

Towards Data-Driven Nonlinear Filtering Algorithms

*Presented at the 1st MMS Workshop for Young Researchers
Department of Mathematics, Kyoto University, Kyoto, Japan*

Amirhossein Taghvaei

Department of Aeronautics & Astronautics
University of Washington, Seattle

Nov 21, 2024



This talk

References:

- *Data-Driven Approximation of Stationary Nonlinear Filters with Optimal Transport Maps*
Mohammad Al-Jarrah, Bamdad Hosseini, Amirhossein Taghvaei
IEEE Conference on Decision and Control (CDC), Milan, 2024
- *Nonlinear Filtering with Brenier Optimal Transport Maps*
Mohammad Al-Jarrah, Niyizhen Jin, Bamdad Hosseini, Amirhossein Taghvaei
International Conference of Machine Learning (ICML), Vienna, 2024
- *Optimal Transport Particle Filters*
Mohammad Al-Jarrah, Amirhossein Taghvaei, Bamdad Hosseini
IEEE Conference on Decision and Control (CDC), Singapore, 2023
- Computational optimal transport and filtering on Riemannian manifolds
D. Grange, M. Al-Jarrah, R. Baptista, A. Taghvaei, T. Georgiou, S. Phillips, A. Tannenbaum
IEEE Control Systems Letters, 2023
- *An optimal transport formulation of Bayes' law for nonlinear filtering algorithms*
Amirhossein Taghvaei, Bamdad Hosseini
IEEE Conference on Decision and Control (CDC), Cancun, 2022

nonlinear filtering $\xrightarrow{\text{Optimal Transport}}$ machine learning

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- **Part I:** Bayes' law and its fundamental challenges
- **Part II:** Conditioning with optimal transport maps
- **Part III:** Application to nonlinear filtering
- **Part IV:** Extension to data-driven setting

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- **Part II:** Conditioning with optimal transport maps
- **Part III:** Application to nonlinear filtering
- **Part IV:** Extension to data-driven setting

Problem:

- Hidden random variable X
- Observed random variable Y
- What is the conditional probability distribution of X given Y ? (posterior)

$$\text{Bayes' law: } P_{X|Y} = \frac{P_X P_{Y|X}}{P_Y}$$

- Data-driven setting: $P_{X,Y}$ is not available.

$$\text{Given: } (X^i, Y^i)_{i=1}^N \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}$$

$$\text{Approximate: } P_{X|Y=y} \text{ for any given observation } y$$

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Kalman filter (KF):

- Assumes (X, Y) is jointly Gaussian

$$P_{X,Y} = N\left(\begin{bmatrix} m_X \\ m_Y \end{bmatrix}, \begin{bmatrix} \Sigma_X & \Sigma_{X,Y} \\ \Sigma_{Y,X} & \Sigma_Y \end{bmatrix}\right)$$

- Implements the conditioning formula for jointly Gaussian random variables

$$P_{X|Y=y} = N(m_X + K(y - m_Y), \Sigma_X - \Sigma_{X,Y}\Sigma_Y^{-1}\Sigma_{Y,X})$$

- Data-driven counterpart: Fit a Gaussian distribution to the data $(X^i, Y^i)_{i=1}^N$ and implement the conditioning formula → Ensemble Kalman filter (EnKF)
- Widely used in meteorology
- Fundamentally limited to Gaussian settings

G. Evensen. "Data Assimilation. The Ensemble Kalman Filter" (2006)

S. Reich, "A dynamical systems framework for intermittent data assimilation" (2011)

E. Calvello, S. Reich, and A. M. Stuart, "Ensemble kalman methods: a mean field perspective" (2022)

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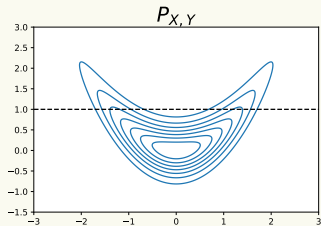
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Illustrative example

Fundamental challenges of EnKF

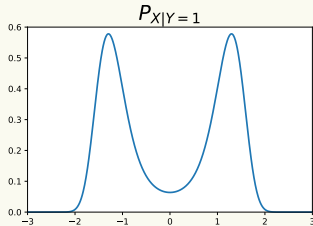
Setup:

- $X \sim \mathcal{N}(0, 1)$
- $Y = \frac{1}{2}X^2 + \epsilon W$
- $P_{X|Y=1} = ?$



EnKF:

- $P_{X|Y=1}$ is not Gaussian
- $P_{X|Y=1}$ is multimodal
- Conditioning formula for EnKF fails

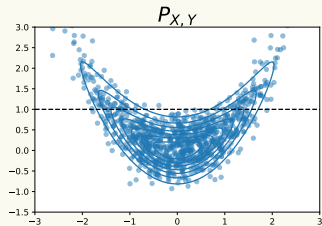


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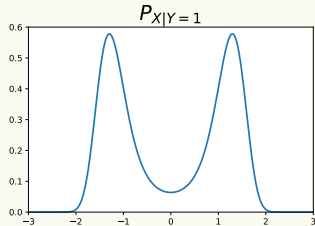
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EnKF:

- $(X^i, Y^i) \sim P_{X,Y}$
- fit a Gaussian
- conditioning formula for Gaussians

