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Multilevel and multi-index EnKF algorithms

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Overview

1. Problem description and motivation
2. New Multilevel EnKF (MLEnKF)
3. Multi-index EnKF (MIEnKF)
4. Conclusion

Problem description and motivation

Problem description

Consider the state-space model with additive Gaussian noise

$$\left.\begin{array}{lr} u_{n+1} = \Psi(u_n) & \text{Markov chain} \\ y_{n+1} = Hu_{n+1} + \gamma_{n+1} & \text{observation} \end{array}\right\} \quad n = 0, 1, \ldots$$

with non-linear $\Psi : \mathbb{R}^d \times \Omega \to \mathbb{R}^d$, linear $H \in \mathbb{R}^{m \times d}$ and

$$\gamma_j \overset{iid}{\sim} N(0, \Gamma) \quad \text{with} \quad \{\gamma_j\} \perp \{u_j\}$$

on filtered probability space $(\Omega, \{\mathcal{F}_t\}_{t \geq 0}, \mathcal{F}, \mathbb{P})$.

Objective: For a given **fixed observation** $Y_n := (y_1, ..., y_n)$, approximate $u_n | Y_n$ weakly by an efficient EnKF method.

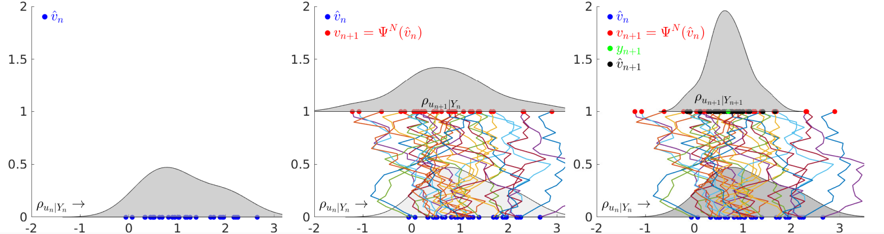
Dynamics constraint: Ψ needs to be sampled by numerical methods, e.g., from an SDE

$$\Psi(u_n) = u_n + \int_0^1 a(u_{n+s}) ds + \int_0^1 b(u_{n+s}) dW_{s+n},$$

Ensemble Kalman filtering (EnKF)

Notation: P ensemble size, N discretization parameter for Ψ.

Prediction: Given ensemble $\hat{v}_{n,1}, \dots \hat{v}_{n,P}$ with $\hat{v}_{n,i} \sim \mathbb{P}_{u_n|Y_n}$, approximate $\mathbb{P}_{u_{n+1}|Y_n}$ by the empirical measure of $v_{n+1,i} = \Psi^N(v_{n,i})$.



Update: Assimilate observation y_{n+1} into $v_{n+1,i}$ by

$$\hat{v}_{n+1,i} = (I - K_{n+1}H)v_{n+1,i} + K_{n+1}(y_{n+1} + \gamma_{n+1,i}).$$

$$\mathbb{P}_{u_{n+1}|y_{1:n+1}} \approx \mu_{n+1}^{N,P} := \frac{1}{P}\sum_{k=1}^{P} \delta_{\hat{v}_{n+1,i}}.$$

Cost of EnKF

For a quantity of interest (QoI) $\varphi : \mathbb{R}^d \to \mathbb{R}$, at each time n,

EnKF estimator:

$$\mathbb{E}[\varphi(u_n)|Y_n] \approx \int_{\mathbb{R}^d} \varphi(x)\, \mu_n^{N,P}(\mathrm{d}x) =: \mu_n^{N,P}[\varphi]$$

Theorem. [Le Gland et al. (2009); H.Hoel et al. (2016)]

Under sufficient regulatory assumptions, for any $p \geq 2$ and $n \geq 0$ we achieve

$$\|\mu_n^{N,P}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_{L^P(\Omega)} = \mathcal{O}(\epsilon)$$

at the compuational cost bounded by

$$\textbf{Cost}(\mu_n^{N,P}[\varphi]) \eqsim P \times \underbrace{\mathrm{Cost}(\Psi_n^N(v))}_{\eqsim N} = \mathcal{O}(\epsilon^{-3}).$$

- Question: Can we improve the cost rate of EnKF?
- Answer: Yes, by **Multilevel EnKF (MLEnKF).**

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Multilevel EnKF ideas

MLEnKF (Original, 2016):

$$\mathbb{E}[\varphi(u_n)|Y_n] \approx \mu_n^{\mathrm{ML}}[\varphi] := \sum_{\ell=0}^{L} (\mu_n^{N_\ell, P_\ell, K_n^{ML}} - \mu_n^{N_{\ell-1}, P_\ell, K_n^{ML}})[\varphi; \omega_\ell]$$

for $N_\ell \eqsim 2^\ell$, P_ℓ exponentially decreasing and $(\mu_n^{N_\ell, P_\ell, K_n^{ML}} - \mu_n^{N_{\ell-1}, P_\ell, K_n^{ML}})[\varphi; \omega_\ell]$ coupled through using the same Kalman gain and driving noise.

MLEnKF (New, 2020):

$$\mathbb{E}[\varphi(u_n)|Y_n] \approx \mu_n^{\mathrm{ML}^{\mathrm{NEW}}}[\varphi]$$

$$:= \sum_{\ell=0}^{L} \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} (\mu_n^{N_\ell, P_\ell, K_n^{\ell}} - \mu_n^{N_{\ell-1}, P_\ell, K_n^{\ell-1}})[\varphi; \omega_{\ell,m}]$$

for $N_\ell \eqsim 2^\ell$, $P_\ell \eqsim 2^\ell$, M_ℓ exponentially decreasing and $(\mu_n^{N_\ell, P_\ell, K_n^{\ell}} - \mu_n^{N_{\ell-1}, P_\ell, K_n^{\ell-1}})[\varphi; \omega_{\ell,m}]$ pairwise-coupled samples of EnKF estimators at different resolution levels.

