n+1}^{(j)} \sim N(0, h^{-1}\Sigma) \tag{4b}$$

for $\Sigma \in \{0, \Gamma\}$.

Define operator (empirical covariance matrix for fluctuation of $\mathcal{G}(u)$ about its mean)

$$C^{pp}(u) = \frac{1}{J}\sum_{j=1}^J \left(\mathcal{G}(u^{(j)} - \overline{\mathcal{G}}\right) \otimes \left(\mathcal{G}(u^{(j)}) - \overline{\mathcal{G}}\right) \tag{5}$$

and empirical covariance matrix of fluctuation of u about its mean with fluctuation of $\mathcal{G}(u)$ about its mean

$$C^{up}(u) = \frac{1}{J}\sum_{j=1}^J \left(u^{(j)} - \overline{u}\right) \otimes \left(\mathcal{G}(u^{(j)}) - \overline{\mathcal{G}}\right). \tag{6}$$

Main message: formulation of EnKF as SMC algorithm with equal weights and particles evolving according to (4), (5), (6).

Invariant subspace property of EnKF:

Lemma 2.1. *If $\mathcal{S} = span\left\{u_0^{(j)},\ j = 1, \ldots, J\right\}$, then $u_n^{(j)} \in \mathcal{S}$ for all $(n, j) \in \mathbb{N} \times \{1, \ldots, J\}$.*

3. Continuous time limit

Limit: send parameter h appearing in (2) to zero.

3.1. **Nonlinear problem.** Assume: $u_n \approx u(nh)$ in (4) in the limit $h \to 0$. Then update step (4) can be written as time-stepping scheme

$$\begin{aligned} u_{n+1}^{(j)} &= u_n^{(j)} + hC^{up}(u_n)\left(hC^{pp}(u_n) + \Gamma\right)^{-1}(y - \mathcal{G}(u_n^{(j)}) + \xi_{n+1}^{(j)}) \\ &= u_n^{(j)} + hC^{up}(u_n)\left(hC^{pp}(u_n) + \Gamma\right)^{-1}\underbrace{(y - \mathcal{G}(u_n^{(j)}) + h^{-1/2}\Sigma^{1/2}\zeta_{n+1}^{(j)})}_{=:arg} \end{aligned}$$

using (4a) and (4) in the first equation, and using (4b) in the second equation with $\zeta_{n+1}^{(j)} \sim N(0, I)$. Assuming that the operator $\mathcal{A}^h(u_n) := C^{up}(u_n)\left(hC^{pp}(u_n) + \Gamma\right)^{-1}$ acts linearly on arg, rearranging the last equation yields

$$u_{n+1}^{(j)} = u_n^{(j)} + h\mathcal{A}^h(y - \mathcal{G}(u_n^{(j)})) + \mathcal{A}^h\left(h^{1/2}\Sigma^{1/2}\right)\zeta_{n+1}^{(j)}.$$

Since $\mathcal{A}^h(u_n) \to C^{up}(u_n)\Gamma^{-1}$ as $h \to 0$, the limiting equation as $h \to 0$ (if it exists) is the system of coupled Ito SDEs

$$du_t^{(j)} = C^{up}(u_t)\Gamma^{-1}(y - \mathcal{G}(u_t^{(j)}))dt + C^{up}(u_t)\Gamma^{-1}\Sigma^{1/2}dW_t. \tag{7}$$

(coupled because $C^{up}(u_t)$ depends on $u_t^{(j)}$ for all j).

Define inner product

$$\langle\cdot,\cdot\rangle_\Gamma := \left\langle\Gamma^{-1/2}\cdot, \Gamma^{-1/2}\cdot\right\rangle_{\mathcal{Y}} \tag{8}$$

and let $W^{(j)}$ be independent, $\mathcal{X}$-valued cylindrical Brownian motions. Then by (6) and definition of tensor product, we may rewrite (7) as

$$du_t^{(j)} = \frac{1}{J}\sum_{k=1}^{J}\left\langle\mathcal{G}(u_t^{(k)}) - \overline{\mathcal{G}}_t, \left[y - \mathcal{G}(u_t^{(j)})\right]dt + \Sigma^{1/2}dW_t^{(j)}\right\rangle_\Gamma\left(u_t^{(k)} - \overline{u}_t\right) \tag{9}$$

with $\overline{u}_t$ and $\overline{\mathcal{G}}_t$ defined as in (3a) for the ensemble u_t.