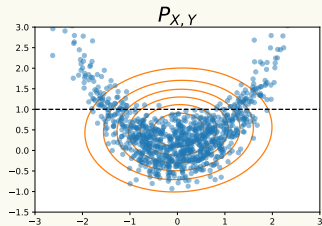


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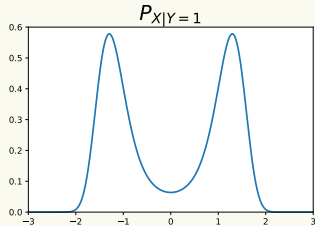
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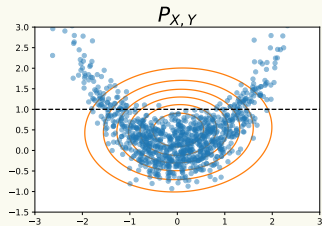


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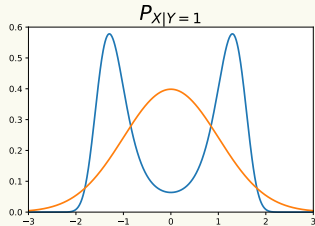
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Importance sampling (IS) particle filter:

- Requires samples/particles $(X^i)_{i=1}^N \stackrel{\text{i.i.d}}{\sim} P_X$ and likelihood function $P_{Y|X}$
- Compute the weights

$$w^i \propto P_{Y=y|X=X^i}$$

- Approximate the posterior as weighted empirical distribution

$$P_{X|Y=y} \approx \sum_{i=1}^N w^i \delta_{X^i}$$

- Asymptotically exact as $N \rightarrow \infty$
- Suffers from weight degeneracy issue

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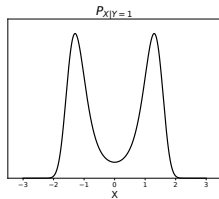
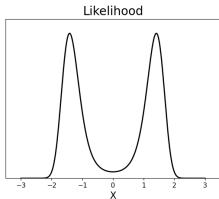
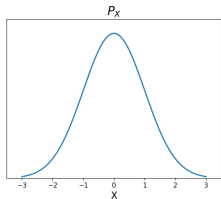
Fundamental challenges of importance sampling

Example:

- $X \sim \mathcal{N}(0, 1)$
- $Y = \frac{1}{2}X^2 + \epsilon W$
- $P_{X|Y=1} = ?$

Importance sampling (IS):

- $q(x) = \mathcal{N}(0, 1)$
- $w(x) = \frac{P_{X|Y=1}(x)}{q(x)}$
- $\int w(x) q(x) dx = 1$



small noise regime: $\epsilon \rightarrow 0$

This is the main reason for the curse of dimensionality of IS-based particle filters

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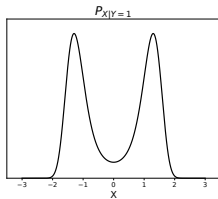
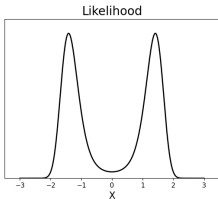
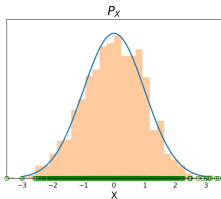
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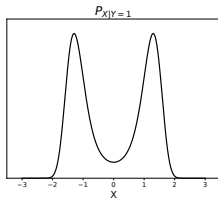
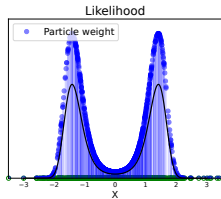
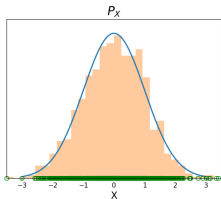
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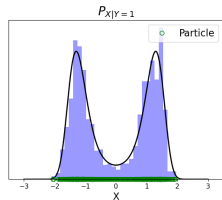
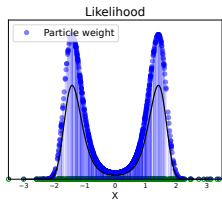
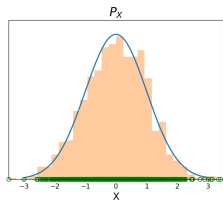
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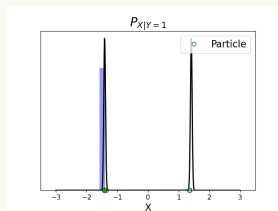
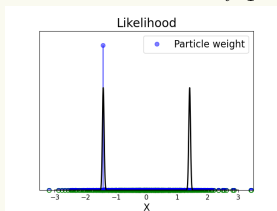
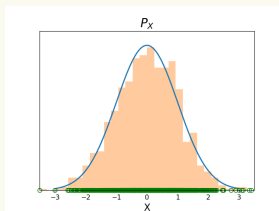
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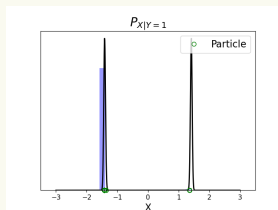
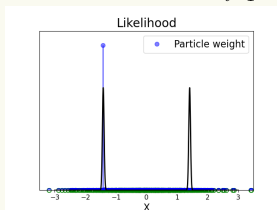
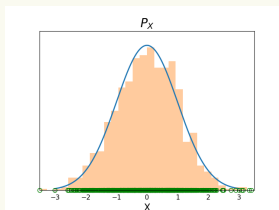
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Control and coupling techniques

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- A dynamical systems framework for data assimilation [Reich. 2011]
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→ Feedback Particle Filter (FPF)
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- Ensemble Kalman methods: a mean field perspective [Calvello et. al. 2022]
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This talk: Conditioning with optimal transport map

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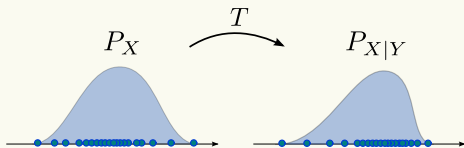
This talk: Conditioning with optimal transport map