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for $N_\ell \eqsim 2^\ell$, $P_\ell \eqsim 2^\ell$, M_ℓ exponentially decreasing and $(\mu_n^{N_\ell, P_\ell, K_n^{\ell}} - \mu_n^{N_{\ell-1}, P_\ell, K_n^{\ell-1}})[\varphi; \omega_{\ell,m}]$ pairwise-coupled samples of EnKF estimators at different resolution levels.

New Multilevel EnKF (MLEnKF)

Multilevel sample estimators

1. Introduce a hierarchy of numerical solvers $\{\Psi^{N_\ell}\}_{\ell=0}^{\infty}$ with $N_\ell \eqsim 2^\ell$.
2. Note that

$$\mathbb{E}\left[\Psi^{N_L}(v)\right] = \sum_{\ell=0}^{L} \mathbb{E}\left[\Psi^{N_\ell}(v) - \Psi^{N_{\ell-1}}(v)\right], \quad (\text{with } \Psi^{N_{-1}}(\cdot) := 0),$$

3. Gives rise to the multilevel Monte Carlo estimator (Giles 2008),

$$\mathbb{E}\left[\Psi^{N_L}(v)\right] \approx \sum_{\ell=0}^{L} E_{P_\ell}[\Psi^{N_\ell}(v) - \Psi^{N_{\ell-1}}(v)],$$

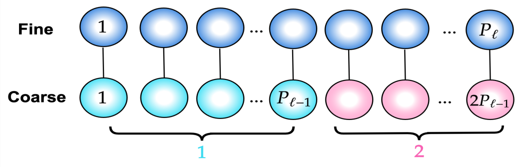
and ... the MLEnKF estimator (H.Hoel et.al., 2016)

$$\mu_n^{\mathrm{ML}}[\varphi] := \sum_{\ell=0}^{L} (\mu_n^{N_\ell, P_\ell} - \mu_n^{N_{\ell-1}, P_\ell})[\varphi]$$

An alternative MLEnKF method

New MLEnKF approach is based on *a sample average of independent and pairwise-coupled samples of EnKF estimators* at different resolution levels.

- **Pairwise coupling of particles.** Set $P_\ell = 2P_{\ell-1}$.



- For $\ell \geq 1$, denote an updated ensemble at time n coupled to the two coarser-level updated ensembles as follows

$$\hat{v}^{\ell}_{n,i} \xleftrightarrow{\text{coupling}} \begin{cases} \hat{v}^{\ell-1,1}_{n,i} & \text{if} \quad i \in \{1, \dots, P_{\ell-1}\}, \\ \hat{v}^{\ell-1,2}_{n,i-P_{\ell-1}} & \text{if} \quad i \in \{P_{\ell-1}+1, \dots, P_\ell\}. \end{cases}$$

- Impose the particle-wise shared initial condition:

$$\hat{v}^{\ell}_{0,i} = \begin{cases} \hat{v}^{\ell-1,1}_{0,i} & \text{if} \quad i \in \{1, \dots, P_{\ell-1}\} \\ \hat{v}^{\ell-1,2}_{0,i-P_{\ell-1}} & \text{if} \quad i \in \{P_{\ell-1}+1, \dots, P_\ell\}. \end{cases}$$

Prediction step

- Simulate for $i = 1, \dots, P_\ell$ on hierarchy levels $\ell = 0, 1, \dots, L$

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

- Compute sample covariances of the ensembles as follows

$$C^{\ell}_{n+1} = \overline{\mathrm{Cov}}[v^{\ell}_{n+1,1:P_\ell}], \; C^{\ell-1,1}_{n+1} = \overline{\mathrm{Cov}}[v^{\ell-1}_{n+1,1:P_{\ell-1}}], \; C^{\ell-1,2}_{n+1} = \overline{\mathrm{Cov}}[v^{\ell-1}_{n+1,P_{\ell-1}+1:P_\ell}]$$

Update step

- Compute the respective Kalman gains by formula[1]

$$K^{\ell}_{n+1} = \mathbf{K}(v^{\ell}_{n+1,1:P_\ell}), \quad K^{\ell-1,1}_{n+1} = \mathbf{K}(v^{\ell-1}_{n+1,1:P_{\ell-1}}), \quad K^{\ell-1,2}_{n+1} = \mathbf{K}(v^{\ell-1}_{n+1,P_{\ell-1}+1:P_\ell}).$$

- For hierarchy levels $\ell = 0, 1, \dots, L$, update the particles

$$\tilde{y}^{\ell}_{n+1,i} = y_{n+1} + \gamma^{\ell}_{n+1,i}, \qquad i = 1, \dots, P_\ell,$$

$$\hat{v}^{\ell}_{n+1,i} = (I - K^{\ell}_{n+1}H)v^{\ell}_{n+1,i} + K^{\ell}_{n+1}\tilde{y}^{\ell}_{n+1,i}, \qquad i = 1, \dots, P_\ell,$$

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$$\hat{v}^{\ell-1,2}_{n+1,i} = (I - K^{\ell-1,2}_{n+1}H)v^{\ell-1}_{n+1,i+P_{\ell-1}} + K^{\ell-1,2}_{n+1}\tilde{y}^{\ell}_{n+1,i+P_{\ell-1}}, \qquad i = 1, \dots, P_{\ell-1}.$$

[1] $\mathbf{K}(\mathbf{x}) = \overline{\mathrm{Cov}}[\mathbf{x}]H^{\mathsf{T}}(H\overline{\mathrm{Cov}}[\mathbf{x}]H^{\mathsf{T}} + \Gamma)^{-1}$

Prediction step

- Simulate for $i = 1, \dots, P_\ell$ on hierarchy levels $\ell = 0, 1, \dots, L$

