Application of learning algorithms to nonlinear filtering and MCMC

PhD Dissertation defense

Nov 6, 2019

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COGNITION & CONTROL IN COMPLEX SYSTEMS

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Thanks to friends & family

Outline

1. PhD Proposal - Recap
2. Poisson's Equation
3. Differential LSTD learning
4. Applications to Nonlinear filtering
5. Applications to MCMC
6. Conclusions and Future Work

great that you went through this fast

PhD Proposal - Recap

Work till then

- Presented the feedback particle filter (FPF) - an approximation of the nonlinear filter that requires computing a gain function by solving a version of *Poisson's equation*.
- Proposed a differential TD-learning algorithm to approximate the gradient of the solution to Poisson's equation. [R et al. 16]

PhD Proposal - Recap

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- Presented the feedback particle filter (FPF) - an approximation of the nonlinear filter that requires computing a gain function by solving a *Poisson's equation*.
- Proposed a differential TD-learning algorithm to approximate the gradient of the solution to Poisson's equation. [R et al. 16]
- Presented numerical examples for gain approximation and state estimation for scalar systems.

PhD Proposal - Recap

Tasks promised and accomplished

- Extend the algorithm to a multidimensional setting.

PhD Proposal - Recap

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delete

- Extend the algorithm to a multidimensional setting. - ✓ [R et al. 18]
- Explore appropriate basis selection for these algorithms.

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New direction Kernel methods

- Simplified differential LSTD algorithm for Langevin diffusion. [R et al. 18]
- Improvements for online gain estimation. [R et al. 19]
- Explored the application to MCMC algorithms. [Brosse et al. 19]

Poisson's Equation

$$0 = \tilde c + \mathcal{D}h$$

$$h(x) = \mathsf{E}\Big[\int_0^\tau \tilde c(X(t))\,dt\Big]$$

with $X(0) = x$

Optimal FPF Gain

$$\mathsf{K} = \nabla h$$

Optimal Control

$$\phi_{n+1}(x) = \arg\min_u \Big\{ c(x,u) + \mathcal{D}_u h_n(x) \Big\}$$

Optimal MCMC CV

$$\gamma^2_{\text{CLT}} = \langle 2\nabla h, \tilde c\rangle$$
$$\gamma^2_\theta = 2\langle h_\theta, \tilde c_\theta\rangle$$
$$= 2\|\nabla h_\theta\|^2$$

Poisson's Equation

Poisson's Equation

- Second order partial differential equation with applications in various fields.
- General form in stochastic systems

delete (no "equal by definition")

$$\mathcal{D}h := -f$$

$\mathcal{D}$ - differential operator
f - forcing function, usually centered

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$$\mathcal{D}h := -f$$

$\mathcal{D}$ - differential operator
f - forcing function, usually centered
h - solution to Poisson's equation

Poisson's Equation

Stochastic optimal control

delete?
or introduce P_*

Example: In average cost optimal control problems,

$$\min_u \{c(x,u) + P_u h^*(x)\} = h^*(x) + \eta^*$$

$c(x,u)$	- Cost function associated with state x and action u.
P_u	- Transition kernel of the controlled Markov chain.
η^*	- Optimal average cost.
$h^*\cancel{(x)}$	- Relative value function

delete

Where is D? f?

$\boxed{Dh^* = -\tilde{c}}$

Poisson's Equation

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$h^*(x)$ - Relative value function

Poisson's equation is the dynamic programming equation.

Poisson's Equation

Langevin Diffusion

Langevin diffusion is given by the SDE,

$$\mathrm{d}\Phi_t = \underbrace{-\nabla U(\Phi_t)\,\mathrm{d}t}_{\text{Drift term}} + \underbrace{\sqrt{2}\,\mathrm{d}W_t}_{\text{Diffusion term}}, \qquad \Phi \in \mathbb{R}^d$$

$U \in C^1$ is called the *potential function*.

$\boldsymbol{W} = \{W_t : t \geq 0\}$ is a standard Brownian motion on $\mathbb{R}^d$.

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$\boldsymbol{W} = \{W_t : t \geq 0\}$ is a standard Brownian motion on $\mathbb{R}^d$.

- May be regarded as a d-dimensional gradient flow with "noise".
- Diffusion is reversible, with unique *invariant density* $\rho = e^{-U+\Lambda}$, where Λ is a normalizing constant.

Poisson's Equation

Langevin Diffusion

delete

Differential generator $\mathcal{D}$~~,~~ :

$$\mathcal{D}f := \lim_{t\to 0} \frac{\mathsf{E}[f(\Phi_t)|\Phi_0 = x] - f(x)}{t}$$

Poisson's Equation

Langevin Diffusion

Differential generator $\mathcal{D}$,

$$\begin{aligned}\mathcal{D}f &:= \lim_{t\to 0} \frac{\mathsf{E}[f(\Phi_t)|\Phi_0 = x] - f(x)}{t} \\ &= -\nabla U \cdot \nabla f + \Delta f, \qquad f \in C^2,\end{aligned}$$

where ∇ is the gradient and Δ is the Laplacian.

Poisson's Equation

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where ∇ is the gradient and Δ is the Laplacian.
Let $c\colon \mathbb{R}^d \to \mathbb{R}$ be a function of interest, and

$$\eta = \int c(x)\rho(x)dx = \langle c, 1\rangle_{L^2}.$$

Poisson's Equation

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Let $c\colon \mathbb{R}^d \to \mathbb{R}$ be a function of interest, and

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Function $h \in C^2$ solves Poisson's equation with forcing function c if

need this earlier with sum for dis. time

$$\left\{ \begin{aligned} &\mathcal{D}h := -\tilde{c}, \qquad \tilde{c} = c - \eta. \\ &h := \int_0^\infty \mathsf{E}[\tilde{c}(\Phi_t)]\mathrm{d}t \end{aligned} \right.$$

Poisson's Equation

Existence of a solution

- A solution exists under weak assumptions on U and c [Glynn 96, Kontoyiannis 12].
- Representations for the gradient of h and bounds are obtained in [Laugesen 15, Devraj 18].
- A smooth solution $h \in C^2$ exists under stronger conditions in [Pardoux 01], subject to growth conditions on c similar to [Glynn 96].

Poisson's Equation

Approximate solution to Poisson's equation

Obtaining an analytical solution for h is difficult outside special cases.
Hence approximation.

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Goal: For a given function class $\mathcal{H}$, find the minimizer of

$$g^* := \arg\min_{g \in \mathcal{H}} \|h - g\|_{L^2}^2$$

Such minimum norm optimization problems can be solved using *TD learning* [Tsitsikilis 99, CTCN].

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$$g^* := \arg\min_{g \in \mathcal{H}} \|h - g\|^2_{L^2} \qquad (*)$$

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to solve (*) if the process

Challenge - No algorithm exists ~~for state spaces of dimension > 1~~.

does not regenerate (for diffusions, dim > 1 ruled out).

LSTD learning

Discounted cost case

I prefer color, but o.k.

Discounted-cost value function:

$$h^\gamma(x) := \int_0^\infty e^{-\gamma t} \mathsf{E}_x[c(\Phi_t)] \mathrm{d}t, \qquad \gamma > 0 \ \cancel{\ } \text{ discount factor}$$

Discounted-cost optimality equation:

$$\gamma h^\gamma = c + \mathcal{D} h^\gamma$$

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LSTD learning

Discounted cost case

$$\text{LSTD goal - } g^* := \arg\min_{g\in\mathcal{H}} \|h^\gamma - g\|_{L^2}^2$$

For a linear parameterization

$$g = h^\theta := \sum_{i=1}^{\ell} \theta_i \psi_i$$

$$\theta^* = M^{-1} b$$

$$M_{ij} = \langle \psi_i, \psi_j \rangle_{L^2}, \quad b_i = \langle \psi_i, h^\gamma \rangle_{L^2}$$

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$$= \langle \psi_i, \ R_\gamma c \rangle_{L^2}$$

$$\text{Resolvent kernel - } R_\gamma c\,(x) := \int_0^\infty \mathsf{E}_x \Big[e^{-\gamma t} c(\Phi_t) \Big] \mathrm{d}t$$

$$R_\gamma c = (I_\gamma - \mathcal{D})^{-1} c$$

why subscript?

$[I\gamma - D]^{-1}$

LSTD learning

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$$= \langle R_\gamma^\dagger \psi_i,\, c \rangle_{L^2}$$

Using an adjoint operation and applying the stationarity of Φ.