- **Part I:** Bayes' law and its fundamental challenges
- **Part II:** Conditioning with optimal transport maps
- **Part III:** Application to nonlinear filtering
- **Part IV:** Extension to data-driven setting

Outline

- Part I: Bayes' law and its fundamental challenges
- **Part II: Conditioning with optimal transport maps**
- Part III: Application to nonlinear filtering
- Part IV: Extension to data-driven setting

Conditioning with transport maps



$$X^i \sim P_X \longrightarrow T(X^i, y) \sim P_{X|Y=y}$$

Example:

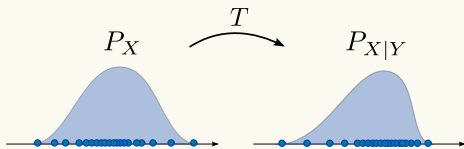
- Consider $X \sim \mathcal{N}(\mu, \sigma^2)$. Then $P_{X|Y=y}$ is represented by the map $T(x, y) = x - \frac{\sigma^2}{y}$.
- Consider jointly Gaussian (X, Y) . Then $P_{X|Y=y}$ is represented by the (deterministic) map $T(x, y) = \frac{\sigma_X^2 - \rho \sigma_X \sigma_Y}{\sigma_Y^2} y + x$.

Questions:

 In a general setting,

- does the map exist?
- how do we explicitly find it?

Conditioning with transport maps



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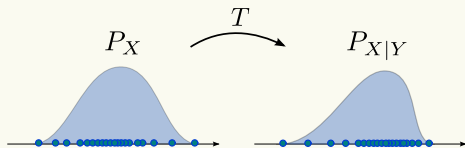
Example:

- Consider $Y = X$. Then, $P_{X|Y=y} = \delta_y$ is represented by the map $T(x, y) = y$
- Consider jointly Gaussian (X, Y) . Then $P_{X|Y=y}$ is represented by the (stochastic) map $X \mapsto X + K(y - Y)$

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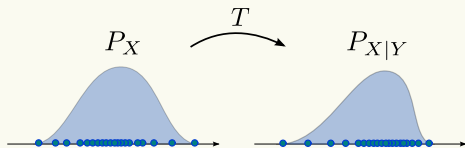
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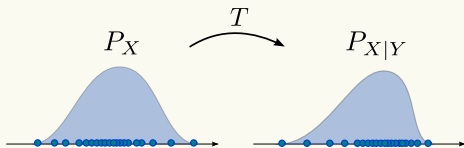
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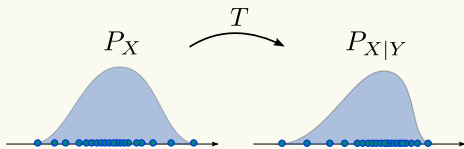
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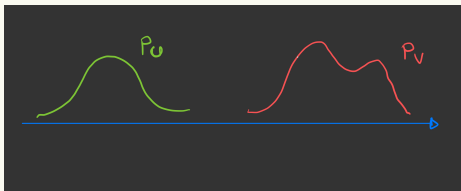
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Background on optimal transportation theory

Monge problem and Brenier's result



- Given two random variables $U \sim P_U$ and $V \sim P_V$
- find a map $x \mapsto T(x)$ that transports P_U to P_V , i.e. $T_{\#}P_U = P_V$
- with minimal transportation cost $\|T(x) - x\|^2$

Questions:

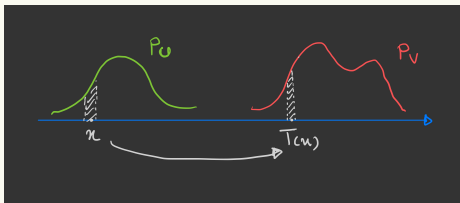
- Does the optimal map exist? Yes, as long as P_V admits Lebesgue density
- How to numerically find it? semi-dual Kantorovich problem

Amirhossein Taghvaei, MIT, EE-6.035, Fall 2016

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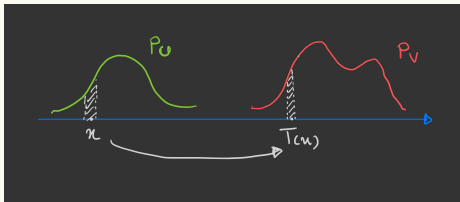
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$$\min_{T: P_U \rightarrow P_V} \int \|T(x) - x\|^2 dP_U(x)$$

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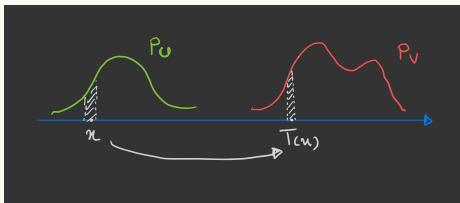
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$$T(x) = \arg \min_{y \in \mathbb{R}^d} \|y - x\|^2 \quad \text{s.t. } T_{\#}P_U = P_V$$

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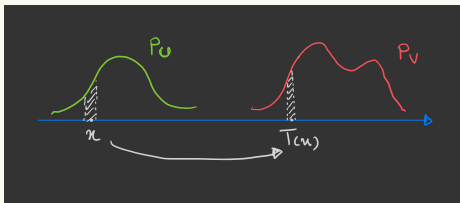
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$$\max_{f \in \mathcal{C}\text{-concave}} \min_T \mathbb{E} \left[\frac{1}{2} \|T(U) - U\|^2 - f(T(U)) + f(V) \right]$$

