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. Poisson's Equation
2. Differential TD learning
3. Applications to Nonlinear filtering
4. Applications to MCMC

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

$$\phi_{n+1}(x) = \operatorname*{argmin}_u \{c(x,u) + \mathcal{D}_u h_n(x)\}$$

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
h	- solution to Poisson's equation.

Poisson's Equation

Stochastic optimal control

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.

$h^*(x)$ - Infinite horizon expected average cost or relative value function.

Poisson's Equation

Langevin Diffusion

Langevin diffusion is given by the SDE,

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

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

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

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$\boldsymbol{W} \quad = \{W_t : t \geq 0\}$ 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 $\mathcal{D}$,

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

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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

$$\mathcal{D}h := -\tilde{c}, \qquad \tilde{c} = c - \eta.$$

$$h := \int_0^\infty \mathsf{E}[\tilde{c}(\Phi_s)]ds$$

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 16].
- A smooth solution $h \in C^2$ exists under stronger conditions in [Pardoux 01], subject to growth conditions on c similar to [Glynn 96].

Approximating 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* [T99, CTCN].

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

Differential TD learning

Idea : Approximate the gradient of h directly [RDM16, DM 16]:

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

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- A reproducing kernel Hilbert space (RKHS).

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- A reproducing kernel Hilbert space (RKHS).
  Choice of basis is not an easy task

  $\Longrightarrow$ RKHS framework is far easier to implement.

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

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Old approach: For a linear parameterization

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

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

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

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

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

Using an adjoint operation and applying the stationarity of Φ.

Differential TD learning

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

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Differential TD learning using RKHS

Basics of RKHS

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

A kernel function $K(\cdot\,,\,\cdot)$ defines an RKHS if

- *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.

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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 TD learning using 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 TD learning using RKHS

Empirical risk minimization (ERM)

Recall 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):

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

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

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

Regularization parameter $\lambda > 0$ introduced to avoid overfitting.

Differential TD learning using 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.

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

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

Differential TD learning using RKHS

Solution in one dimension

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

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

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

$$M = \frac{1}{N}\left[\begin{array}{c} M_y \\ \hline M_{xy}\end{array}\right][M_x\,|M_{xy}] + \lambda\left[\begin{array}{c|c} M_0 & M_y \\ \hline M_x & M_{xy}\end{array}\right]$$

$$b = \frac{1}{N}\left[\begin{array}{c} M_0 \\ \hline M_x\end{array}\right]\varsigma\,, \qquad \varsigma^{\mathsf{T}} = [\tilde{c}_N(x^1),\dots,\tilde{c}_N(x^N)]$$

$$\beta^{\mathsf{T}} = [\beta_1^0,\dots,\beta_N^0\,,\,\beta_1^1,\dots,\beta_N^1]$$

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

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

- $X_t \in \mathbb{R}^d$ 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.

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- $a(.)$,$c(.)$ 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.

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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.

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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]):

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

I_t^i : Innovations process

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

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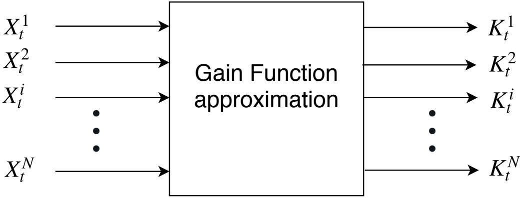
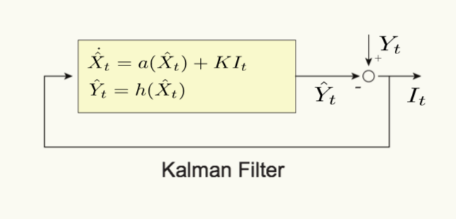


Finite-N implementation

Applications to Nonlinear filtering

Feedback Particle Filter

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



Applications to Nonlinear filtering

Feedback Particle Filter

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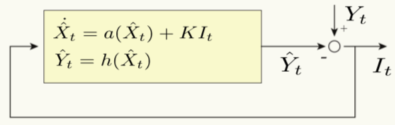
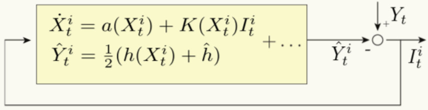
FPF: $$\mathrm{d}X^i_t = a(X^i_t)\mathrm{d}t + \mathrm{d}B^i_t + \underbrace{\mathsf{K}_t(X^i_t) \circ (\mathrm{d}Z_t - \tfrac{1}{2}[c(X^i_t) + \hat{c}_t]\mathrm{d}t)}_{\text{update}}$$



