Design and Analysis of Particle-based Algorithms for Nonlinear Filtering and Sampling

Doctoral Final Examination

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Outline

Part I: Analysis of the feedback particle filter (FPF)

- Background (9 slides)
- (1) Gain function approximation (12 slides)
- (2) Optimal transport FPF (back-up slides)
- (3) Error analysis of linear FPF (back-up slides)

Part II: Accelerated flow for probability distributions (8 slides)

Common theme

- Control problem on the space of probability distributions (mean-field control)
- Numerical algorithm as a system of interacting particles

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Background:

- Filtering problem in discrete time
- Monte-Carlo approximation
- Filtering problem in continuous time
- Feedback particle filter (FPF)

Analysis of FPF

- Gain function approximation (this talk)
- Optimal transport FPF (back-up slides)
- Error analysis of linear FPF (back-up slides)

Objective: Motivate the three topics of contribution

Background: Filtering problem

Mathematical formulation in discrete-time

$$\begin{tikzcd}
\arrow[r] & X_{k-1} \arrow[r] \arrow[d] & X_k \arrow[r] \arrow[d] & X_{k+1} \arrow[r] \arrow[d] & \\
& Z_{k-1} & Z_k & Z_{k+1} &
\end{tikzcd}$$

State process: $X_k \sim a(\cdot|X_{k-1}), \qquad X_0 \sim \pi_0(\cdot)$

Observation process: $Z_k \sim l(\cdot|X_k)$

Filtering objective: Compute the posterior distribution $\pi_k(\cdot) := \mathsf{P}(X_k \in \cdot|Z_{1:k})$

Solution:

$$\pi_{k-1}(x) \quad \longrightarrow \quad \tilde{\pi}_k(x) = \int a(x|x')\pi_{k-1}(x')\mathrm{d}x'$$

$$\longrightarrow \quad \pi_k(x) = \frac{l(Z_k|x)\tilde{\pi}_k(x)}{\gamma} \quad \text{(Bayes rule)}$$

- In general, no finite-dimensional solution $\Rightarrow$ approximations

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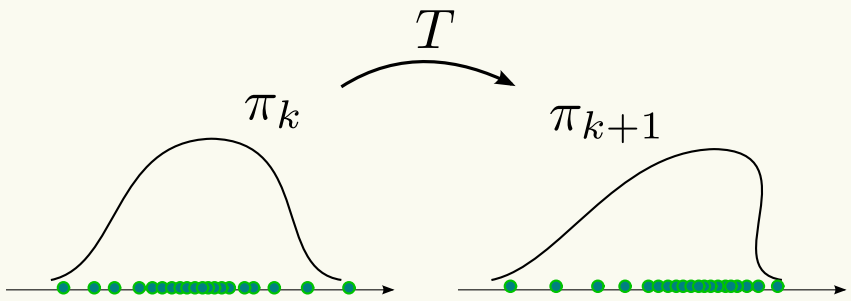
Background: Monte-Carlo approximation

Coupling viewpoint

- Approximate π_k with empirical distribution of particles $\frac{1}{N}\sum_{i=1}^{N}\delta_{X_k^i}$
- Transform particles $\{X_k^i\}_{i=1}^N \sim \pi_k$ to particles $\{X_{k+1}^i\}_{i=1}^N \sim \pi_{k+1}$



Coupling viewpoint:

- Find a coupling $\gamma(x, y)$ between π_k and π_{k+1}

$$\{X_k^i\}_{i=1}^N \longrightarrow \{X_{k+1}^i\}_{i=1}^N$$

- Update the particles with the transition kernel

$$X_{k+1}^i \sim T(X_k^i, \cdot)$$

There are infinitely many couplings!

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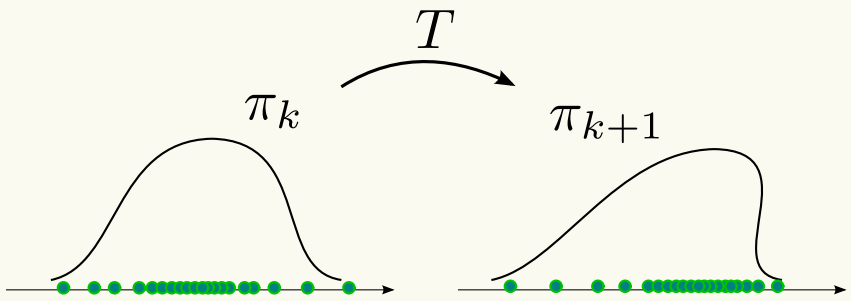

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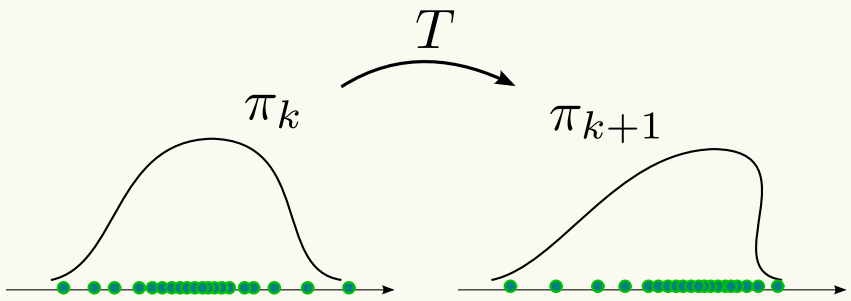

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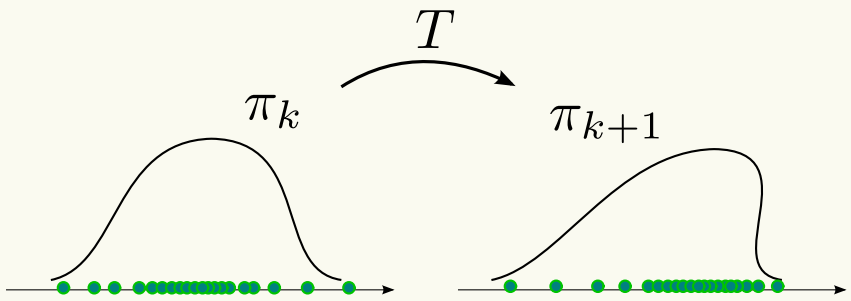

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There are infinitely many couplings!

Background: Brief review of algorithms

Coupling viewpoint

Assume there is no dynamics: $\pi_{k+1}(x) = \dfrac{l_k(x)\pi_k(x)}{\gamma}$

SIR particle filter: (Gordon et al., 1993, Doucet, 2009)

- Sample from the independent coupling:

$$\mathbb{P}(x_k^i, x_k^j) = \pi_{k+1}(x_k^i)\pi_{k+1}(x_k^j) \quad \text{for } i, j = 1, \ldots, N$$

  But π_{k+1} is not explicitly known!

- Approximate $\pi_{k+1} \approx \sum_{i=1}^{N} w_k^i \delta_{x_k^i}$ where $w_k^i = \dfrac{l_k(x_k^i)}{\sum_{j=1}^{N} l_k(x_k^j)}$

(Variations of) SIR particle filter: (Del Moral 2004, Bain & Crisan 2009, Van Leeuwen 2015, Nakamura & Potthast 2015)

- Sample from a coupling that is optimal with respect to some optimality criteria

Ensemble transform particle filters:

- Sample from optimal transport coupling (Cheng & Reich, 2013)
- Sample from Schrodinger bridge coupling (Reich, 2018)

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Background: Monte-Carlo approximation

Three questions

1. Approximation: Numerical approximate of a coupling

$$\textbf{Given:} \quad \{X_k^1, \ldots, X_k^N\} \sim \pi_k \quad \text{and} \quad l_k(\cdot)$$

$$\textbf{Approximate:} \quad \text{a coupling between } \pi_k \text{ and } \pi_{k+1}$$

2. Design: Which coupling to choose?

3. Error analysis: Analysis of the error between empirical distribution $\frac{1}{N}\sum_{i=1}^{N}\delta_{X_k^i}$ and exact filter π_k

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Background: Filtering problem

Mathematical formulation in continuous-time

State process: $\mathrm{d}X_t = a(X_t)\mathrm{d}t + \sigma_B(X_t)\mathrm{d}B_t, \qquad X_0 \sim p_0(\cdot)$

Observation process: $\mathrm{d}Z_t = h(X_t)\mathrm{d}t + \mathrm{d}W_t$

Filtering objective: Compute the posterior distribution $\pi_t(\cdot) := \mathrm{P}(X_t \in \cdot | Z_{[0,t]})$

Solution:

$$\mathrm{d}\pi_t = (\text{Kushner-Stratonovic eq.})$$

- In general, no finite-dimensional solution $\Rightarrow$ approximations

J. Xiong, An introduction to stochastic filtering theory, 2008

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Background: Monte-Carlo approximation

Continuous-time setting

Idea:

- Approximate π_t with empirical distribution of particles $\frac{1}{N}\sum_{i=1}^{N}\delta_{X_t^i}$
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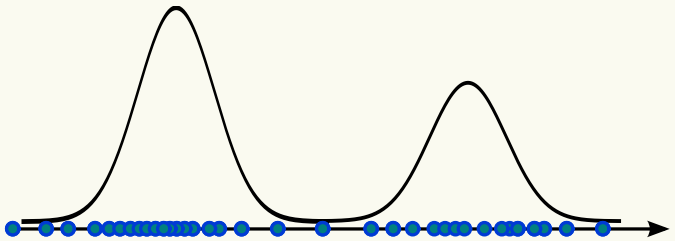

$\{X_t^1, \ldots, X_t^N\}$

Control viewpoint: Find a control law

$$\mathrm{d}X_t^i = (\text{control law}) \quad \text{such that} \quad \underbrace{X_t^i \sim \pi_t}_{\text{exactness}}$$

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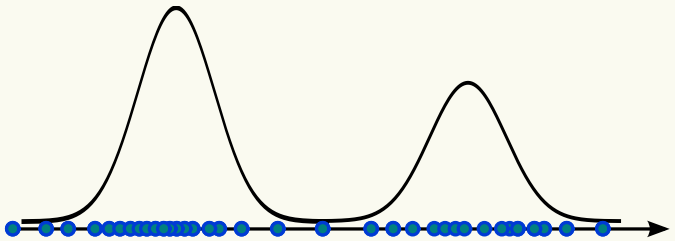

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Background: Feedback particle filter (FPF)

Update formula:

$$\mathrm{d}X_t^i = \text{(dynamic model)} + \underbrace{\mathsf{K}_t(X_t^i) \circ (\mathrm{d}Z_t - \frac{h(X_t^i) + \hat{h}_t}{2}\mathrm{d}t)}_{\text{correction}}, \quad X_0^i \overset{\text{i.i.d}}{\sim} \pi_0$$

- Gain function $\mathsf{K}_t(x) = \nabla\phi_t(x)$ where ϕ_t solves the Poisson eq.

$$\frac{1}{\rho_t(x)}\nabla \cdot (\rho_t(x)\nabla\phi_t(x)) = h(x) - \hat{h}_t$$

- $\hat{h}_t = \mathsf{E}[h(X_t^i)|\mathcal{Z}_t]$
- ρ_t is probability density for X_t^i

FPF is exact: $X_t^i \sim \pi_t$

T. Yang, P. G. Mehta, and S. P. Meyn. Feedback particle filter, *TAC*, 2013
T. Yang, R. S. Laugesen, P. G. Mehta, and S. P. Meyn. Multivariable feedback particle filter, *Automatica*, 2016

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Background: Feedback particle filter

Three questions

1. Approximation: Numerical approximation of the gain function

$$\textbf{Given:} \quad \{X_t^1, \ldots, X_t^N\}_{i=1}^N \sim \rho_t$$

$$\textbf{Approximate:} \quad \{\mathsf{K}_t(X_t^1), \ldots, \mathsf{K}(X_t^N)\}_{i=1}^N$$

2. Design: How to construct a control law that is exact?

3. Error analysis: Analysis of the error between empirical distribution $\frac{1}{N}\sum_{i=1}^N \delta_{X_t^i}$ and exact filter π_t

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  - A. Taghvaei and P. G. Mehta, Gain function approximation in the feedback particle filter, in Conference on Decision and Control (CDC), 2016, pp. 5446–5452.
  - A. Taghvaei, P. G. Mehta, and S. P. Meyn, Error estimates for the kernel gain function approximation in the feedback particle filter, in American Control Conference (ACC), 2017, pp. 4576–4582.
  - A. Taghvaei, P. G. Mehta, and S. P. Meyn, Gain function approximation in the feedback particle filter, SIAM journal on Uncertainty Quantification (under review),
- Optimal transport FPF
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Part II: Accelerated flow for probability distributions

FPF update formula:

$$\mathrm{d}X_t^i = \text{(dynamic model)} + \mathsf{K}_t(X_t^i) \circ (\mathrm{d}Z_t - \frac{1}{2}(h(X_t^i) + \hat{h}_t)\mathrm{d}t)$$

Gain function $\quad \mathsf{K}_t(x) = \nabla\phi_t(x) \quad$ where ϕ_t solves the Poisson eq.

