

Variational Optimal Transport Methods for Nonlinear Filtering

*Presented at 7th Workshop on Cognition and Control
Univ. of Florida, Gainsville, Jan. 2024*

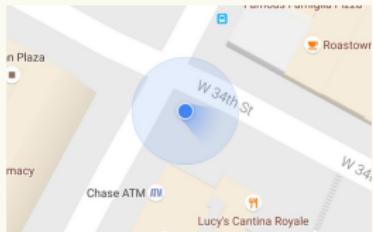
Amirhossein Taghvaei

Department of Aeronautics & Astronautics
University of Washington, Seattle

Jan 26, 2024

W

Uncertainty is everywhere



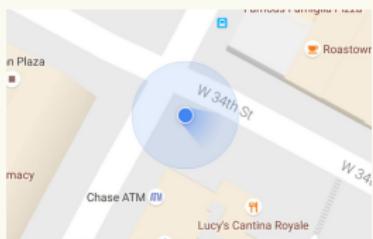
Weather forecast

COVID-19

Navigation

How to quantify uncertainty
and how to use data to reduce it

Uncertainty is everywhere



Navigation

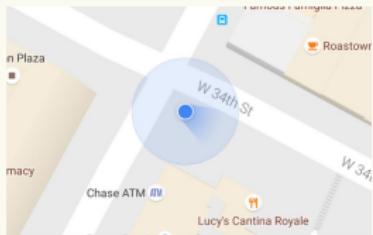


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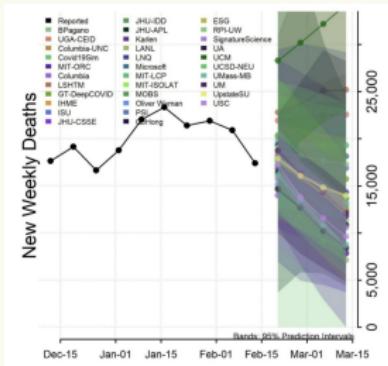
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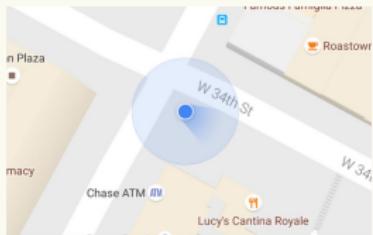
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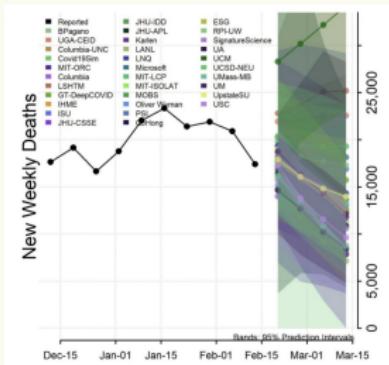
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and how to use data to reduce it

Mathematics of uncertainty

Probability theory: (quantify uncertainty)



Optimal transport (OT) theory: (geometry for distributions)

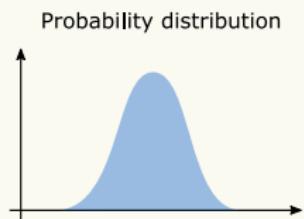
Global geometry

Local model fitting

This talk: application of OT to uncertainty quantification

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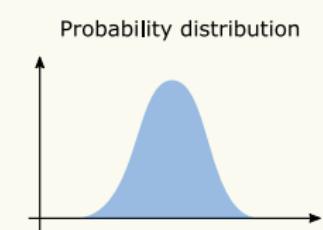
Distance between distributions

Smoothness of distributions

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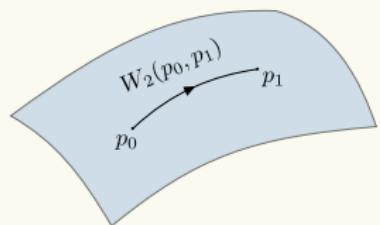
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Nobel prize (1975)



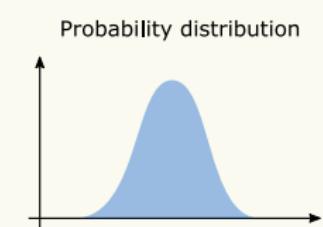
Fields medal (2010)



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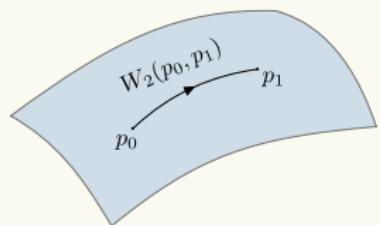
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This talk: application of OT to uncertainty quantification

Outline

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

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Bayes' law

Problem:

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

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

Simple to express, but difficult to implement, both intuitively and numerically

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When intuition fails

Two children puzzle:

- Smiths family has two children
- At least, one of them is a girl
- What is the probability that Smiths have two girls?
- What if you are told she is born on Tuesday?
- And her name is Florida.

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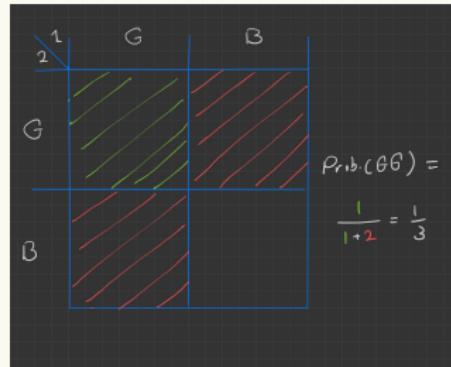
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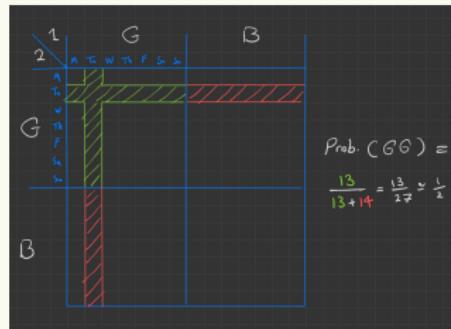
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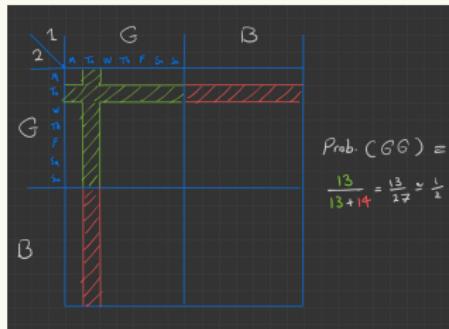