LSTD learning

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$$\text{Eligibility vector - } \varphi(t) := \int_0^\infty e^{-\gamma r} \psi(\Phi_{t-r}) \mathrm{d}r \qquad \phi(t)$$

$$R_\gamma^\dagger \psi_i(x) = \mathsf{E}[\cancel{\varphi_i}(t) | \Phi_t = x]$$

$$\phi_i$$

LSTD learning

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For a linear parameterization

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$$\begin{aligned} M_{ij} = \langle \psi_i, \psi_j \rangle_{L^2}, \quad b_i &= \langle R_\gamma^\dagger \psi_i, c \rangle_{L^2} \\ &= \mathsf{E}[\cancel{\varphi_{\psi_i}}(t) c(\Phi_t)] \end{aligned}$$

φ_i

LSTD learning

Discounted cost case

ODE formulation of the LSTD algorithm:

$$
\begin{aligned}
\frac{d}{dt}M(t) &= \psi(\Phi_t)\psi^{\intercal}(\Phi_t) \\
\frac{d}{dt}\varphi_\psi(t) &= -\gamma\,\varphi_\psi(t) + \psi(\Phi_t) \\
\frac{d}{dt}b(t) &= \varphi_\psi(t)c(\Phi_t) \\
\theta(t) &:= M(t)^{-1}b(t)
\end{aligned}
$$

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By law of large numbers,

$$\lim_{t\to\infty} \theta(t) = \theta^*$$

LSTD learning

Discounted cost case

ODE formulation of the LSTD algorithm:

$M(T) = M(0) + \int_0^T \psi \, \psi^T \, dt$

$$
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$$

By law of large numbers, be able to defend this.

$$\lim_{t\to\infty} \theta(t) = \theta^*$$

~~Drawback!~~ For average-cost, LSTD requires the existence of a regenerating state.

Differential LSTD learning (∇-LSTD)

Poisson's equation

Idea: Approximate the gradient of h directly [R et al. 16, Devraj et al. 16]:

$$g^* := \arg\min_{g \in \mathcal{H}} \|\nabla h - \nabla g\|_{L^2}^2$$

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Need to choose a function class $\mathcal{H}$ for g (or ∇g)

- A finitely parameterized family of functions.
- A reproducing kernel Hilbert space (RKHS).

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- A finitely parameterized family of functions.
- A reproducing kernel Hilbert space (RKHS).
  Choice of basis is not an easy task
  $\Longrightarrow$ RKHS framework is far easier to implement.

great independent work here. Brag about it!

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∇-LSTD goal - $g^* := \arg\min_{g \in \mathcal{H}} \|\nabla h - \nabla g\|^2_{L^2}$

Challenge: the function h is not known,
and hence the objective function is not observable

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∇-LSTD: For a linear parameterization

$$g = h^\theta := \sum_{i=1}^{\ell} \theta_i \psi_i \implies \nabla g = \sum_{i=1}^{\ell} \theta_i \nabla \psi_i$$

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$$M_{ij} = \langle \nabla \psi_i, \nabla \psi_j \rangle_{L^2}, \quad b_i = \langle \nabla \psi_i, R_{U''} \nabla c \rangle_{L^2}$$

Resolvent kernel - $R_{U''} \nabla c\,(x) := \int_0^\infty \mathsf{E}_x \Big[\exp\Big(- \int_0^t U''(\Phi_s)\, \mathrm{d}s \Big) \nabla c(\Phi_t) \Big] \mathrm{d}t$

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∇-LSTD-L: For Langevin diffusion, if $f, g \in L^2(\rho)$

$$\langle \nabla f, \nabla g \rangle_{L^2} = -\langle f, \mathcal{D} g \rangle_{L^2} = -\langle \mathcal{D} f, g \rangle_{L^2}.$$

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Applying this and Poisson's equation $\mathcal{D}h = -\tilde{c}$:

$$\begin{aligned} \|\nabla h - \nabla g\|_{L^2}^2 &= \|\nabla h\|_{L^2}^2 + \|\nabla g\|_{L^2}^2 - 2\langle \nabla h, \nabla g \rangle_{L^2} \\ &= \|\nabla h\|_{L^2}^2 + \|\nabla g\|_{L^2}^2 + 2\langle \mathcal{D} h, g \rangle_{L^2} \end{aligned}$$

use color so transformation is clear

Differential LSTD learning (∇-LSTD)

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Differential LSTD learning (∇-LSTD $-\ L$)

Poisson's equation

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Differential LSTD learning (∇-LSTD $- L$)

Poisson's equation

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Differential LSTD learning (∇-LSTD $- L$)

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$$M_{ij} = \langle \nabla\psi_i, \nabla\psi_j \rangle_{L^2} \approx \frac{1}{t}\int_0^t \nabla\psi(\Phi_s)\,\nabla\psi^{\intercal}(\Phi_s)\,ds$$

\,

small space

$$b_i = \langle \nabla\psi_i, \nabla h \rangle_{L^2} = \langle \psi_i, \tilde{c} \rangle_{L^2} \approx \frac{1}{t}\int_0^t \psi_i(\Phi_s)\,\tilde{c}(\Phi_s)\,ds$$

Differential LSTD learning on RKHS (∇-LSTD-RKHS)

Basics of RKHS

Choose a kernel function $K(x,y)$ that is

- *Symmetric*: $K(x,y) = K(y,x)$ for any $x, y \in \mathbb{R}^d$
- *Positive definite*: For any finite subset $\{x^i\} \subset \mathbb{R}^d$, the matrix $\{M_{ij} := K(x^i, x^j)\}$ is positive definite.
- *Smooth*: $K \in C^2$

raises questions

K defines a ~~unique~~ reproducing kernel Hilbert space (RKHS) $\mathcal{H}$ [Moore-Aronszajn theorem].

Inner product: If $g_\alpha = \sum_i \alpha_i K(x^i, \cdot\,)$ and $g_\beta = \sum_j \beta_j K(y^j, \cdot\,)$,

$$\langle g_\alpha, g_\beta \rangle_{\mathcal{H}} := \sum_{i,j} \alpha_i \beta_j K(x^i, y^j)$$

Reproducing property: $g_\alpha(x) = \langle g_\alpha, K(x, \cdot\,) \rangle_{\mathcal{H}}\,, \quad x \in \mathbb{R}^d.$

Differential LSTD learning on RKHS

Empirical risk minimization (ERM)

Recall ∇-LSTD -L ? goal: $\boxed{\text{∇-LSTD-L goal}}$?

$$g^* = \arg\min_{g \in \mathcal{H}} \Big\{ \|\nabla g\|_{L^2}^2 - 2\langle \tilde{c}, g \rangle_{L^2} \Big\}$$

Approximation via empirical risk minimization (ERM):

$$\arg\min_{g \in \mathcal{H}} \underbrace{\frac{1}{N} \sum_{i=1}^{N} \Big[\|\nabla g(x^i)\|^2 - 2\tilde{c}_N(x^i) g(x^i) \Big]}_{\text{Empirical risk}} + \underbrace{\lambda \|g\|_{\mathcal{H}}^2}_{\text{Regularization}}$$

where $\tilde{c}_N(x) = c(x) - \frac{1}{N} \sum_{i=1}^{N} c(x^i)\,, \quad x \in \mathbb{R}^d$

Differential LSTD learning on RKHS

Empirical risk minimization (ERM)

Extended Representer Theorem [Zhou 08]

If loss function $L(x, \cdot, \cdot)$ is convex on $\mathbb{R}^{d+1}$ for each $x \in \mathbb{R}^d$, then the optimizer g^* over $g \in \mathcal{H}$ exists:

$$g^*(\cdot) = \sum_{i=1}^{N} \Big[\beta_i^{0*} K(x^i, \cdot) + \sum_{k=1}^{d} \beta_i^{k*} \frac{\partial}{\partial x_k} K(x^i, \cdot) \Big]$$

Differential LSTD learning on RKHS

Empirical risk minimization (ERM)

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Our loss function is convex: $L(x, g, \nabla g) = \|\nabla g(x)\|^2 - 2\tilde{c}(x) g(x)$

Differential LSTD learning on RKHS

Optimal solution in one dimension

∇-LSTD-RKHS ERM:

$$g^* = \arg\min_{g\in\mathcal{H}} \frac{1}{N}\sum_{i=1}^{N}\Big\{(g'(x^i))^2 - 2\tilde{c}_N(x^i)g(x^i)\Big\} + \lambda\|g\|_{\mathcal{H}}^2$$

Solution: $g^*(y) = \sum_{i=1}^{N}\Big\{\beta_i^{0*}K(x^i,y) + \beta_i^{1*}\partial_x K(x^i,y)\Big\}, \quad y\in\mathbb{R}$