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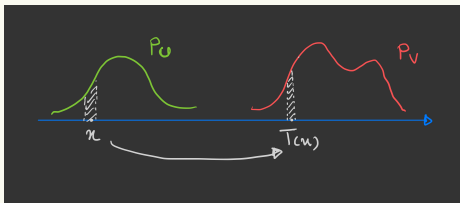
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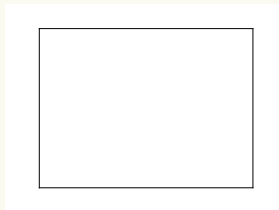
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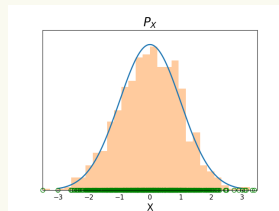
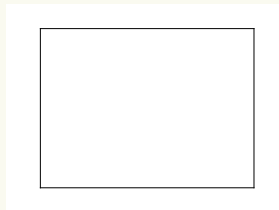
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Conditioning with optimal transport map

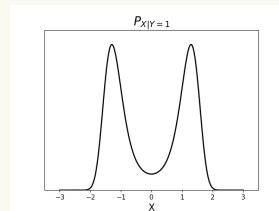
Illustrative example



→

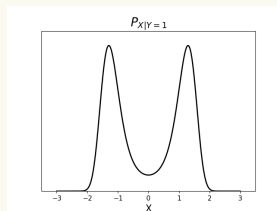
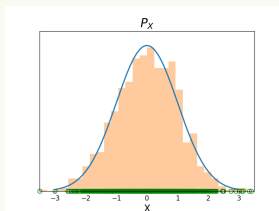
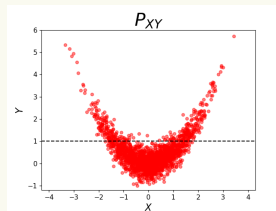
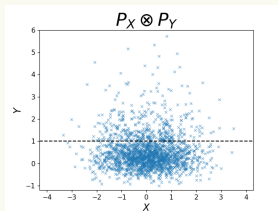


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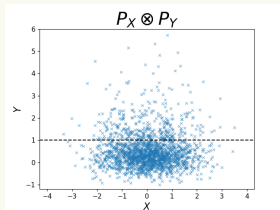
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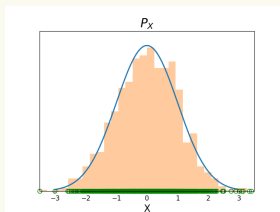
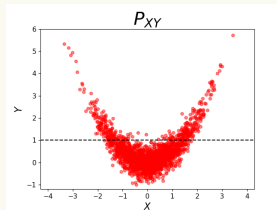


Conditioning with optimal transport map

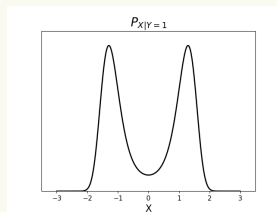
Illustrative example



$$\xrightarrow{(T(X,Y), Y)}$$

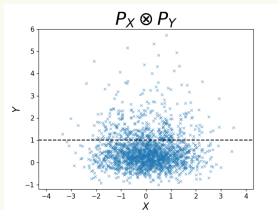


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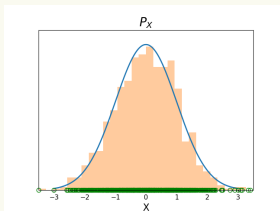
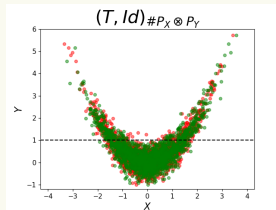


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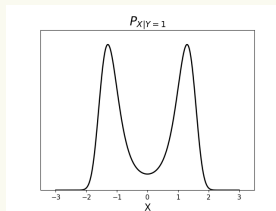
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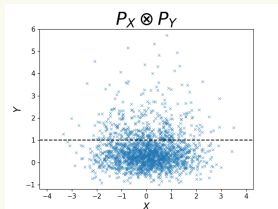


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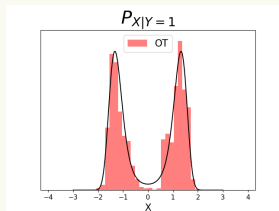
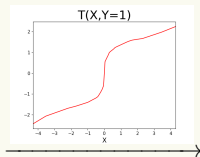
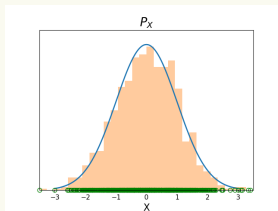
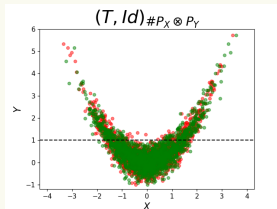


Conditioning with optimal transport map

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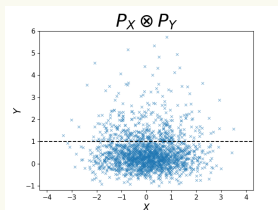


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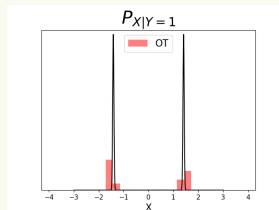
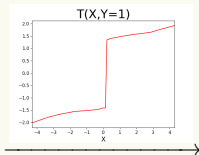
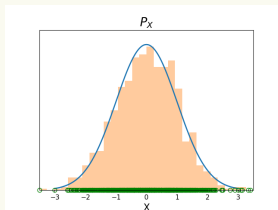
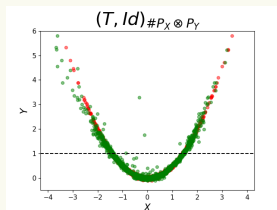