Poisson equation:

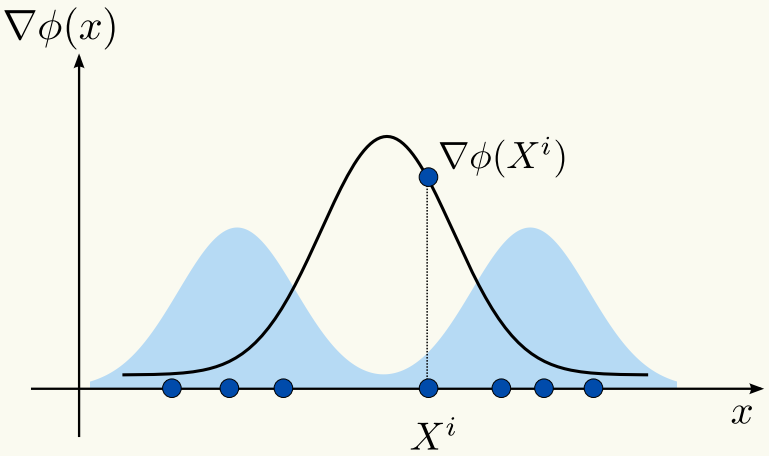
$$-\Delta_\rho \phi(x) = h(x) - \hat{h}$$

where $\Delta_\rho \phi := \frac{1}{\rho}\nabla \cdot (\rho \nabla \phi)$

Computational problem:

Given: $\{X^1, \ldots, X^N\} \overset{\text{i.i.d}}{\sim} \rho$

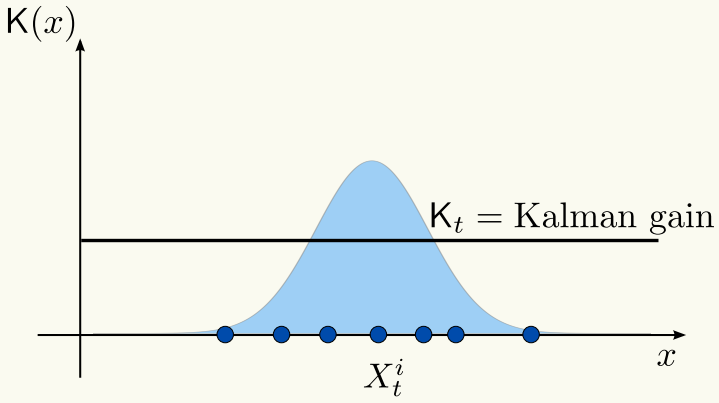
Approximate: $\{\mathsf{K}(X^1), \ldots, \mathsf{K}(X^N)\}$



Linear Gaussian setting

- ρ is Gaussian $\mathcal{N}(m, \Sigma)$
- $h(x) = Hx$

$$\mathsf{K}(x) = \Sigma H^\top \quad \text{(Kalman gain)}$$



FPF $\xrightarrow{\text{linear Gaussian}}$ Ensemble Kalman filter (EnKF)

A. Taghvaei, J de Wiljes, P. G. Mehta, and S. Reich. Kalman filter and its modern extensions for the continuous-time nonlinear filtering problem. ASME, 2017

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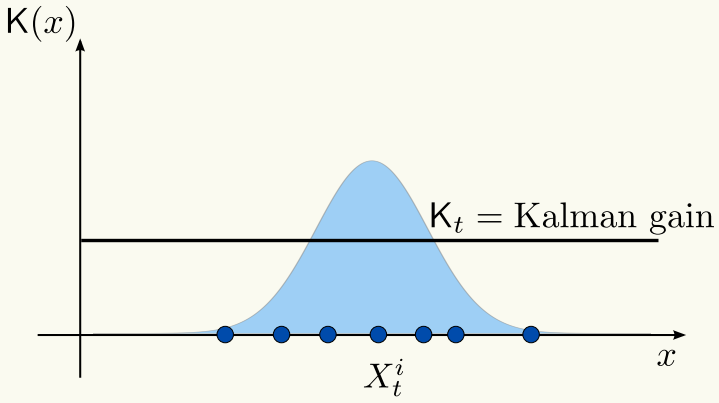

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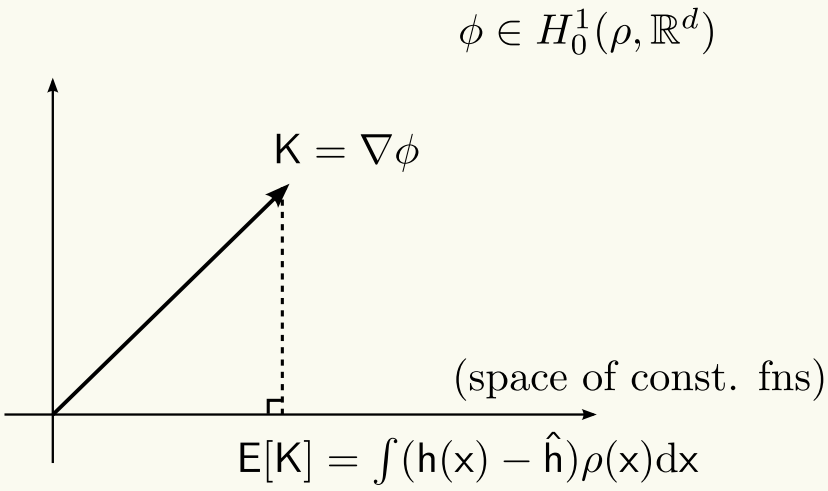
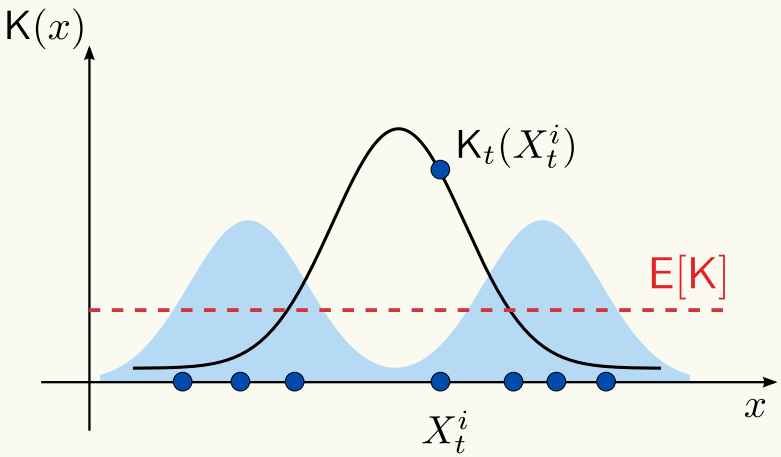
Idea: Projection to space of constant functions





A closed-form formula:

$$\mathsf{K}_{\mathsf{const}} = \int (h(x) - \hat{h}_t) x \rho(x) \mathrm{d}x \approx \frac{1}{N} \sum_{i=1} (h(X^i) - \hat{h}^{(N)}) X^i$$

Can we improve this approximation?

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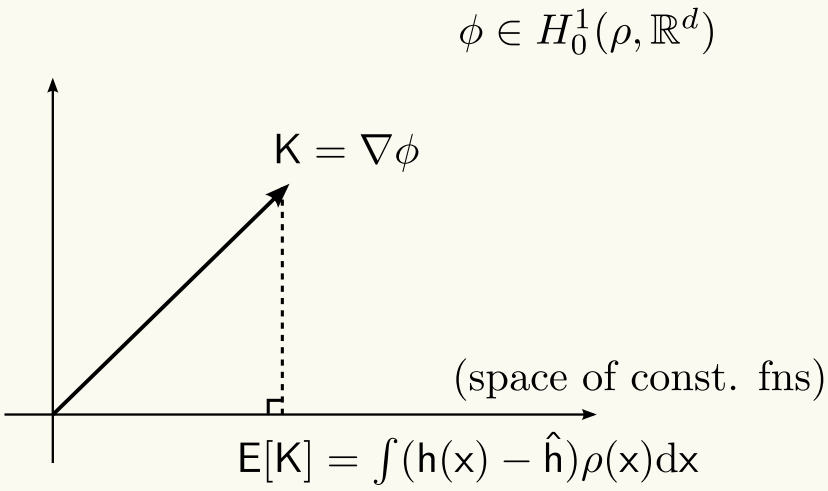

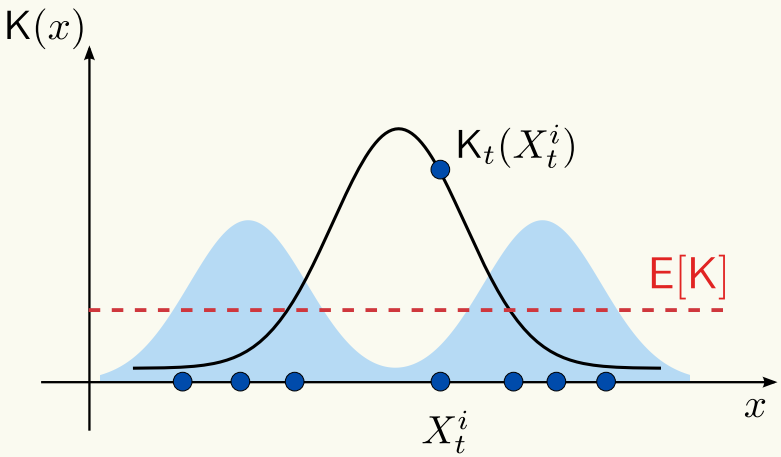

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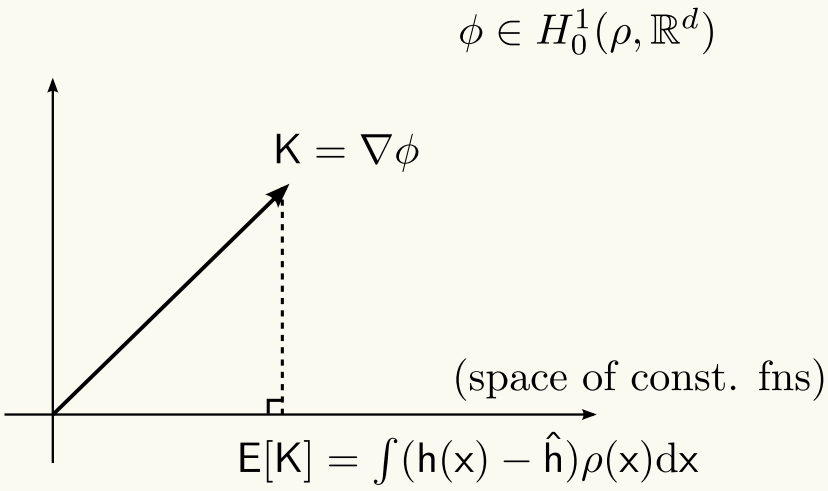

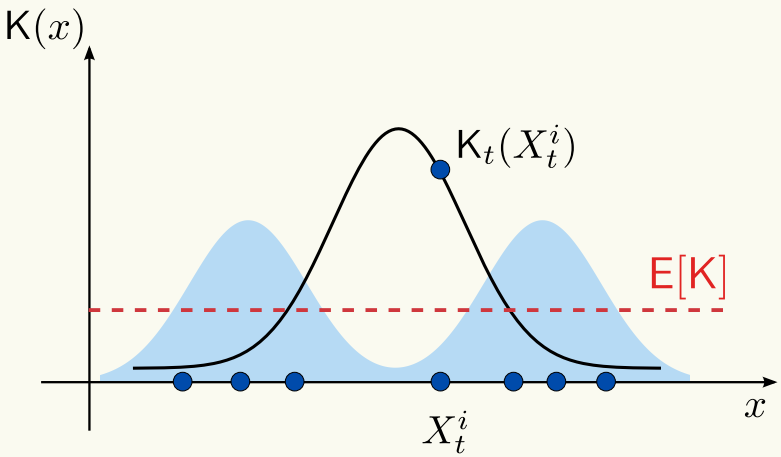

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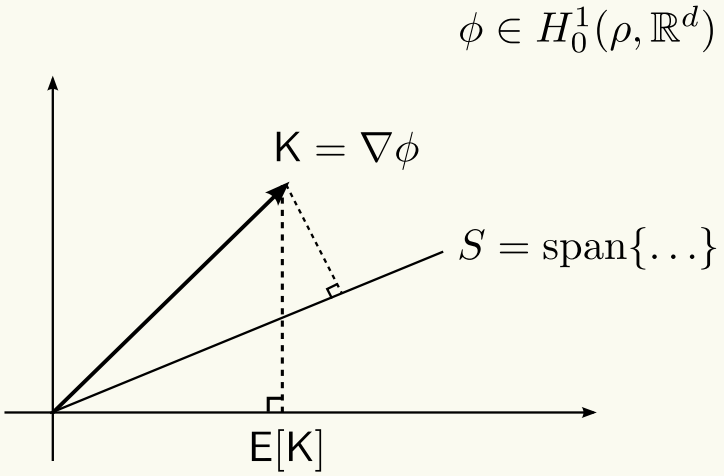
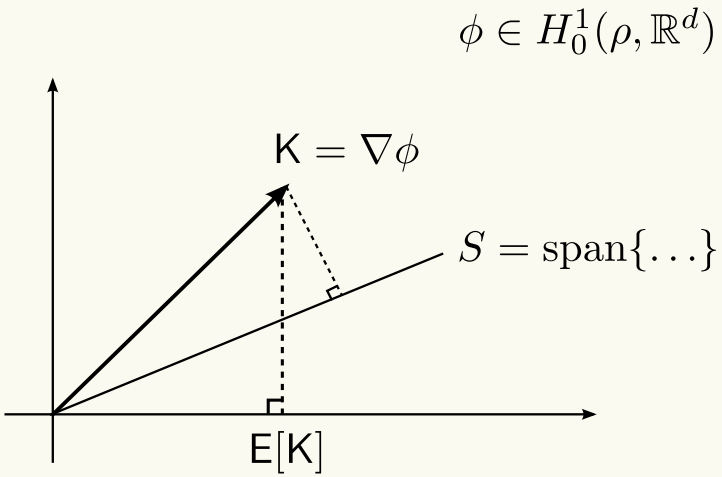
Gain function approximation
Galerkin approximation

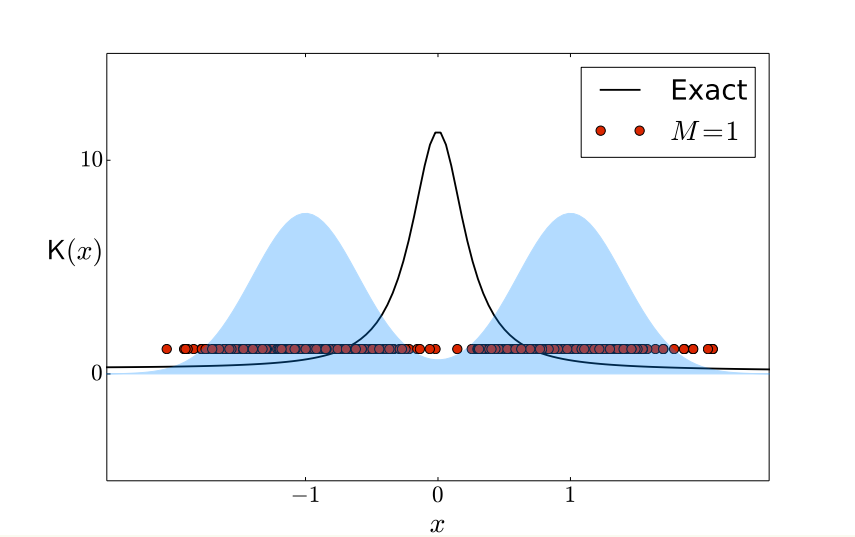
Idea: Projection into a finite-dim subspace



Choice of basis function is difficult

Idea: Projection into a finite-dim subspace





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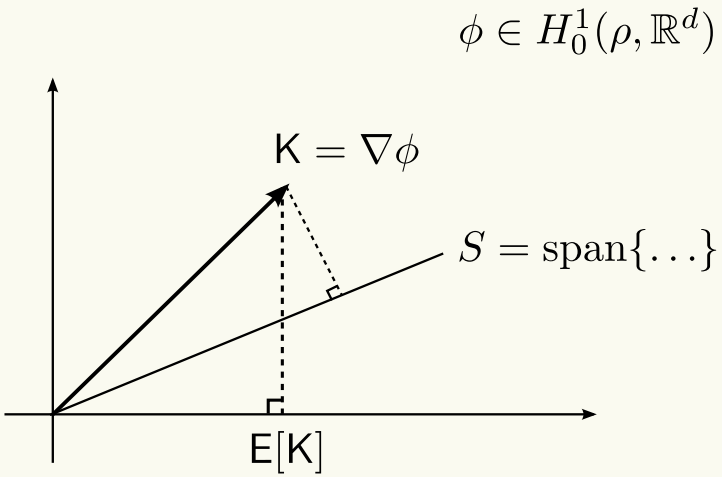