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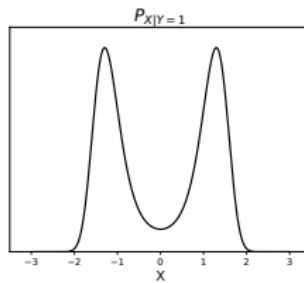
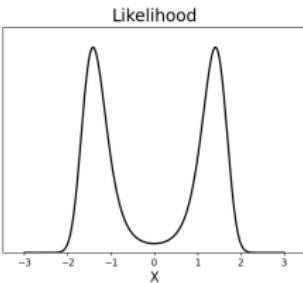
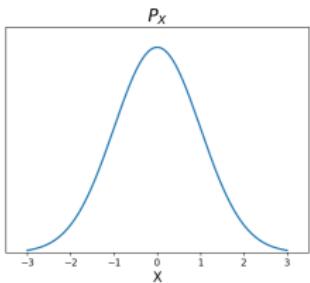
When numerics fail

Example:

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

Importance sampling (IS):

- $P_{X|Y=1}$ is a bimodal distribution
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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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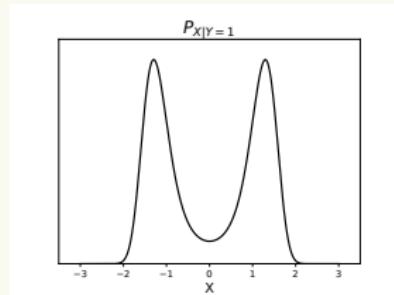
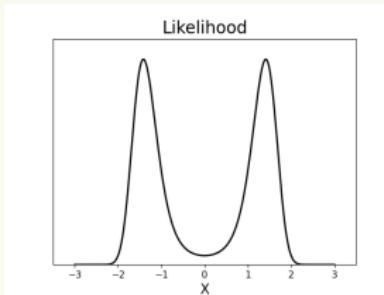
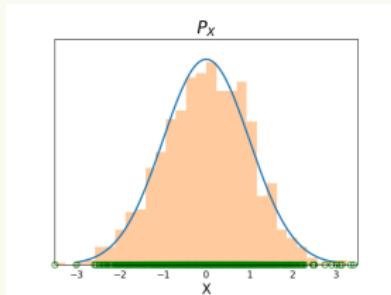
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- $X^i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$
- $w^i \propto P(Y = 1|X^i)$
- $P_{X|Y=1} \approx \sum_{i=1}^N w^i \delta_{X^i}$



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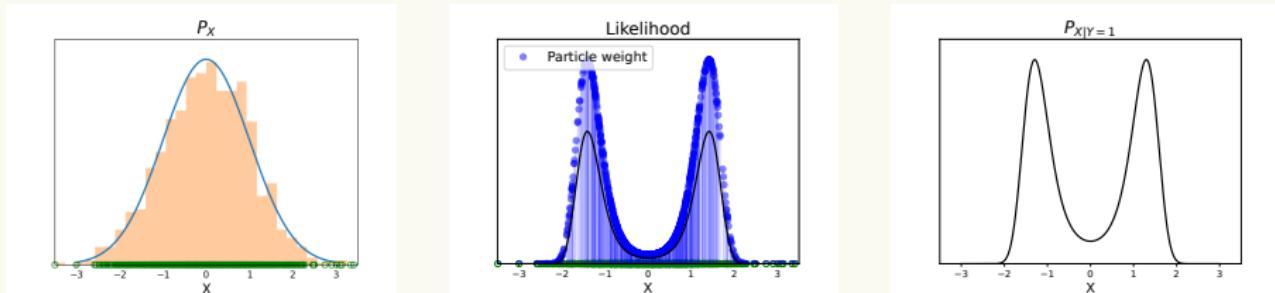
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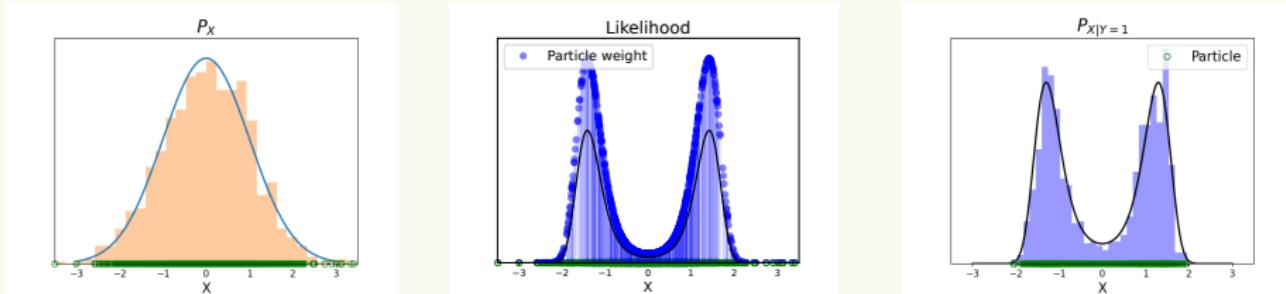
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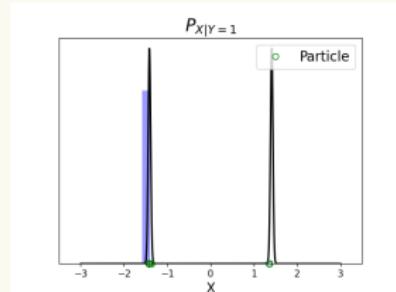
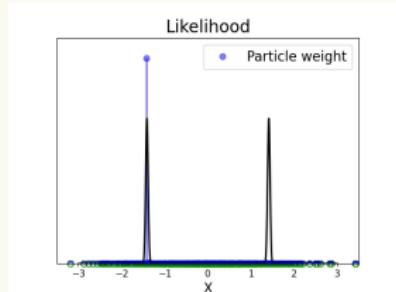
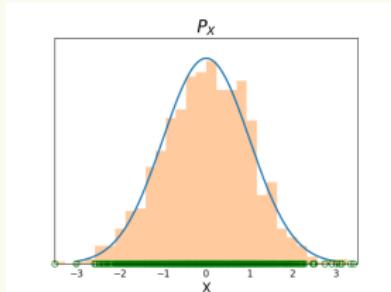
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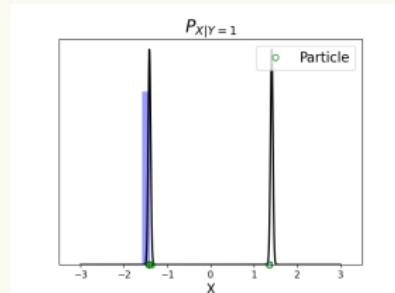
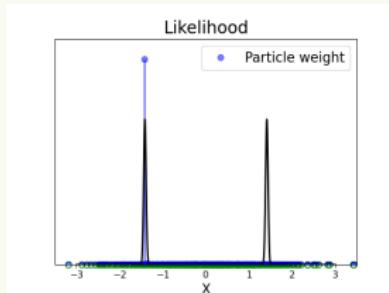
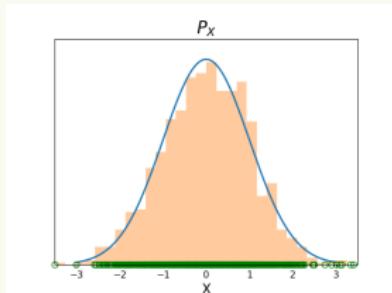
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Curse of dimensionality in particle filters

