Multilevel ensemble Kalman filtering

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11th International EnKF Workshop, Ulvik







Overview

- Problem description
- 2 Ensemble Kalman Filtering
- 3 Multilevel ensemble Kalman filtering
- 4 Numerical examples
- 5 Extension of MLEnKF and conclusion

Problem description

Consider the underlying and unobservable dynamics

$$u_{n+1} = \underbrace{u_n + \int_n^{n+1} a(u_t) dt + \int_n^{n+1} b(u_t) dW(t)}_{=:\Psi(u_n)}$$

with $u_n \in \mathbb{R}^d$, and Lipschitz continuous $a : \mathbb{R}^d \to \mathbb{R}^d$ and $b : \mathbb{R}^d \to \mathbb{R}^{d \times \hat{d}}$.

And noisy observations

$$y_n = Hu_n + \gamma_n,$$

with i.i.d. $\gamma \sim N(0,\Gamma)$ and $H \in \mathbb{R}^{k \times d}$.

Objective: Let $Y_n := (y_1, y_2, ..., y_n)$ and let Y_n^{obs} be a sequence of *fixed* observations. Construct an efficient method for tracking $u_n|(Y_n = Y_n^{\text{obs}})$. That is approximate

$$\mathbb{E}\left[\phi(u_n)|Y_n=Y_n^{\mathrm{obs}}\right]$$

for an observable $\phi: \mathbb{R}^d \to \mathbb{R}$.

Abuse of notation: will write $u_n|Y_n^{\text{obs}}$ to represent $u_n|(Y_n=Y_n^{\text{obs}})$.

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Ensemble Kalman Filtering

Predict

1 Compute (numerical solutions of) M particle paths one step forward

$$\widehat{v}_{n+1,i} = \Psi(v_{n,i}, \omega_i)$$
 for $i = 1, 2, \dots, M$.

2 Compute sample mean and covariance

$$\begin{split} \widehat{m}_{n+1}^{\text{MC}} &= E_M[\widehat{v}_{n+1}] \\ \widehat{C}_{n+1}^{\text{MC}} &= \text{Cov}_M[\widehat{v}_{n+1}] \end{split}$$

where
$$E_M[\widehat{v}_{n+1}] := \frac{1}{M} \sum_{i=1}^{M} \widehat{v}_{n+1,i}$$

and
$$\operatorname{Cov}_M[\widehat{v}_{n+1}] := E_M[\widehat{v}_{n+1}\widehat{v}_{n+1}^T] - E_M[\widehat{v}_{n+1}](E_M[\widehat{v}_{n+1}])^T$$
.

Ensemble Kalman Filtering II

Update

Generate signal observations for the ensemble of particles

$$\tilde{y}_{n+1,i} = y_{n+1}^{\text{obs}} + \gamma_{n+1,i} \quad \text{for } i = 1, 2 \dots, M,$$

with i.i.d. $\gamma_{n+1,1} \sim N(0,\Gamma)$.

2 Use signal observations to update particle paths

$$\begin{aligned} v_{n+1,i} &= (I - \underbrace{K_{n+1}^{\text{MC}}H})\widehat{v}_{n+1,i} + \underbrace{K_{n+1}^{\text{MC}}}\widehat{y}_{n+1,i}, \\ \text{where} \quad \underbrace{K_{n+1}^{\text{MC}}} &= \widehat{C}_{n+1}^{\text{MC}}H^T(H\widehat{C}_{n+1}^{\text{MC}}H^T + \Gamma)^{-1}. \end{aligned}$$

Note: After the first step, all particles are correlated due to K_{n+1}^{MC} .