Differential LSTD learning on RKHS

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Notation:

$$M_{00}(i,j) := K(x^i, x^j), \qquad M_{10}(i,j) := \frac{\partial K}{\partial x}(x^i, x^j)$$

$$M_{01}(i,j) := \frac{\partial K}{\partial y}(x^i, x^j), \qquad M_{11}(i,j) := \frac{\partial^2 K}{\partial x \partial y}(x^i, x^j)$$

$$\tilde{\varsigma}_j := \tilde{c}_N(x^j), \qquad \beta^{\intercal} = [\beta_1^0, \ldots, \beta_N^0, \beta_1^1, \ldots, \beta_N^1]$$

Differential LSTD learning on RKHS

Optimal solution in one dimension

∇-LSTD-RKHS ERM:

$$g^* = \arg\min_{g\in\mathcal{H}} \frac{1}{N}\sum_{i=1}^{N}\Big\{(g'(x^i))^2 - 2\breve{c}_N(x^i)g(x^i)\Big\} + \lambda\|g\|_{\mathcal{H}}^2$$

Solution: $g^*(y) = \sum_{i=1}^{N}\Big\{\beta_i^{0*}K(x^i,y) + \beta_i^{1*}\partial_x K(x^i,y)\Big\}, \quad y \in \mathbb{R}$

Computation: $\beta^* = M^{-1}b$

Boring

$$M = \frac{1}{N}\left[\frac{M_{01}}{M_{11}}\right]\left[M_{10}\,|M_{11}\right] + \lambda\left[\begin{array}{c|c} M_{00} & M_{01} \\ \hline M_{10} & M_{11}\end{array}\right]$$

$$b = \frac{1}{N}\left[\frac{M_{00}}{M_{10}}\right]$$

Differential LSTD learning on RKHS

Simplified solution

Drawback : Complexity grows linearly with d, since $\beta^* \in \mathbb{R}^{(d+1)\times N}$

Simplified solution : By considering the finite-dimensional function class - $\mathcal{H}_N :=$ span$\{K_{x^j} : 1 \leq j \leq N\}$

$$g^*(y) = \sum_{j=1}^{N} \beta_j^* K(x^j, y)$$

$$\beta^* = M^{-1} b$$

where, $\cancel{M := N^{-1} M_{01} M_{10} + \lambda M_{00}, \qquad b := N^{-1} M_{00} \tilde{\varsigma}}$

Surprising empirical observation : Simplified solution does as good as the optimal solution for $d \leq 5$.

Applications to Nonlinear filtering

Feedback Particle Filter

needs color
A figure

Goal : To obtain estimates of the state of a stochastic dynamical system based on noisy partial observations. figure here of a plane or...

Kalman filter is optimal for a linear Gaussian system.

For nonlinear systems, conditional distribution fails to be Gaussian, cannot be captured by a finite set of parameters.

Particle filters are Monte-Carlo approximations of the nonlinear filter.

Applications to Nonlinear filtering

Feedback Particle Filter

Problem:

Signal: $$\mathrm{d}X_t = a(X_t)\mathrm{d}t + \mathrm{d}B_t, \quad X_0 \sim \rho_0^*,$$

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

- $X_t \in \mathbb{R}^d$ is the state at time t.
- $\{Z_t : t \geq 0\}$ is the observation process.
- $a(.)$,$c(.)$ are C^1 functions.
- $\{B_t\}$,$\{W_t\}$ are mutually independent Wiener processes.

Applications to Nonlinear filtering

Feedback Particle Filter

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- $\{Z_t : t \geq 0\}$ is the observation process.
- $a(.)$,$c(.)$ are C^1 functions.
- $\{B_t\}$,$\{W_t\}$ are mutually independent Wiener processes.
- $\rho_t^* := P(X_t | \cancel{\{} Z_s : s \leq t \cancel{\}})$ is the posterior distribution.

no brackets

Applications to Nonlinear filtering

Feedback Particle Filter

et. al. (mainly Prashant)

Feedback particle filter (FPF) [Yang 13] is motivated by techniques from mean-field optimal control.

Applications to Nonlinear filtering

Feedback Particle Filter

Feedback particle filter (FPF) [Yang 13] is motivated by techniques from mean-field optimal control.

N *particles* are propagated in the form of a controlled system.

$$\mathrm{d}X_t^i = \underbrace{a(X_t^i)dt + \mathrm{d}B_t^i}_{\text{Propagation}} + \underbrace{\mathrm{d}U_t^i}_{\text{Update}}, \quad i = 1 \text{ to } N$$

- $X_t^i \in \mathbb{R}$ is the state of the i^{th} particle at time t
- U_t^i is the control input applied to i^{th} particle
- $\{B_t^i\}$ are mutually independent standard Wiener processes.

Applications to Nonlinear filtering

Feedback Particle Filter

Feedback particle filter (FPF) [Yang 13] is motivated by techniques from mean-field optimal control.

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- U_t^i is the control input applied to i^{th} particle
- $\{B_t^i\}$ are mutually independent standard Wiener processes.

Approximation of ρ_t^* :

$$\rho_t^* \approx \rho_t^{(N)}(A) = \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}\{X_t^i \in A\}, \quad A \subset \mathbb{R}.$$

block or color or something to wake audience

Applications to Nonlinear filtering

Feedback Particle Filter

~~Asymptotically exact filter obtained by minimizing the KL divergence between ρ_t^* and ρ_t (see [Yang 13]):~~

$$\mathsf{d}U_t^i = \mathsf{K}_t(X_t^i) \circ \overbrace{\left(\mathsf{d}Z_t - \tfrac{1}{2}[c(X_t^i) + \hat{c}_t]\mathsf{d}t\right)}^{\mathsf{d}I_t^i},$$

I_t^i : Innovations process.

K_t : FPF gain, similar in nature to the Kalman gain.

Applications to Nonlinear filtering

Feedback Particle Filter

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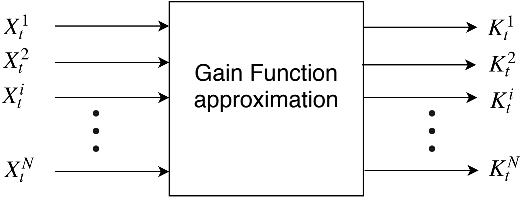
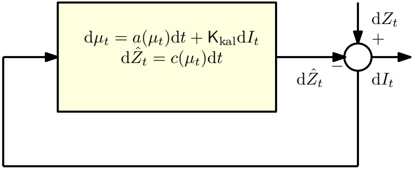


Figure: Finite-N implementation

Applications to Nonlinear filtering

Feedback Particle Filter

KF: $$\mathsf{d}\mu_t = a(\mu_t)\mathsf{d}t + \underbrace{\mathsf{K}_{\mathsf{kal}}(\mathsf{d}Z_t - c(\mu_t)\mathsf{d}t)}_{\text{update}}$$



Kalman filter

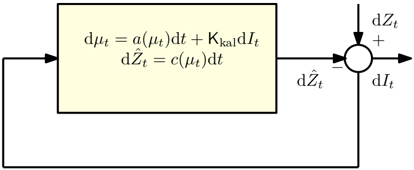
Applications to Nonlinear filtering

Feedback Particle Filter

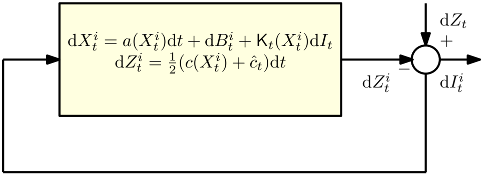
go through this fast
unnecessary review.

KF: $$\mathsf{d}\mu_t = a(\mu_t)\mathsf{d}t + \underbrace{\mathsf{K}_{\mathsf{kal}}(\mathsf{d}Z_t - c(\mu_t)\mathsf{d}t)}_{\text{update}}$$

FPF: $$\mathsf{d}X_t^i = a(X_t^i)\mathsf{d}t + \mathsf{d}B_t^i + \underbrace{\mathsf{K}_t(X_t^i) \circ (\mathsf{d}Z_t - \tfrac{1}{2}[c(X_t^i) + \hat{c}_t]\mathsf{d}t)}_{\text{update}}$$



Kalman filter



Feedback particle filter (FPF)

Applications to Nonlinear filtering

FPF Gain function

Representation: $\mathsf{K}_t = \nabla h$

h solves Poisson's equation: $\mathcal{D}h = -\nabla U \cdot \nabla h + \Delta h = -\tilde{c}$.