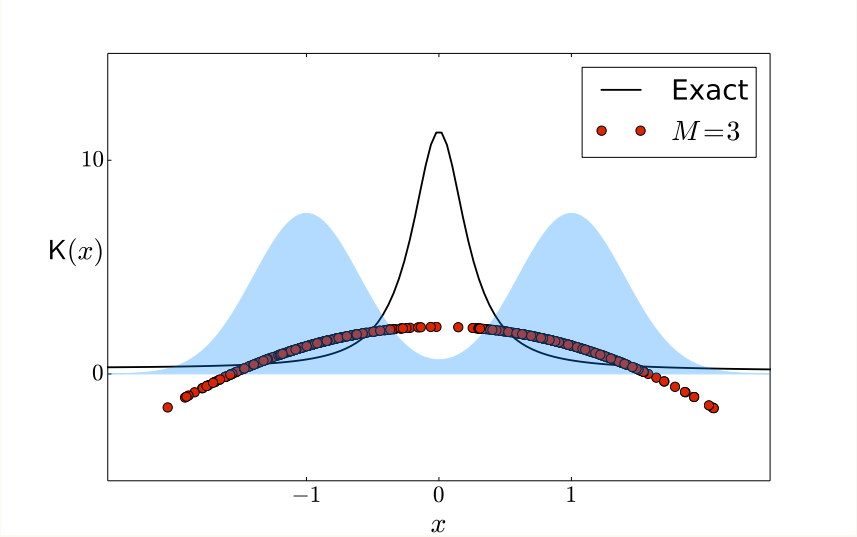

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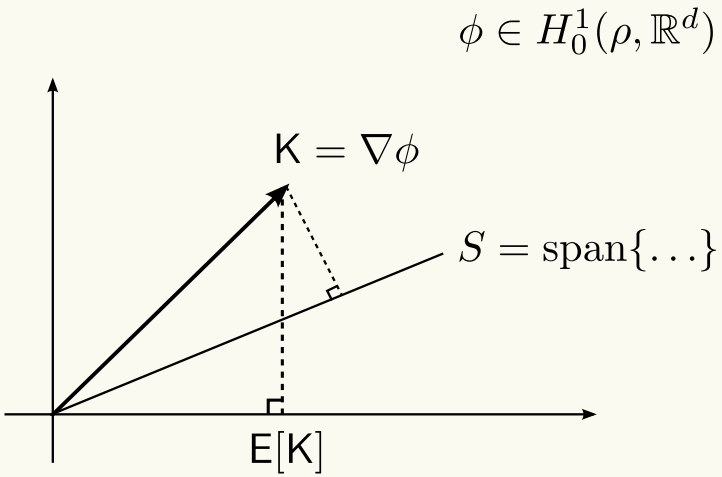

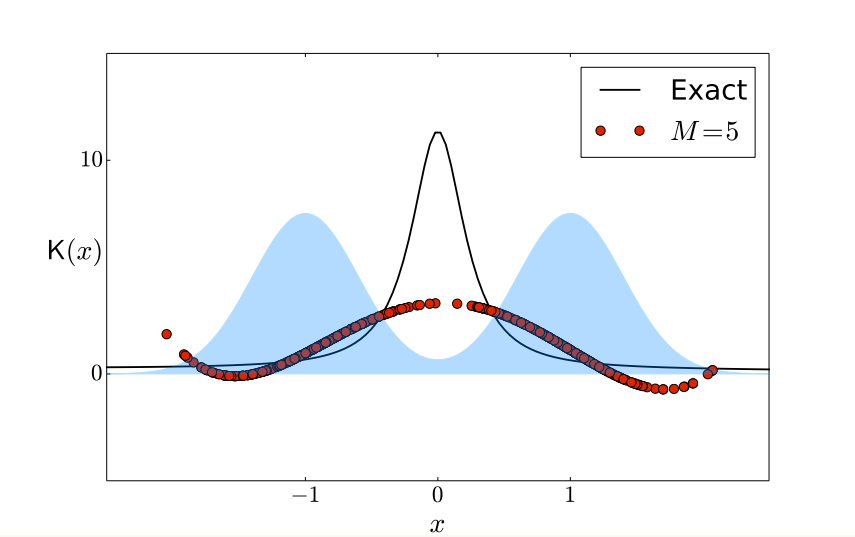

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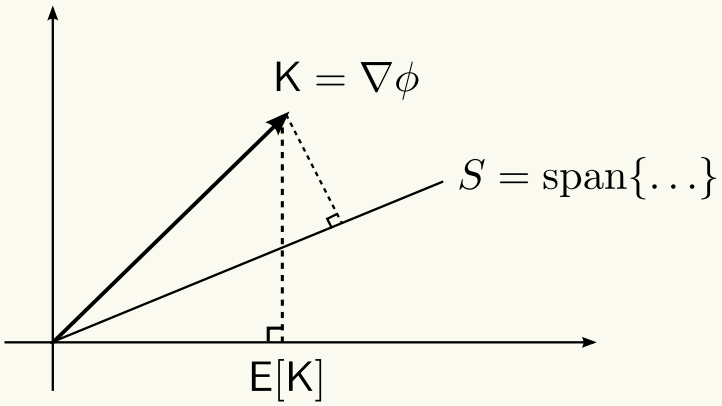
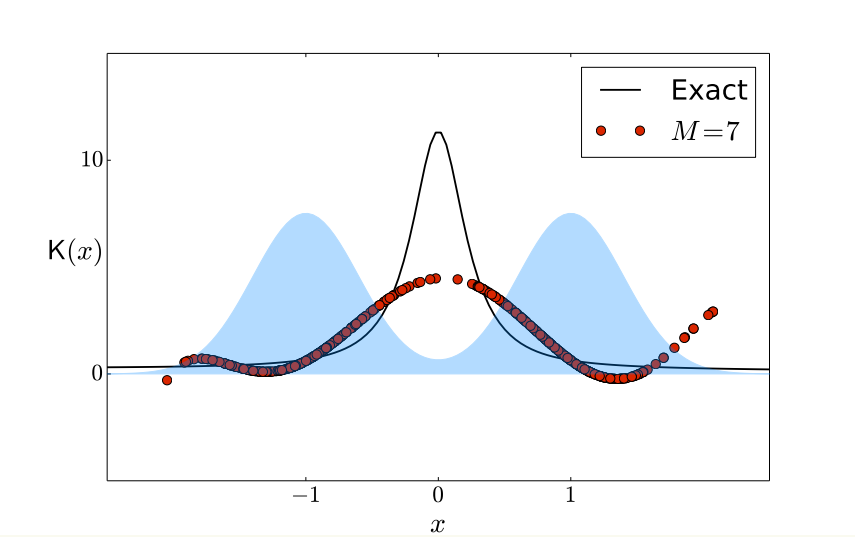
$\phi \in H_0^1(\rho, \mathbb{R}^d)$





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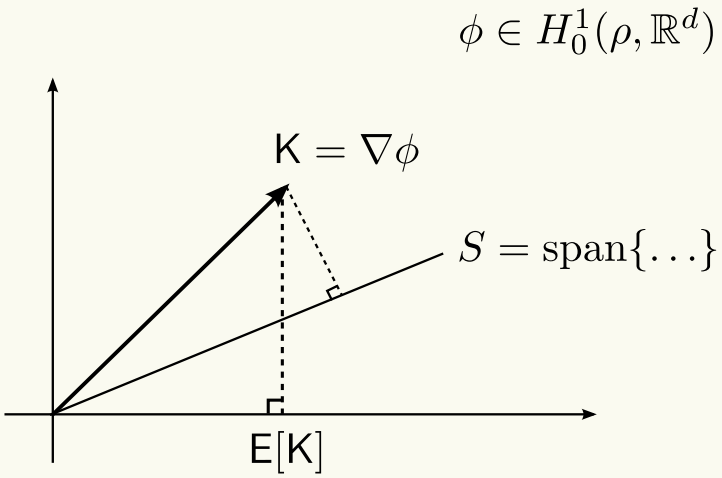

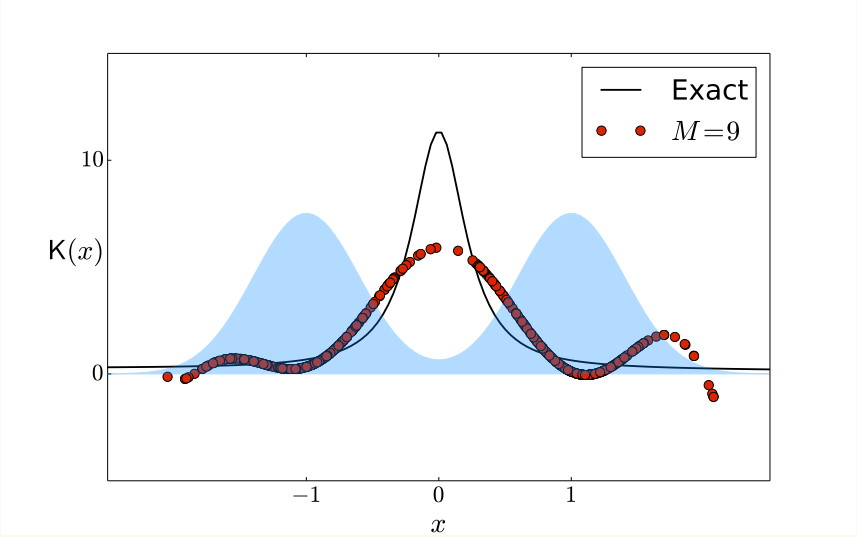

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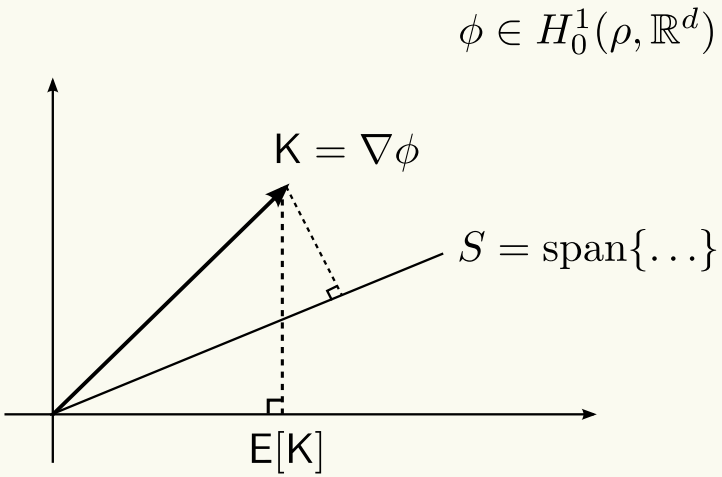

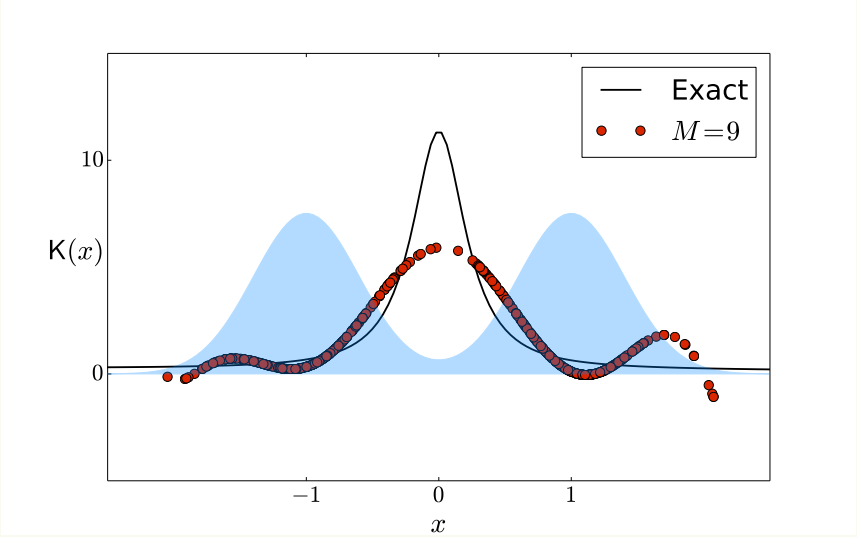

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Choice of basis function is difficult

Gain function approximation: Diffusion map-based algorithm

Overview

Poisson eq.: $-\Delta_\rho \phi = h - \hat{h}, \quad \phi \in H_0^1(\rho)$

(approximation steps)

Finite-dim eq.: $\Phi = \mathsf{T}\Phi + \epsilon(\mathsf{h} - \pi(h)), \quad \Phi \in \mathbb{R}_0^N$

- T is a $N \times N$ Markov matrix
- $k_\epsilon^{(N)}(x, y)$ is the diffusion map kernel (Coifman & Lafon, 2006)
- The solution $\Phi \approx (\phi(X^1), \ldots, \phi(X^N))$

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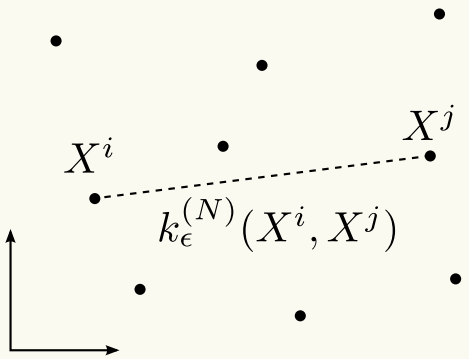
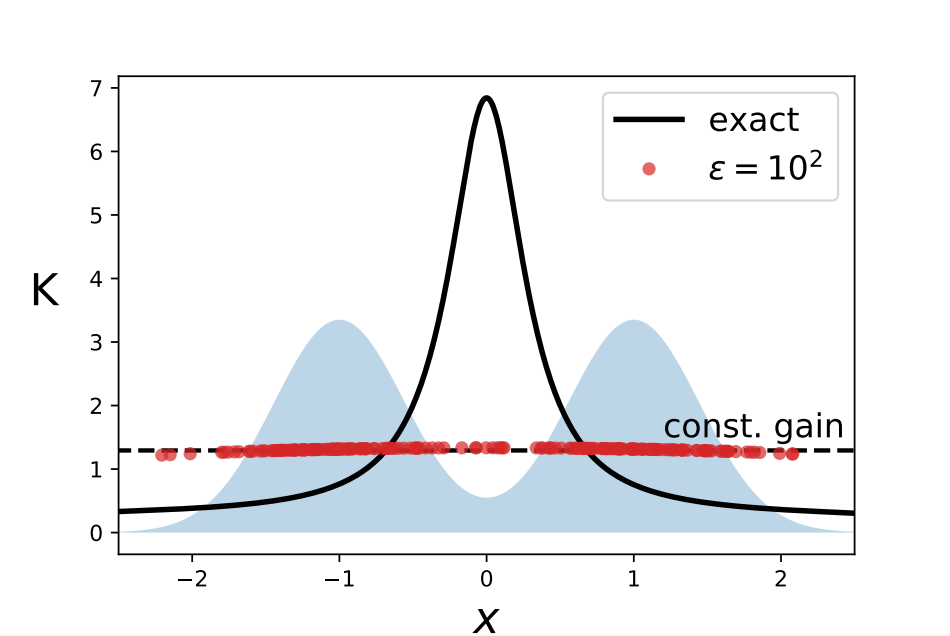