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

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$$\hat{v}_{n+1,i}^{\ell-1,2} = (I - K_{n+1}^{\ell-1,2} H) v_{n+1,i+P_{\ell-1}}^{\ell-1} + K_{n+1}^{\ell-1,2} \tilde{y}_{n+1,i+P_{\ell-1}}^{\ell}, \qquad i = 1, ..., P_{\ell-1}.$$

[1] $\mathbf{K}(\mathbf{x}) = \overline{\mathrm{Cov}}[\mathbf{x}] H^{\mathsf{T}} (H \overline{\mathrm{Cov}}[\mathbf{x}] H^{\mathsf{T}} + \Gamma)^{-1}$

- **Pairwise coupling of EnKF estimators.** Correspondingly, define the fine-level EnKF estimator coupled to the two coarse-level EnKF estimators by

$$\mu_n^{N_\ell, P_\ell}[\varphi] := \sum_{i=1}^{P_\ell} \frac{\varphi(\hat{v}_{n,i}^\ell)}{P_\ell} \xleftrightarrow{\text{coupling}} \begin{cases} \mu_n^{N_{\ell-1}, P_{\ell-1}, 1}[\varphi] := \sum_{i=1}^{P_{\ell-1}} \frac{\varphi(\hat{v}_{n,i}^{\ell-1,1})}{P_{\ell-1}}, \\ \mu_n^{N_{\ell-1}, P_{\ell-1}, 2}[\varphi] := \sum_{i=1}^{P_{\ell-1}} \frac{\varphi(\hat{v}_{n,i}^{\ell-1,2})}{P_{\ell-1}}. \end{cases}$$

- Introduce a decreasing sequence $\{M_\ell\}_{\ell=0}^L \subset \mathbb{N}$ with M_ℓ representing the number of i.i.d. and pairwise-coupled EnKF estimators and define the new MLEnKF estimator as

$$\mu_n^{\mathrm{ML^{NEW}}}[\varphi] = \sum_{\ell=0}^{L} \sum_{m=1}^{M_\ell} \frac{\left(\mu_n^{N_\ell, P_\ell, m} - (\mu_n^{N_{\ell-1}, P_{\ell-1}, 1, m} + \mu_n^{N_{\ell-1}, P_{\ell-1}, 2, m})/2\right)[\varphi]}{M_\ell}.$$

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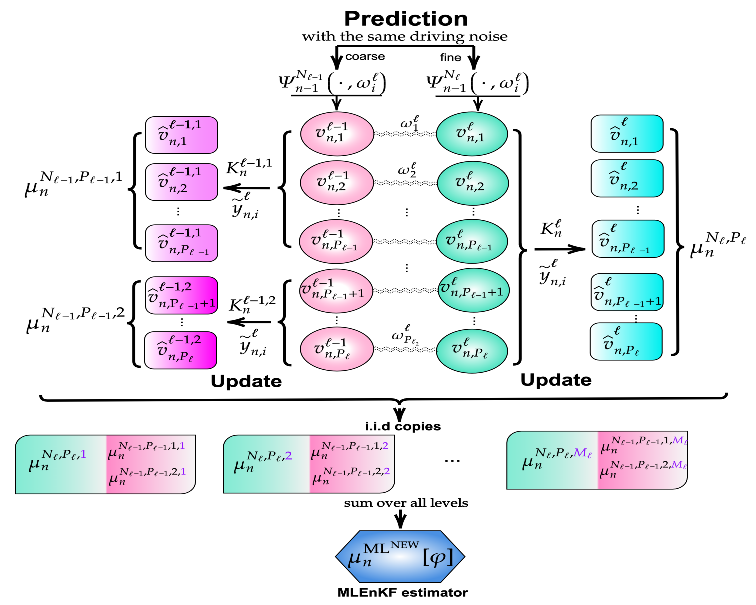
Visual description of couplings



Convergence of new MLEnKF

Theorem. (MLEnKF convergence)

Under sufficient regularity, for $\epsilon > 0$, there exists an $L(\epsilon) > 0$ and triplet of sequences $\{P_\ell\}$, $\{N_\ell\}$, $\{M_\ell\}$ such that

$$\|\mu_n^{\mathrm{ML}^{\mathrm{NEW}}}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_p = \mathcal{O}(\epsilon),$$

is achieved at cost

$$\mathrm{Cost}\left(\mu_n^{\mathrm{ML}^{\mathrm{NEW}}}\right) = \mathcal{O}(\epsilon^{-2})$$

! Compare with the original MLEnKF, where cost is

$$\mathrm{Cost}\left(\mu_n^{\mathrm{ML}}[\varphi]\right) = \mathcal{O}(|\log(\epsilon)|^{1-n}\epsilon^{-2}).$$

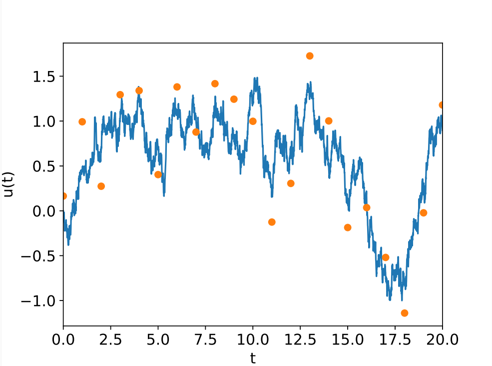
Numerical example

Stochastic dynamics in a double-well

$$u_{n+1} = \Psi(u_n) := \int_n^{n+1} -V'(u_t)dt + \int_n^{n+1} \frac{1}{2} dW_t, \qquad (1)$$

with the potential function and observations given by

$$V(u_t) = \frac{1}{2+4u_t^2} + \frac{u_t^2}{4}, \qquad y_{n+1} = u_{n+1} + 0.1\mathcal{N}(0,1)$$



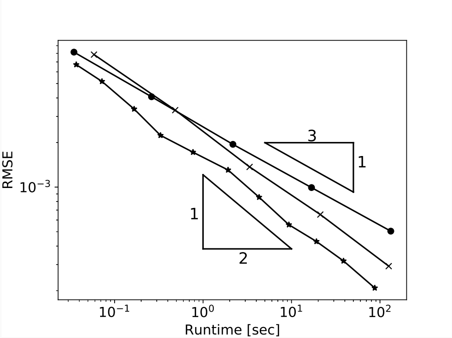


Figure 1: Runtime vs root-MSE for the QoI $\varphi(x) = x$. Original MLEnKF (solid-asterisked), new MLEnKF (solid-crossed) and EnKF (solid-bulleted).