Applications to Nonlinear filtering

FPF Gain function

Representation: $\mathsf{K}_t = \nabla h$

h solves Poisson's equation: $\mathcal{D}h = -\nabla U \cdot \nabla h + \Delta h = -\tilde{c}$.

Approximations to K can be obtained by

$$\min_{g\in\mathcal{H}} \|\mathsf{K} - \hat{\mathsf{K}}\|^2_{L^2} = \min_{g\in\mathcal{H}} \|\nabla h - \nabla g\|^2_{L^2}$$

Applications to Nonlinear filtering

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Can be solved using ∇-LSTD learning

Applications to Nonlinear filtering

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FPF implementation requires online gain estimation for each t.

- ∇-LSTD-RKHS with optimal mean
- ∇-LSTD-RKHS with memory

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Constant gain approximation for K is the minimizer obtained over all deterministic vectors:

$$\widehat{\mathsf{K}}^* := \arg\min_{\widehat{\mathsf{K}} \in \mathbb{R}^d} \|\mathsf{K} - \widehat{\mathsf{K}}\|_{L^2}^2$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

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$$\widehat{\mathsf{K}}^* := \arg\min_{\widehat{\mathsf{K}}\in\mathbb{R}^d} \|\mathsf{K} - \widehat{\mathsf{K}}\|^2_{L^2}$$

Solution is evidently the mean, $\widehat{\mathsf{K}}^* = \mathsf{E}[\mathsf{K}]$.

$$\widehat{\mathsf{K}}^*_k = \langle \mathsf{K},\, e_k\rangle_{L^2}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

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Solution is evidently the mean, $\widehat{\mathsf{K}}^* = \mathsf{E}[\mathsf{K}]$.

$$\begin{aligned} \widehat{\mathsf{K}}_k^* &= \langle \mathsf{K}, e_k \rangle_{L^2} \\ &= \langle \nabla h, e_k \rangle_{L^2} \end{aligned}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Constant gain approximation for K is the minimizer obtained over all deterministic vectors:

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Solution is evidently the mean, $\widehat{\mathsf{K}}^* = \mathsf{E}[\mathsf{K}]$.

∇x_k

$$\begin{aligned} \widehat{\mathsf{K}}_k^* &= \langle \mathsf{K}, e_k \rangle_{L^2} \\ &= \langle \nabla h, e_k \rangle_{L^2} \\ &= -\langle \mathcal{D}h, x_k \rangle_{L^2} = \langle \tilde{c}, x_k \rangle_{L^2} \end{aligned}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Constant gain approximation for K is the minimizer obtained over all deterministic vectors:

$$\widehat{\mathsf{K}}^* := \operatorname*{arg\,min}_{\widehat{\mathsf{K}} \in \mathbb{R}^d} \|\mathsf{K} - \widehat{\mathsf{K}}\|_{L^2}^2$$

Solution is evidently the mean, $\widehat{\mathsf{K}}^* = \mathsf{E}[\mathsf{K}]$.

$$\begin{aligned}\widehat{\mathsf{K}}_k^* &= \langle \mathsf{K},\, e_k \rangle_{L^2} \\ &= \langle \nabla h,\, e_k \rangle_{L^2} \\ &= -\langle \mathcal{D}h,\, x_k \rangle_{L^2} = \langle \tilde{c},\, x_k \rangle_{L^2}\end{aligned}$$

Empirical approximation:

$$\widehat{\mathsf{K}}_k^* \approx \frac{1}{N} \sum_{i=1}^{N} [c(x^i) - \hat{c}] x_k^i$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Redefine the approximation to K as,

$$\nabla g = \widehat{\mathsf{K}}^* + \nabla \tilde{g}$$

Modified ERM with constaints is:

$$\begin{aligned} \tilde{g}^* := \arg\min_{\tilde{g}\in\mathcal{H}} \quad & \|\nabla h - \widehat{\mathsf{K}}^* - \nabla \tilde{g}\|_{L_2}^2 \\ \text{s.t.} \quad & \langle \partial_{x_k} \tilde{g}, 1 \rangle_{L_2} = 0, \quad 1 \le k \le d \end{aligned}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Redefine the approximation to K as,

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Modified ERM with constaints is:

$$\begin{aligned} \tilde{g}^* := \underset{\tilde{g}\in\mathcal{H}}{\arg\min} \quad & \|\nabla h - \widehat{\mathsf{K}}^* - \nabla \tilde{g}\|_{L_2}^2 \\ \text{s.t.} \quad & \langle \partial_{x_k} \tilde{g}, 1 \rangle_{L_2} = 0, \quad 1 \le k \le d \end{aligned}$$

Solution obtained by finding a saddle point for the Lagrangian

$$L(\tilde{g}, \mu) := \|\nabla h - \widehat{\mathsf{K}}^* - \nabla \tilde{g}\|_{L_2}^2 + \langle \mu, \nabla \tilde{g} \rangle_{L_2}$$

where $\mu \in \mathbb{R}^d$ are the Lagrange multipliers.

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Redefine the approximation to K as,

$$\nabla g = \widehat{\mathsf{K}}^* + \nabla \tilde{g}$$

Modified ERM with constaints is:

$$\tilde{g}^* := \arg\min_{\tilde{g}\in\mathcal{H}} \ \|\nabla h - \widehat{\mathsf{K}}^* - \nabla \tilde{g}\|_{L_2}^2$$

$$\text{s.t.} \quad \langle \partial_{x_k} \tilde{g}, 1\rangle_{L_2} = 0, \quad 1 \leq k \leq d$$

Using $\mathcal{H}_N := \text{span}\{K_{x^j} : 1 \leq j \leq N\}$, β and μ can be obtained by solving $N + d$ linear equations

$$\mathsf{K} = \widehat{\mathsf{K}}^* + \nabla \tilde{g}^*$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-memory

Gain updates are done at $t = n\delta$, where δ is the inter-sampling time.
Continuity : $\mathsf{K}_n = \mathsf{K}_{t_n} \approx \mathsf{K}_{t_{n-1}}$ if $\delta \approx 0$.

Applications to Nonlinear filtering

∇-LSTD-RKHS-memory

Gain updates are done at $t = n\delta$, where δ is the inter-sampling time.
Continuity : $\mathsf{K}_n = \mathsf{K}_{t_n} \approx \mathsf{K}_{t_{n-1}}$ if $\delta \approx 0$.
Adding a regularizer term to the loss function:

$$g_n^* := \arg\min_{g \in \mathcal{H}} \frac{1}{N} \sum_{j=1}^{N} L_n(x_n^j, g, \nabla g) + \lambda \|g\|_{\mathcal{H}}^2$$

$$L_n(x, g, \nabla g) := \|\nabla g(x)\|^2 - 2\tilde{c}_N(x) g(x) + \underbrace{\lambda_{mem} \|\nabla g(x) - \nabla g_{n-1}(x)\|^2}_{\text{continuity penalty}}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-memory

Gain updates are done at $t = n\delta$, where δ is the inter-sampling time.
Continuity : $\mathsf{K}_n = \mathsf{K}_{t_n} \approx \mathsf{K}_{t_{n-1}}$ if $\delta \approx 0$.

$$\beta_n^* = M^{-1} b$$

where,
$$M = (1 + \lambda_{mem}) \sum_{k=1}^{d} M_{10}^T M_{10} + \lambda N M_{00}$$

$$b = M_{00}\tilde{\varsigma} + \lambda_{mem} \sum_{k=1}^{d} M_{10}^T \mathsf{K}_{n-1,k}$$

Applications to Nonlinear filtering

∇-LSTD-RKHS-memory

Gain updates are done at $t = n\delta$, where δ is the inter-sampling time.
Continuity : $\mathsf{K}_n = \mathsf{K}_{t_n} \approx \mathsf{K}_{t_{n-1}}$ if $\delta \approx 0$.

$$\beta_n^* = M^{-1} b$$ ok, but no details.

where, $$M = \cancel{(1+\lambda_{mem})\sum_{k=1}^{d} M_{10}^{T} M_{10} + \lambda} N M_{00}$$

$$b = \cancel{M_{00}\tilde{\varsigma} + \lambda_{mem}\sum_{k=1}^{d} M_{10}^{T}} \mathsf{K}_{n-1,k}$$

Both these improvements can be applied independently or simultaneously.

Applications to Nonlinear filtering

Markov kernel approximation [Taghvaei 16]

No time

Approximates the transition kernel of the Langevin diffusion:

$$h = P_\epsilon h + \int_0^\epsilon P_s(c - \hat{c})\mathrm{d}s,$$

Give the expression for kernel approx. Empirical approximation on particle locations x^i:

$$h_i = \sum_{j=1}^{N} \mathsf{T}_{ij} h_j + \epsilon(c - \hat{c}), \text{ for } i = 1 \text{ to } N$$

Gain K is then obtained by approximating the gradient ∇h_i.