Conditioning with optimal transport map

Illustrative example



$$\xrightarrow{(T(X,Y), Y)}$$



small noise limit

Conditioning with optimal transport map

Variational formulation of the Bayes' law

$$\begin{aligned}\text{Bayes law: } P_{X|Y} &= \frac{P_X P_{Y|X}}{P_Y} \\ &= T(\cdot; Y) \# P_X\end{aligned}$$

Conditional max-min formulation:

$$\max_{f \in \mathcal{C}\text{-concave}_x} \min_T \mathbb{E} \left[\frac{1}{2} \|T(\bar{X}, Y) - \bar{X}\|^2 - f(T(\bar{X}, Y), Y) + f(X; Y) \right]$$

Computational properties:

- Only requires samples $(X_i, Y_i) \sim P_{XY}$ (data-driven/simulation based)
- Enables construction of “approximate” posterior distributions
- Allows application of ML tools (stochastic optimization and neural nets)

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Conditioning with optimal transport map

Theoretical analysis

- Variational problem: $\max_f \min_T J(f, T; P_{X,Y})$
- max-min optimality gap: $\epsilon(f, T)$

(Conditional) Brenier's theorem

- (Well-posedness) If P_X admits (Lebesgue) density, then, there exists a unique pair (\bar{f}, \bar{T}) that solves the variational problem and

$$\bar{T}(\cdot, y) \# P_X = P_{X|Y=y}, \quad \text{a.e. } y$$

- (Sensitivity) Let (f, T) be a possibly non-optimal pair. Assume $x \mapsto \frac{1}{2} \|x\|^2 - f(x, y)$ is α -strongly convex for all y . Then,

$$d(T(\cdot, Y) \# P_X, P_{X|Y}) \leq \sqrt{\frac{4}{\alpha} \epsilon(f, T)}.$$

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About convexity assumption

- Ensuring the assumption that

$$x \mapsto \frac{1}{2}\|x\|^2 - f(x, y) \text{ is } \alpha\text{-strongly convex for all } y$$

is computationally challenging

- In practice, we do not enforce a convexity constraint
- The optimizer outputs f that is, sometimes, slightly non-convex

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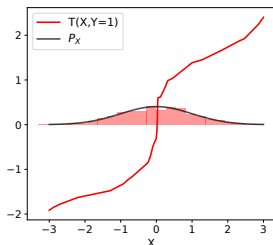
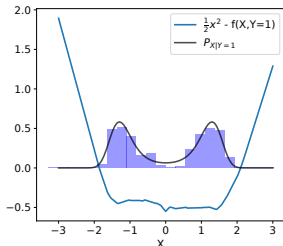
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Nonlinear filtering problem

Model:

$$X_t \sim a(\cdot | X_{t-1}), \quad X_0 \sim \pi_0$$
$$Y_t \sim h(\cdot | X_t)$$

- X_t is the state
- Y_t is the observation
- dynamic and observation models are available as simulators

Questions: Given history of observation $Y_{1:t} := \{Y_1, \dots, Y_t\}$,

- What is the most likely value of X_t ?
- What is the probability of $X_t \in A$?
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Answer: given by the conditional distribution $\pi_t = P_{X_t|Y_{1:t}}$ (posterior)

Nonlinear filtering: numerical approximation of the posterior π_t for all t .

Nonlinear filtering problem

Model:

$$X_t \sim a(\cdot | X_{t-1}), \quad X_0 \sim \pi_0$$
$$Y_t \sim h(\cdot | X_t)$$

- X_t is the state
- Y_t is the observation
- dynamic and observation models are available as simulators

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Filtering equations

- $\pi_t := P(X_t|Y_{1:t})$
- Two important operations:

$$\text{Propagation: } \pi \xrightarrow{\text{dynamics}} \mathcal{A}\pi$$

$$\text{Conditioning: } \pi \xrightarrow{\text{Bayes law}} \mathcal{B}_y(\pi)$$

- Recursive update law for the posterior

$$\pi_{t-1} \xrightarrow{\text{dynamics}} \pi_{t|t-1} := \mathcal{A}\pi_{t-1} \xrightarrow{\text{Bayes law}} \pi_t = \mathcal{B}_{Y_t}(\pi_{t|t-1}) =: \mathcal{T}_{t,t-1}(\pi_{t-1})$$

- (Exponential) filter stability : $\exists \lambda \in (0, 1)$ s.t.

$$d(\mathcal{T}_{t,0}(\pi_0), \mathcal{T}_{t,0}(\tilde{\pi}_0)) \leq C\lambda^k d(\pi_0, \tilde{\pi}_0), \quad \forall \pi_0, \tilde{\pi}_0.$$

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Optimal Transport Filter

Filter design steps:

exact posterior: $\pi_{t-1} \longrightarrow \pi_{t|t-1} = \mathcal{A}\pi_{t-1} \longrightarrow \pi_t = \mathcal{B}_{Y_t}(\pi_{t|t-1})$

mean-field process: $\bar{X}_{t-1} \longrightarrow \bar{X}_{t|t-1} \sim a(\cdot | \bar{X}_{t-1}) \longrightarrow \bar{X}_t = \bar{T}_t(\bar{X}_{t|t-1}, Y_t)$

particle system: $X_{t-1}^i \longrightarrow X_{t|t-1}^i \sim a(\cdot | X_{t-1}^i) \longrightarrow X_t^i = \hat{T}_t(X_{t|t-1}^i, Y_t)$