Observation:

$$\|\mu_n^{\mathrm{EnKF}}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_{L^2(\Omega)} \lesssim \text{Runtime}^{-1/3},$$

$$\|\mu_n^{\mathrm{ML}}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_{L^2(\Omega)} \lesssim \text{Runtime}^{-1/2}.$$

Summary on new MLEnKF

Main motivations to develop the new MLEnKF:

- In many settings, the (theoretical) convergence results in the new MLEnKF is better than those obtained in the original MLEnKF.
- The approach is closer to classic EnKF $\implies$ easier to implement for practioners.
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Multi-index EnKF (MIEnKF)

A brief overview of Multi-index EnKF

- Introduce a multi-index $\boldsymbol{\ell} := (\ell_1, \ell_2) \in \mathbb{N}_0^2$.
- Define the four-coupled EnKF estimator using the first-order mixed difference:

$$\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi] := \Delta_2(\Delta_1 \mu_n^{N_{\ell_1}, P_{\ell_2}}[\varphi]) = \Delta_2(\mu_n^{N_{\ell_1}, P_{\ell_2}} - \mu_n^{N_{\ell_1 - 1}, P_{\ell_2}})[\varphi]$$

$$= \Bigg(\mu_n^{N_{\ell_1}, P_{\ell_2}} - \left(\mu_n^{N_{\ell_1}, P_{\ell_2 - 1}, 1} + \mu_n^{N_{\ell_1}, P_{\ell_2 - 1}, 2} \right)/2$$

$$- \mu_n^{N_{\ell_1 - 1}, P_{\ell_2}} + \left(\mu_n^{N_{\ell_1 - 1}, P_{\ell_2 - 1}, 1} + \mu_n^{N_{\ell_1 - 1}, P_{\ell_2 - 1}, 2} \right)/2 \Bigg)[\varphi]$$

- Introduce a shorter notation as follows

$$\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi] := \left(\mu_n^{\boldsymbol{\ell}} - \frac{\mu_n^{\boldsymbol{\ell} - \mathbf{e}_2, 1} + \mu_n^{\boldsymbol{\ell} - \mathbf{e}_2, 2}}{2} - \mu_n^{\boldsymbol{\ell} - \mathbf{e}_1} + \frac{\mu_n^{\boldsymbol{\ell} - \mathbf{1}, 1} + \mu_n^{\boldsymbol{\ell} - \mathbf{1}, 2}}{2} \right)[\varphi],$$

with shorthands $\boldsymbol{e}_1 := (1, 0)$, $\boldsymbol{e}_2 := (0, 1)$, and $\mathbf{1} := (1, 1)$.

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$$= \Bigg(\mu_n^{N_{\ell_1}, P_{\ell_2}} - \left(\mu_n^{N_{\ell_1}, P_{\ell_2 - 1}, 1} + \mu_n^{N_{\ell_1}, P_{\ell_2 - 1}, 2} \right)/2$$

$$- \mu_n^{N_{\ell_1 - 1}, P_{\ell_2}} + \left(\mu_n^{N_{\ell_1 - 1}, P_{\ell_2 - 1}, 1} + \mu_n^{N_{\ell_1 - 1}, P_{\ell_2 - 1}, 2} \right)/2 \Bigg)[\varphi]$$

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MIEnKF estimator

- For a properly selected index set $\mathcal{I}$, the MIEnKF estimator is defined by

$$\mu_n^{\mathrm{MI}}[\varphi] := \sum_{\ell \in \mathcal{I}} \sum_{m=1}^{M_\ell} \frac{\boldsymbol{\Delta}\mu_n^{\ell,m}[\varphi]}{M_\ell},$$

where $\{\boldsymbol{\Delta}\mu_n^{\ell,m}[\varphi]\}_{m=1}^{M_\ell}$ are i.i.d. copies of $\boldsymbol{\Delta}\mu_n^{\ell}[\varphi]$, and $\{\boldsymbol{\Delta}\mu_n^{\ell,m}[\varphi]\}_{(\ell,m)}$ are mutually independent.

- Note that multi-index here refers to a two-index method, consisting of a **hierarchy of EnKF estimators** that are coupled in two degrees of freedom: time discretization N_{ℓ_1} and ensemble size P_{ℓ_2}.
- Sampling four-coupled EnKF estimators may lead to **a stronger variance reduction** than that achieved by pairwise-coupling in MLEnKF.

MIEnKF algorithm

Prediction step

- Given the four-coupled $(\hat{v}^{\boldsymbol{\ell}}_{n,i}, \hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n,i}, \hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n,i}, \hat{v}^{\boldsymbol{\ell}-\boldsymbol{1}}_{n,i})$ updated states for $i = 1, \dots, P_{\ell_2}$, the prediction states are given by

$$v^{\boldsymbol{\ell}}_{n+1,i} = \Psi_n^{N_{\ell_1}}(\hat{v}^{\boldsymbol{\ell}}_{n,i}), \qquad v^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1,i} = \Psi_n^{N_{\ell_1-1}}(\hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n,i}),$$

$$v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,i} = \Psi_n^{N_{\ell_1}}(\hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n,i}), \qquad v^{\boldsymbol{\ell}-\boldsymbol{1}}_{n+1,i} = \Psi_n^{N_{\ell_1-1}}(\hat{v}^{\boldsymbol{\ell}-\boldsymbol{1}}_{n,i}),$$