Gain function approximation: Diffusion map-based algorithm

Numerical analysis



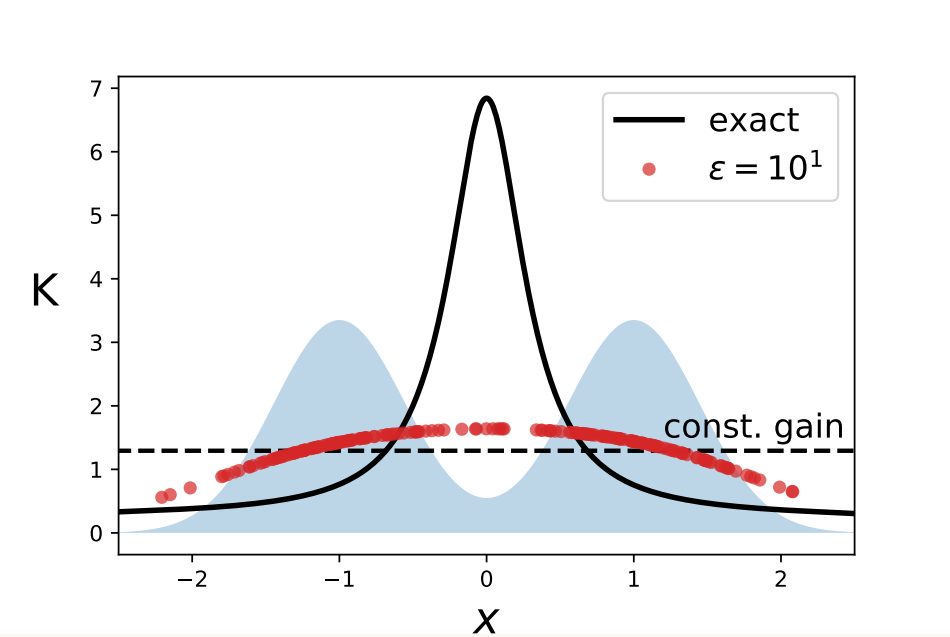
Properties:

- No basis function selection
- Reduces to constant gain in the limit as $\epsilon \to \infty$

Objective: Error analysis of bias and variance

Gain function approximation: Diffusion map-based algorithm

Numerical analysis



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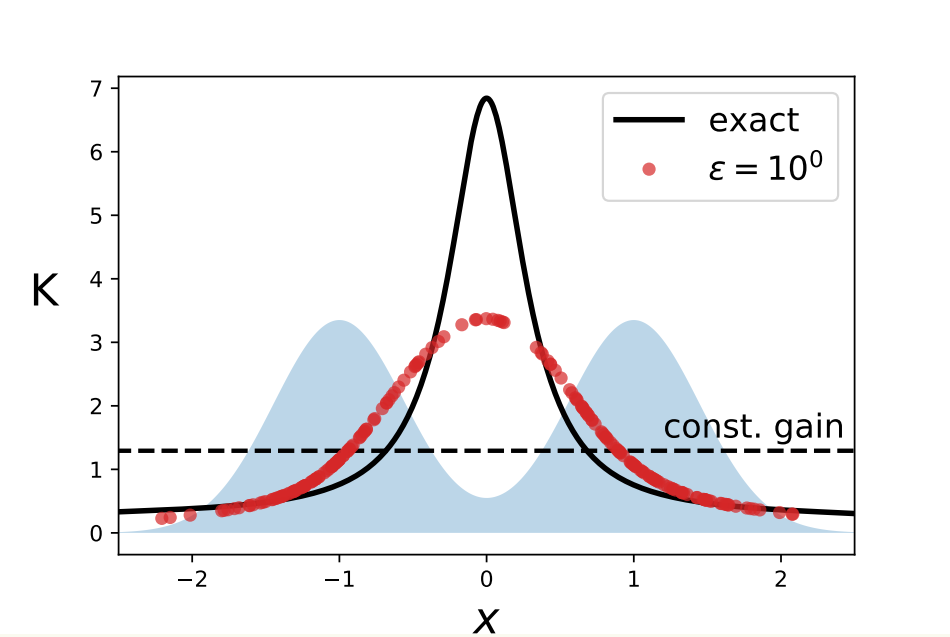

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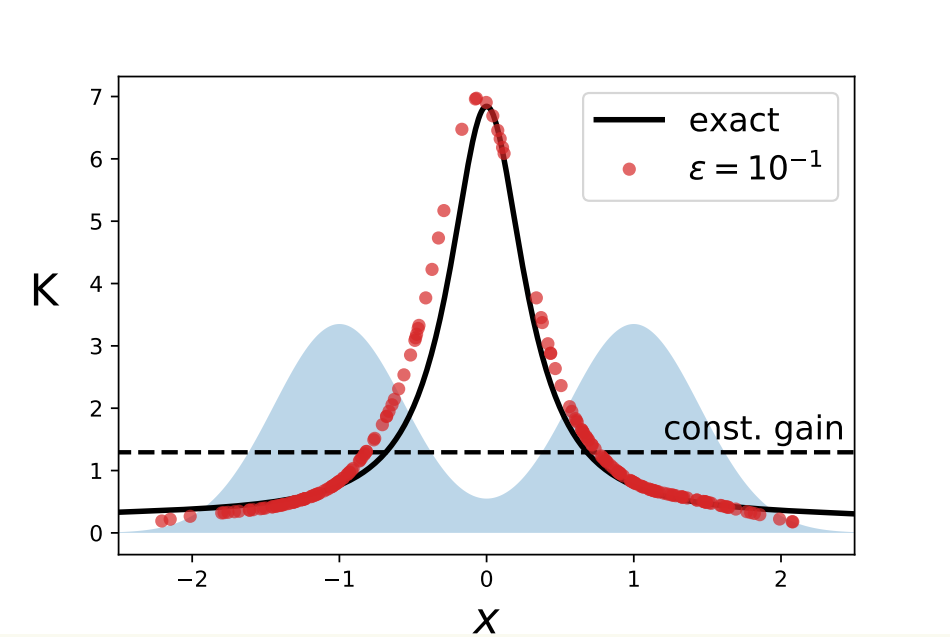

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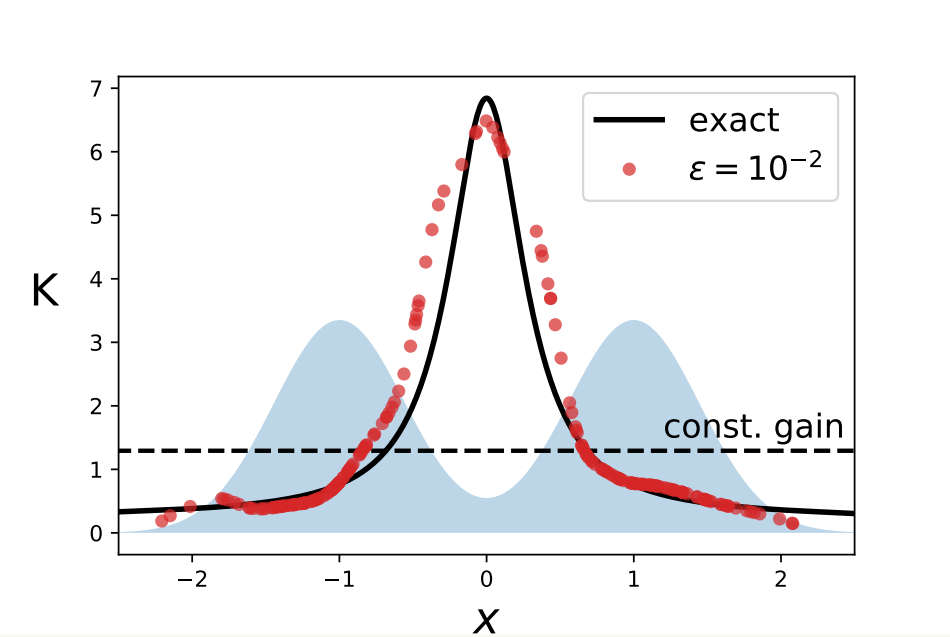

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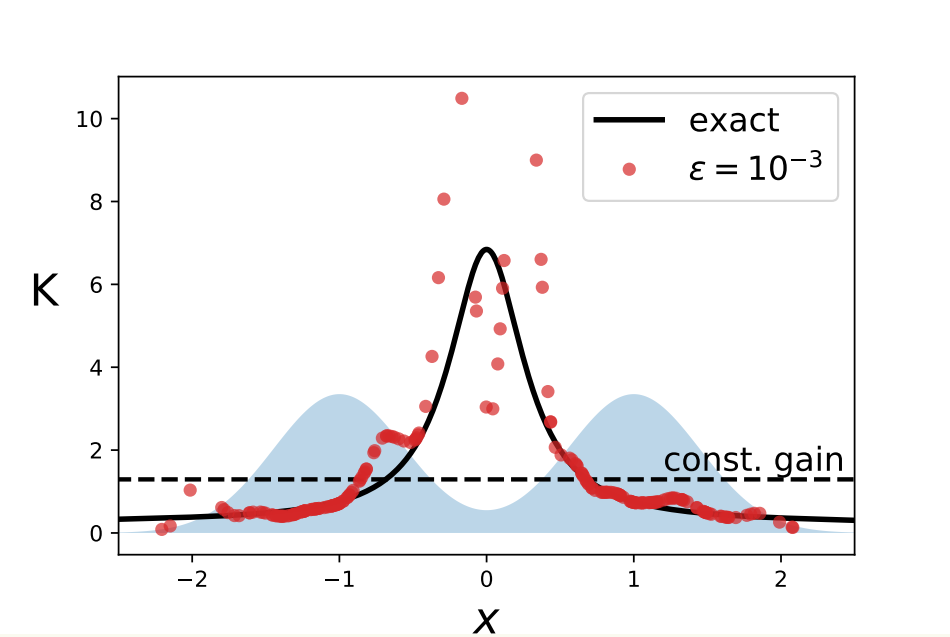

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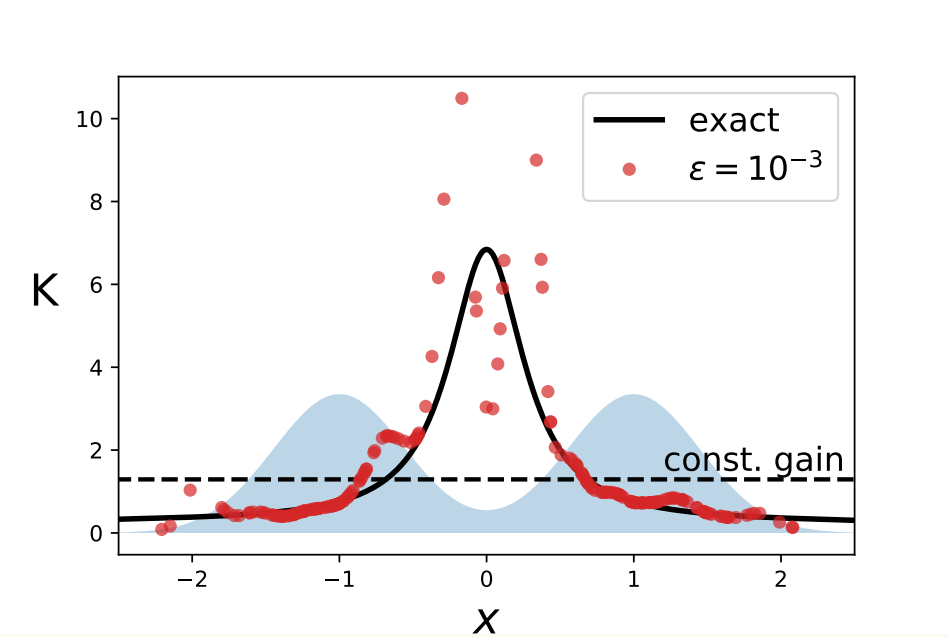

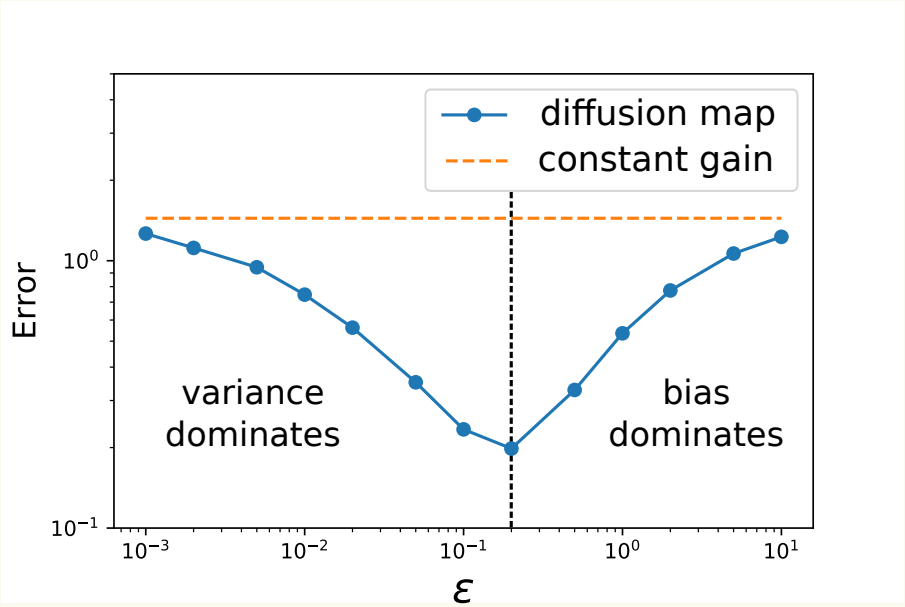

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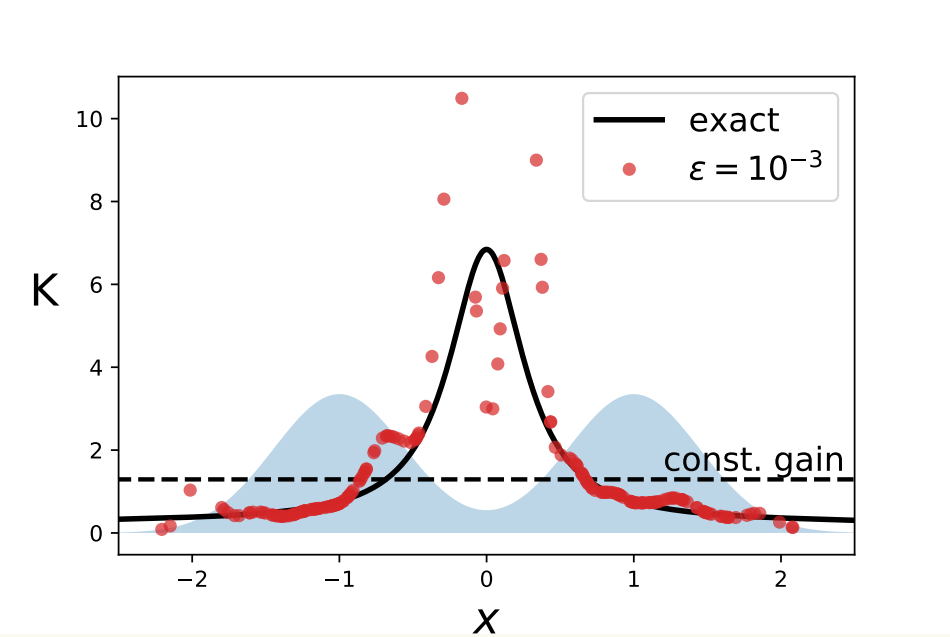