Kalman Filter



Feedback Particle Filter

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

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

Can be solved using differential TD learning

- Finite dimensional function space
- RKHS

Application to Nonlinear filtering

Example: For a fixed t, ρ_t a Gaussian mixture
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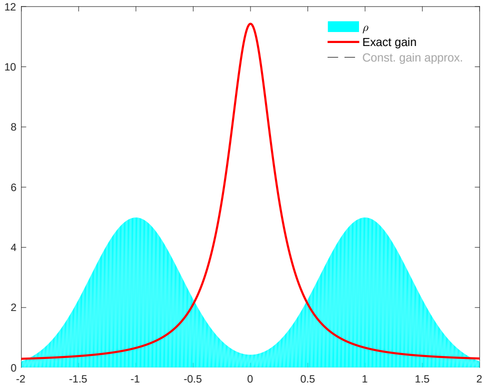

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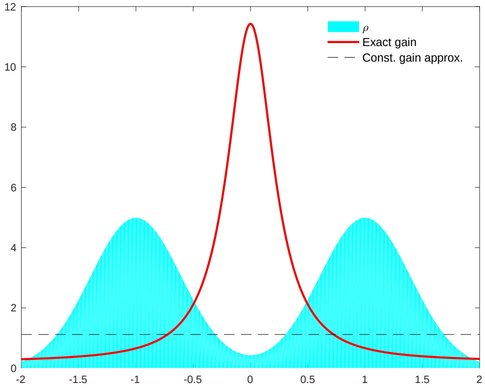

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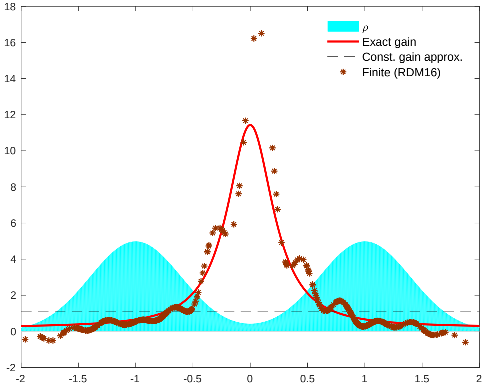

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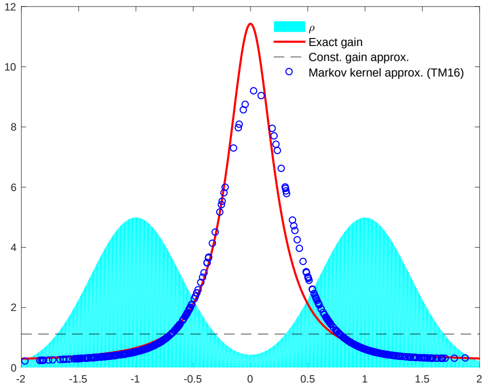

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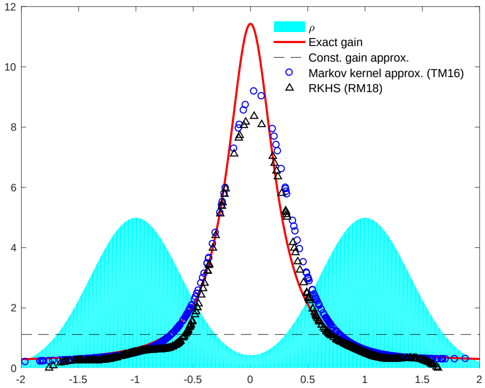
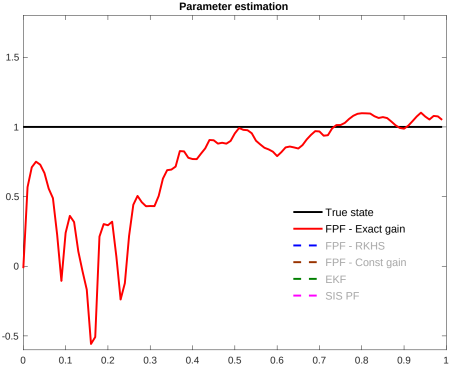