- $X, Y \in \mathbb{R}^n$ with i.i.d. components.
- Exact posterior: π_{exact}
- IS approximation: $\pi_{\text{IS}}^{(N)}$
- Asymptotic limit as $N \rightarrow \infty$:

$$\lim_{N \rightarrow \infty} \sqrt{N} d(\pi_{\text{exact}}, \pi_{\text{IS}}^{(N)}) = C \gamma^n$$

where $d(\cdot, \cdot)$ is the dual bounded metric.

- Good news: accurate as $N \rightarrow \infty$ (universal for any prior and likelihood)
- Bad news: error scales exponentially with the dimension n
- Remedy: exploit problem specific properties (e.g. spatial correlation decay in localization methods)
- Alternative method: replacing IS with control or coupling-based techniques

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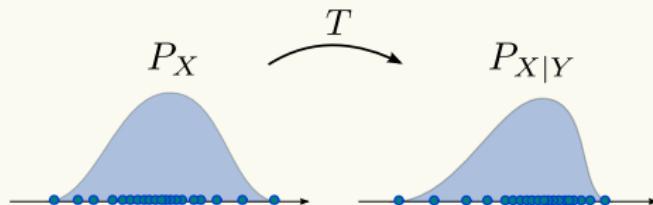
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Coupling/Control viewpoint



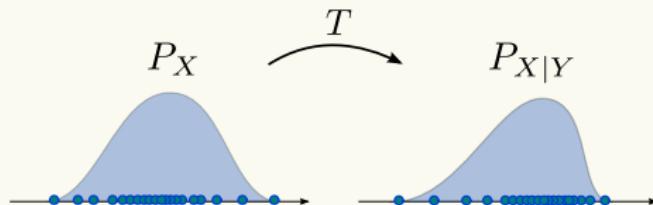
$$X^i \sim P_X \longrightarrow T(X^i, y) \sim P_{X|Y=y}$$

Example:

- Consider $X \sim P_X$. Then $T(X, y)$ is the random variable obtained by applying T to X .
- If T is a deterministic function, then $T(X, y)$ is a deterministic function of X and y .

How to numerically find the map T in a general setting?

Coupling/Control viewpoint



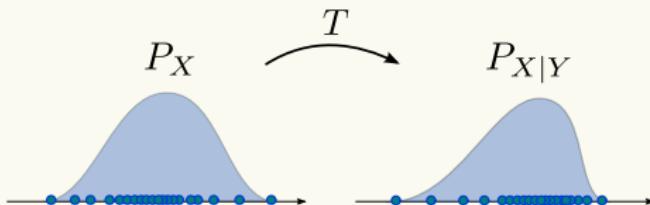
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Example:

- 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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Literature survey

Control and coupling techniques for filtering and Bayesian inference

- Particle flow filters [Daum et. al. 2010]
- A dynamical systems framework for data assimilation [Reich. 2011]
- Mean-field control approach [Yang, Mehta, Meyn, 2011]
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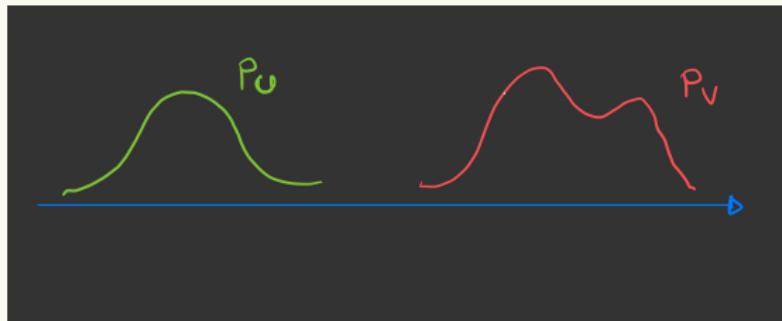
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Background on optimal transportation theory