- Compute sample covariances of the following ensembles

$$C^{\boldsymbol{\ell}}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}}_{n+1,1:P_{\ell_2}}],\ C^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1,1:P_{\ell_2}}],$$

$$C^{\boldsymbol{\ell}-\boldsymbol{e}_2,1}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,1:P_{\ell_2-1}}],\ C^{\boldsymbol{\ell}-\boldsymbol{e}_2,2}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,P_{\ell_2-1}+1:P_{\ell_2}}],$$

$$C^{\boldsymbol{\ell}-\boldsymbol{1},1}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}-\boldsymbol{1}}_{n+1,1:P_{\ell_2-1}}],\ C^{\boldsymbol{\ell}-\boldsymbol{1},2}_{n+1} = \overline{\mathrm{Cov}}[v^{\boldsymbol{\ell}-\boldsymbol{1}}_{n+1,P_{\ell_2-1}+1:P_{\ell_2}}].$$

Update step

- The respective Kalman gains are

$$K^{\boldsymbol{\ell}}_{n+1} = \mathbf{K}(v^{\boldsymbol{\ell}}_{n+1,1:P_{\ell_2}}),\ K^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1} = \mathbf{K}(v^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1,1:P_{\ell_2}}),$$

$$K^{\boldsymbol{\ell}-\boldsymbol{e}_2,1}_{n+1} = \mathbf{K}(v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,1:P_{\ell_2-1}}),\ K^{\boldsymbol{\ell}-\boldsymbol{e}_2,2}_{n+1} = \mathbf{K}(v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,P_{\ell_2-1}+1:P_{\ell_2}}),$$

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MIEnKF algorithm

Update step

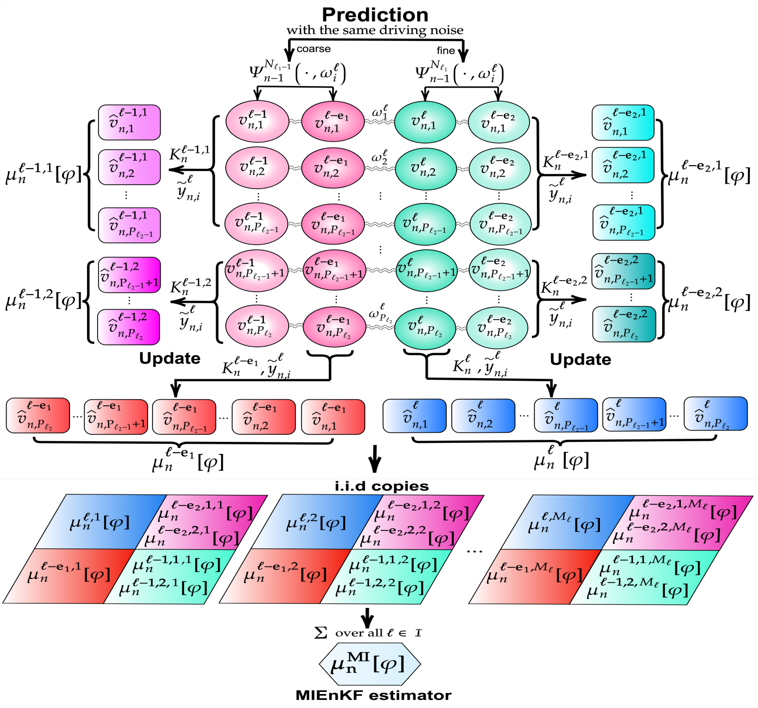
- The perturbed observations are also particle-wise coupled, so that the updated particle states are:

$$\left.\begin{aligned}
\tilde{y}^{\boldsymbol{\ell}}_{n+1,i} &= y_{n+1} + \eta^{\boldsymbol{\ell}}_{n+1,i},\\
\hat{v}^{\boldsymbol{\ell}}_{n+1,i} &= (I - K^{\boldsymbol{\ell}}_{n+1}H)v^{\boldsymbol{\ell}}_{n+1,i} + K^{\boldsymbol{\ell}}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i},\\
\hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1,i} &= (I - K^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1}H)v^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1,i} + K^{\boldsymbol{\ell}-\boldsymbol{e}_1}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i},
\end{aligned}\right\}$$

for $i = 1, \ldots, P_{\ell_2}$, $\{\eta^{\ell_2}_{n+1,i}\}_{i=1}^{P_{\ell_2}}$ are i.i.d. with $\eta^{\ell_2}_{n+1,1} \sim N(0, \Gamma)$,

$$\left.\begin{aligned}
\hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_2,1}_{n+1,i} &= (I - K^{\boldsymbol{\ell}-\boldsymbol{e}_2,1}_{n+1}H)v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,i} + K^{\boldsymbol{\ell}-\boldsymbol{e}_2,1}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i},\\
\hat{v}^{\boldsymbol{\ell}-\boldsymbol{e}_2,2}_{n+1,i} &= (I - K^{\boldsymbol{\ell}-\boldsymbol{e}_2,2}_{n+1}H)v^{\boldsymbol{\ell}-\boldsymbol{e}_2}_{n+1,i+P_{\ell_2-1}} + K^{\boldsymbol{\ell}-\boldsymbol{e}_2,2}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i+P_{\ell_2-1}},\\
\hat{v}^{\boldsymbol{\ell}-\boldsymbol{1},1}_{n+1,i} &= (I - K^{\boldsymbol{\ell}-\boldsymbol{1},1}_{n+1}H)v^{\boldsymbol{\ell}-\boldsymbol{1}}_{n+1,i} + K^{\boldsymbol{\ell}-\boldsymbol{1},1}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i},\\
\hat{v}^{\boldsymbol{\ell}-\boldsymbol{1},2}_{n+1,i} &= (I - K^{\boldsymbol{\ell}-\boldsymbol{1},2}_{n+1}H)v^{\boldsymbol{\ell}-\boldsymbol{1}}_{n+1,i+P_{\ell_2-1}} + K^{\boldsymbol{\ell}-\boldsymbol{1},2}_{n+1}\tilde{y}^{\boldsymbol{\ell}}_{n+1,i+P_{\ell_2-1}},
\end{aligned}\right\}$$

for $i = 1, \ldots, P_{\ell_2-1}$.