Applications to Nonlinear filtering

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



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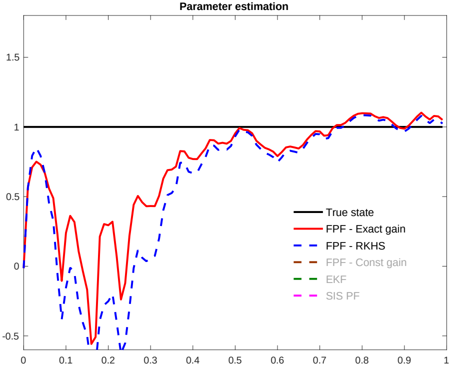

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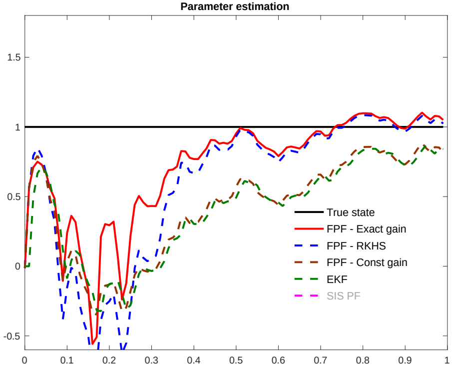

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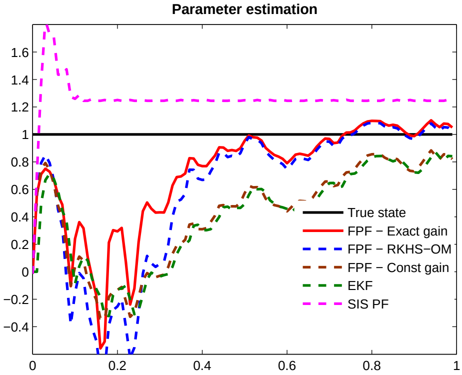

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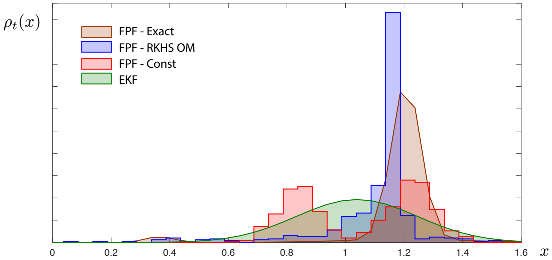
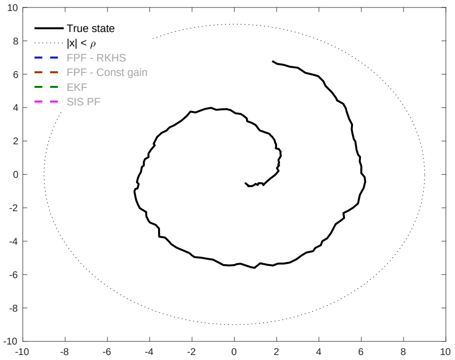


Posterior estimates at $t = 1$.

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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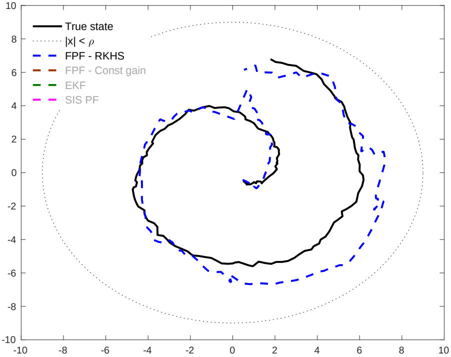

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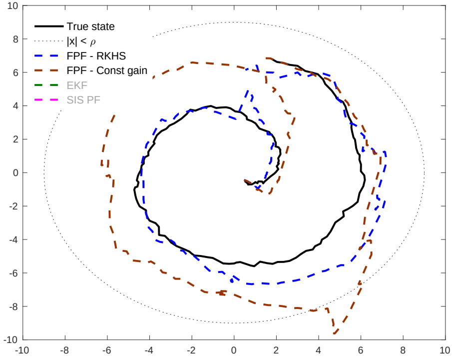

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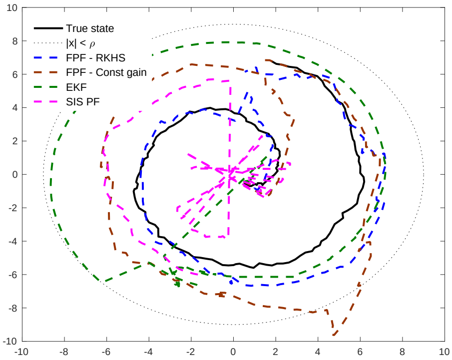