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. $T_{\#}P_U = P_V$ or $T(U) \stackrel{d}{=} V$
- with minimal transportation cost $\|T(x) - x\|^2$

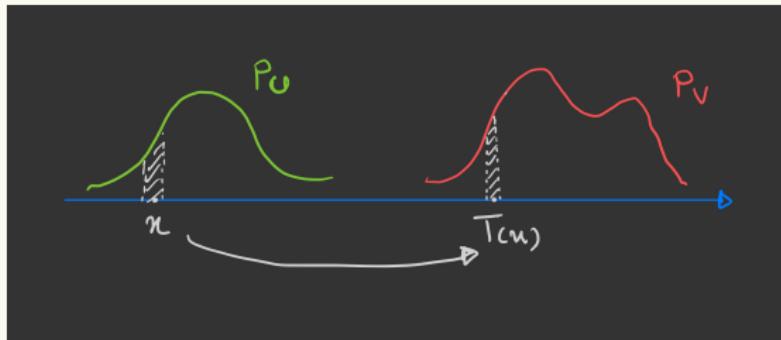
Brenier's result

If P_U admits (Lebesgue) density, the optimal map $\bar{T} = \nabla \bar{f}$ where \bar{f} minimizes

$$\min_{f \text{ is convex}} \mathbb{E}[f(U) + f^*(V)]$$

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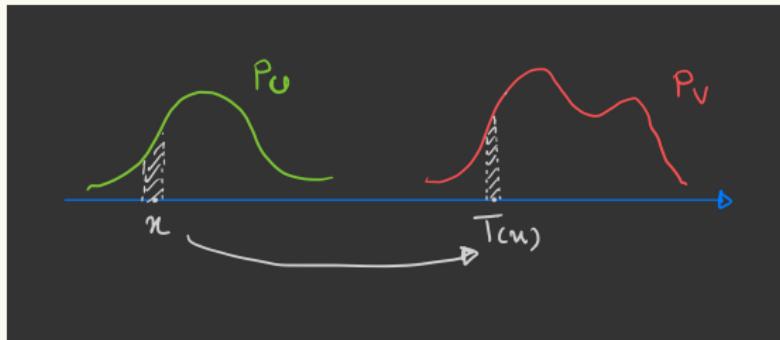
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If P_U admits (Lebesgue) density, the optimal map $\bar{T} = \nabla \bar{f}$ where \bar{f} minimizes

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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. $T_{\#}P_U = P_V$ or $T(U) \stackrel{d}{=} V$
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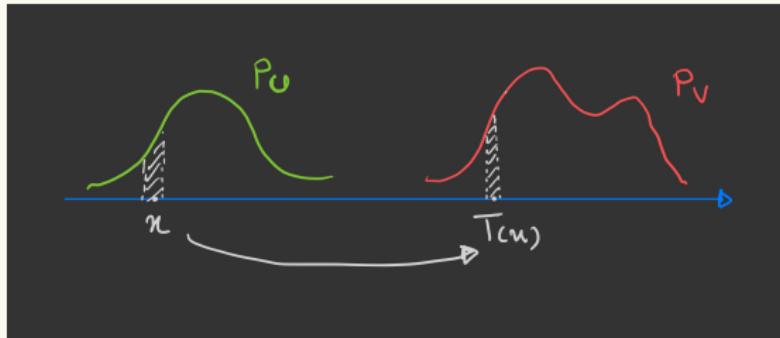
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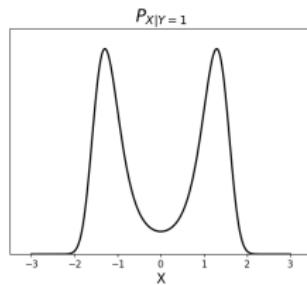
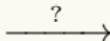
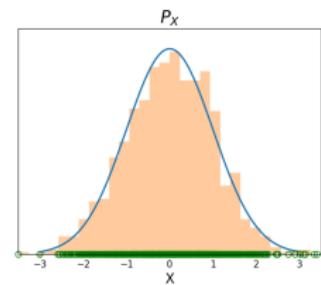
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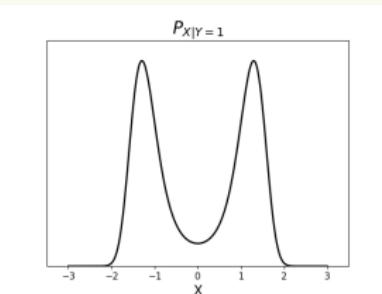
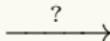
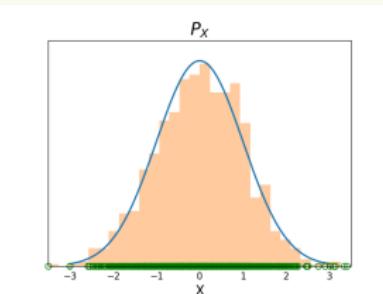
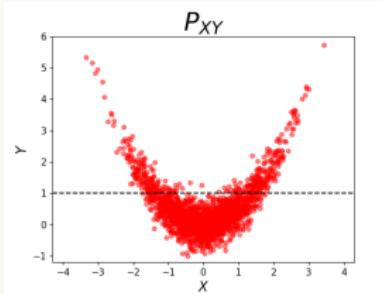
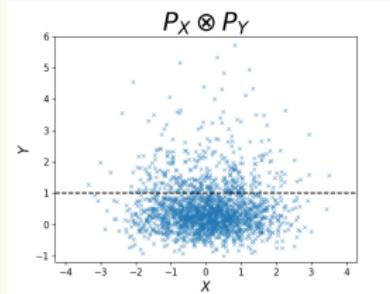
Conditioning with optimal transport map