From EnKF to mean field EnKF

For studying convergence properties of EnKF it is useful to introduce the mean field EnKF (MFEnKF)

$$\Pr \begin{cases} \widehat{\boldsymbol{v}}_{n+1,i}^{\mathrm{MF}} &= \boldsymbol{\Psi}(\boldsymbol{v}_{n,i}^{\mathrm{MF}}, \boldsymbol{\omega}_i) \\ \widehat{\boldsymbol{m}}_{n+1}^{\mathrm{MF}} &= \mathbb{E}\left[\widehat{\boldsymbol{v}}_{n+1,i}^{\mathrm{MF}}\right] \\ \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MF}} &= \mathrm{Cov}[\widehat{\boldsymbol{v}}_{n+1,i}^{\mathrm{MF}}], \end{cases} \quad \mathsf{Up} \begin{cases} K_{n+1}^{\mathrm{MF}} &= \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MF}} \boldsymbol{H}^{T} (\boldsymbol{H} \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MF}} \boldsymbol{H}^{T} + \boldsymbol{\Gamma})^{-1} \\ \widetilde{\boldsymbol{y}}_{n+1,i} &= \boldsymbol{y}_{n+1}^{\mathrm{obs}} + \gamma_{n+1,i} \\ \boldsymbol{v}_{n+1,i}^{\mathrm{MF}} &= (\boldsymbol{I} - K_{n+1}^{\mathrm{MF}} \boldsymbol{H}) \boldsymbol{v}_{n+1,i}^{\mathrm{MF}} + K_{n+1}^{\mathrm{MF}} \widetilde{\boldsymbol{y}}_{n+1,i}. \end{cases}$$

and in comparison, EnKF

$$\Pr \begin{cases} \widehat{\boldsymbol{v}}_{n+1,i} &= \boldsymbol{\Psi}(\boldsymbol{v}_{n,i}, \boldsymbol{\omega}_i) \\ \widehat{\boldsymbol{m}}_{n+1}^{\mathrm{MC}} &= \boldsymbol{E}_{\boldsymbol{M}}[\widehat{\boldsymbol{v}}_{n+1}] \\ \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MC}} &= \operatorname{Cov}_{\boldsymbol{M}}[\widehat{\boldsymbol{v}}_{n+1}] \end{cases} \ \mathsf{Up} \begin{cases} K_{n+1}^{\mathrm{MC}} &= \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MC}} \boldsymbol{H}^{T} (\boldsymbol{H} \widehat{\boldsymbol{C}}_{n+1}^{\mathrm{MC}} \boldsymbol{H}^{T} + \boldsymbol{\Gamma})^{-1} \\ \widetilde{\boldsymbol{y}}_{n+1,i} &= \boldsymbol{y}_{n+1}^{\mathrm{obs}} + \gamma_{n+1,i} \\ \boldsymbol{v}_{n+1,i} &= (\boldsymbol{I} - K_{n+1}^{\mathrm{MC}} \boldsymbol{H}) \widehat{\boldsymbol{v}}_{n+1,i} + K_{n+1}^{\mathrm{MC}} \widetilde{\boldsymbol{y}}_{n+1,i}. \end{cases}$$

- When underlying dynamics is linear with Gaussian additive noise and u_0 Gaussian, it holds that $\mu_n^{\mathrm{MF}}(dx) = \mathbb{P}\left(u_n \in dx | Y_n^{\mathrm{obs}}\right)$, where $\mu_n^{\mathrm{MF}} = \mathrm{Law}(v_{n,i}^{\mathrm{MF}})$.
- In nonlinear settings, we use as approximation goal

$$\int_{\mathbb{R}^d} \phi(x) \mu_n^{\mathrm{MF}}(dx). \quad \mathsf{NB!}(\mu_n^{\mathrm{MF}} \neq \mathbb{P}\left(u_n \in \cdot | Y_n^{\mathrm{obs}}\right).)$$

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Convergence of EnKF

Theorem 1 (Le Gland et al. (2009))

Consider the dynamics and observations,

$$u_{n+1} = f(u_n) + \xi_{n+1}, \quad \xi_{n+1} \sim N(0, \Sigma),$$

 $y_{n+1} = Hu_{n+1} + \gamma_{n+1}, \quad \gamma_{n+1} \sim N(0, \Gamma),$

 $\max(|f(x)-f(x')|, |\phi(x)-\phi(x')|) \le C|x-x'|(1+|x|^s+|x'|^s), \text{ for an } s \ge 0.$

and assume $u_0 \in L^p(\Omega)$ for any $p \geq 1$, and that

and assume
$$u_0 \in L$$
 (31) for any $p \ge 1$, and the

Then, for the EnKF update ensemble
$$\{v_{n,i}\}_{i=1}^{M}$$
,

for any order $p \ge 1$ and finite n.