Prediction
with the same driving noise
coarse
fine
Update
Update
i.i.d copies
Σ over all ℓ ∈ I
MIEnKF estimator

MIEnKF complexity

Assumption

For $N_{\ell_1} \eqsim 2^{\ell_1}, P_{\ell_2} \eqsim 2^{\ell_2} \quad \forall \boldsymbol{\ell} \in \mathbb{N}_0^2$ and $\varphi : \mathbb{R}^d \to \mathbb{R}$, the four-coupled EnKF estimator $\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi]$ satisfies:

$$\begin{aligned} \left|\mathbb{E}\left[\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi]\right]\right| &\lesssim N_{\ell_1}^{-1} P_{\ell_2}^{-1}, \\ \mathbb{V}[\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi]] &\lesssim N_{\ell_1}^{-2} P_{\ell_2}^{-2}, \\ \mathrm{Cost}(\boldsymbol{\Delta}\mu_n^{\boldsymbol{\ell}}[\varphi]) &\eqsim N_{\ell_1} P_{\ell_2}. \end{aligned}$$

Theorem 1 (MIEnKF complexity)

Under sufficient regulatory assumptions, for any $\epsilon > 0$ and $n \geq 0$, the index set $\mathcal{I} = \{\boldsymbol{\ell} \in \mathbb{N}_0^2 \mid \ell_1 + \ell_2 \leq L\}$, with $L \simeq \lceil \log \epsilon^{-1} + \log\log \epsilon^{-1} \rceil$ and $M_{\boldsymbol{\ell}} \eqsim \epsilon^{-2} N_{\ell_1}^{-3/2} P_{\ell_2}^{-3/2}$ ensures that

$$\mathbb{E}\left[\left(\mu_n^{\mathrm{MI}}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\right)^2\right] = \mathcal{O}(\epsilon^2),$$

$$\mathrm{Cost}(\mu_{\mathrm{n}}^{\mathrm{MI}}[\varphi]) = \mathcal{O}(\epsilon^{-2}).$$

Numerical example

- Again consider nonlinear dynamics with a double well potential

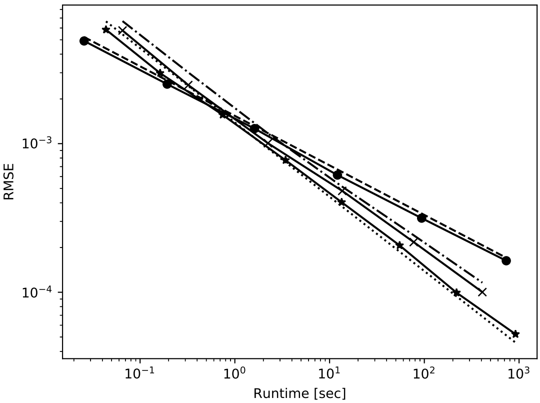


Figure 2: Runtime vs root-MSE for the QoI $\varphi(x) = x$. MIEnKF (solid-asterisked), new MLEnKF (solid-crossed) and EnKF (solid-bulleted).

Comparison of computational costs

Methods	**EnKF**	**New MLEnKF**	**MIEnKF**
MSE	$\mathcal{O}(\epsilon^2)$	$\mathcal{O}(\epsilon^2)$	$\mathcal{O}(\epsilon^2)$
Cost	$\mathcal{O}(\epsilon^{-3})$	$\mathcal{O}(\epsilon^{-2}\left\|\log(\epsilon)\right\|^3)$	$\mathcal{O}(\epsilon^{-2})$

Table 1: Comparison of computational costs versus errors for EnKF, original MLEnKF, new MLEnKF and MIEnKF methods

Conclusion

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- Presented different ideas of combining **multilevel and multi-index Monte Carlo with EnKF** to produce new filtering methods that display **efficiency gains** over standard single-level EnKF.
- A new multi-level EnKF method is based on a sample average of independent samples of **pairwise-coupled EnKF estimators**.
- Multi-index EnKF method is based on independent samples of **four-coupled EnKF estimators** on a multi-index hierarchy of resolution levels.
- **Under certain assumptions**, the MIEnKF method is proven to be more tractable than EnKF and MLEnKF, and this is also verified numerically.
- We believe that MIEnKF will often outperform alternative methods prominently when **more than two degrees of freedom** need to be discretized.

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References

1. **H. Hoel, K. JH Law, and R. Tempone**, **Multilevel ensemble Kalman filtering**, **SIAM J. Numer. Anal., 54(3), pp. 1813–1839 (2016).**
2. **H. Hoel, G. Shaimerdenova, and R. Tempone, Multilevel ensemble Kalman filtering based on a sample average of independent EnKF estimators. Foundations of Data Science 2, 4 (2020), 351.**
3. **H. Hoel, G. Shaimerdenova, and R. Tempone, Multi-index ensemble Kalman filtering. Preprint, 2021, arXiv:2104.07263**

THANK YOU!