Illustrative example



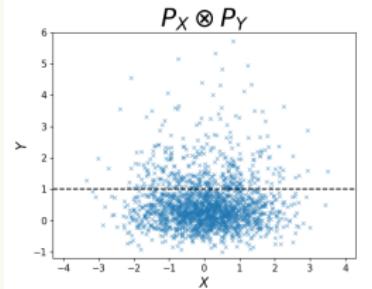
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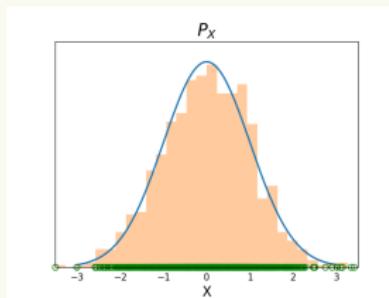
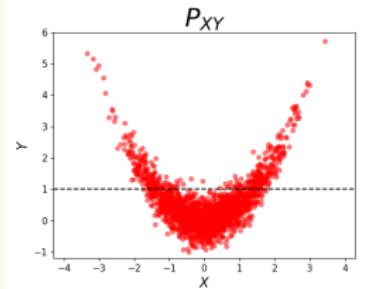


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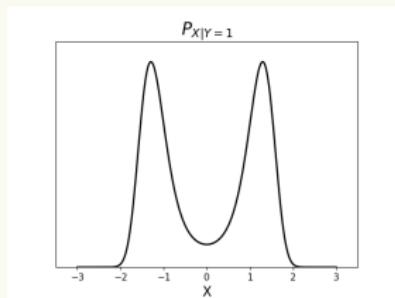
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$$\xrightarrow{(T(X,Y), Y)}$$

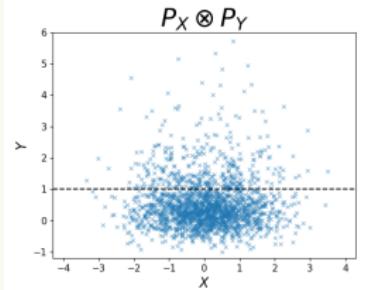


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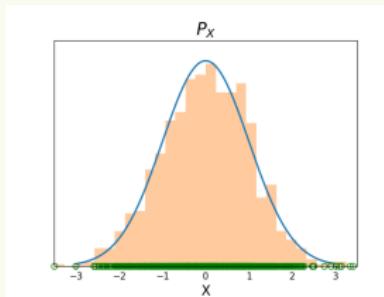
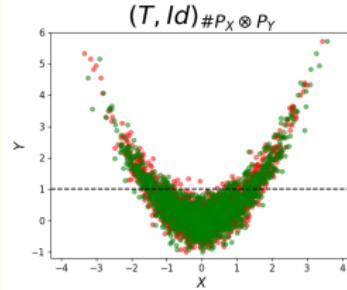


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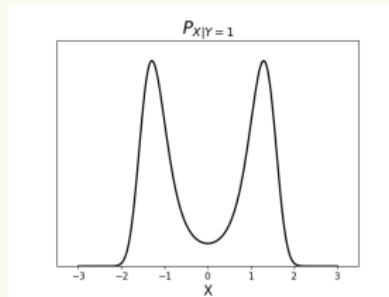
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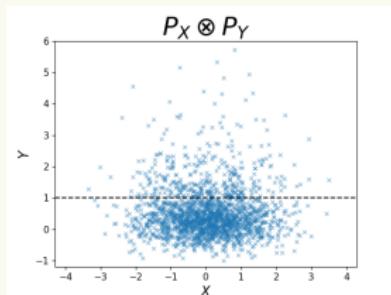


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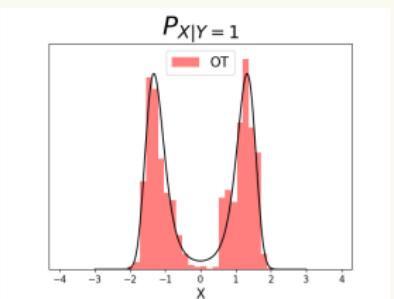
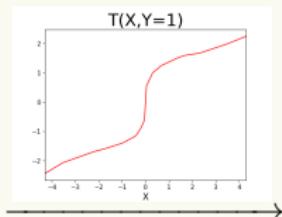
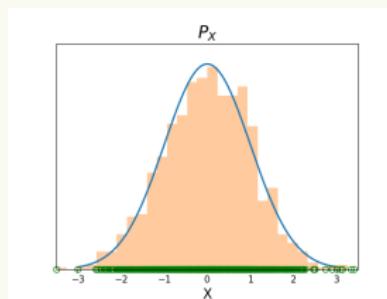
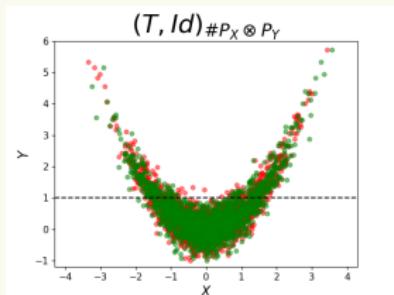


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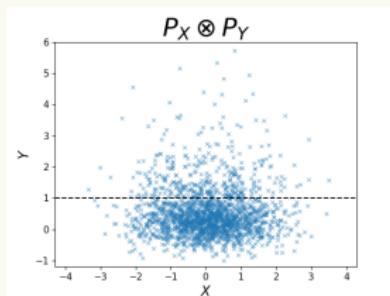