3.2. **Linear noise-free case.** Suppose $\mathcal{G}h = Ah$ for linear operator $A : \mathcal{X} \to \mathcal{Y}$, and $\Sigma \equiv 0$. Then (9) becomes

$$du_t^{(j)} = \frac{1}{J}\sum_{k=1}^{J}\left\langle A(u_t^{(k)} - \overline{u}_t), y - Au_t^{(j)}\right\rangle_\Gamma(u_t^{(k)} - \overline{u}_t). \tag{10}$$

Given empirical covariance operator

$$C(u) := \frac{1}{J}\sum_{j=1}^{J}\left(u^{(k)} - \overline{u}\right)\otimes\left(u^{(k)} - \overline{u}\right),$$

(10) becomes

$$du_t^{(j)} = -C(u_t)D_u\Phi(u_t^{(j)}; y)dt \tag{11}$$

for data-model misfit

$$\Phi(u; y) = \frac{1}{2}\left\|\Gamma^{-1/2}(y - Au)\right\|_{\mathcal{Y}}^2.$$

Interpretation: Each particle $u_t^{(j)}$ performs gradient descent for $\Phi(\cdot\ ; y)$, where the gradient is preconditioned by the empirical covariance operator C. The preconditioning for each gradient flow is the same. Preconditioning makes gradient flow nonlinear, even though $\mathcal{G} = A$ is linear. Since C is positive semidefinite,

$$\frac{d}{dt}\Phi(u_t; y) \leq 0.$$

Question (global existence of gradient flow): does a solution $(u_t)_{0\leq t\leq T}$ exist for all $T > 0$?

4. Asymptotic behaviour in linear setting

Recall $A : \mathcal{X} \to \mathcal{Y}$ is linear.

4.1. **Noise-free case.** Suppose data y is image of truth $u^\dagger \in \mathcal{X}$ under A. Define: deviation of particle / ensemble member from ensemble mean

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

deviation of particle / ensemble member from truth underlying data

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

and matrices $E, R, F \in \mathbb{R}^{J\times J}$ by

$$E_{ij} = \left\langle Ae^{(i)}, Ae^{(j)} \right\rangle_\Gamma, \quad R_{ij} = \left\langle Ar^{(i)}, Ar^{(j)} \right\rangle_\Gamma, \quad F_{ij} = \left\langle Ar^{(j)}, Ae^{(j)} \right\rangle_\Gamma.$$

Properties

- E, R symmetric
- $E(0) = X\Lambda(0)X^\top$ for X orthogonal matrix of eigenvectors of $E(0)$,
- $E1 = F1 = 0$ for vector of 1's in $\mathbb{R}^J$.

Theorem 4.1. [1, Theorem 2] *Let* $\mathcal{X}_0 = span\left\{u_0^{(j)},\ 1 \le j \le J\right\}$. *Then (10) has a unique solution* $u^{(j)}(\cdot) \in C([0,\infty); \mathcal{X}_0)$ *for* $1 \le j \le J$.

Interpretation: invariant subspace property holds for continuous case (compare with Lemma 2.1).

Proof. (Sketch only): RHS of (11) is locally Lipschitz $\rightsquigarrow$ local existence in $C([0,T); \mathcal{X}_0$ for some $T > 0$ since $\dim \mathcal{X}_0 < \infty$. Can show that E_t and F_t are bounded by a constant depending on u_0 but not on $t \rightsquigarrow$ global bound on u with constant depending on u_0 and growing exponentially with $t \rightsquigarrow$ global existence. □

Next result show ensemble collapse to mean at algebraic rate. Rate slows down linearly as ensemble size J increases.

Theorem 4.2. [1, Theorem 3] *The matrix-valued process converges to zero, with* $\|E_t\| = O(J^{-1}t)$.

Proof. (Sketch only) Can show that

$$\frac{dE}{dt} = -\frac{2}{J}E^2, \quad E_0 = X\Lambda(0)X^\top.$$

with $\Lambda(0) = \operatorname{diag}(\lambda_0^{(1)}, \dots \lambda_0^{(J)})$. Then

$$E_t = X\Lambda(t)X^\top,$$

with k-th diagonal entry of $\Lambda(t)$ being $(2t/J + \lambda^(k)_0)^{-1}$ if $\lambda_0^{(k)} \neq 0$ and is zero otherwise. □

Theorem 4 in paper characterises relation between approximation quality of initial ensemble $(u_0^{(j)})_{j=1}^J$ and convergence behaviour of residuals $(r_t^{(j)})_{t\ge 0}$ for $1 \le j \le J$. Roughly: under suitable conditions, $Ar_t^{(j)}$ decomposes as orthogonal sum of terms in span of $(Ae_0^{(j)})_{j=1}^J$ and orthogonal complement of this span in $\langle\cdot,\cdot\rangle_\Gamma$. Terms in the span converge to zero as $t \to \infty$ for all j; terms in orthogonal complement remain constant.

4.2. **Noisy observational data.** Suppose (0a) holds, where $\mathcal{G} = A$, additive noise $\eta \in \mathbb{R}^K$. Similar results as Theorems 2 and 3 above hold.

References

1. Schillings, Claudia and Stuart, Andrew M., *Analysis of the Ensemble Kalman Filter for Inverse Problems.*
2. T. J. Sullivan, *Uncertainty Quantification*, Springer, Heidelberg, 2015.

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