Appendix

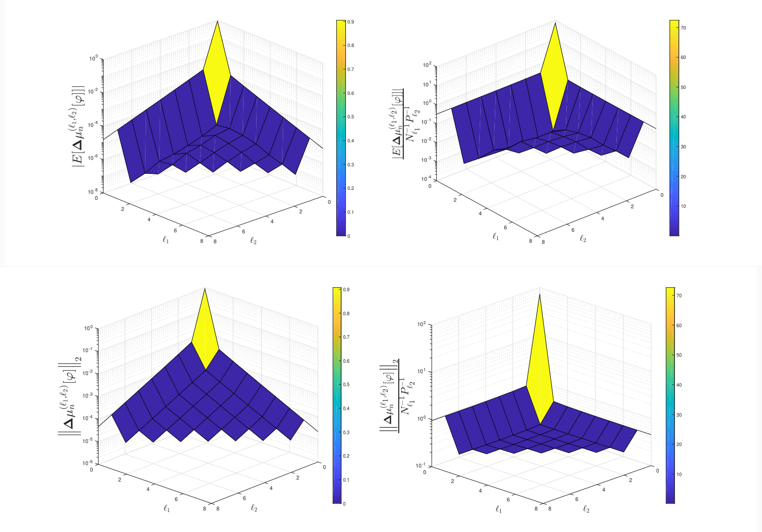

Figure 3: Double Well problem. Estimates based on $S = 10^6$ independent runs. Top row: Numerical evidence of weak rate assumption. Bottom row: Similar plots for verifying strong rate assumption.

EnKF convergence

Assumption 1.

For all $p \geq 2$,

1. $\|\Psi^N(v)\|_{L^p(\Omega,\mathbb{R}^d)} \lesssim 1 + \|v\|_{L^p(\Omega,\mathbb{R}^d)}$,
2. $\|\Psi^N(u) - \Psi^N(v)\|_{L^p(\Omega,\mathbb{R}^d)} \lesssim \|u - v\|_{L^p(\Omega,\mathbb{R}^d)}$,
3. there exists $\alpha > 0$ s.t. if

$$\left|\mathbb{E}\left[\varphi(u) - \varphi(v^N)\right]\right| \lesssim N^{-\alpha} \implies \left|\mathbb{E}\left[\varphi(\Psi(u)) - \varphi(\Psi^N(v^N))\right]\right| \lesssim N^{-\alpha}$$

Theorem. [Le Gland et al. (2009); H.Hoel et al. (2016)]

If Assumption 1 holds and $u_0|Y_0 \in \cap_{r\geq 2} L^r(\Omega, \mathbb{R}^d)$, then for any $\varphi \in \mathbb{F}$, $\|\mu_n^{N,P}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_{L^p(\Omega)} \lesssim P^{-1/2} + N^{-\alpha}$.

- In order to achieve $\mathcal{O}(\epsilon)$ accuracy $P \eqsim \epsilon^{-2}$ and $N \eqsim \epsilon^{-1/\alpha}$.
- Then the cost of EnKF is bounded by **Cost**$(\mu_n^{N,P}[\varphi]) \eqsim \epsilon^{-(2+1/\alpha)}$.

Original MLEnKF – the pairwise coupling

Prediction step

- Simulate pairwise coupled particles

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

  for $i = 1, \ldots, P_\ell$ on hierarchy levels $\ell = 0, 1, \ldots, L$.

- MLMC approximation of prediction covariance:

$$C_{n+1}^{\mathrm{ML}} = \sum_{\ell=0}^{L} \mathrm{Cov}_{P_\ell}[v_{n+1}^{\ell}] - \mathrm{Cov}_{P_\ell}[v_{n+1}^{\ell-1}]$$

Update step

For $\ell = 0, 1, \ldots, L$ and $i = 1, 2, \ldots, P_\ell$,

$$\tilde{y}_{n+1,i}^{\ell} = y_{n+1} + \gamma_{n+1,i}^{\ell}, \qquad \text{i.i.d. } \gamma_{n+1,i}^{\ell} \sim N(0, \Gamma)$$

$$\hat{v}_{n+1,i}^{\ell-1} = (I - K_{n+1}^{\mathrm{ML}} H) v_{n+1,i}^{\ell-1} + K_{n+1}^{\mathrm{ML}} \tilde{y}_{n+1,i}^{\ell},$$

$$\hat{v}_{n+1,i}^{\ell} = (I - K_{n+1}^{\mathrm{ML}} H) v_{n+1,i}^{\ell} + K_{n+1}^{\mathrm{ML}} \tilde{y}_{n+1,i}^{\ell},$$

where $K_{n+1}^{\mathrm{ML}} = C_{n+1}^{\mathrm{ML}} H^{\mathsf{T}} (H C_{n+1}^{\mathrm{ML}} H^{\mathsf{T}} + \Gamma)^{-1}$.

Original MLEnKF accuracy vs. cost

Theorem. [H.Hoel et al., 2016]

If, in addition to Assumption 1 for EnKF, there exists a $\beta > 0$ such that for all $p \geq 2$ and $v \in \cap_{r \geq 2} L^r(\Omega, \mathbb{R}^d)$,

$$\|\Psi^{N_\ell}(v) - \Psi^{N_{\ell-1}}(v)\|_{L^p(\Omega)} \lesssim (1 + \|v\|_{L^p(\Omega)}) N_\ell^{-\beta/2}.$$

Then, for any $u_0 | Y_0 \in \cap_{r \in \mathbb{N}} L^r(\Omega)$, $\varphi \in \mathbb{F}$ and $\epsilon > 0$, there exists an $L(\epsilon) > 0$ and $\{P_\ell\}_{\ell=0}^{L}$ such that

$$\|\mu_n^{\mathrm{ML}}(\varphi) - \mu_n^{\infty,\infty}(\varphi)\|_p \lesssim \epsilon.$$

And

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

! Compare with EnKF, where $\mathrm{Cost}\left(\mu_n^{N,P}(\varphi)\right) \eqsim \epsilon^{-\left(2+\frac{1}{\alpha}\right)}$.

Assumption 2.