Variational problem:

$$\min_{\pi_t} \int \int \ell(x, y) d\pi_t(x, y) \quad \text{subject to}$$
$$\pi_t \llcorner \mathcal{X}_t = \pi_{t-1} \llcorner \mathcal{X}_{t-1} \quad \pi_t \llcorner \mathcal{Y}_t = \delta_{Y_t}$$

Posterior approximation:

$$\pi_t \approx \hat{\pi}_t^{(N)} = \frac{1}{N} \sum_{i=1}^N \delta_{X_t^i}$$

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Variational problem:

$$\bar{T}_t \leftarrow \max_f \min_T J(f, T; P_{X_t, Y_t | Y_{1:t-1}})$$

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Algorithm

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Remarks:

- The need for analytical forms of the dynamic and observation models
- In practice, only a few iterations of the optimization are performed

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Remarks:

- The cost function J is a function of the distance and the number of particles
- The particles with the lowest cost are the optimal transport particles

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Remarks:

- The cost function $J(f, T)$ is the expected cost of the particles
- The particles $X_{t|t-1}^i$ are the particles of the optimal transport filter

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Optimal Transport Filter

Error Analysis

Theorem

Assume

- 1 The exact filter is exponentially stable
- 2 Uniform bound $\epsilon_{\mathcal{F},\mathcal{T},N}$ on the max-min optimality gap
- 3 The function $x \mapsto \frac{1}{2}\|x\|^2 - \hat{f}_t(x, y)$ is α -strongly convex for all t and y .
- 4 Particles are resampled at each step

Then,

$$d\left(\frac{1}{N} \sum_{i=1}^N \delta_{X_t^i}, \pi_t\right) \leq C \left(\sqrt{\frac{2}{\alpha} \epsilon_{\mathcal{F},\mathcal{T},N}} + \frac{1}{\sqrt{N}} \right), \quad \forall t.$$

- Optimality gap $\epsilon_{\mathcal{F},\mathcal{T},N}$ has the decomposition

$$\epsilon_{\mathcal{F},\mathcal{T},N} \leq \underbrace{\epsilon_{\mathcal{F},\mathcal{T}}}_{\text{approx. theory}} + \underbrace{\frac{C_{\mathcal{F},\mathcal{T}}}{\sqrt{N}}}_{\text{statistical generalization}} + \text{optimization error}$$

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Optimal Transport Filter

Numerical example

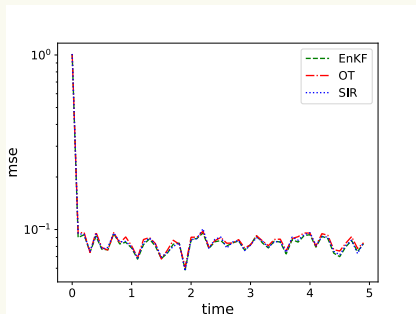
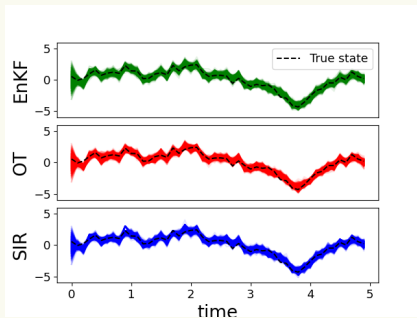
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$$Y_t = X_t + \sigma_W W_t,$$

- Ensemble Kalman filter (EnKF)
- sequential importance re-sampling (SIR)
- Optimal Transport (OT)

Optimal Transport Filter

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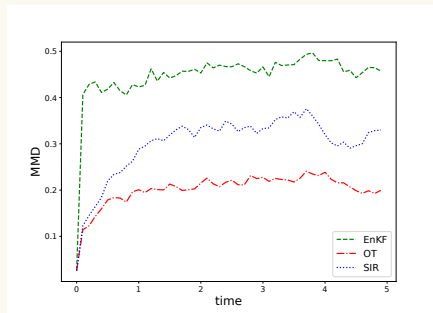
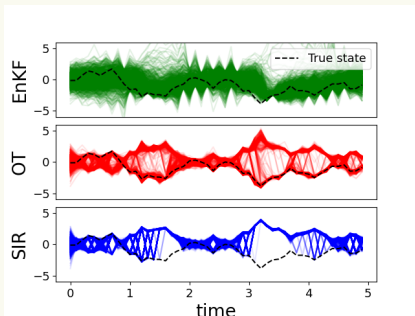
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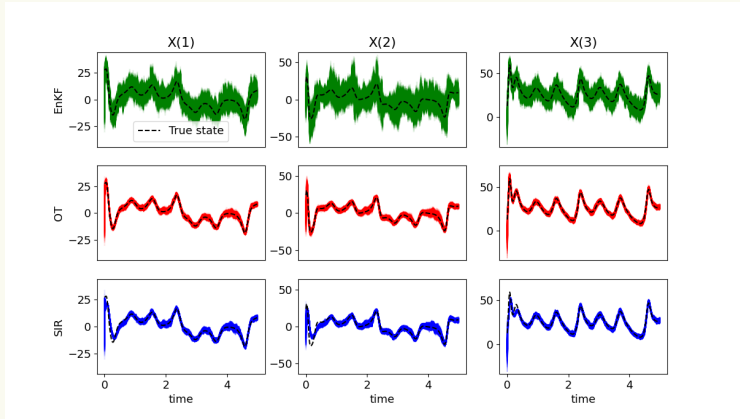
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Optimal Transport Filter