$$\sup_{M\geq 1} \sqrt{M} \left(\mathbb{E}\left[\left| \sum_{i=1}^{M} \frac{\phi(v_{n,i})}{M} - \int_{\mathbb{R}^d} \phi(x) \mu_n^{\mathrm{MF}}(dx) \right|^p \right] \right)^{1/p} < \infty.$$

Computational cost of EnKF

To meet the constraint

$$\left(\mathbb{E}\left[\left|\sum_{i=1}^{M} \frac{\phi(v_{n,i})}{M} - \int_{\mathbb{R}^d} \phi(x) \mu_n^{\mathrm{MF}}(dx)\right|^p\right]\right)^{1/p} = \mathcal{O}(\epsilon),$$

one thus needs ensemble of size $M = \mathcal{O}(\epsilon^{-2})$.

- How does the computational cost increase if the EnKF dynamics has to be sampled using a numerical solver for which $|\mathbb{E}[\Psi_{\Delta t} \Psi]| = \mathcal{O}(\Delta t^{\alpha})$?
- Short answer (under additional assumptions): the cost increases to $\mathcal{O}(\epsilon^{-(2+1/\alpha)})$.

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Multilevel EnKF (MLEnKF)

Prediction

■ Compute an ensemble of particle paths on a hierarchy of accuracy levels

$$\widehat{v}_{n+1,i}^{\ell-1} = \Psi^{\ell-1}(v_{n,i}^{\ell-1}, \omega_{\ell,i}), \quad \widehat{v}_{n+1,i}^{\ell} = \Psi^{\ell}(v_{n,i}^{\ell}, \omega_{\ell,i}),$$

for the levels $\ell = 0, 1, \dots, L$ and $i = 1, 2, \dots, M_{\ell}$.

■ Multilevel approximation of mean and covariance matrices:

$$\widehat{m}_{n+1}^{\mathrm{ML}} = \sum_{\ell=0}^{L} E_{\mathbf{M}_{\ell}} [\widehat{v}_{n+1}^{\ell} - \widehat{v}_{n+1}^{\ell-1}],$$

$$\widehat{C}_{n+1}^{\mathrm{ML}} = \sum_{\ell=0}^{L} \mathrm{Cov}_{\mathbf{M}_{\ell}} [\widehat{v}_{n+1}^{\ell}] - \mathrm{Cov}_{\mathbf{M}_{\ell}} [\widehat{v}_{n+1}^{\ell-1}]$$

Notice the telescoping properties $\mathbb{E}\left[\widehat{m}_{n+1}^{\mathrm{ML}}\right] = \mathbb{E}\left[\widehat{v}_{n+1}^{L}\right]$ and $\mathbb{E}\left[\widehat{C}_{n+1}^{\mathrm{ML}}\right] = \mathrm{Cov}(\widehat{v}_{n+1}^{L}) + O(1/M_{L})$.

MLEnKF update step

Update

Convergence of MLEnKF

For observables $\phi: \mathbb{R}^d \to \mathbb{R}$, introduce notation

$$\mu_n^{\mathrm{ML}}(\phi) := \sum_{\ell=0}^L rac{1}{M_\ell} \sum_{i=1}^{M_\ell} \phi(v_{n,i}^\ell) - \phi(v_{n,i}^{\ell-1}).$$

and

$$\mu_n^{\mathrm{MF}}(\phi) := \int_{\mathbb{R}^d} \phi(x) \mu_n^{\mathrm{MF}}(dx).$$

Question: Under what assumptions and at what cost can one achieve

$$\|\mu_n^{\mathrm{ML}}(\phi) - \mu_n^{\mathrm{MF}}(\phi)\|_{L^p(\Omega)} = \mathcal{O}(\epsilon)$$
?