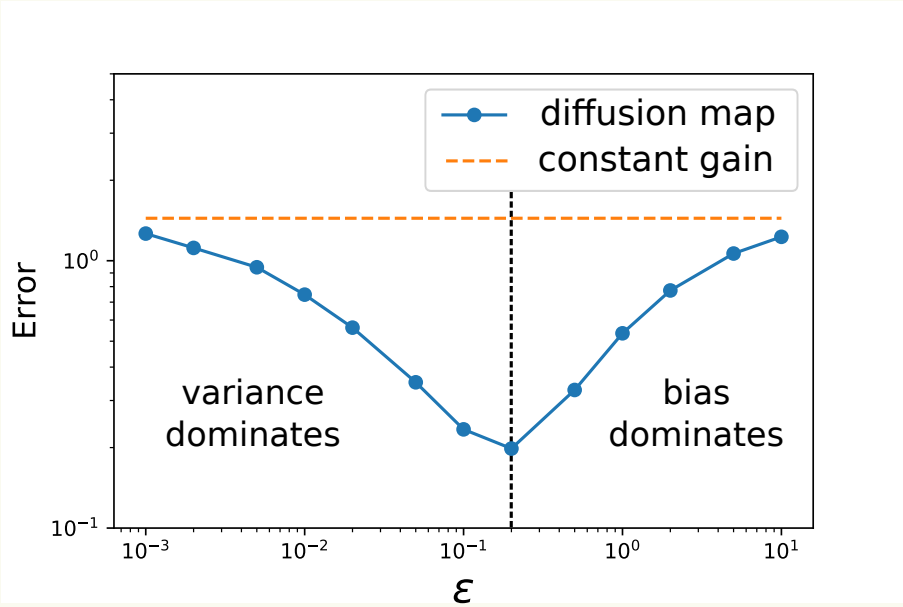

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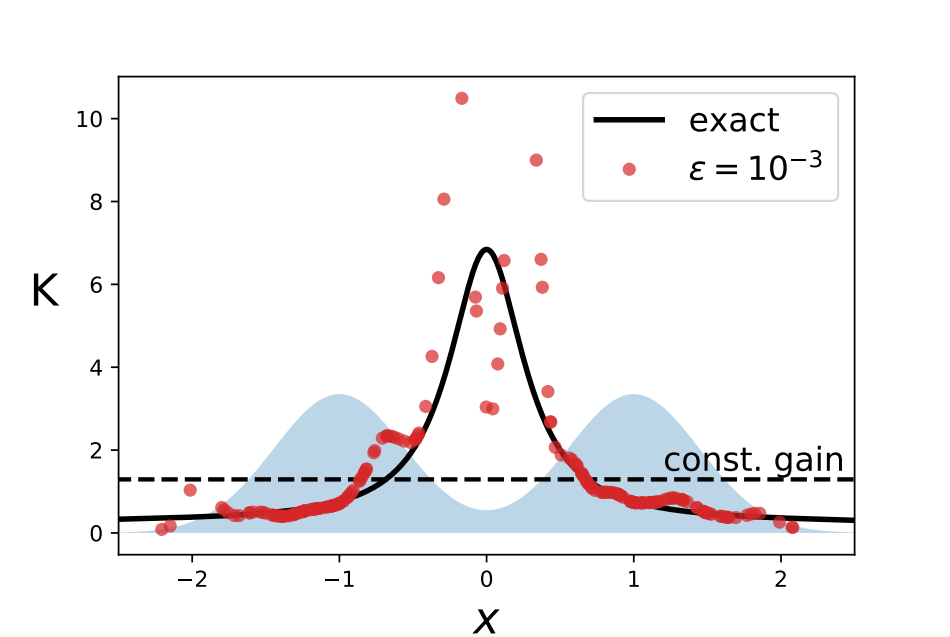

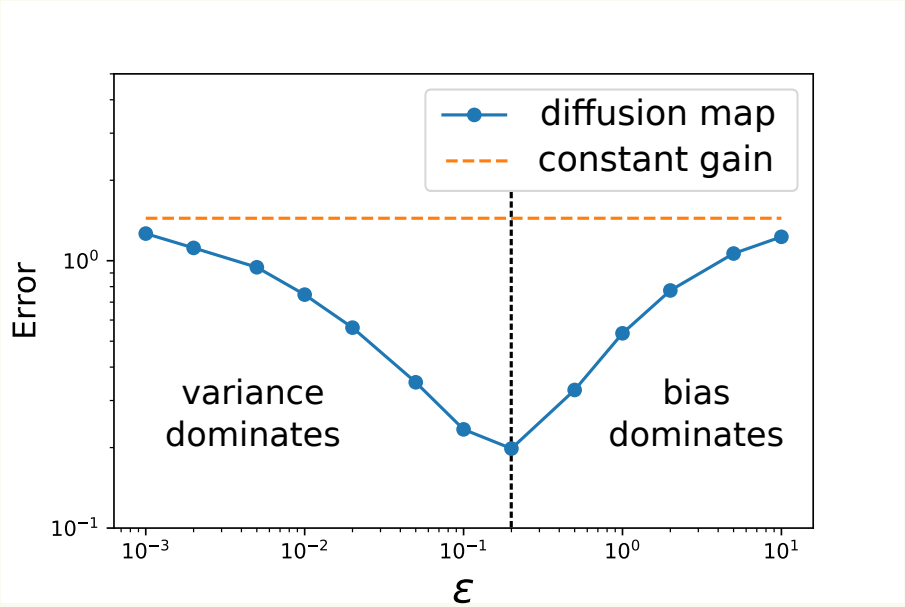

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Gain function approximation: Diffusion map-based algorithm

Four Markov operators

- Semigroup $P_t = e^{t\Delta_\rho}$

$$\frac{\partial}{\partial t} P_t f = P_t \Delta_\rho f$$

- Diffusion map T_ϵ

$$T_\epsilon f(x) := \frac{1}{n_\epsilon(x)} \int g_\epsilon(x,y) \frac{f(y)\rho(y)}{\sqrt{(g_\epsilon * \rho)(y)}} \mathrm{d}y$$

- Empirical approximation $T_\epsilon^{(N)}$

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R. Coifman and S. Lafon, Diffusion maps, Applied and computational harmonic analysis, 21 (2006)
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Gain function approximation: Diffusion map-based algorithm

Approximation steps overview

(1) Poisson equation: $$-\Delta_\rho \phi = h - \hat{h}$$

(2) Semigroup formulation: $$\phi = P_\epsilon \phi + \int_0^\epsilon P_s(h - \hat{h})\mathrm{d}s$$

(3) Diffusion map approx: $$\phi_\epsilon = T_\epsilon \phi_\epsilon + \epsilon(h - \hat{h}_\epsilon)$$

(4) Empirical approx: $$\phi_\epsilon^{(N)} = T_\epsilon^{(N)} \phi_\epsilon^{(N)} + \epsilon(h - \hat{h}_\epsilon^{(N)})$$

(5) Finite-dim: $$\mathsf{\Phi} = \mathsf{T}\mathsf{\Phi} + \epsilon(\mathsf{h} - \hat{h}_\epsilon^{(N)})$$

$$(1) \Leftrightarrow (2) \overset{\epsilon\downarrow 0}{\approx} (3) \overset{N\uparrow\infty}{\approx} (4) \Leftrightarrow (5)$$

Error analysis:

- Bias: Study convergence $\phi_\epsilon \to \phi$
- Variance: Study convergence $\phi_\epsilon^{(N)} \to \phi_\epsilon$

Gain function approximation: Diffusion map-based algorithm

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(2) Semigroup formulation: $$\phi = P_\epsilon \phi + \int_0^\epsilon P_s(h - \hat{h})\mathrm{d}s$$

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(4) Empirical approx: $$\phi_\epsilon^{(N)} = T_\epsilon^{(N)} \phi_\epsilon^{(N)} + \epsilon(h - \hat{h}_\epsilon^{(N)})$$

(5) Finite-dim: $$\mathsf{\Phi} = \mathsf{T}\mathsf{\Phi} + \epsilon(\mathsf{h} - \hat{h}_\epsilon^{(N)})$$

$$(1) \Leftrightarrow (2) \overset{\epsilon\downarrow 0}{\approx} (3) \overset{N\uparrow\infty}{\approx} (4) \Leftrightarrow (5)$$

Error analysis:

- Bias: Study convergence $\phi_\epsilon \to \phi$
- Variance: Study convergence $\phi_\epsilon^{(N)} \to \phi_\epsilon$

Assumptions:

(A1) (Density has Gaussian tail) $\rho = e^{-V}$ where $V(x) = \frac{1}{2}(x-\bar{x})^\top \Sigma^{-1}(x-\bar{x}) + W(x)$ with $W \in C_b^\infty(\mathbb{R}^d)$

(A2) (h has linear growth) $h(x) = c^\top x + w(x)$ where $w \in C_b^\infty(\mathbb{R}^d)$

Function spaces: $L^2(\rho)$, $H^1(\rho)$, $L_0^2(\rho) := \left\{ f \in L^2(\rho); \int f \rho \mathrm{d}x = 0 \right\}$, $H_0^1(\rho)$

Poincaré inequality: Under Assumption (A1), $\exists \lambda > 0$ such that

$$\int (f - \hat{f})^2 \rho \mathrm{d}x \leq \frac{1}{\lambda} \int |\nabla f|^2 \rho \mathrm{d}x, \quad \forall f \in H^1(\rho)$$

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Gain function approximation: Error analysis
Bias

$$\phi = P_t\phi + \int_0^t P_s(h-\hat{h})\mathrm{d}s \quad \text{and} \quad \phi_\epsilon = T_\epsilon\phi_\epsilon + \epsilon(h-\hat{h}_\epsilon)$$

Proposition

1. For all functions $f, \nabla f \in L^4(\rho)$

$$\|T^n_{\frac{t}{n}} f - P_t f\|_{L^2(\rho)} \leq \frac{(\text{const.})}{n}(\|f\|_{L^4(\rho)} + \|\nabla f\|_{L^4(\rho)})$$

2. $T^n_{\frac{t}{n}}$ admits a uniform spectral gap on $L^2_0(\rho_\epsilon)$ and

$$\|\phi_\epsilon\|_{L^2(\rho_\epsilon)} \leq (\text{const.})\|h\|_{L^2(\rho_\epsilon)}$$

3. In the asymptotic limit as $\epsilon \to 0$

$$\|\phi_\epsilon - \phi\|_{L^2(\rho)} \leq O(\epsilon)$$

1. Proof of 1: Feynman-Kac representation of semigroup
2. Proof of 2: Foster-Lyapunov condition from stochastic stability theory

S. P. Meyn and R. L. Tweedie. Markov chains and stochastic stability. 2012.

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Variance

$$\phi_\epsilon^{(N)} = T_\epsilon^{(N)} \phi_\epsilon^{(N)} + \epsilon(h - \hat{h}_\epsilon^{(N)}) \quad \text{and} \quad \phi_\epsilon = T_\epsilon \phi_\epsilon + \epsilon(h - \hat{h}_\epsilon)$$

Proposition

- For any bounded function f and for all $x \in \mathbb{R}^d$:

$$\lim_{N\to\infty} T_\epsilon^{(N)} f(x) = T_\epsilon f(x), \quad \text{a.s}$$

- For any $\delta \in (0,1)$

$$\|T_\epsilon^{(N)} f - T_\epsilon f\|_{L^2(\rho)}^2 \leq O(\frac{\log(\frac{N}{\delta})}{N\epsilon^d})$$

  with probability larger than $1-\delta$

- If the distribution ρ has compact support

$$\lim_{N\to\infty} \|\phi_\epsilon^{(N)} - \phi_\epsilon\|_\infty = 0, \quad \text{a.s}$$

Approach: Numerical analysis of integral equations on a grid (Anselone, 1971, Atkinson, 1976)

Gain function approximation: Error analysis
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Gain function approximation: Numerical analysis

Error estimate:

$$\text{r.m.s.e} \leq \underbrace{O(\epsilon)}_{\text{bias}} + \underbrace{O\left(\frac{1}{\epsilon^{1+d/2} N^{1/2}}\right)}_{\text{variance}}$$

Setup: $\rho(x) = \rho_{\text{bimodal}}(x_1) \prod_{n=2}^{d} \rho_{\text{Gaussian}}(x_n)$ and $h(x) = x_1$.

Convergence to const. gain approx.:

$$\lim_{\epsilon \to \infty} \mathsf{K}_{\epsilon}^{(N)} = \text{const. gain approximatoin}$$

Gain function approximation: Numerical analysis

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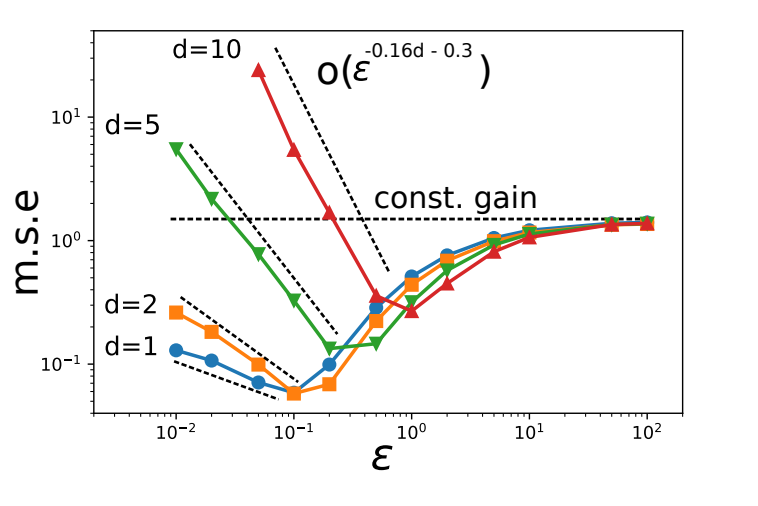

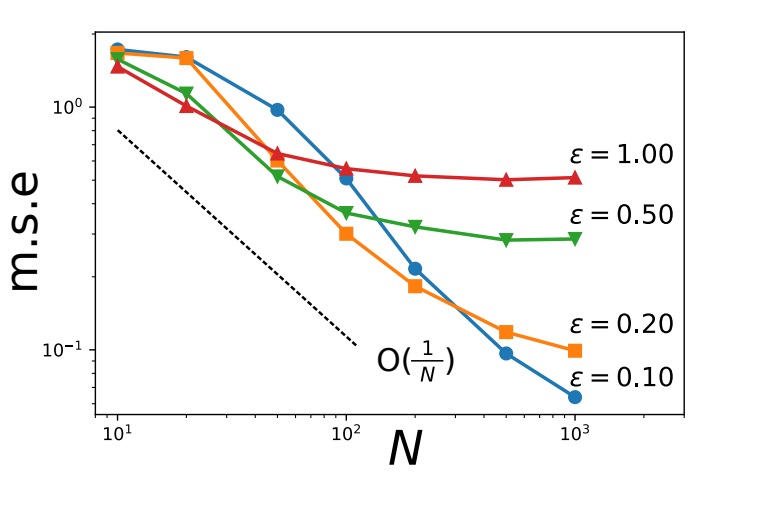

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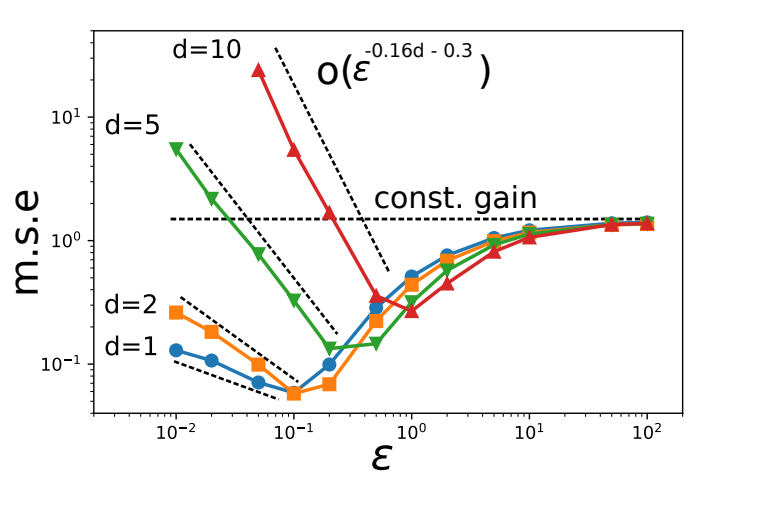