Let $|\kappa|_1 := \sum_{i=1}^{d} \kappa_i$ for any $\kappa \in \mathbb{N}_0^d$. For all $\ell \in \mathbb{N}_0 \cup \{\infty\}$ and $p \geq 2$,

(i) for all $|\kappa|_1 \leq 1$,

$$\left\|\partial^\kappa \Psi^{N_\ell}(u)\right\|_{L^p(\Omega,\mathbb{R}^d)} \lesssim (1 + \|u\|_{L^p(\Omega,\mathbb{R}^d)}),$$

(ii) for all $|\kappa|_1 = 2$,

$$\left\|\partial^\kappa \Psi^{N_\ell}(u)\right\|_{L^{2p}(\Omega,\mathbb{R}^d)} \lesssim (1 + \|u\|_{L^{2p}(\Omega,\mathbb{R}^d)}),$$

(iii) for all $|\kappa|_1 \leq 1$,

$$\left\|\partial^\kappa \Psi^{N_{\ell+1}}(u) - \partial^\kappa \Psi^{N_\ell}(u)\right\|_{L^p(\Omega,\mathbb{R}^d)} \lesssim (1 + \|u\|_{L^p(\Omega,\mathbb{R}^d)}) N_\ell^{-\beta/2}.$$

Convergence of new MLEnKF

Theorem. (MLEnKF convergence)

If Assumptions 1 and 2 hold, then for any $u_0|Y_0 \in \cap_{r\in\mathbb{N}} L^r(\Omega)$, $\varphi \in \mathbb{F}$, $n \geq 0$, $p \geq 2$ and $\epsilon > 0$, there exists an $L(\epsilon) > 0$ and triplet of sequences $\{P_\ell\}$, $\{N_\ell\}$, $\{M_\ell\}$ such that

$$\|\mu_n^{\mathrm{ML}^{\mathrm{NEW}}}[\varphi] - \mu_n^{\infty,\infty}[\varphi]\|_p \lesssim \epsilon.$$

$$\mathrm{Cost}\left(\mu_n^{\mathrm{ML}^{\mathrm{NEW}}}\right) \lesssim \begin{cases} \epsilon^{-2} & \text{if } \beta > 1, \alpha > 1, \\ \epsilon^{-2}|\log(\epsilon)|^3 & \text{if } (\beta > 1, \alpha = 1) \text{ or } (\beta = 1, \alpha \geq 1), \\ \epsilon^{-(1+1/\alpha)} & \text{if } (\beta \geq 1, \alpha < 1) \text{ or } (\beta < 1, \alpha \leq \beta), \\ \epsilon^{-(2+(1-\beta)/\alpha)} & \text{if } \beta < 1, \alpha > \beta. \end{cases}$$

with the configuration $P_\ell \eqsim 2^\ell$, $N_\ell \eqsim 2^{s\ell}$ for any $s > 0$.

! Compare with old MLEnKF, where cost is

$$\mathrm{Cost}\left(\mu_n^{\mathrm{ML}}[\varphi]\right) \lesssim \begin{cases} \left(|\log(\epsilon)|^{1-n}\epsilon\right)^{-2}, & \text{if} \quad \beta > 1, \\ \left(|\log(\epsilon)|^{1-n}\epsilon\right)^{-2} |\log(\epsilon)|^3, & \text{if} \quad \beta = 1, \\ \left(|\log(\epsilon)|^{1-n}\epsilon\right)^{-\left(2+\frac{1-\beta}{\alpha}\right)}, & \text{if} \quad \beta < 1. \end{cases}$$

Choosing the index set $\mathcal{I}$

- We assume $\mathcal{I} = \{\boldsymbol{\ell} \in \mathbb{N}_0^2 \mid \ell_1 + \ell_2 \leq L\}$.

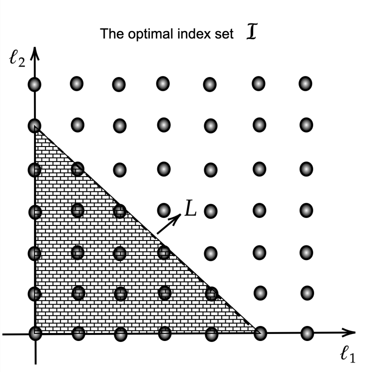

Figure 4: Illustration of multi-index set $\mathcal{I}$.

- The problem of optimizing the set $\mathcal{I}$ may be recast as a knapsack optimization problem.

DMFEnKF algorithm

• The initial updated density $\rho_{\hat{v}_0} = \rho_{u_0|Y_0}$, the number of time steps N_t, the number of spatial steps N_x, the discretization interval $[x_0, x_1]$, the simulation length $\mathcal{N}$.

• The prediction and updated density, $\rho_{\bar{v}_n}$ and $\rho_{\hat{v}_n}$, respectively.

$\Delta t = \frac{1}{N_t}$, $\Delta x = \frac{x_1 - x_0}{N_x}$.

For n=1 : $\mathcal{N}$

1. Compute the prediction density $\rho_{\bar{v}_n}(x) = \mathcal{S}^1 \rho_{\hat{v}_{n-1}}$ by a numerical method (e.g., Crank-Nicolson) with the discretization steps $(\Delta t, \Delta x)$.
2. Compute the prediction covariance $\bar{C}_n = \int x^2 \rho_{\bar{v}_n}(x) dx - (\int x \rho_{\bar{v}_n}(x) dx)^2$ using a quadrature rule.
3. Compute the Kalman gain $\bar{K}_n = \bar{C}_n H^\mathsf{T} (H \bar{C}_n H^\mathsf{T} + \Gamma)^{-1}$.
4. Compute the updated density $\rho_{\hat{v}_n} = \rho_X * \rho_Y$ by discrete convolution of the two functions represented on the spatial mesh.

end

Bayes filter vs MFEnKF

Illustration of contracting property: given nonlinear Ψ defined by the SDE $du = -(u + \pi \cos(\pi u/5)/5)dt + \sigma dW$ and having different update densities at time n, we have almost identical prediction densities at time $n+1$ for both Bayes filter and MFEnKF.