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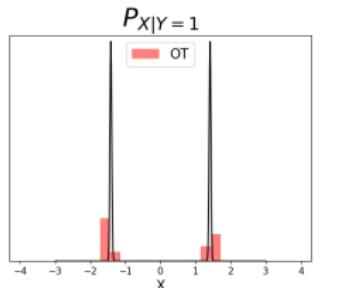
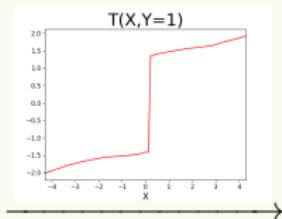
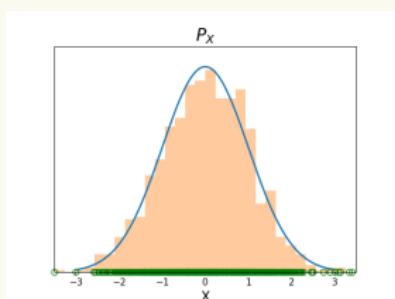
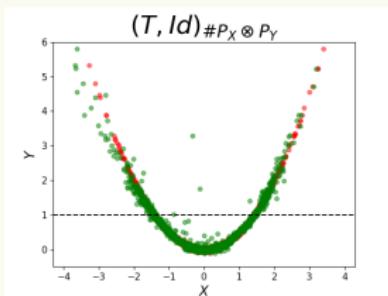


Conditioning with optimal transport map

Illustrative example



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



small noise limit

Conditioning with optimal transport map

Variational formulation of the Bayes' law

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

where $\bar{f} = \arg \min_{f \in L^1(\mathcal{X} \times \mathcal{Y})} \mathbb{E}_{(X,Y) \sim P_X \otimes P_Y} [f(X; Y)] + \mathbb{E}_{(X,Y) \sim P_{XY}} [f^*(X; Y)]$

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

- $(X, Y) \sim P_{X,Y}$ and $(\bar{X}, Y) \sim P_X \otimes P_Y$
- Variational problem: $\min_f J(f, P_{X,Y}) := \mathbb{E}[f(\bar{X}, Y) + f^*(X, Y)]$

(Conditional) Brenier's theorem

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

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

- (Sensitivity) Let f be a possibly non-optimal function. Assume $x \mapsto f(x, y)$ is convex and β -smooth for all y . Then,

$$d(\nabla f(\cdot, Y) \# P_X, P_{X|Y}) \leq \sqrt{2\beta (J(f) - J(\bar{f}))}.$$

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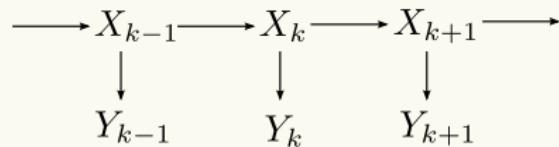
Outline

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

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Nonlinear filtering problem



- X_t is the state (unknown)
- Y_t is the observation

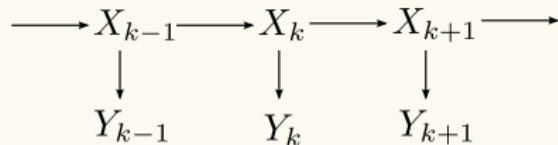
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Answer: given by the conditional distribution $\pi_t = P_{X_t|Y_{1:t}}$ (posterior, belief)

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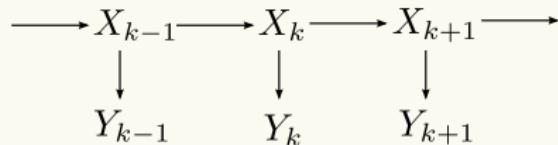
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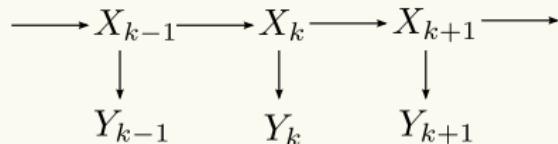
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Filtering equations

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

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

$$\text{Conditioning: } \pi \xrightarrow{\text{Bayes law}} B_y(\pi)$$

- Recursive update law for the posterior

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

- (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

No dynamics setting (for simplicity)

Filter design steps:

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

$$\text{mean-field process: } \bar{X}_t = \nabla \bar{f}_t(\bar{X}_{t-1}, Y_t)$$

$$\text{particle system: } X_t^i = \nabla \hat{f}_t(X_{t-1}^i, Y_t)$$

Variational problem:

$$\min_{\pi_t} \mathbb{E}[\mathcal{L}(\pi_t, \bar{X}_t)] + \beta \mathbb{E}[\mathcal{D}_{\text{OT}}(\pi_t, \delta_{\bar{X}_t})]$$
$$\mathcal{L}(\pi_t, \bar{X}_t) = \frac{1}{N} \sum_{i=1}^N \ell(\pi_t(x_i), \bar{X}_t)$$
$$\mathcal{D}_{\text{OT}}(\pi_t, \delta_{\bar{X}_t}) = \inf_{\pi_{\text{OT}}} \mathbb{E}_{\pi_{\text{OT}}}[d(x, \bar{X}_t)]$$

Posterior approximation:

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

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Optimal Transport Filter

Error Analysis

Theorem

Assume

- 1 The exact filter is exponentially stable
- 2 Uniform bound $\epsilon_{\mathcal{F},N}$ on the optimality gap $J(\hat{f}_t) - J(\bar{f}_t)$
- 3 The function $\hat{f}_t(\cdot, y)$ is convex and β -smooth for all t and y .
- 4 Particles are resampled at each step

Then,

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

- Optimality gap $\epsilon_{\mathcal{F},N}$ has bias-variance decomposition

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

Optimal Transport Filter

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- 2 Uniform bound $\epsilon_{\mathcal{F},N}$ on the optimality gap $J(\hat{f}_t) - J(\bar{f}_t)$
- 3 The function $\hat{f}_t(\cdot, y)$ is convex and β -smooth for all t and y .
- 4 Particles are resampled at each step