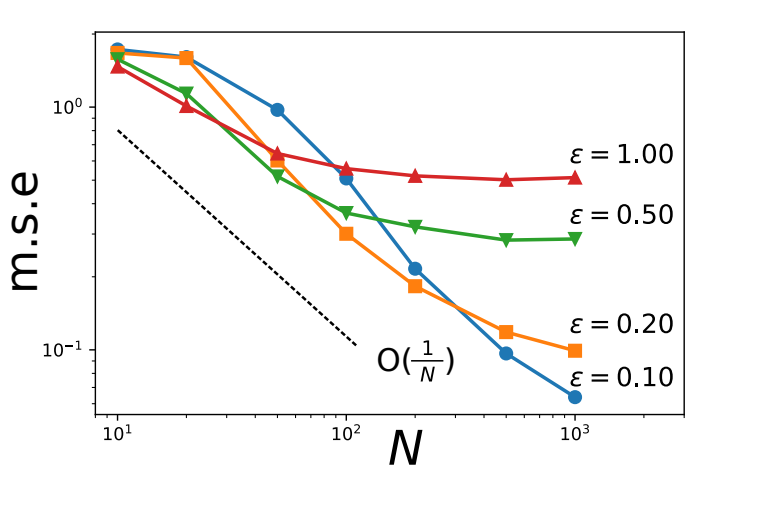

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Outline

Part I: Analysis of the feedback particle filter (FPF)

- Introduction
- Gain function approximation
- Optimal transport FPF
  - A. Taghvaei and P. G. Mehta, An optimal transport formulation of the linear feedback particle filter, in American Control Conference (ACC), 2016, pp. 3614–3619.

    Summary:
  - Developed a principled approach to construct a unique control law
  - Carry out the approach in linear Gaussian setting
- Error analysis of linear FPF

Part II: Accelerated flow for probability distributions

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  - A. Taghvaei and P. G. Mehta, Error analysis of the linear feedback particle filter, in Conference on Decision and Control (CDC), 2018, pp. 7194-7199

  Summary:

  - Error analysis of two types of FPF algorithms in linear Gaussian setting
  - Convergence of the empirical distribution to the exact filter given by Kalman filter

Part II: Accelerated flow for probability distributions

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Part I: Analysis of the feedback particle filter (FPF)

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Part II: Accelerated flow for probability distributions

- A. Taghvaei and P. G. Mehta, Accelerated flow for probability distributions, International Conference on Machine Learning (ICML), 2019

Part II: Motivation and objective

- Many machine learning problems are modeled as an optimization problem on the space of probability distributions
  - Bayesian inference
  - Learning generative models
  - Policy optimization in reinforcement learning
- This motivates application of optimization algorithms to solve these problems
- **Objective:** Construct accelerated gradient flows for probability distribution

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Part II: Proposed Approach

Euclidean space	Space of probability distributions
Gradient descent	Wasserstein gradient flow
Accelerated methods	?

- (Wibisono, et. al. 2017) proposed a variational formulation to construct accelerated flows on Euclidean space
- Our approach is to extend the variational formulation for probability distributions

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Part II: Review of variational formulation in Euclidean space

- Optimization problem:

$$\min_{x\in\mathbb{R}^d} \; f(x) \quad \text{(Assume } f \text{ is convex)}$$

- Gradient flow:

$$\frac{\mathrm{d}x_t}{\mathrm{d}t} = -\nabla f(x_t)$$

- Accelerated gradient flow (ode limit of Nesterov method) (Su, et. al. 2014):

$$\frac{\mathrm{d}x_t}{\mathrm{d}t} = \frac{2}{t^3} y_t,$$
$$\frac{\mathrm{d}y_t}{\mathrm{d}t} = -\frac{t^3}{2}\nabla f(x_t)$$

- Variational formulation (Wibinoso, et. al. 2016):

$$\begin{aligned} \text{Minimize} \quad & \int_0^\infty t^3\left(\frac{1}{2}|u_t|^2 - f(x_t)\right)\mathrm{d}t \\ \text{Subject to} \quad & \frac{\mathrm{d}x_t}{\mathrm{d}t} = u_t \end{aligned}$$

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Part II: Summary

	vector variables $\mathbb{R}^d$	probability distribution $\mathcal{P}_2(\mathbb{R}^d)$
Objective funct.	$f(x)$	?
Gradient flow	$\dot{x}_t = -\nabla f(x_t)$	?
Lagrangian	$t^3(\frac{1}{2}\lvert u_t\rvert^2 - f(x_t))$	?
Accelerated flow	$\frac{\mathrm{d}x_t}{\mathrm{d}t} = \frac{2}{t^3} y_t$ $\frac{\mathrm{d}y_t}{\mathrm{d}t} = -\frac{t^3}{2}\nabla f(x_t)$	?

Part II: Wasserstein gradient flow

- Optimization problem:

$$\min_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \mathsf{F}(\rho) = D(\rho|\rho_\infty)$$

where $\rho_\infty = e^{-f}$.

- Wasserstein gradient flow (Jordan, et. al. 1998):

$$\text{pde form:} \quad \frac{\partial \rho_t}{\partial t} = \nabla \cdot (\rho_t \nabla f) + \Delta \rho_t, \quad \text{(Fokker-Planck eq.)}$$

$$\text{probabilistic form:} \quad \mathrm{d}X_t = -\nabla f(X_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \quad \text{(Langevin eq.)}$$

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- The goal is to build accelerated version of this sde

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	vector variables $\mathbb{R}^d$	probability distribution $\mathcal{P}_2(\mathbb{R}^d)$
Objective funct.	$f(x)$	$\mathsf{F}(\rho) = \mathsf{D}(\rho \| \rho_\infty)$
Gradient flow	$\dot{x}_t = -\nabla f(x_t)$	$\mathrm{d}X_t = -\nabla f(X_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t$
Lagrangian	$t^3(\frac{1}{2}\lvert u_t\rvert^2 - f(x_t))$	?
Accelerated flow	$\frac{\mathrm{d}x_t}{\mathrm{d}t} = \frac{2}{t^3}y_t$ $\frac{\mathrm{d}y_t}{\mathrm{d}t} = -\frac{t^3}{2}\nabla f(x_t)$	?

PDE form:

$$\begin{aligned} &\text{Minimize} && \int_0^\infty t^3 \left(\int_{\mathbb{R}^d} \frac{1}{2} |u_t(x)|^2 \rho_t(x) \mathrm{d}x - D(\rho_t | \rho_\infty) \right) \mathrm{d}t \\ &\text{Subject to} && \frac{\partial \rho_t}{\partial t} + \nabla \cdot (\rho_t u_t) = 0 \end{aligned}$$

Probabilistic form:

$$\begin{aligned} &\text{Minimize} && \mathsf{E}\left[\int_0^\infty t^3 \left(\frac{1}{2} |U_t|^2 - \log\left(\frac{\rho_t(X_t)}{\rho_\infty(X_t)}\right) \right) \mathrm{d}t \right] \\ &\text{Subject to} && \frac{\mathrm{d}X_t}{\mathrm{d}t} = U_t \end{aligned}$$

- It is a mean-field optimal control problem (Bensoussan, et al. 2013, Carmona & Delarue, 2017)

Part II: Variational formulation for probability distributions

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Part II: Main result

Proposition (ICML'19)

1. Accelerated flow (probabilistic form):

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} = \frac{2}{t^3} Y_t$$
$$\frac{\mathrm{d}Y_t}{\mathrm{d}t} = -\frac{t^3}{2}(\nabla f(X_t) + \nabla \log(\rho_t(X_t)))$$

   where $\rho_t = \mathsf{Law}(X_t)$

2. (Convergence) If $\mathsf{F}(\rho) = D(\rho|\rho_\infty)$ is displacement convex, and the dimension $d = 1$. Then

$$D(\rho_t|\rho_\infty) \leq O(\frac{1}{t^2})$$

3. If ρ_∞ is Gaussian, then X_t is also Gaussian and the mean evolves according to the accelerated gradient flow in Euclidean space

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Accelerated flow	$\frac{\mathrm{d}x_t}{\mathrm{d}t} = \frac{2}{t^3}y_t$ $\frac{\mathrm{d}y_t}{\mathrm{d}t} = -\frac{t^3}{2}\nabla f(x_t)$	$\frac{\mathrm{d}X_t}{\mathrm{d}t} = \frac{2}{t^3}Y_t$ $\frac{\mathrm{d}Y_t}{\mathrm{d}t} = -\frac{t^3}{2}(\nabla f(X_t) + \nabla \log(\rho_t(X_t)))$

Procedure: Simulate N particles $\{(X_t^1, Y_t^1), \ldots, (X_t^N, Y_t^N)\}$

$$\frac{\mathrm{d}X_t^i}{\mathrm{d}t} = \frac{2}{t^3} Y_t^i, \quad X_0^i \sim \rho_0$$
$$\frac{\mathrm{d}Y_t^i}{\mathrm{d}t} = -\frac{t^3}{2}(\nabla f(X_t^i) + \underbrace{\nabla \log(\rho_t(X_t^i))}_{\text{interaction term}})$$

Approximation: Interaction term is approximated with particles

- (parametric) Gaussian approximation

$$\nabla \log(\rho(x)) \approx -\Sigma^{-1}(x - m), \quad m, \Sigma = \text{empirical mean and covariance}$$

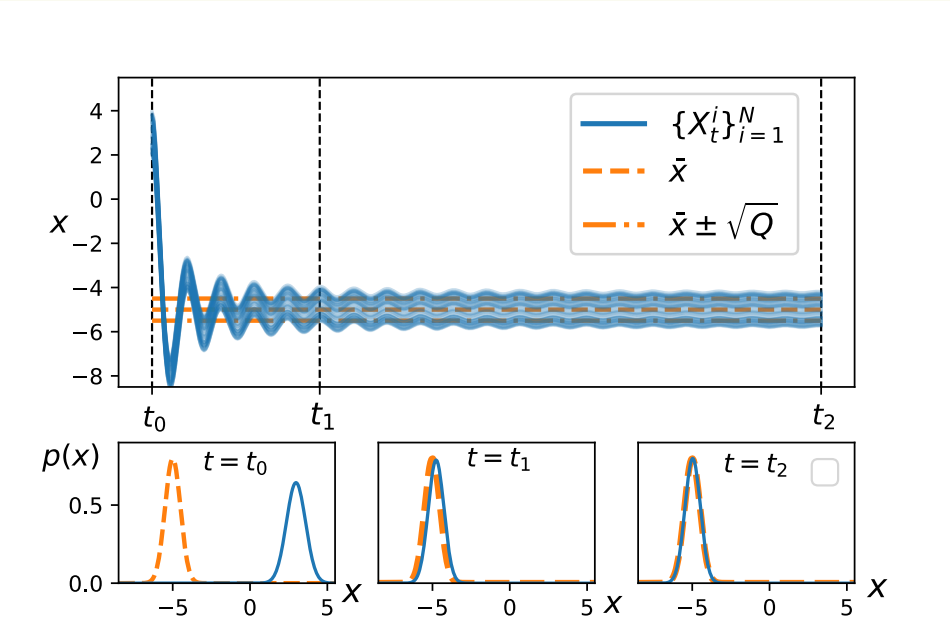
- (non-parametric) Diffusion-map approximation

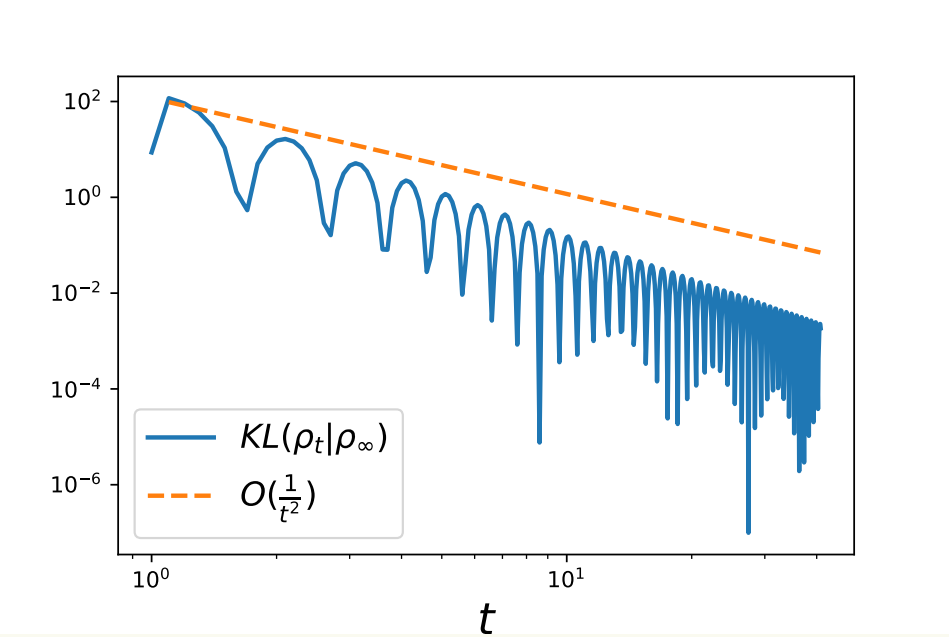
$$\nabla \log(\rho(x)) = \Delta_\rho(x) \approx -\frac{1}{\epsilon} \frac{\sum_{i=1}^N k_\epsilon(x, X^i)(x - X^i)}{\sum_{i=1}^N k_\epsilon(x, X^i)}$$

where $k_\epsilon(\cdot, \cdot)$ is the <u>diffusion-map kernel</u>

Part II: Numerical example

- The target distribution is Gaussian
- The target distribution is mixture of two Gaussians





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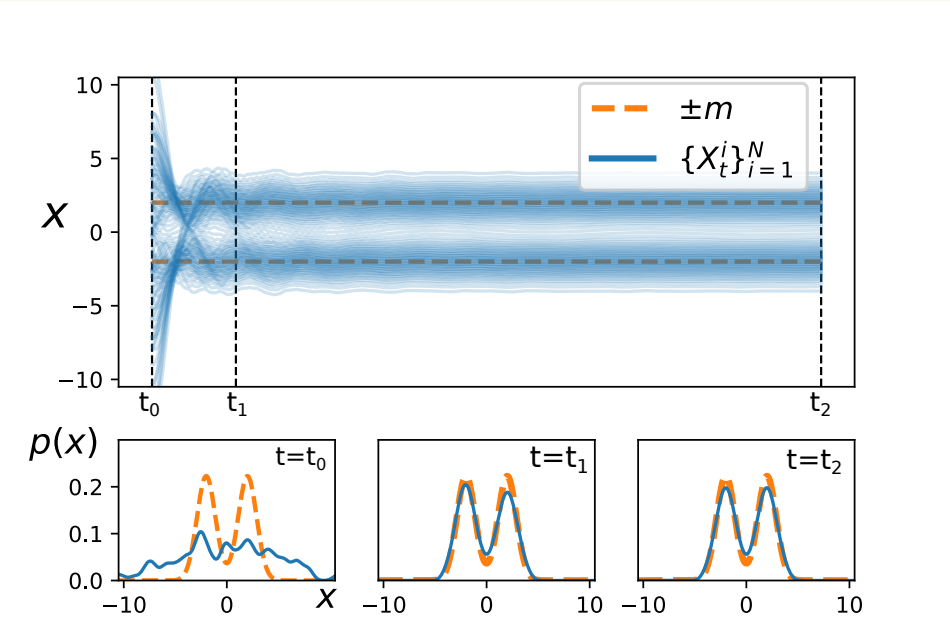