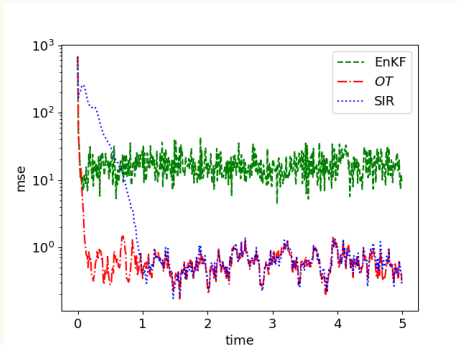
Numerical example: Lorenz 63



- Trajectory of the particles
- mean-squared error (mse) in estimating the state

Optimal Transport Filter

Numerical example: Lorenz 63



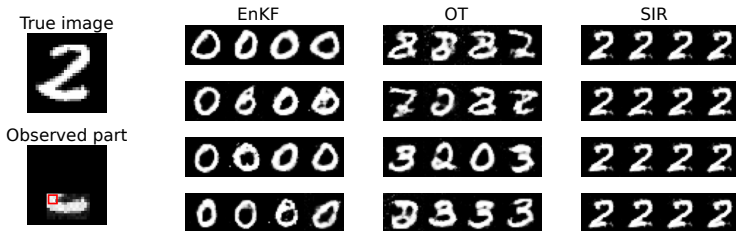
- Trajectory of the particles
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Numerical example: Image in-painting

$$X \sim N(0, I_{100}),$$

$$Y_t = h(G(X), c_t) + W_t,$$

$$G : \mathbb{R}^{100} \rightarrow \mathbb{R}^{28 \times 28} \text{ (pre-trained generator)}$$

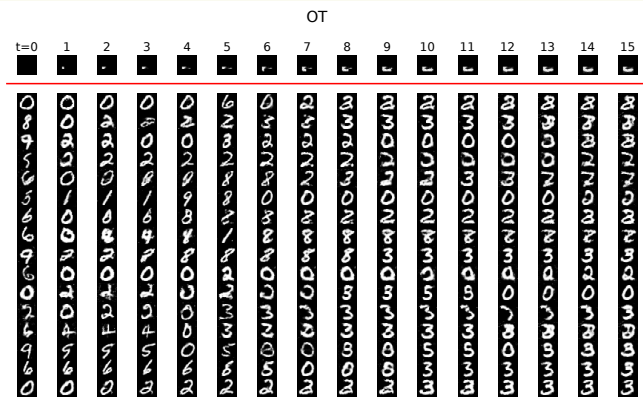


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Extension to Riemannian manifolds

McCann's result

- Assume $X \in \mathcal{M}$ with metric g and geodesic distance d_g
- Replace the Euclidean distance with the geodesic distance
- Replace $T(x, y)$ with $\exp_x(U(x, y))$ where $U(x, y) \in T_x M$

$$\max_{f: \mathcal{M} \rightarrow \mathbb{R}} \min_{U: \mathcal{M} \rightarrow T\mathcal{M}} \mathbb{E} \left[\frac{1}{2} d_g(\exp_{\bar{X}}(U(\bar{X}, Y)), \bar{X})^2 - f(\exp_{\bar{X}}(U(\bar{X}, Y)), Y) + f(X; Y) \right]$$

Extension to Riemannian manifolds

McCann's result

- Assume $X \in \mathcal{M}$ with metric g and geodesic distance d_g
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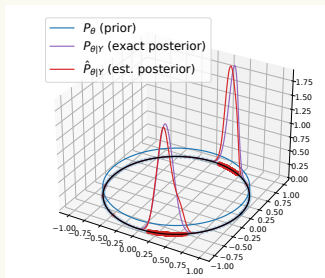
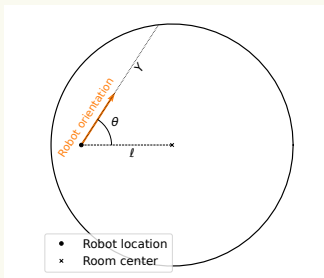
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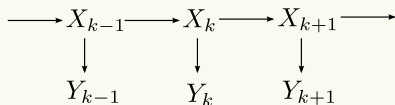
Numerical example: $\mathcal{M} = S^1$

- $\theta \in \mathcal{M}$ is robot's orientation and Y is noisy measurement of distance to the wall

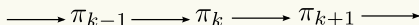


Summary

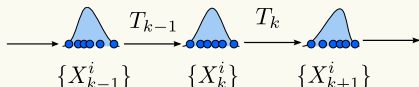
■ Mathematical model:



■ Nonlinear filtering: compute the posterior $\pi_k = P(X_k | Y_{1:k})$



■ OT approach:



■ Variational problem:

$$T_k \leftarrow \max_{f \in \mathcal{F}} \min_{T \in \mathcal{T}} J(f, T; \frac{1}{N} \sum_{i=1}^N \delta_{(X_k^i, Y_k^i)})$$

Outline

- **Part I:** Bayes' law and fundamental challenges of importance sampling
- **Part II:** Conditioning with optimal transport maps
- **Part III:** Application to nonlinear filtering
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Problem setup:

$$X_t \sim a(\cdot | X_{t-1}), \quad X_0 \sim \pi_0$$
$$Y_t \sim h(\cdot | X_t)$$

- X_t is the state
- Y_t is the observation
- the dynamic and observation models are unknown

Objective:

given: $\{X_0^j, (X_1^j, Y_1^j), \dots, (X_{t_f}^j, Y_{t_f}^j)\}_{j=1}^J$

compute: $\pi_t := P(X_t | Y_t, \dots, Y_1), \quad \forall t \geq 0$
for a new set of observations $\{Y_t, \dots, Y_1\}$