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture
$c(x) \equiv x$
$T = 10^4, 10^5, 10^6$ with $\delta = 0.01$, $N = 1000$

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

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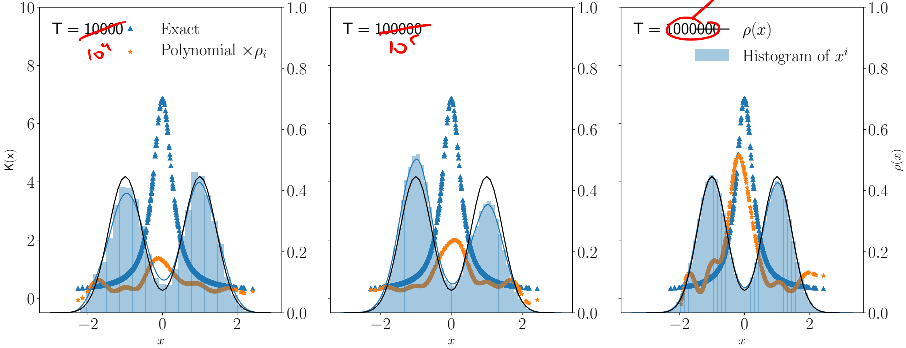


∇-LSTD with $\psi_i = x^i \rho_1(x)$, $\psi_{i+1} = x^i \rho_2(x)$ with $1 \le i \le 5$.

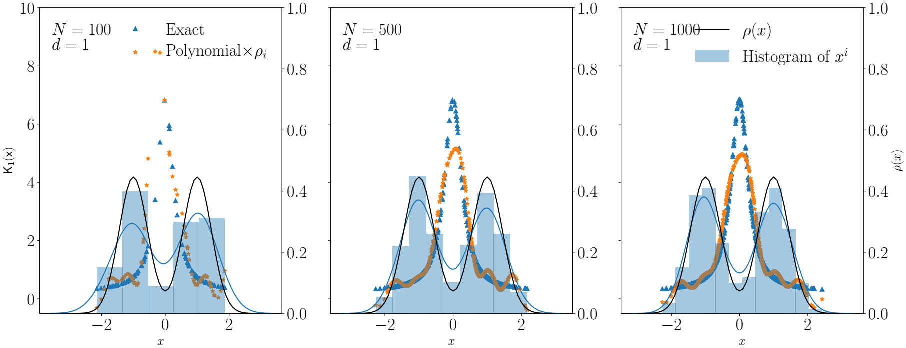
Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture

$c(x) \equiv x$

$N = 100, 500, 1000$



∇-LSTD-L with $\psi_i = x^i \rho_1(x)$, $\psi_{i+1} = x^i \rho_2(x)$ with $1 \leq i \leq 5$.

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

kill

Example: For a fixed t, ρ_t a Gaussian mixture
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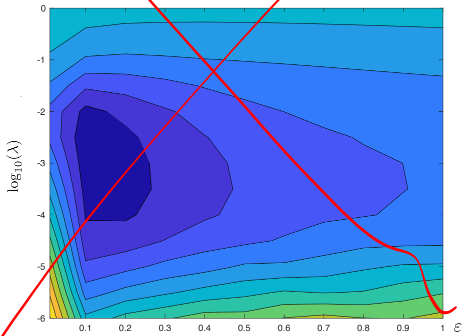
$N = 100, 500, 1000$



Grid-search using $K_\varepsilon := e^{-\frac{\|x-x'\|^2}{4\varepsilon}}$, yields and $\varepsilon = 0.1$ and $\lambda = 10^{-2}$.

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

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$c(x) \equiv x$
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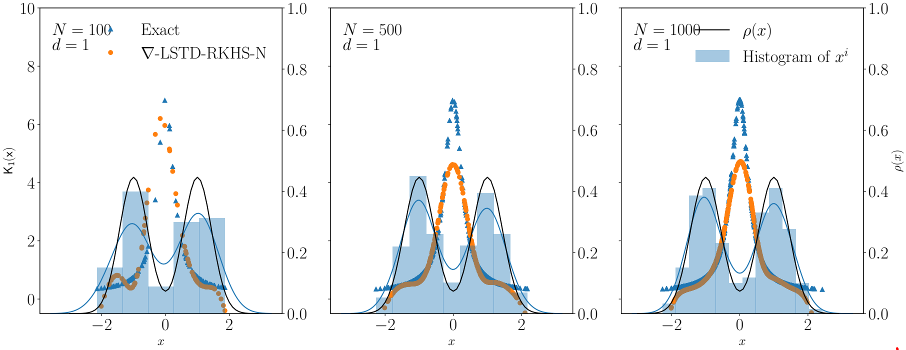
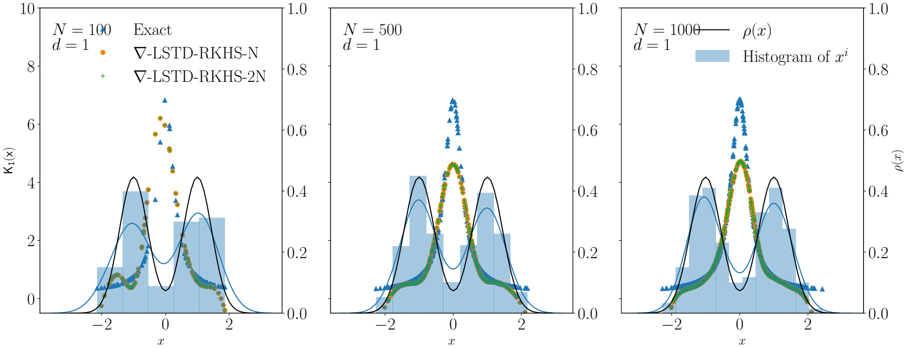


∇-LSTD-RKHS-N with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$ (best)

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture
$c(x) \equiv x$
$N = 100, 500, 1000$

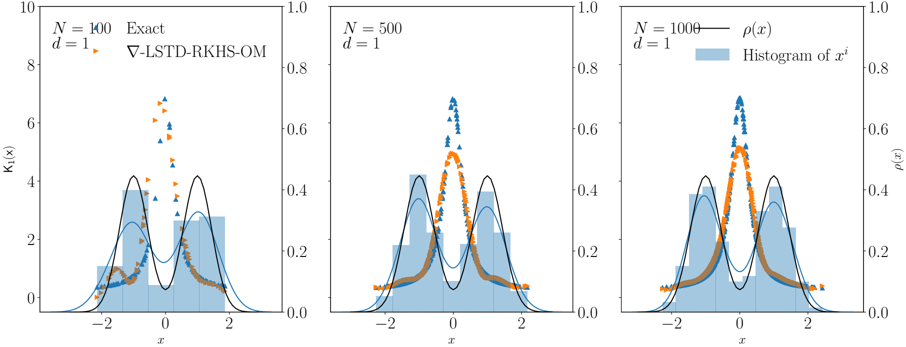


∇-LSTD-RKHS-2N with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture
$c(x) \equiv x$
$N = 100, 500, 1000$



∇-LSTD-RKHS-OM with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture
$c(x) \equiv x$
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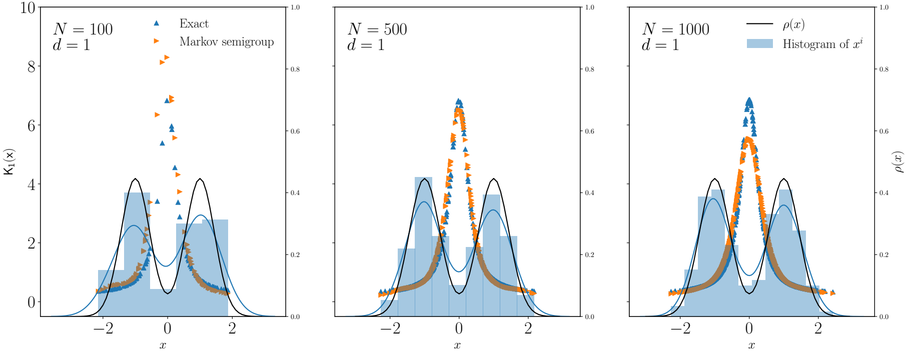


Markov kernel approximation with $\epsilon = 0.1$

Application to nonlinear filtering

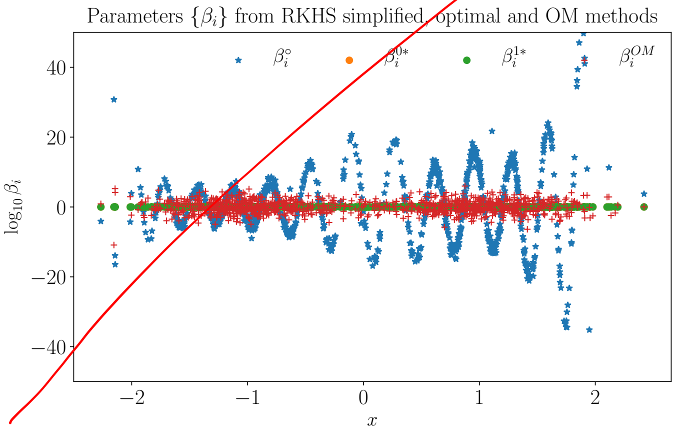
Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture

$c(x) \equiv x$

$N = 100, 500, 1000$

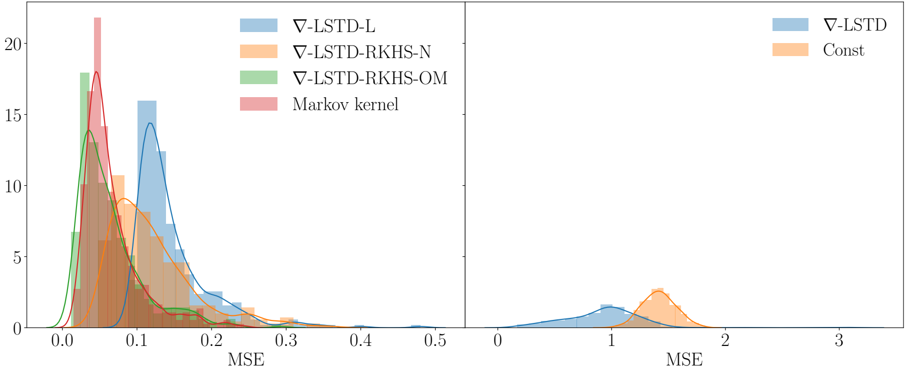
kill



Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: For a fixed t, ρ_t a Gaussian mixture
$c(x) \equiv x$
$N = 100, 500, 1000$

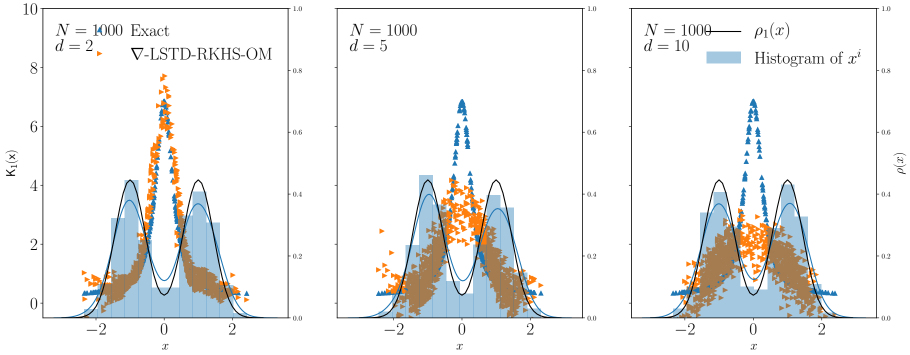


Histogram of MSEs obtained from 400 independent trials

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

Example: $\rho(x) = \prod_{k=1}^{d} \rho_k(x_k)$
$c(x) = C^T x$, where $C = \mathbb{I}_d$
$d = 2, 5, 10, \quad N = 1000$



∇-LSTD-RKHS-OM

Application to nonlinear filtering

Numerical example - Gain approximation for a fixed t

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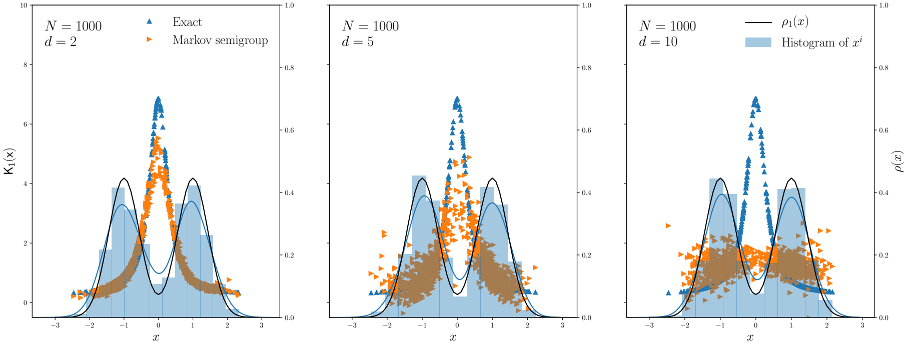

Markov kernel approximation

Application to nonlinear filtering

Numerical example - Gain for a nonlinear oscillator model

Example: $\rho(x)$ is a mixture of von Mises densities on a circle

$$\mathrm{d}\vartheta = \omega \mathrm{d}t + \sigma_B \mathrm{d}B_t \mod 2\pi,$$

$$\mathrm{d}Z_t = c(\vartheta)\mathrm{d}t + \sigma_W \mathrm{d}W_t, \quad c(\vartheta) = \tfrac{1}{2}[1 + \cos(\vartheta)]$$

kill?

Application to nonlinear filtering

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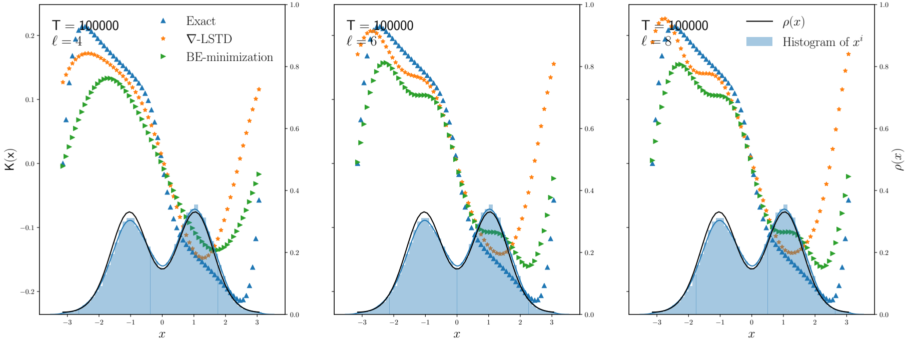
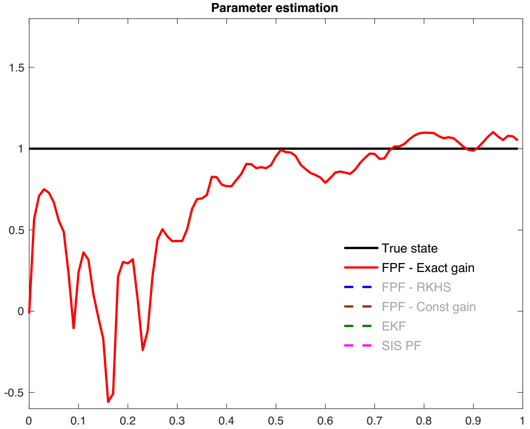


∇-LSTD-L with $\psi_i = \sin(ix), \psi_{i+1} = \cos(ix)$ with $1 \le i \le \ell/2$, $\ell = 4, 6, 8.$

Applications to Nonlinear filtering

Numerical example - Parameter estimation

Example: Parameter estimation with bimodal prior
Observations: parameter plus additive noise with $\sigma_W = 1$.



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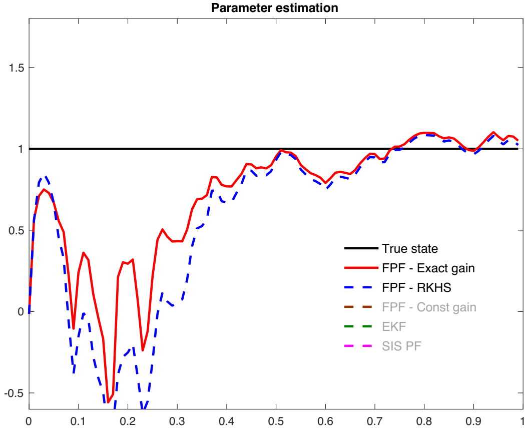

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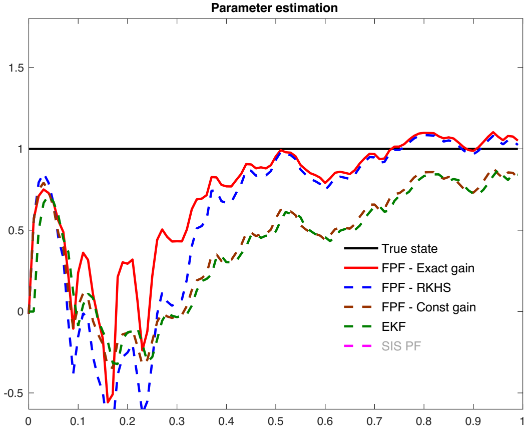

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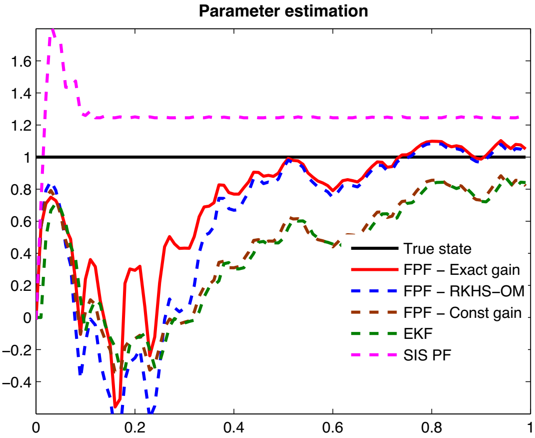

Applications to Nonlinear filtering

Numerical example - Parameter estimation

?

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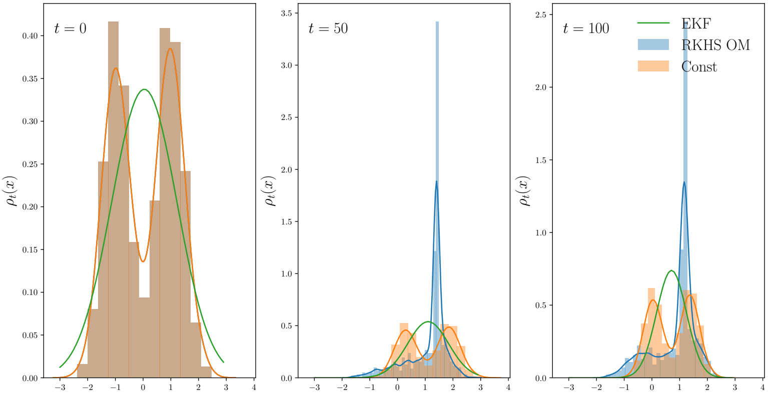
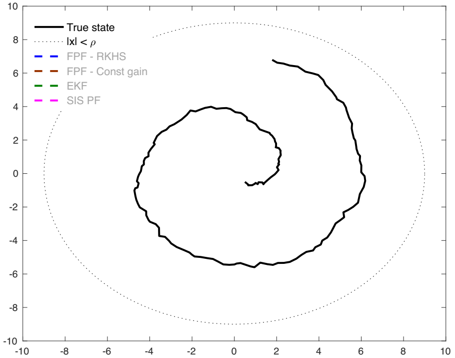


Applications to Nonlinear filtering

Numerical example - Nonlinear $2d$ ship dynamics model

Example: Nonlinear ship dynamics model in $2d$.
Observations: $c(x) = \arctan(x_1/x_2)$ with std. deviation $\approx 18°$.

10 secs



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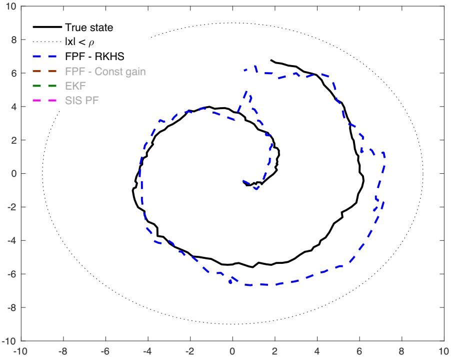

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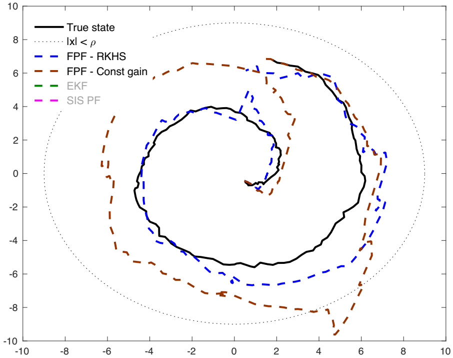

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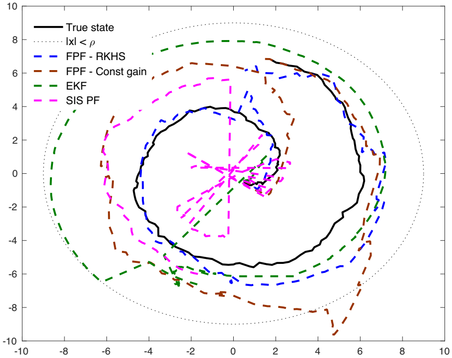

Applications to Nonlinear filtering

Numerical example - Nonlinear $2d$ ship dynamics model

Summary table of RMSEs from 100 trials

Type of filter	$\Sigma_1 = I_{2\times 2}$	$\Sigma_2 = 5I_{2\times 2}$	Lost track (Σ_2)
FPF RKHS-OM	0.9023	1.6254	4 times
FPF RKHS mem.	0.9162	1.9408	7 times
FPF const. gain	1.3060	2.3231	14 times
SIR PF	3.1481	4.2648	57 times
EKF	6.5203	18.441	93 times

Applications to MCMC

Introduction to MCMC

In many applications, we need to compute

$$\eta = \int c(x)\rho(x)\,\mathrm{d}x$$

- $c\colon \mathbb{R}^\ell \to \mathbb{R}$ is a measurable function.
- ρ is a target probability density in $\mathbb{R}^\ell$.

Markov-Chain Monte Carlo (MCMC) methods provide numerical algorithms to obtain estimates:

$$\eta_t = \frac{1}{t}\int_0^t c(\Phi(s))\,ds$$

$\boldsymbol{\Phi}$ is a Markov process with steady state distribution ρ.

Applications to MCMC

Asymptotic Variance

Estimates η_t obey a Central Limit Theorem,

$$\sqrt{t}(\eta_t - \eta) \xrightarrow{d} N(0, \gamma^2)$$

γ^2 a. variance

Rate of convergence captured by asymptotic variance

$$\gamma^2 = \lim_{t\to\infty} \mathsf{E}\left[\left(\frac{1}{\sqrt{t}}\int_0^t (c(\Phi(s)) - \eta)\, ds\right)^2\right]$$

Alternate representation in terms of covariance

$$\gamma^2 := \int_{-\infty}^{\infty} R(s)ds, \qquad R(s) = \mathsf{E}[\tilde{c}(\Phi_0)\tilde{c}(\Phi_s)]$$

Applications to MCMC

Asymptotic Variance

Slide I

+ M

Representation in terms of h [Glynn 96]:

$$\gamma^2 = 2\langle h, \tilde{c}\rangle$$

$Dh = -\tilde{c}$

Applications to MCMC

Asymptotic Variance

Slide I

Representation in terms of h [Glynn 96]:

$$\gamma^2 = 2\langle h, \tilde{c}\rangle$$
$$= 2\|\nabla h\|_{L^2}$$

(For Langevin diffusion)

Applications to MCMC

Control Variates

Goal: To minimize asymptotic variance.

Applications to MCMC

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Goal: To minimize asymptotic variance.

Idea: Modify the estimator using control variates [Henderson 01, CTCN]

$$c_g = c + \underbrace{\mathcal{D}g}_{\text{Control variate}}, \quad \textit{where} \quad g \in \mathcal{H}$$

$$\eta_t^g = \frac{1}{t}\int_0^t c_g(\Phi_s)\, ds$$

For asymptotically unbiased estimates, control variate needs to have zero-mean with respect to ρ.

Too many word

Applications to MCMC

Control Variates

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For asymptotically unbiased estimates, control variate needs to have zero-mean with respect to ρ.

For any $g \in C^2$, ~~P_g is invariant with $\rho \iff$~~ $\langle \mathcal{D}g,\, 1\rangle_{L^2} = 0$.

L_2

Applications to MCMC

Optimal control variates

Let $\tilde{h}_g = h - g$,

$$\begin{aligned} \mathcal{D}\tilde{h}_g &= \mathcal{D}h - \mathcal{D}g \\ &= -c_g + \eta \end{aligned}$$

Thus $\tilde{h}_g$ is the solution to Poisson's equation with forcing function c_g.

Applications to MCMC

Optimal control variates

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Asymptotic variance of the new estimator:

$$\gamma_g^2 = 2\langle \tilde{h}_g, \tilde{c}_g \rangle_{L^2}$$

Applications to MCMC

Optimal control variates

Slide III

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Asymptotic variance of the new estimator:

h-g

$$\begin{aligned}\gamma_g^2 &= 2\langle \tilde{h}_g, \tilde{c}_g \rangle_{L^2} \\ &= 2\|\nabla h - \nabla g\|_{L^2}^2 \text{ (For Langevin diffusion)}\end{aligned}$$

no line break

Applications to MCMC

Optimal control variates

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(For Langevin diffusion)

Can be minimized using ∇-LSTD algorithms.

Applications to MCMC

Numerical Examples - Sample variance v Asymptotic variance

Sample variance v Asymptotic variance

$$\sigma^2 = \langle \tilde{c}, \tilde{c} \rangle_{L^2} = R(0)$$ - Sample variance

Applications to MCMC

Numerical Examples - Sample variance v Asymptotic variance

$R(t) = \langle \tilde{c}, P^t \tilde{c} \rangle$

Sample variance v Asymptotic variance

$$\sigma^2 = \langle \tilde{c}, \tilde{c} \rangle_{L^2} = R(0) \qquad \text{- ~~Sample~~ Variance}$$

$$\gamma^2 = 2\langle h, \tilde{c} \rangle_{L^2} = \int_{-\infty}^{\infty} R(s)ds \qquad \text{- Asymptotic variance}$$

Applications to MCMC

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Minimizing σ^2 is easier than minimizing γ^2 [Oates 14, Papamarkou 14]

~~Appropriate only if samples are i.i.d.~~

Minimizing σ^2 also minimizes γ^2 ?

Applications to MCMC

Numerical Examples - Sample variance v Asymptotic variance

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Appropriate only if samples are i.i.d.

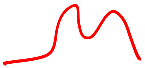
Minimizing σ^2 also minimizes γ^2 ? NO !

Applications to MCMC

Numerical Examples - Sample variance vs Asymptotic variance

Example: Unadjusted Langevin algorithm (ULA)

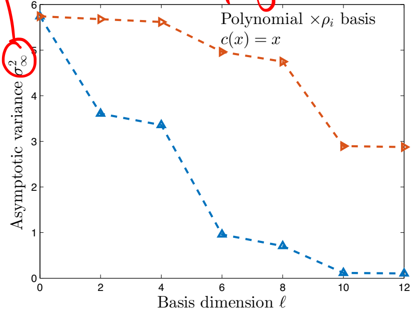
$c(x) \equiv x$

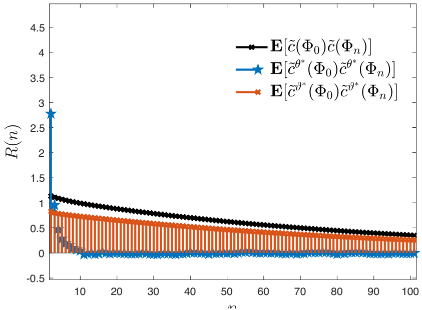


show bimodal density

ℓ

legend ok?





Applications to MCMC

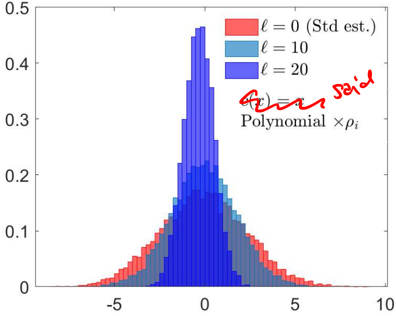
Numerical Examples - ULA

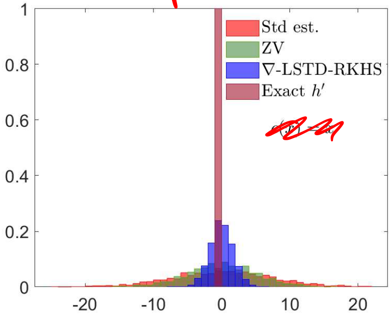
Plot would be better.

Example: Unadjusted Langevin algorithm (ULA)

$c(x) \equiv x$, $\rho \sim 0.5\mathcal{N}(-1, 0.4472) + 0.5\mathcal{N}(1, 0.4472)$

Same density as prev. page?



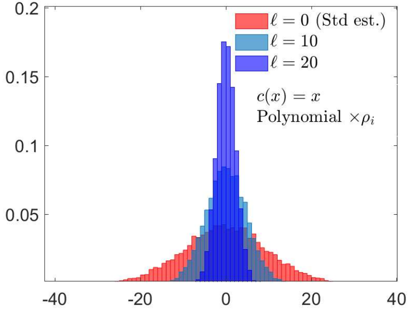


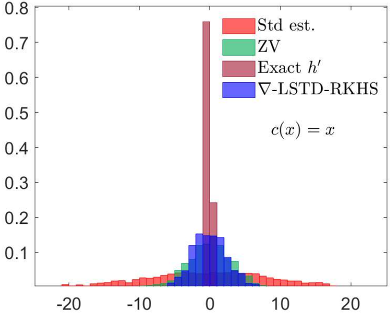
Applications to MCMC

Numerical Examples - RWM

kill ?

Example: Random walk Metropolis (RWM)
$c(x) \equiv x$, $\rho \sim 0.5\mathcal{N}(-1, 0.4472) + 0.5\mathcal{N}(1, 0.4472)$
Theoretical justification based on [Brosse et al. 19]

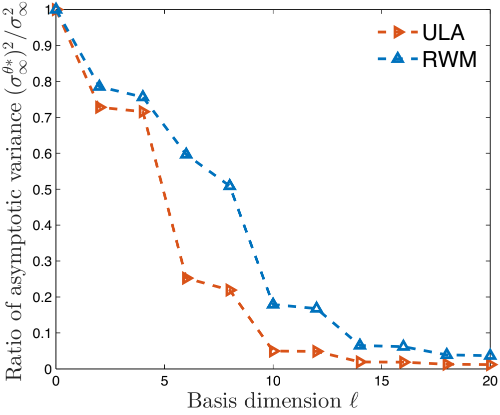




Applications to MCMC

Numerical Examples - ULA v RWM

Unadjusted Langevin algorithm (ULA) vs Random walk Metropolis (RWM)



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Applications to MCMC

Numerical Examples - Logistic regression with RWM sampling

(other stuff list)

~~Example~~: Logistic Regression for Swiss bank notes

$X \in \mathbb{R}^{200\times 4}$ - Covariates measurements of four features of 200 bank notes.

$\{Y_i \in \{0,1\}, 1 \leq i \leq 200\}$ - Binary response variables.

$\Theta \in \mathbb{R}^4$ - Regression coefficients for classification.

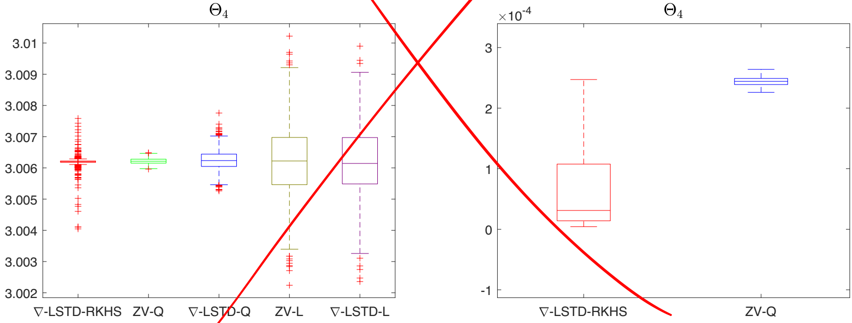
$$\rho(\Theta|\{X_i, Y_i\}_1^N) \propto$$

$$\exp\left(\underbrace{\sum_{i=1}^{N}\{Y_i\Theta^T X_i - \log(1 + e^{\Theta^T X_i})\}}_{\text{Likelihood}} - \underbrace{\frac{\Theta^T\Sigma^{-1}\Theta}{2}}_{\text{Prior}}\right)$$

Applications to MCMC

Numerical Examples - Logistic Regression with RWM sampling

Example: Logistic Regression for Swiss bank notes
RWM sampling



Box plots of estimates of Θ_4.

Conclusions

- Differential LSTD learning based approaches to approximate solution to Poisson's equation for the Langevin diffusion.
  - Finite dimensional basis.
  - RKHS.
- Two interesting applications
  - Asymptotic variance reduction in MCMC algorithms.
  - Gain function approximation in Feedback particle filter.
- Extended the approach to include reversible Markov chains.

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Thank You!

Questions?