Assumption 1

Consider the dynamics

$$u_{n+1} = \Psi(u_n) = u_n + \int_n^{n+1} a(u_t)dt + \int_n^{n+1} b(u_t)dW(t), \quad n = 0, 1, \dots$$

with $u_0 \in \bigcap_{p \in \mathbb{N}} L^p(\Omega)$ and a hierarchy of numerical solvers $\{\Psi^\ell\}_{\ell=0}^{\infty}$. Furthermore, assume the observable $\phi : \mathbb{R}^d \to \mathbb{R}$ satisfies

$$|\phi(x) - \phi(x')| \le C|x - x'|(1 + |x|^s + |x'|^s)$$
, for an $s \ge 0$,

that there exists positive constants $\alpha, \beta > 0$, and an positive exponentially increasing sequence $\{N_\ell\}_\ell$ such that for all $u, v \in \cap_{p \in \mathbb{N}} L^p(\Omega)$,

- (i) $\left| \mathbb{E} \left[\phi(\Psi^{\ell}(u)) \phi(\Psi(v)) \right] \right| \lesssim N_{\ell}^{-\alpha}$, provided that $\left| \mathbb{E}[u-v] \right| \lesssim N_{\ell}^{-\alpha}$,
- (ii) $\|\phi(\Psi^{\ell}(v)) \phi(\Psi^{\ell-1}(v))\|_p \lesssim N_{\ell}^{-\beta}$, for all $p \geq 1$,
- (iii) Cost $(\Psi^{\ell}(v)) \lesssim N_{\ell}$.

Theorem 2 (MLEnKF accuracy vs. cost)

Suppose Assumption 1 holds. Then, for any $\epsilon>0$ and $p\geq 2$, there exists an L>0 and $\{M_\ell\}_{\ell=0}^L$ such that

$$\|\mu_n^{\mathrm{ML}}(\phi) - \mu_n^{\mathrm{MF}}(\phi)\|_{p} \lesssim \epsilon.$$

And

$$\operatorname{Cost}\left(\operatorname{MLEnKF}\right) \lesssim \begin{cases} \left(|\log(\epsilon)|^{1-n} \epsilon \right)^{-2}, & \text{if } \beta > 1, \\ \left(|\log(\epsilon)|^{1-n} \epsilon \right)^{-2} |\log(\epsilon)|^{3}, & \text{if } \beta = 1, \\ \left(|\log(\epsilon)|^{1-n} \epsilon \right)^{-\left(2 + \frac{1-\beta}{\alpha}\right)}, & \text{if } \beta < 1. \end{cases}$$
(1)

In comparison

$$\|\mu_n^{
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In comparison,

$$\|\mu_n^{\text{EnKF}}(\phi) - \mu_n^{\text{MF}}(\phi)\|_p \lesssim \epsilon,$$

is achieved at cost $\mathcal{O}\left(\epsilon^{-\left(2+\frac{1}{\alpha}\right)}\right)$.

Central idea in the proof

Introduce

$$\mu_n^{\text{MLMF}}(\phi) := \sum_{\ell=0}^L \frac{1}{M_\ell} \sum_{i=1}^{M_\ell} \phi(v_n^{\text{MF},\ell}(\omega_{i,\ell})) - \phi(v_n^{\text{MF},\ell-1}(\omega_{i,\ell}))$$
$$\mu_n^{\text{MF},L}(\phi) := \mathbb{E}\left[\phi(v_n^{\text{MF},L})\right],$$

and bound MLEnKF error by

$$\begin{split} &\|\mu_{n}^{\mathrm{ML}}(\phi) - \mu_{n}^{\mathrm{MF}}(\phi)\|_{p} \leq \|\mu_{n}^{\mathrm{ML}}(\phi) - \mu_{n}^{\mathrm{MLMF}}(\phi)\|_{p} \\ &+ \|\mu_{n}^{\mathrm{MLMF}}(\phi) - \mu_{n}^{\mathrm{MF},\mathrm{L}}(\phi)\|_{p} + \|\mu_{n}^{\mathrm{MF},\mathrm{L}}(\phi) - \mu_{n}^{\mathrm{MF}}(\phi)\|_{p} \\ &\leq c \sum_{\ell=0}^{L} \left[\|v_{n}^{\ell} - v_{n}^{\mathrm{MF},\ell}\|_{\hat{p}} + \frac{\|v_{n}^{\mathrm{MF},\ell} - v_{n}^{\mathrm{MF},\ell-1}\|_{\hat{p}}}{M_{\ell}^{1/2}} \right] + \left| \mathbb{E} \left[\phi(v_{n}^{\mathrm{MF},\mathrm{L}}) - \phi(v_{n}^{\mathrm{MF}}) \right] \right| \\ &\leq c \left(\epsilon + \sum_{\ell=0}^{L} M_{\ell}^{-1/2} N_{\ell}^{-\beta/2} + N_{L}^{-\alpha} \right) \end{split}$$