Then,

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

- Optimality gap $\epsilon_{\mathcal{F},N}$ has bias-variance decomposition

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

Optimal Transport Filter

Error Analysis

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Optimal Transport Filter

Numerical example

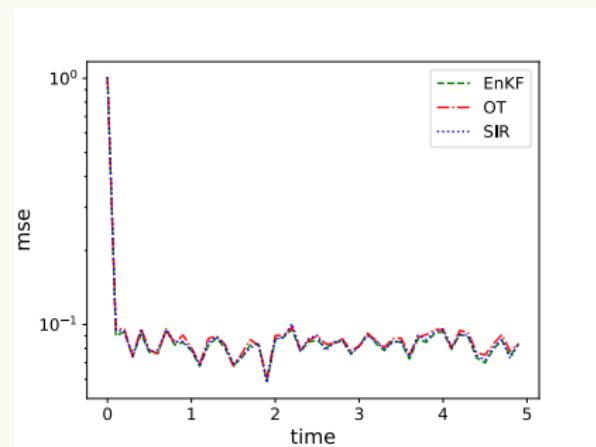
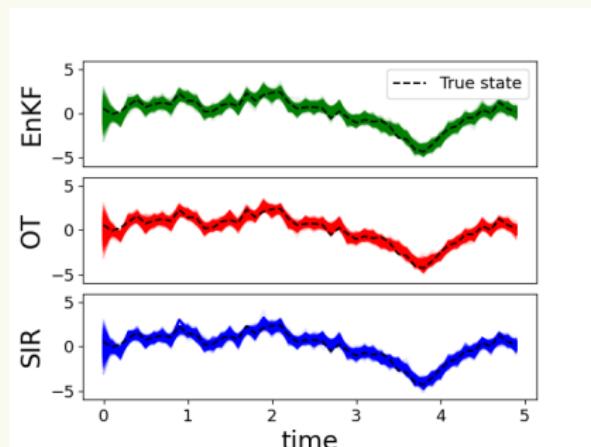
$$X_t = (1 - \alpha)X_{t-1} + \sigma_V V_t, \quad X_0 \sim \mathcal{N}(0, I_n),$$
$$Y_t = \textcolor{red}{X_t} + \sigma_W W_t,$$

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

Optimal Transport Filter

Numerical example

$$X_t = (1 - \alpha)X_{t-1} + \sigma_V V_t, \quad X_0 \sim \mathcal{N}(0, I_n), \\ Y_t = \textcolor{red}{X_t} + \sigma_W W_t,$$

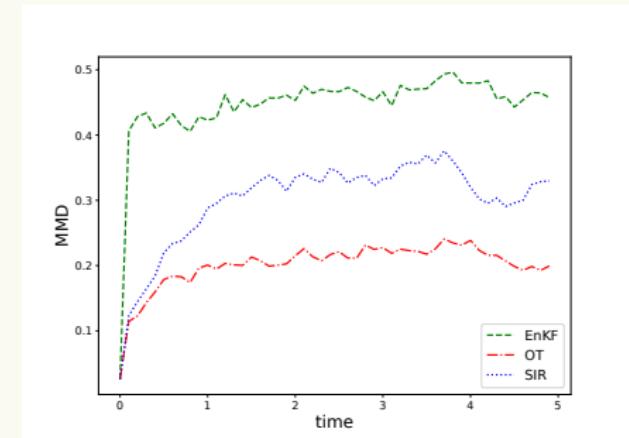
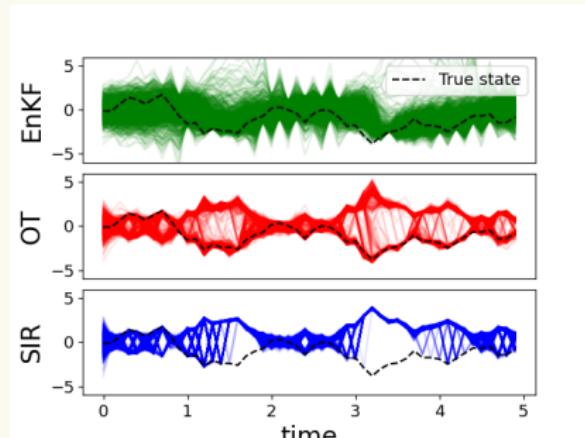


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Optimal Transport Filter

Numerical example

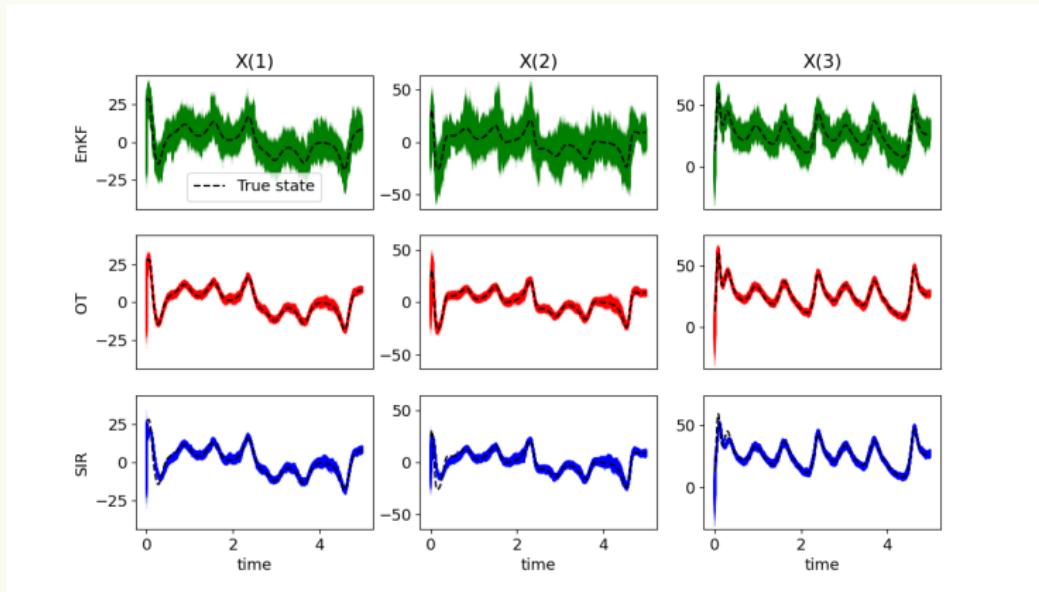
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Optimal Transport Filter