Applications to MCMC

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:

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

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

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

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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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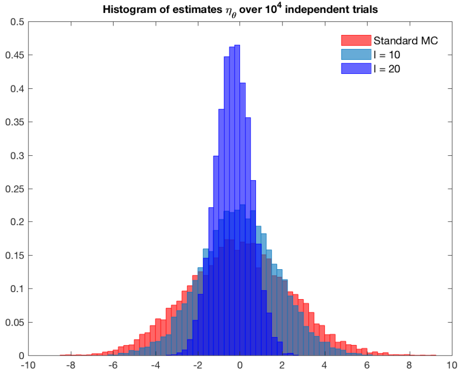
Can be minimized using differential TD-learning.

Applications to MCMC

Numerical Examples

Example: Unadjusted Langevin algorithm (ULA)

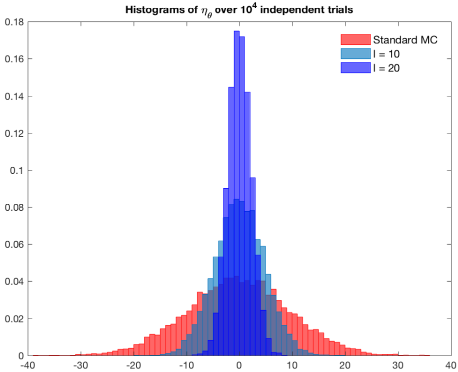


Histograms over 10000 independent trials of $\sqrt{T}(\eta^i - \eta)$ for $\ell = 0, 10, 20$

Applications to MCMC

Numerical Examples

Example: Random walk Metropolis (RWM)



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Applications to MCMC

Numerical Examples

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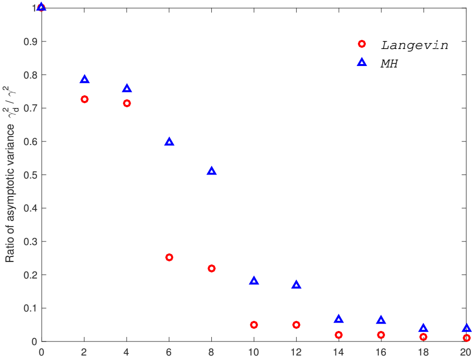

Applications to MCMC

Numerical Examples

Variance vs Asymptotic variance

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

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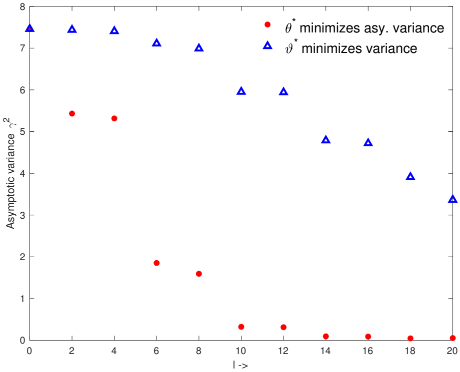

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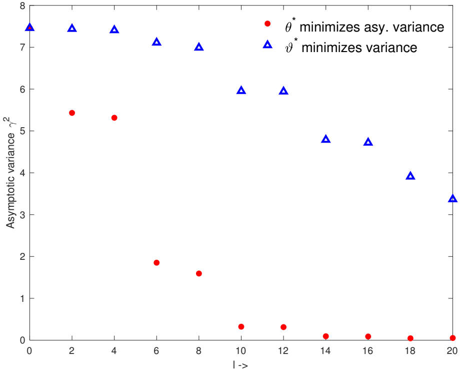

Applications to MCMC

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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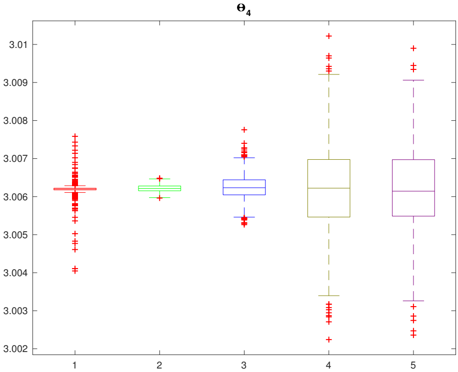

Box plots of estimates of Θ_4.

Conclusions

- Differential TD 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?