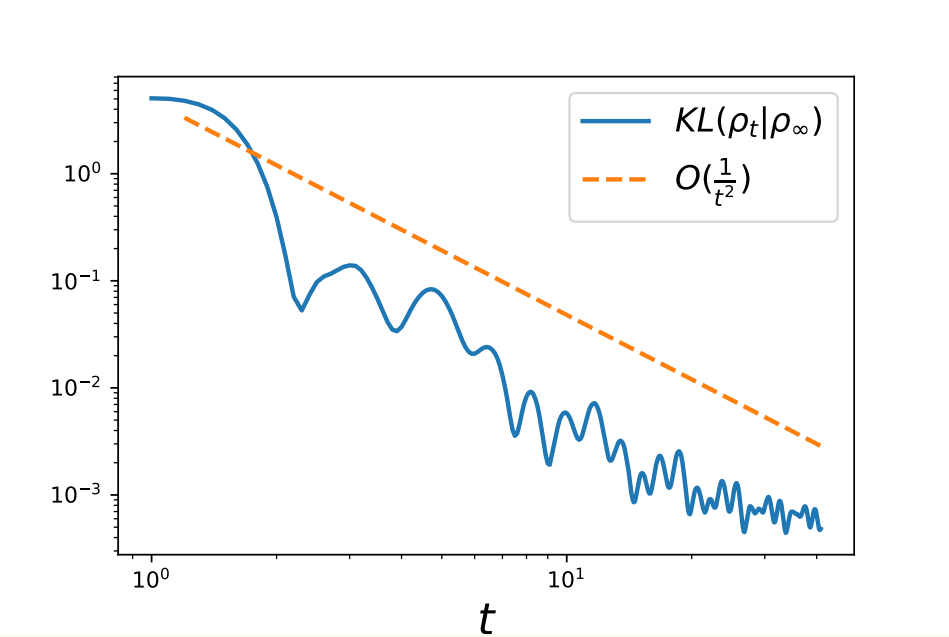

Summary and future work

Part I: Analysis of FPF

- Gain function approximation: Diffusion map-based algorithm and its error analysis
- Optimal transport FPF: An optimal transportation-based approach to construct FPF control law
- Error analysis of linear FPF: Convergence in linear Gaussian setting

Question: Can the three questions be addressed in a single framework?

Part II: Accelerated flow for probability distributions

Variational problem: $$\int_0^\infty t^3 \left(\int_{\mathbb{R}^d} \frac{1}{2} |u_t(x)|^2 \rho_t(x) \mathrm{d}x - D(\rho_t | \rho_\infty) \right) \mathrm{d}t$$

Accelerated flow: $$\frac{\mathrm{d}X_t}{\mathrm{d}t} = \ldots, \quad \frac{\mathrm{d}Y_t}{\mathrm{d}t} = \ldots + \nabla \log(\rho_t(X_t))$$

Future work: Obtain approximation from variational formulation

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- NSF, ME, Math, ECE, CSE, CSL
- Collaborators: S. P. Meyn, S. Reich, C. Zhang, J. Kim, J. de Wiljes
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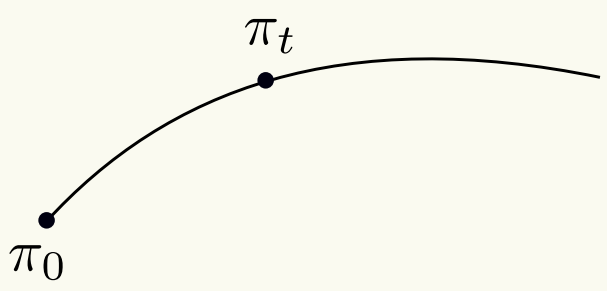
Optimal transport FPF
Problem overview

Control viewpoint:

$$\mathrm{d}\bar{X}_t = \text{(control law)}$$

Objective: Find the control law s.t $\bar{X}_t$ follows the posterior π_t



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Non-uniqueness: There are infinitely many solutions

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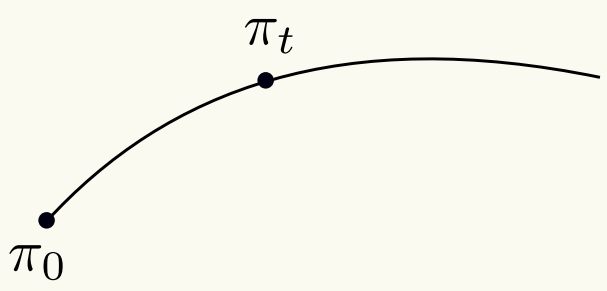

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Optimal transport FPF

Non-uniqueness example

Example:

State process: $\mathrm{d}X_t = \mathrm{d}B_t, \quad X_0 \sim N(0,1)$

Objective: compute $\pi_t(\cdot) = \mathsf{P}(X_t \in \cdot)$

Two solutions:

(I) $\mathrm{d}X_t^i = \mathrm{d}B_t^i$

(II) $\frac{\mathrm{d}}{\mathrm{d}t} X_t^i = \frac{X_t^i}{\frac{2}{N}\sum_{j=1}^N (X_t^i)^2}$

They both produce the same distribution $N(0, 1+t)$.

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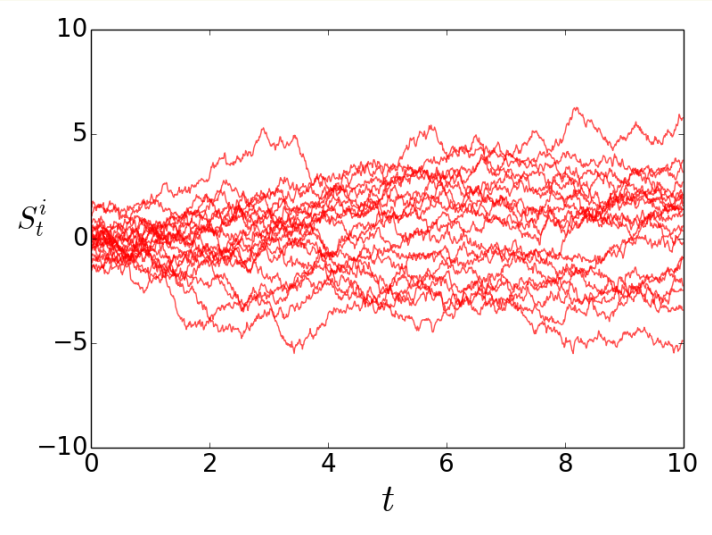

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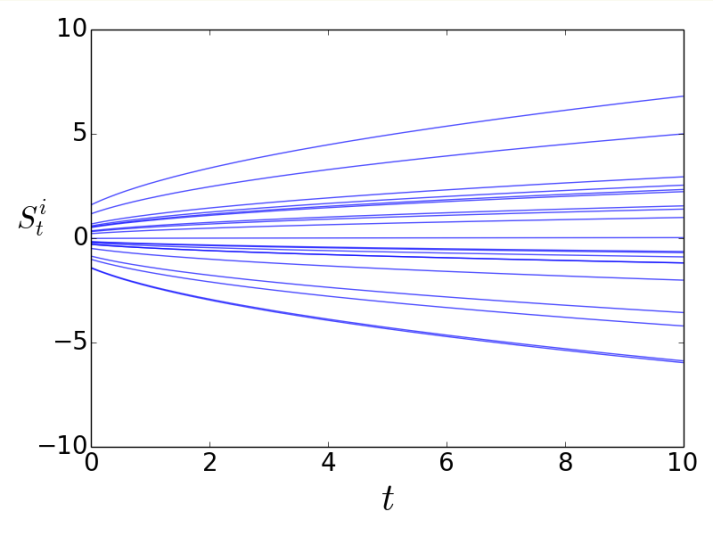

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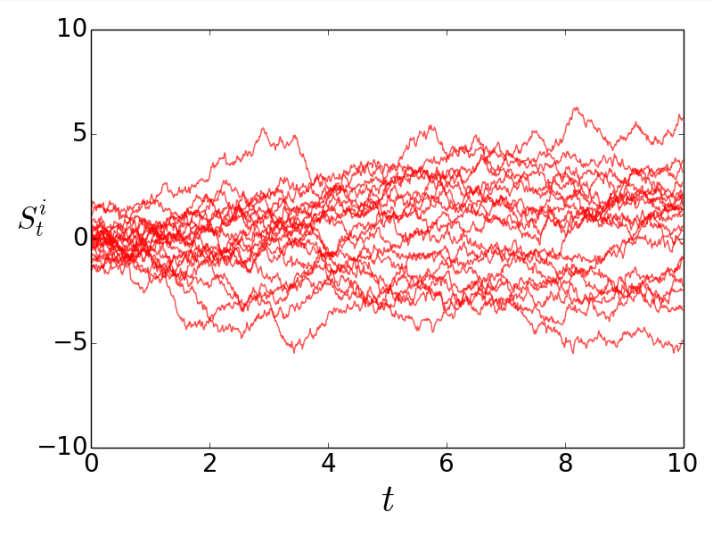

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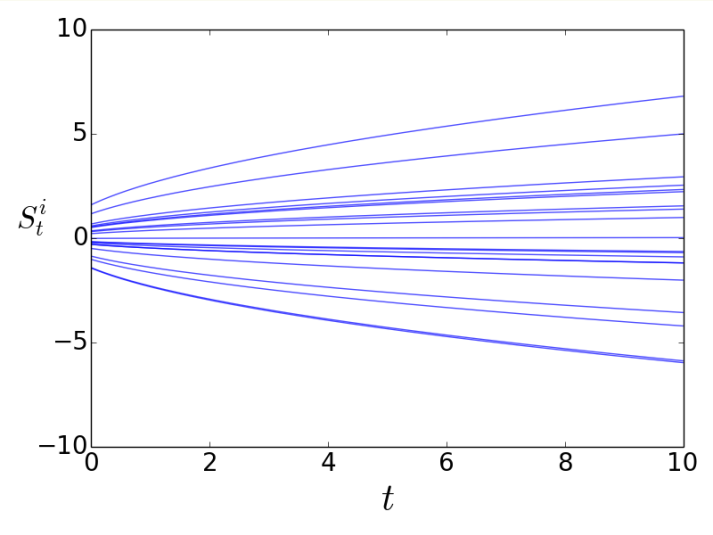

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Optimal transport FPF

Optimal transportation approach

- Reason for non-uniqueness: Only the marginal distributions, at each time instant, are specified
- Optimal transport maps provide a way to uniquely couple two distributions.

Proposed solution: Infinitesimal optimal transport maps

$$\bar{X}_{t+\Delta t} = T_t(\bar{X}_t),$$

- T_t is the optimal transport map between π_t and $\pi_{t+\Delta t}$
- Take the limit as $\Delta t \to 0$

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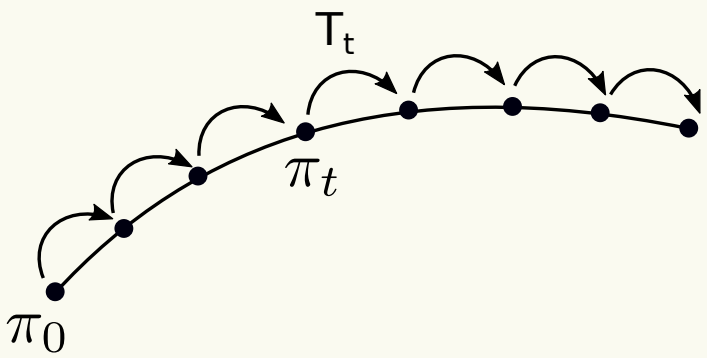

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Optimal transport FPF

Linear Gaussian setting

The procedure is carried out in linear Gaussian setting.

$$\textbf{FPF:} \quad \mathrm{d}\bar{X}_t = A\bar{X}_t\mathrm{d}t + \mathrm{d}\bar{B}_t + \bar{\mathsf{K}}_t(\mathrm{d}Z_t - \frac{H\bar{X}_t + H\bar{m}_t}{2}\mathrm{d}t),$$

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- The process noise term is replaced with a deterministic term
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$$\Omega_t\bar{\Sigma}_t^{-1} + \bar{\Sigma}_t^{-1}\Omega_t = A^T - A + \frac{1}{2}(\bar{\mathsf{K}}_t H - H^T\bar{\mathsf{K}}_t^T)$$

Extension: Developed an approach that does not require invertible covariance matrix

A. Taghvaei, P. G. Mehta, An optimal transport formulation for the linear feedback particle filter, (ACC) 2016

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$$\textbf{FPF:} \quad \mathrm{d}\bar{X}_t = A\bar{X}_t\mathrm{d}t + \mathrm{d}\bar{B}_t + \bar{\mathsf{K}}_t(\mathrm{d}Z_t - \frac{H\bar{X}_t + H\bar{m}_t}{2}\mathrm{d}t),$$

$$\textbf{Opt. FPF:} \quad \mathrm{d}\bar{X}_t = A\bar{X}_t\mathrm{d}t + \frac{1}{2}\bar{\Sigma}_t^{-1}(\bar{X}_t - \bar{m}_t)\mathrm{d}t + \bar{\mathsf{K}}_t(\mathrm{d}Z_t - \frac{H\bar{X}_t + H\bar{m}_t}{2}\mathrm{d}t) + \Omega_t\bar{\Sigma}_t^{-1}(\bar{X}_t - \bar{m}_t)\mathrm{d}t,$$

- The process noise term is replaced with a deterministic term
- Ω_t is the (skew symmetric) solution to the matrix equation:

$$\Omega_t\bar{\Sigma}_t^{-1} + \bar{\Sigma}_t^{-1}\Omega_t = A^T - A + \frac{1}{2}(\bar{\mathsf{K}}_t H - H^T\bar{\mathsf{K}}_t^T)$$

Extension: Developed an approach that does not require invertible covariance matrix

A. Taghvaei, P. G. Mehta, An optimal transport formulation for the linear feedback particle filter, (ACC) 2016

Linear Gaussian setting:

$$\mathrm{d}X_t = AX_t\mathrm{d}t + \sigma_B \mathrm{d}B_t$$
$$\mathrm{d}Z_t = HX_t\mathrm{d}t + \mathrm{d}W_t$$

Kalman-Bucy filter: $P(X_t|Z_{[0,t]})$ is Gaussian $\mathcal{N}(m_t, \Sigma_t)$

Update for mean: $\mathrm{d}m_t = \underbrace{Am_t\mathrm{d}t}_{\text{dynamics}} + \underbrace{\mathsf{K}_t(\mathrm{d}Z_t - Hm\mathrm{d}t)}_{\text{correction}}$

Update for covariance: $\dfrac{\mathrm{d}\Sigma_t}{\mathrm{d}t} =$ (Ricatti equation)

Kalman gain: $\mathsf{K}_t := \Sigma_t H^\top$

R. E Kalman and R. S Bucy. New results in linear filtering and prediction theory, 1961

Error analysis of linear FPF

Linear Gaussian filtering problem: Kalman-Bucy Filter

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Error analysis of linear FPF
Problem formulation

Stochastic linear FPF:

$$\mathrm{d}X_t^i = AX_t^i + \sigma_B \mathrm{d}B_t^i + \Sigma_t^{(N)} H^\top (\mathrm{d}Z_t - \frac{1}{2}H(X_t^i + m_t^{(N)})\mathrm{d}t), \quad X_0^i \overset{\text{i.i.d}}{\sim} p_0$$

Deterministic linear FPF:

$$\begin{aligned}\mathrm{d}X_t^i =& AX_t^i + \frac{1}{2}\Sigma_B(\Sigma^{(N)})^{-1}(X_t^i - m_t^{(N)})\mathrm{d}t \\ &+ \Sigma_t^{(N)} H^\top (\mathrm{d}Z_t - \frac{1}{2}H(X_t^i + m_t^{(N)})\mathrm{d}t), \quad X_0^i \overset{\text{i.i.d}}{\sim} p_0\end{aligned}$$

where $m_t^{(N)}, \Sigma_t^{(N)}$ are empirical mean and covariance

Exactness: If $N = \infty$ (mean-field approximation), then $m_t^{(\infty)} = m_t$ and $\Sigma_t^{(\infty)} = \Sigma_t$

Question: What is the approximation error when $N < \infty$?