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Numerical example

Underlying dynamics is the Ornstein-Uhlenbeck SDE

$$du = -udt + 0.5dW(t),$$

with a set of observations

$$y_n = u_n + \gamma_n$$
, i.i.d. $\gamma_n \sim N(0, 0.04)$

Solvers: Hierarchy of Milstein solution operators $\{\Psi_\ell\}_{\ell=0}^L$ with $\Delta t^\ell = \mathcal{O}\left(2^{-\ell}\right)$.

Compare the approximation errors for the observable $\phi(x)=x$ in terms of the RMSE

$$\sqrt{\sum_{n=1}^{N} \frac{|\mu_n^{\mathrm{ML}}(\phi) - \mu_n^{\mathrm{MF}}(\phi)|^2}{N}}.$$

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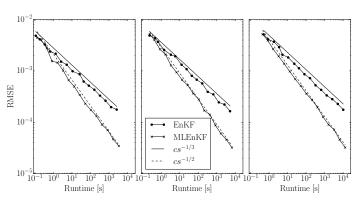
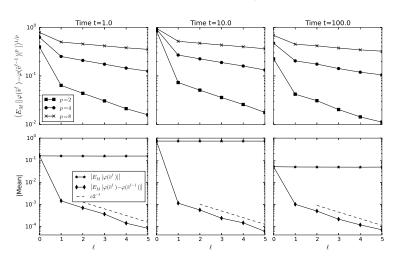


Figure: From left to right: N = 100,200 and 400.

OU example

Consider less regular observable $\phi(x) := \mathbf{1}\{x > 0.1\}$. Outside the scope of our theory since it does not hold that

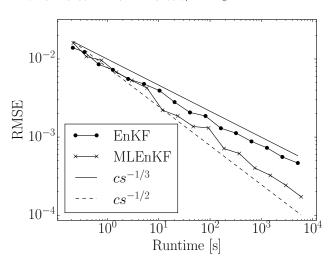
$$\|\phi(\Psi^{\ell}(v)) - \phi(\Psi^{\ell-1}(v))\|_p \lesssim N_{\ell}^{-\beta}, \quad \forall p \geq 2.$$



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Extension of MLEnKF to infinite dimensional state spaces

- Work in progress with Alexey Chernov, Kody Law, Fabio Nobile and Tempone.
- Infinite dimensional stochastic dynamics:

$$u_{n+1} = \Psi(u_n)$$

where $u_n \in L^p(\Omega; \mathcal{H})$ with $\mathcal{H} = \operatorname{Span}(\{\nu_i\}_{i=1}^{\infty})$, and $\Psi: L^p(\Omega; \mathcal{H}) \to L^p(\Omega; \mathcal{H})$.

And finite dimensional observations

$$y_n = Hu_n + \gamma_n,$$

with linear $H:\mathcal{H} \to \mathbb{R}^m$

Introduce nested hierarchy of Hilbert spaces

$$\mathcal{H}_0 \subset \mathcal{H}_1 \subset \ldots \subset \mathcal{H}_\infty = \mathcal{H},$$

where $\mathcal{H}_{\ell} = \operatorname{Span}(\{\nu_i\}_{i=1}^{N_{\ell}})$ and work with a hierarchy of solvers

$$\Psi^{\ell}: L^p(\Omega; \mathcal{H}_{\ell}) \to L^p(\Omega; \mathcal{H}_{\ell}).$$

Conclusion

- Extended EnKF to multilevel EnKF.
- Verified asymptotic efficiency gain for approximations of expectation of observables. We hope to improve result further!
- Further extension of MLEnKF to infinite dimensional state space is work in progress.

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