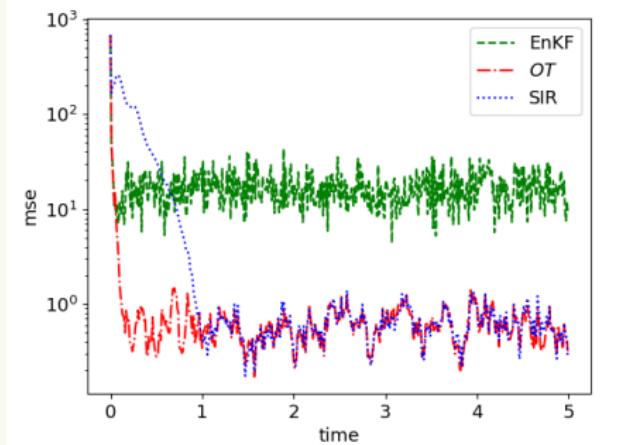
Numerical example: Lorenz 63



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

Optimal Transport Filter

Numerical example: Lorenz 63



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

Numerical example: Image in-painting

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

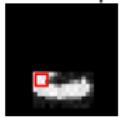
$$Y_t = h(G(X), c_t) + W_t,$$

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

True image



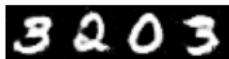
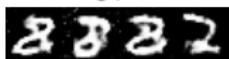
Observed part



EnKF



OT



SIR

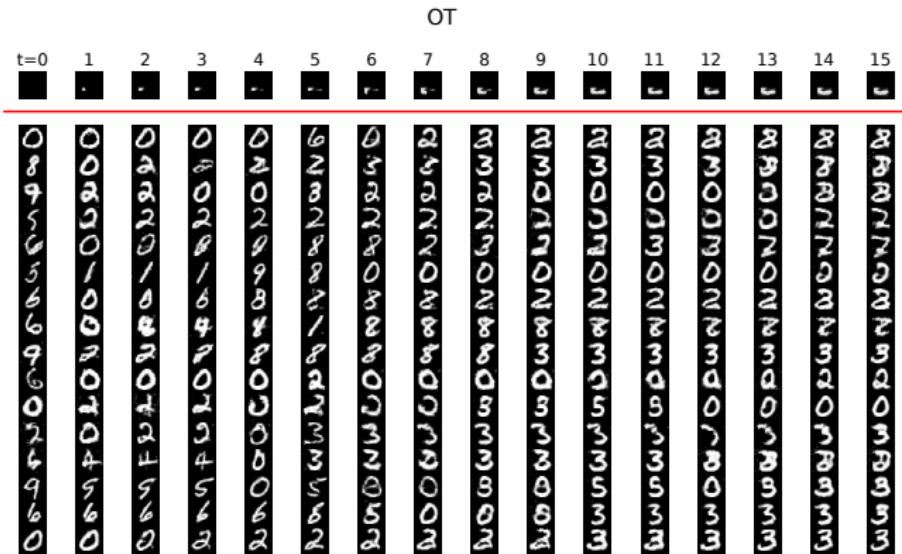


Numerical example: Image in-painting

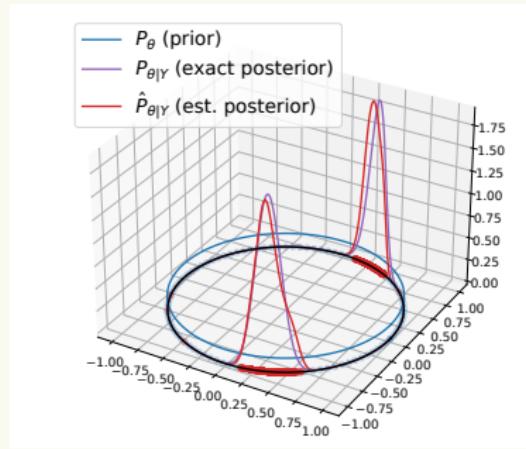
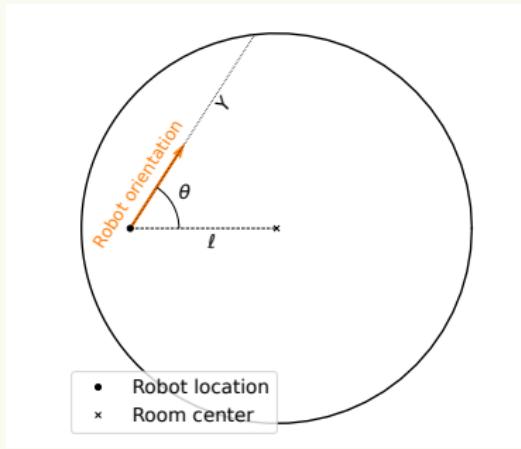
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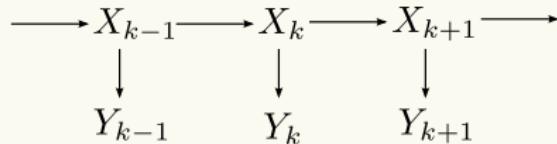


Numerical example: Attitude estimation



Summary

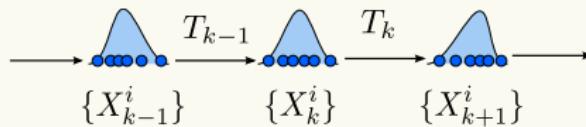
- Mathematical model:



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

$$\xrightarrow{\quad} \pi_{k-1} \xrightarrow{\quad} \pi_k \xrightarrow{\quad} \pi_{k+1} \xrightarrow{\quad}$$

- OT approach:



- Variational problem:

$$T_k = \nabla_x \bar{f}_k, \quad \text{where} \quad \bar{f}_k = \arg \min_{f \in \mathcal{F}} J^{(N)}(f; \{(X_k^i, Y_k^i)\})$$

References

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NSF