G. Evensen. Sequential data assimilation with a nonlinear quasi-geostrophic model . . . 1994.
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Error analysis of linear FPF

Result: Deterministic linear FPF

Evolution of mean and covariance:

$$\mathrm{d}m_t^{(N)} = \underbrace{Am_t^{(N)}\mathrm{d}t + \mathsf{K}_t^{(N)}(\mathrm{d}Z_t - Hm_t^{(N)}\mathrm{d}t)}_{\text{Kalman filter}}$$

$$\mathrm{d}\Sigma_t^{(N)} = \underbrace{(A\Sigma_t^{(N)} + \Sigma_t^{(N)}A^\top + \sigma_B\sigma_B^\top - \Sigma_t^{(N)}H^\top H\Sigma_t^{(N)})\mathrm{d}t}_{\text{Kalman filter}}$$

Assumptions: (i) System is detectable and stabilizable; (ii) $\Sigma_0^{(N)}$ is invertible

Proposition

- Convergence of mean and variance: $\exists \lambda_0 > 0$ s.t

$$\mathsf{E}[|m_t^{(N)} - m_t|^2] \le (\text{const.})\frac{e^{-2\lambda_0 t}}{N}, \quad \mathsf{E}[\|\Sigma_t^{(N)} - \Sigma_t\|_F^2] \le (\text{const.})\frac{e^{-4\lambda_0 t}}{N}$$

- Convergence of the empirical distribution:

$$\mathsf{E}\left[\left|\frac{1}{N}\sum_{i=1}^N f(X_t^i) - \pi_t(f)\right|^2\right] \le \frac{(\text{const})}{N}$$

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Error analysis of linear FPF

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Assumption: The system is stable and the observation matrix is full rank.

Proposition

- Convergence of empirical mean and covariance:

$$\mathsf{E}[|m_t - m_t^{(N)}|^2] \leq \frac{(\text{const.})}{N}, \quad \mathsf{E}[|\Sigma_t - \Sigma_t^{(N)}|^2] \leq \frac{(\text{const.})}{N}$$

- Convergence of empirical distribution: ...

P Del Moral, J Tugaut. On the stability and the uniform propagation of chaos properties of ensemble Kalman–Bucy filters, 2018

Error analysis of linear FPF

Result: Stochastic linear FPF

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PDE viewpoint:

$$\langle \nabla\phi, \nabla\psi \rangle = \langle \psi, h - \hat{h} \rangle$$

- T. Yang, et. al. Automatica, 2015. (Constant gain and Galerkin approximation)
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$$\phi = e^{\epsilon \Delta_\rho} \phi + \tilde{h}$$

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Variational viewpoint:

$$\min_{\phi} \mathsf{E}[\frac{1}{2}|\nabla\phi(X)|^2 - \phi(X)h(X)]$$

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Diffusion map approximation
Mathematical preliminaries

- **Weighted Laplacian:** $\Delta_\rho f := \frac{1}{\rho}\nabla \cdot (\rho \nabla f)$
- **Spectral representation:** $-\Delta_\rho f = \sum_{m=0}^{\infty} \lambda_m \langle \psi_m, f \rangle \psi_m$

$$\text{Eigenvalues:} \quad \lambda_0 = 0 < \lambda_1 \leq \lambda_2 \leq \dots$$
$$\text{Eigenfunctions:} \quad \psi_0 = 1, \psi_1, \psi_2, , \dots$$

- **Diffusion semigroup:** $e^{t\Delta_\rho} f(x) = \sum_{m=0}^{\infty} e^{-t\lambda_m} \langle \psi_m, f \rangle \psi_m(x)$
- **Kernel representation:** $e^{t\Delta_\rho} f(x) = \int \bar{k}_t(x,y) f(y) \rho(y) \mathrm{d}y$

$$\textbf{Poincaré inequality} \quad \Rightarrow \quad \underbrace{\lambda_1 > 0}_{\textbf{Spectral gap}} \quad \Rightarrow \quad \underbrace{\|e^{t\Delta_\rho}\|_{L^2_0(\rho)} = e^{-t\lambda_1} < 1}_{\textbf{Contraction}}$$

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Gaussian example

Assume ρ is Gaussian density $N(0,1)$

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$$e^{t\Delta_\rho} f(x) = \int_{\mathbb{R}^d} \underbrace{\frac{1}{\sqrt{2\pi(1-e^{-2t})}} \exp\left(-\frac{e^{-2t}x^2 + e^{-2t}y^2 + e^{-t}xy}{2(1-e^{-2t})}\right)}_{\bar{k}_t(x,y)} f(y)\rho(y)\mathrm{d}y$$

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Poisson equation to semigroup formulation

Step $(1) \Leftrightarrow (2)$

(1) Poisson equation: $$-\Delta_\rho \phi = h - \hat{h}$$

(2) Semigroup formulation: $$\phi = e^{\epsilon \Delta_\rho}\phi + \int_0^\epsilon e^{s\Delta_\rho}(h - \hat{h})\mathrm{d}s$$

- $(1) \Leftrightarrow (2)$ follows from the semigroup identity

$$\frac{\partial}{\partial t} P_t \phi = P_t \Delta_\rho \phi \quad \Rightarrow \quad P_\epsilon \phi = \phi + \int_0^\epsilon P_s \Delta_\rho \phi \, \mathrm{d}s$$

- P_ϵ is a contraction $\Rightarrow$ A unique solution $\phi \in L_0^2(\rho)$ exists

Proposition

Under Assumptions (A1)-(A2) the unique solution to (1) is the unique solution to (2)

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Under Assumptions (A1)-(A2) the unique solution to (1) is the unique solution to (2)

Poisson equation to semigroup formulation

Step $(1) \Leftrightarrow (2)$

(1) Poisson equation: $$-\Delta_\rho \phi = h - \hat{h}$$

(2) Semigroup formulation: $$\phi = e^{\epsilon \Delta_\rho}\phi + \int_0^\epsilon e^{s\Delta_\rho}(h - \hat{h})\mathrm{d}s$$

- $(1) \Leftrightarrow (2)$ follows from the semigroup identity

$$\frac{\partial}{\partial t} P_t \phi = P_t \Delta_\rho \phi \quad \Rightarrow \quad P_\epsilon \phi = \phi + \int_0^\epsilon P_s \Delta_\rho \phi \, \mathrm{d}s$$

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Proposition

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Empirical approximation to Finit-dim. eq

Step $(4) \Leftrightarrow (5)$

(4) Empirical approx: $$\phi_\epsilon^{(N)} = T_\epsilon^{(N)} \phi_\epsilon^{(N)} + \epsilon(h - \pi(h))$$

(5) Finite-dim. eq: $$\Phi = \mathsf{T}\Phi + \epsilon(\mathsf{h} - \pi(h))$$

where

$$\mathsf{T}_{ij} := \frac{g_\epsilon(X^i, X^j)}{n_\epsilon^{(N)}(X^i)\sqrt{\sum_{l=1}^N g_\epsilon(X^j, X^l)}}$$

$$\mathsf{h} := (h(X^1), \ldots, h(X^N))$$

- T is a reversible $N \times N$ Markov matrix with invariant dist π
- $\pi(h) = \sum_{i=1}^N \pi_i \mathsf{h}_i$

A unique solution $\Phi \in \mathbb{R}_0^N$ exists

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Error analysis: Bias

Study convergence $T^n_{\frac{t}{n}} \to P_t$ as $n \to \infty$

Proposition

- Feynman-Kac representation of the semigroup

$$P_t f(x) = e^{U(x)} \mathsf{E}[e^{-\int_0^t W(B^x_{2s})\mathrm{d}s} e^{-U(B^x_{2t})} f(B^x_{2t})]$$

  where B^x_t is the Brownian motion with $B^x_0 = x$
- Stochastic representation of the Diffusion map

$$T^n_\epsilon f(x) = e^{U_\epsilon(x)} \mathsf{E}[e^{-\epsilon \sum_{k=0}^{n-1} W_\epsilon(B^x_{2k\epsilon})} e^{-U_\epsilon(B^x_{2t})} f(B^x_{2t})]$$

  where $U_\epsilon = U + O(\epsilon)$ and $W_\epsilon = W + O(\epsilon)$
- Convergence: For all functions $f, \nabla f \in L^4(\rho)$

$$\|T^n_{\frac{t}{n}} f - P_t f\|_{L^2(\rho)} \leq (\text{const}) \frac{\sqrt{t}}{n} (\|f\|_{L^4(\rho)} + \|\nabla f\|_{L^4(\rho)})$$

Define $U(x) = \frac{1}{2}\log(\rho(x))$ and $W(x) = |\nabla U(x)|^2 - \Delta U(x)$

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Spectral gap and error bound

$$\phi_\epsilon = T_\epsilon \phi_\epsilon + \epsilon(h - \hat{h}_\epsilon) \quad \Rightarrow \quad \phi_\epsilon = T_\epsilon^n \phi_\epsilon + \epsilon \sum_{k=0}^{n-1} T_\epsilon^k (h - \hat{h}_\epsilon)$$

Proposition

- Foster-Lyapunov condition DV(3): $\exists a, b, R, \delta > 0$ and prob. measure ν such that

$$\log(e^{-U_\epsilon} T_\epsilon^n e^{U_\epsilon}) \leq -atU_\epsilon + bt\mathbf{1}_{[|x| \leq R]}$$
$$T_\epsilon^n \mathbf{1}_{[A]} \geq \delta \nu(A) \quad \forall |x| \leq R$$

- T_ϵ^n admits a spectral gap on $L^2(\rho_\epsilon)$ and

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- In the asymptotic limit as $\epsilon \to 0$

$$\|\phi_\epsilon - \phi\|_{L^2(\rho)} \leq O(\epsilon)$$

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Optimal transport FPF
Singular covariance case

Idea: Modification of the procedure to construct sequence of stochastic maps

Result:

$$\begin{aligned}\mathrm{d}\bar{X}_t =& A\bar{X}_t + \frac{1}{2}(\sigma_B + e_t)u_t^\top(\bar{X}_t - \bar{m}_t)\mathrm{d}t + e_t\mathrm{d}\bar{B}_t \\ &+ \bar{\mathsf{K}}_t(\mathrm{d}Z_t - \frac{HX_t^i + H\bar{m}_t}{2}\mathrm{d}t) + \text{(extra terms)}\end{aligned}$$

- $u_t = \mathsf{Proj}(\sigma_B; \mathsf{Range}(\bar{\Sigma}_t))$
- $e_t = \sigma_B - \bar{\Sigma}_t u_t$
- It simplifies to the previous sde if $\bar{\Sigma}_t$ is invertible
- Important for finite-N implementation when $N < d$ and $\bar{\Sigma}_t$ is singular

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Error analysis of finite-N system
Problem formulation

Finite-N system:

$$\mathrm{d}X_t^i = AX_t^i + \sigma_B \mathrm{d}B_t^i + \mathsf{K}_t^{(N)}(\mathrm{d}Z_t - \frac{1}{2}H(X_t^i + m_t^{(N)})\mathrm{d}t), \quad X_0^i \overset{\text{i.i.d}}{\sim} p_0$$

$$\mathsf{K}_t^{(N)} = \Sigma_t^{(N)} H^\top$$

with empirical mean $m_t^{(N)}$ and covariance $\Sigma_t^{(N)}$

Mean-field limit:

$$\mathrm{d}\bar{X}_t = (\text{linear dynamics}) + \bar{\mathsf{K}}_t(\mathrm{d}\bar{Z}_t - \frac{1}{2}H(X_t^i + \bar{m}_t)\mathrm{d}t), \quad \bar{X}_0 \sim p_0$$

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Error analysis:

1. Analysis of the mean-field system
2. Analysis of the converegnce of the finite-N system to the mean-field limit

$$\text{Finite-}N\text{ system} \overset{(2)}{\approx} \text{mean-field system} \overset{(1)}{=} \text{Kalman filter}$$

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Background: Wasserstein gradient

- Objective functional:

$$\mathsf{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$$

- Wasserstein gradient: $\nabla_W \mathsf{F}(\rho) : \mathbb{R}^d \to \mathbb{R}^d$ is a vector field that satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{F}(\rho_t)\Big|_{t=0} = \langle \nabla_W \mathsf{F}(\rho), u \rangle_{L^2(\rho)},$$

for all path $\{\rho_t\}$ s.t $\quad \dfrac{\partial \rho_t}{\partial t} + \nabla \cdot (\rho_t u) = 0$

- Example:

$$\mathsf{F}(\rho) = \mathsf{D}(\rho \| \rho_\infty) \quad \text{(relative entropy)}$$

$$\Longrightarrow \quad \nabla_W \mathsf{F}(\rho)(x) = \nabla \log(\rho(x)) + \nabla f(x)$$

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Comparison to Hamiltonian MCMC

- Proposed accelerated flow:

$$\ddot{X}_t = -\frac{3}{t}\dot{X}_t - \nabla f(X_t) - \underbrace{\nabla \log(\rho_t(X_t))}_{\text{mean-field term}}$$

- Continuous-time limit of Hamiltonian MCMC (under-damped Langevin eq.)

$$\begin{aligned} \mathrm{d}X_t &= v_t \mathrm{d}t \\ \mathrm{d}v_t &= -\gamma v_t \mathrm{d}t - \nabla f(X_t)\mathrm{d}t + \underbrace{\sqrt{2}\mathrm{d}B_t}_{\text{stochastic term}} \end{aligned}$$

- Trade-off between computational efficiency and accuracy

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Numerical example
comparison with MCMC and HMCMC