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Data-driven setting

Solution approach

- Exact posterior:

$$\pi_t := \mathbb{P}_{X_0 \sim \pi_0}(X_t | Y_t, \dots, Y_1)$$

- Step 1: Truncated posterior

$$\pi_{t,s}^\mu := \mathbb{P}_{X_s \sim \mu}(X_t | Y_t, \dots, Y_{s+1})$$

- Step 2: OT representation

$$\pi_{t,s}^\mu = T(\cdot, Y_t, \dots, Y_s) \# \mu \quad \text{where}$$
$$T \leftarrow \max_{f \in \mathcal{F}} \min_{T \in \mathcal{T}} J(f, T; P_{X_t, Y_t, \dots, Y_{s+1}})$$

- Step 3: Stationary assumption

$$P_{X_t, Y_t, \dots, Y_{s+1}} = P_{X_w, Y_w, \dots, Y_1} \quad \text{where } w := t - s$$

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Error analysis

Assume

- The exact filter is exponentially stable
- The process (X_t, Y_t) is stationary
- μ is equal to the stationary distribution of X_t and $M := \sup_t d(\pi_t, \mu) < \infty$
- (f, T) is a possibly non-optimal pair with max-min gap $\epsilon(f, T)$
- The function $x \mapsto \frac{1}{2}\|x\|^2 - f(x, y_w, \dots, y_1)$ is α -strongly convex for all (y_w, \dots, y_1) .

Then,

$$d(T(\cdot, Y_t, \dots, Y_{t-w}) \# \mu, \pi_t) \leq C\lambda^w M + \sqrt{\frac{4}{\alpha} \epsilon(f, T)}$$

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Numerical example

Model:

$$X_t = aX_{t-1} + \sigma V_t$$

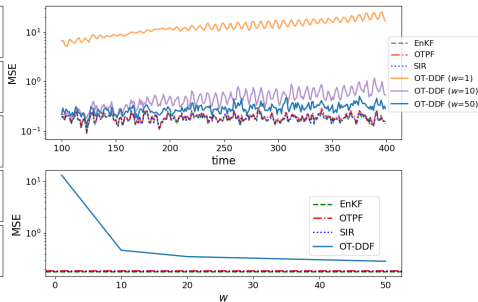
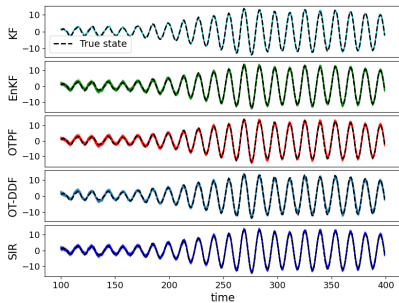
$$Y_t = h(X_t) + \sigma W_t$$

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$$Y_t = X_t + \sigma W_t$$

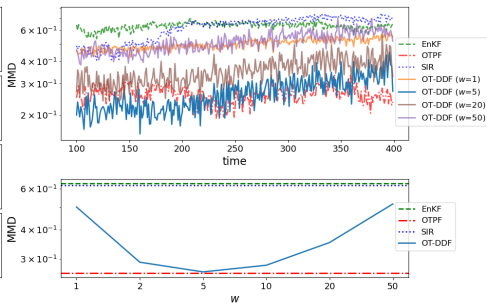
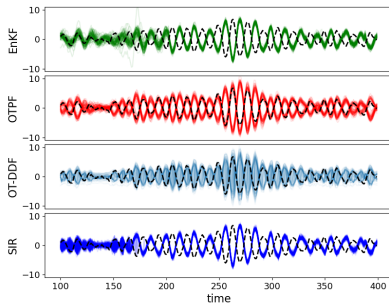


Numerical example

Model:

$$X_t = aX_{t-1} + \sigma V_t$$

$$Y_t = X_t^2 + \sigma W_t$$



Numerical example

Lorenz 63 model

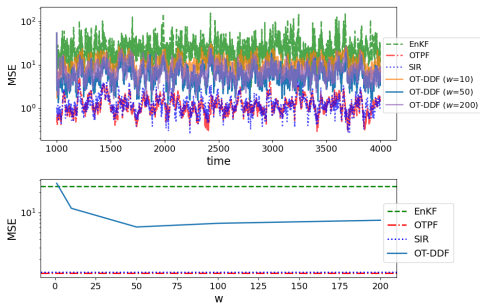
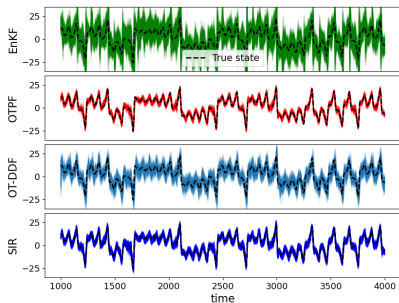
$$\begin{aligned}\dot{X} &= f(X), & X_0 &\sim \mathcal{N}(\mu_0, \sigma_0^2 I_3), \\ Y_t &= X_t(1) + W_t, & W_t &\sim \mathcal{N}(0, \sigma^2), \quad \Delta t = 0.01\end{aligned}$$

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Offline training time: 46.29 seconds

One-time step update:

Method	EnKF	SIR	OTPF	OT-DDF
time	1.7×10^{-4}	2.0×10^{-4}	6.8×10^{-2}	1.5×10^{-4}

Acknowledgments



M. Al-Jarrah



N. Jin



B. Hosseini



NSF

References:

