Application of learning algorithms to nonlinear filtering and MCMC

PhD Dissertation defense

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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

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 *Poisson's equation*.
- Proposed a differential TD-learning algorithm to approximate the gradient of the solution to Poisson's equation.

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.
- 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.

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- Extend the algorithm to a multidimensional setting. - $\checkmark$
- Explore appropriate basis selection for these algorithms.

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New direction

- Simplified version of the algorithm for Langevin diffusion.
- Improvements for online gain estimation.
- Explored the application to MCMC algorithms.

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

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

$$\gamma^2_\theta = 2\langle h_\theta, \tilde{c}_\theta\rangle$$

$$= 2\|\nabla h_\theta\|^2$$

Poisson's Equation

Poisson's Equation

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

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

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

Poisson's Equation

Stochastic optimal control

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

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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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- May be regarded as a d-dimensional gradient flow with "noise".

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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

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

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

where ∇ is the gradient and Δ is the Laplacian.

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

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

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

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

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

LSTD learning

Discounted cost case

Discounted-cost value function:

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

Discounted-cost optimality equation:

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

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

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

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

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Using an adjoint operation and applying the stationarity of Φ.

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Eligibility vector - $\varphi_\psi(r) := \int_0^\infty \exp(-\gamma(t-r))\psi(\Phi_{r-t})\mathrm{d}t$

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

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$$= \mathsf{E}[\varphi_{\psi_i}(0) c(\Phi_0)]$$

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)
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By law of large numbers,

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

Drawback: Requires the existence of a regenerating state.

Poisson's equation

Idea: Approximate the gradient of h directly [RDM 16, DM 16]:

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

Differential LSTD learning (∇-LSTD)

Poisson's equation

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

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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$$= \langle \nabla\psi_i,\, R_{U''} \nabla c \rangle_{L^2}$$

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 $\mathcal{D} h = -\tilde{c}$:

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

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

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

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

Basics of RKHS

A suitable choice of basis functions is a challenging problem [RDM 16, TM 16].

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A kernel function $K(\cdot\,,\,\cdot)$ defines an RKHS if (Moore-Aronsjazn theorem)

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

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

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

Final condition is required for our loss function.

Differential LSTD learning on RKHS

Basics of RKHS

Vector space $\mathcal{H}^\circ$: all finite linear combinations

$$g_\alpha(y) = \sum_{i=1}^{m} \alpha_i K(x^i, y), \quad y \in \mathbb{R}^d,$$

scalars $\{\alpha_i\} \subset \mathbb{R}$ and $\{x^i\} \subset \mathbb{R}^d$ arbitrary.

Inner product: for $g_\alpha, g_\beta \in \mathcal{H}^\circ$,

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

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

Assume $\mathcal{H}^\circ$ admits a completion $\mathcal{H}$

Differential LSTD learning on RKHS

Empirical risk minimization (ERM)

Recall ∇-LSTD goal:

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

Approximation via empirical risk minimization (ERM):

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

$\tilde{c}$ is also approximated as:

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

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, is unique and has the form

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

where $\{\beta_i^{k*} : i = 1, \cdots, N, \ k = 0, \cdots, d\}$ are real numbers.

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, is unique and has the form

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

where $\{\beta_i^{k*} \colon i = 1, \cdots, N,\ k = 0, \cdots, d\}$ are real numbers.

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

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Notation:

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

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

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

Differential LSTD learning on RKHS

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

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

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

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

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

Applications to Nonlinear filtering

Feedback Particle Filter

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

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

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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.
- $\rho_t^* := P(X_t|\{Z_s : s \leq t\})$ is the posterior distribution.

Applications to Nonlinear filtering

Feedback Particle Filter

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

Applications to Nonlinear filtering

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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
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Applications to Nonlinear filtering

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- $\{B_t^i\}$ are mutually independent standard Wiener processes.

Approximation of ρ_t^* :

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

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

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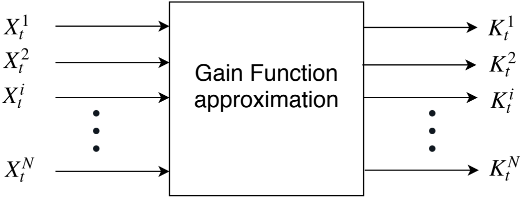
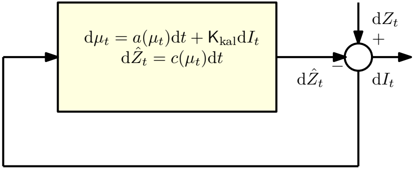


Finite-N implementation

Applications to Nonlinear filtering

Feedback Particle Filter

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



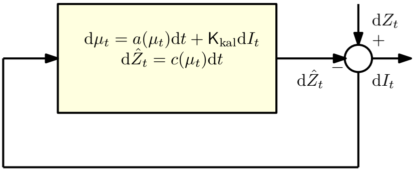
Kalman filter

Applications to Nonlinear filtering

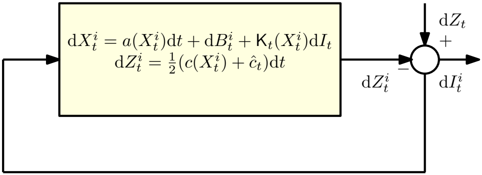
Feedback Particle Filter

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

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



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

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Approximations to K can be obtained by

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

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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:

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

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

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

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Empirical approximation:

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

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:

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

Solution obtained by finding a saddle point for the Lagrangian

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

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

Applications to Nonlinear filtering

∇-LSTD-RKHS-OM

Using the finite-dimensional function class, $\mathcal{H}_N := \text{span}\{K_{x^j} : 1 \leq j \leq N\}$

Applications to Nonlinear filtering
∇-LSTD-RKHS-OM

Using the finite-dimensional function class, $\mathcal{H}_N := \text{span}\{K_{x^j} : 1 \leq j \leq N\}$

β and μ can be obtained by solving $N + d$ linear equations:

$$0 = 2\Big(\frac{1}{N}\sum_{k=1}^{d} M_{x_k}^{\mathsf{T}} M_{x_k} + \lambda M_{00}\Big)\beta^* + \frac{\kappa\mu^*}{N} + \frac{2}{N}\Big(\kappa\widehat{\mathsf{K}}^* - M_{00}\tilde{\varsigma}\Big)$$

$$0 = \kappa^{\mathsf{T}}\beta^*$$

Gain is then computed as $\mathsf{K} = \widehat{\mathsf{K}}^* + \nabla\tilde{g}^*$.

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:

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

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

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

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

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

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Both refinements 1 and 2 can be applied independently or simultaneously.

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$$0 = \kappa^{T}\beta^*$$

Gain is then computed as $\mathsf{K} = \widehat{\mathsf{K}}^* + \nabla\tilde{g}^*$.

Applications to Nonlinear filtering

Markov kernel approximation [Taghvaei 16]

Approximates the transition kernel of the Langevin diffusion:

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

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.

Numerical example

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

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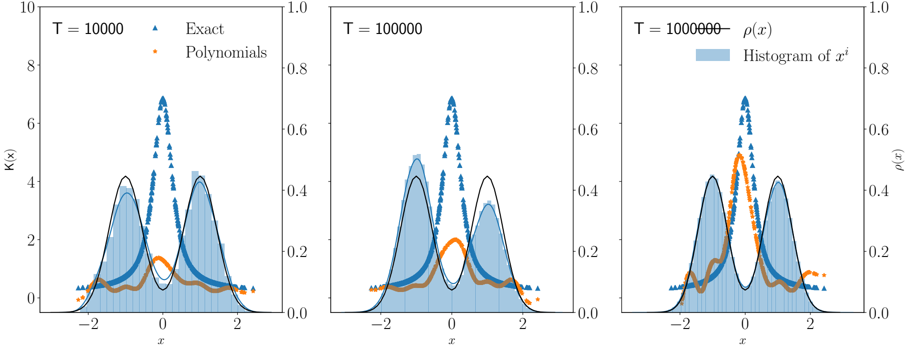

∇-LSTD with $\psi_i = x^i$ with $1 \leq i \leq 10$.

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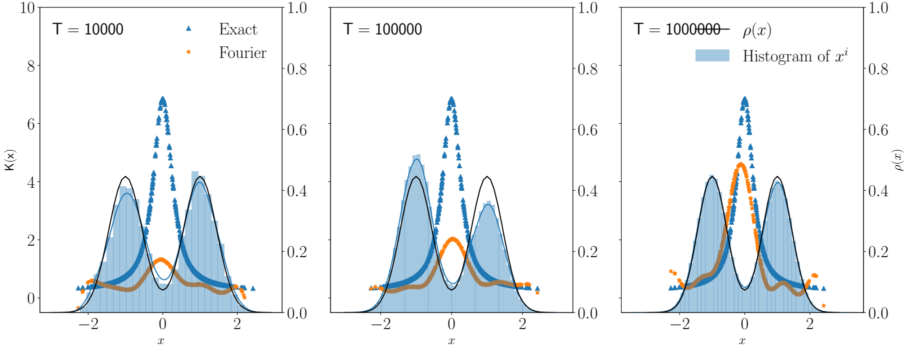

∇-LSTD with $\psi_i = \sin ix$, $\psi_{i+1} = \cos ix$ with $1 \leq i \leq 5$.

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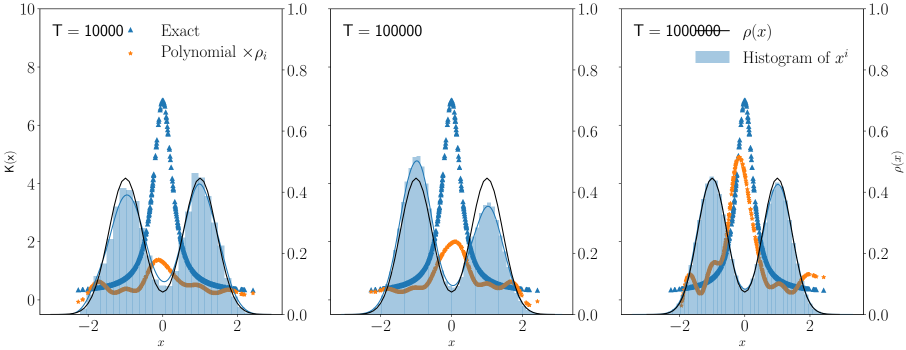
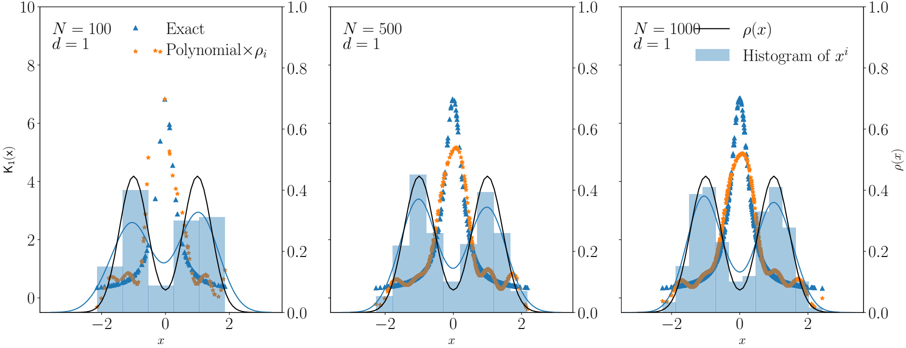


∇-LSTD with $\psi_i = x^i \rho_1(x)$, $\psi_{i+1} = x^i \rho_2(x)$ with $1 \leq i \leq 5$.

Numerical example

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 $1 \leq i \leq 5$.

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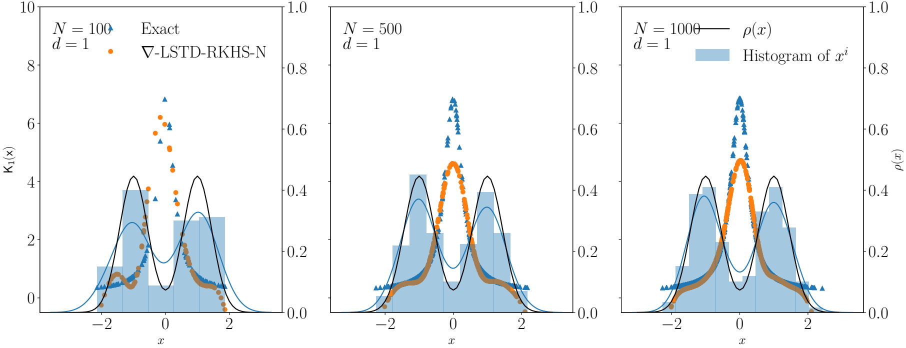

∇-LSTD-RKHS-N with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$

Numerical example

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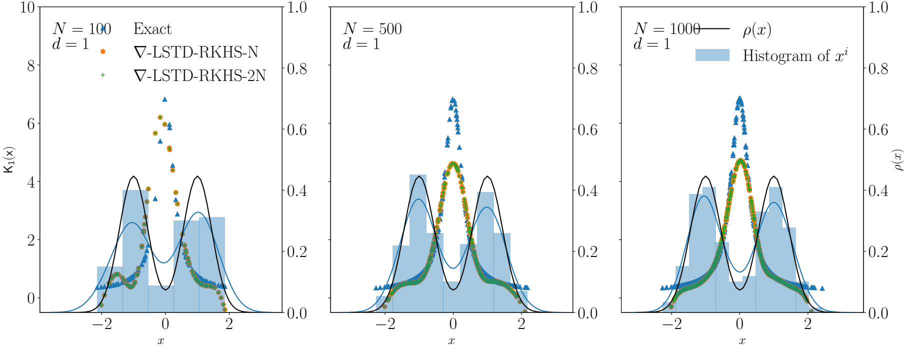

∇-LSTD-RKHS-2N with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$

Numerical example

Example: For a fixed t, ρ_t a Gaussian mixture
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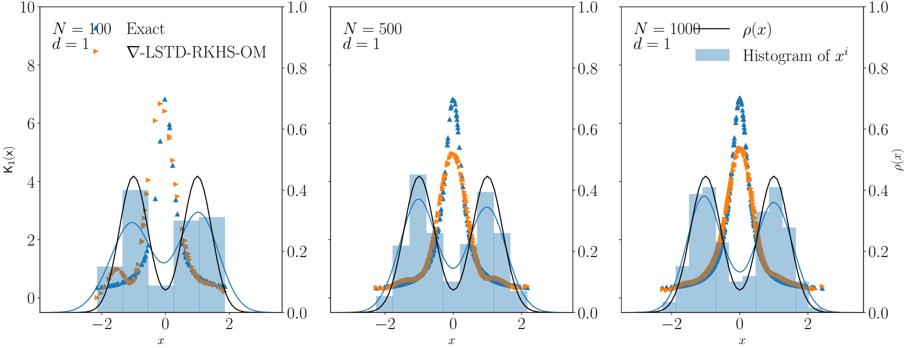

∇-LSTD-RKHS-OM with Gaussian kernel, $\varepsilon = 0.1$ and $\lambda = 10^{-2}$

Numerical example

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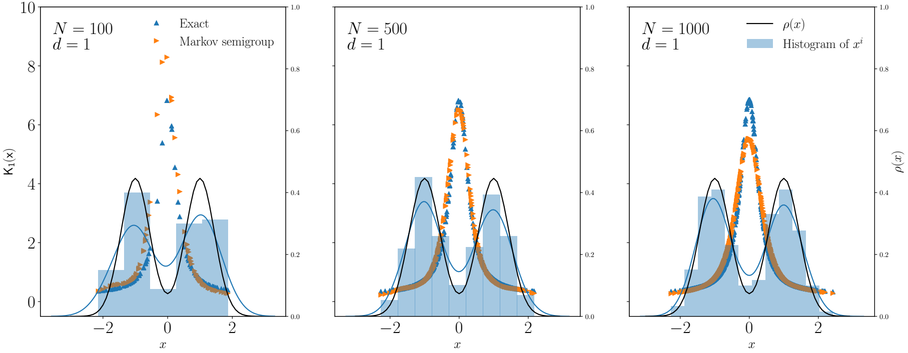
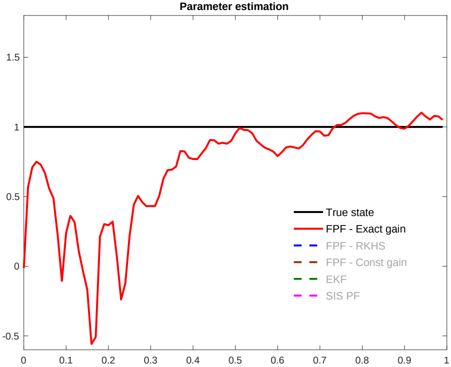


Markov kernel approximation with $\epsilon = 0.1$

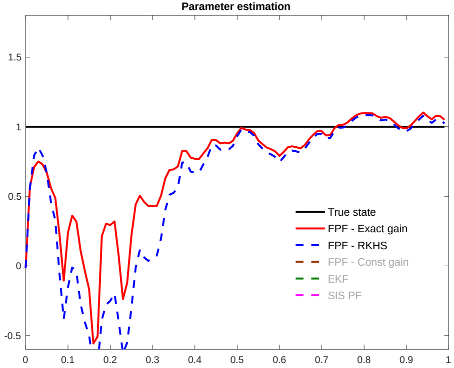
Applications to Nonlinear filtering

Example: Parameter Estimation with bimodal prior
Observations: parameter plus additive noise with $\sigma_W = 0.3$.



Applications to Nonlinear filtering

Example: Parameter Estimation with bimodal prior
Observations: parameter plus additive noise with $\sigma_W = 0.3$.



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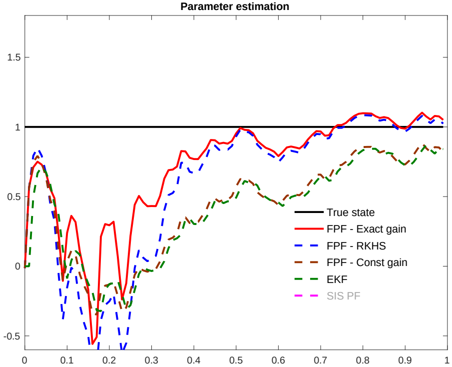

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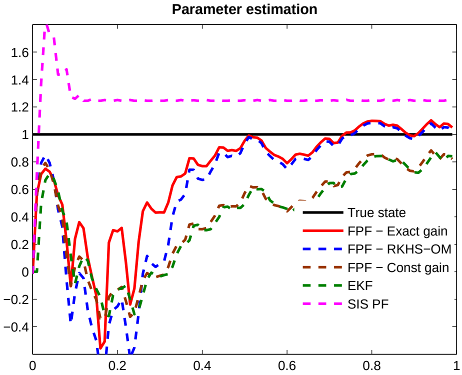

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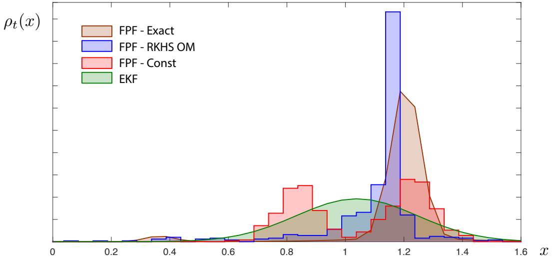
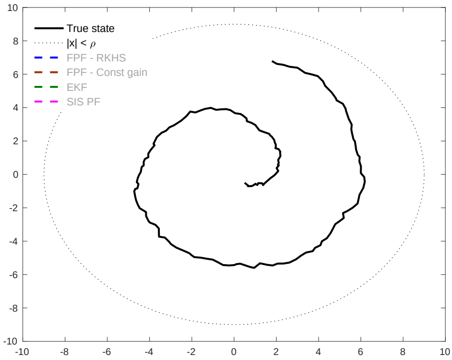


Posterior estimates at $t = 1$.

Applications to Nonlinear filtering

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



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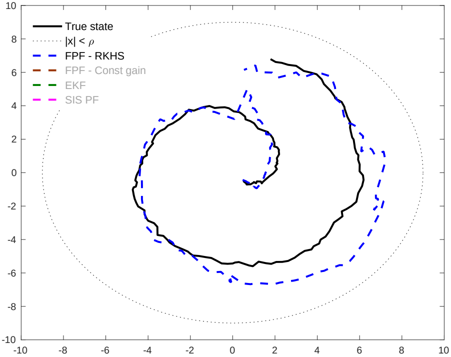

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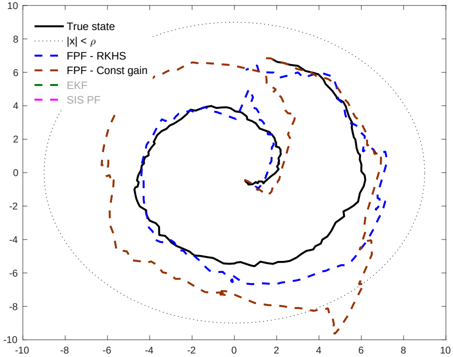

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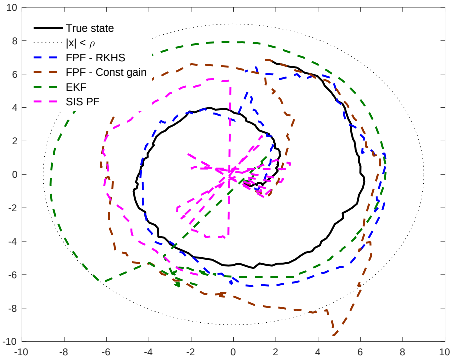

Applications to MCMC

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:

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

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

Applications to MCMC

Asymptotic Variance

Estimates η_t obey a Central Limit Theorem,

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

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

Representation in terms of h:

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

Applications to MCMC

Asymptotic Variance

Representation in terms of h:

$$\begin{aligned}\gamma^2 &= 2\langle h,\, \tilde{c}\rangle \\ &= 2\|\nabla h\|_{L^2} \\ &\text{(For Langevin diffusion)}\end{aligned}$$

Applications to MCMC

Control Variates

Goal: To minimize asymptotic variance.

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Idea: Modify the estimator

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

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

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.

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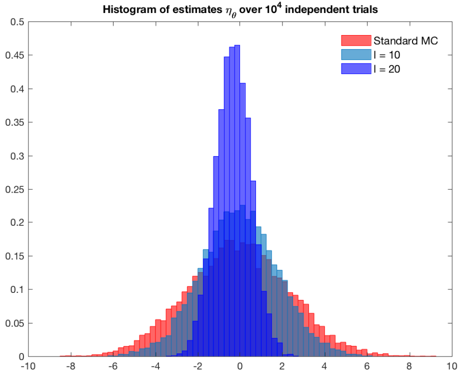
Can be minimized using differential TD-learning.

Applications to MCMC

Numerical Examples

Example: Unadjusted Langevin algorithm (ULA)

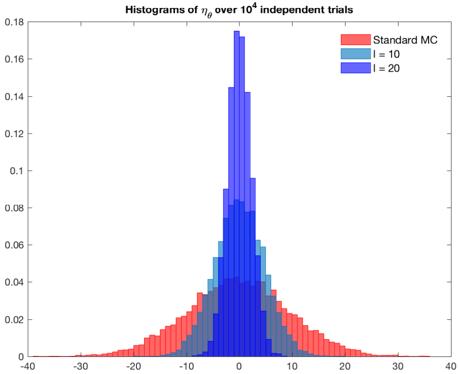


Histograms over 10000 independent trials of $\sqrt{T}(\eta^i - \eta)$ for $\ell = 0, 10, 20$

Applications to MCMC

Numerical Examples

Example: Random walk Metropolis (RWM)



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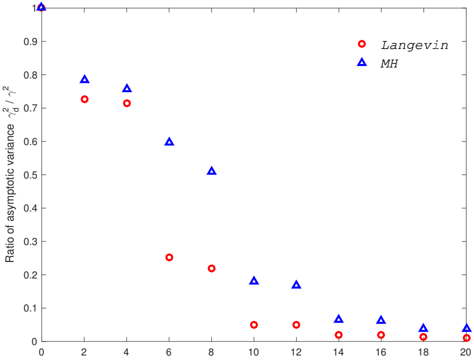
Applications to MCMC

Numerical Examples

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



Applications to MCMC

Numerical Examples

Variance vs Asymptotic variance

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

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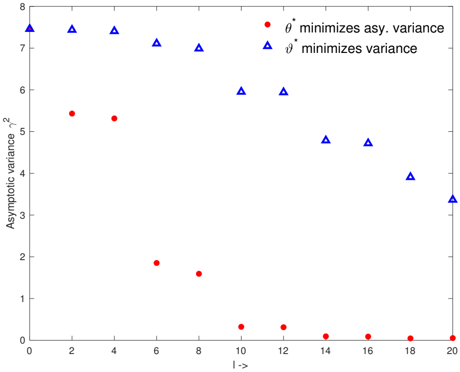

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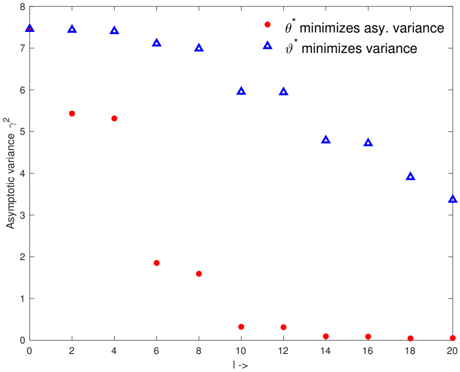

Applications to MCMC

Numerical Examples

Example: Logistic Regression for Swiss bank notes

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

$\{Y_i \in \{0,1\}, 1 \leq i \leq 200\}$ - Labels denoting genuine or counterfeit.

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

$$\rho(\Theta|\{X_i, Y_i\}_1^N) \propto \exp\left(\sum_{i=1}^{N}\{Y_i\Theta^T X_i - \log(1+e^{\Theta^T X_i})\} - \frac{\Theta^T\Sigma^{-1}\Theta}{2}\right)$$

Applications to MCMC

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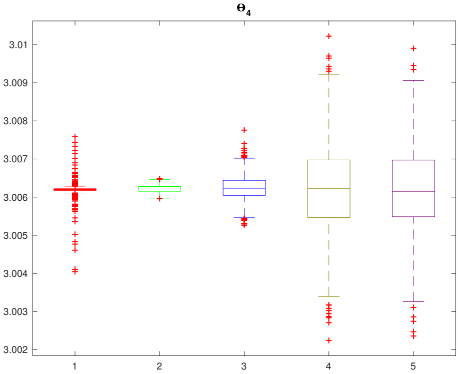

Box plots of estimates of Θ_4.

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?