Newton, Polyak and Nesterov

Quickest Stochastic Approximation and Reinforcement Learning

Reinforcement Learning and Data-Driven Control
INFORMS 2019

Adithya M. Devraj

Department of Electrical and Computer Engineering  University of Florida

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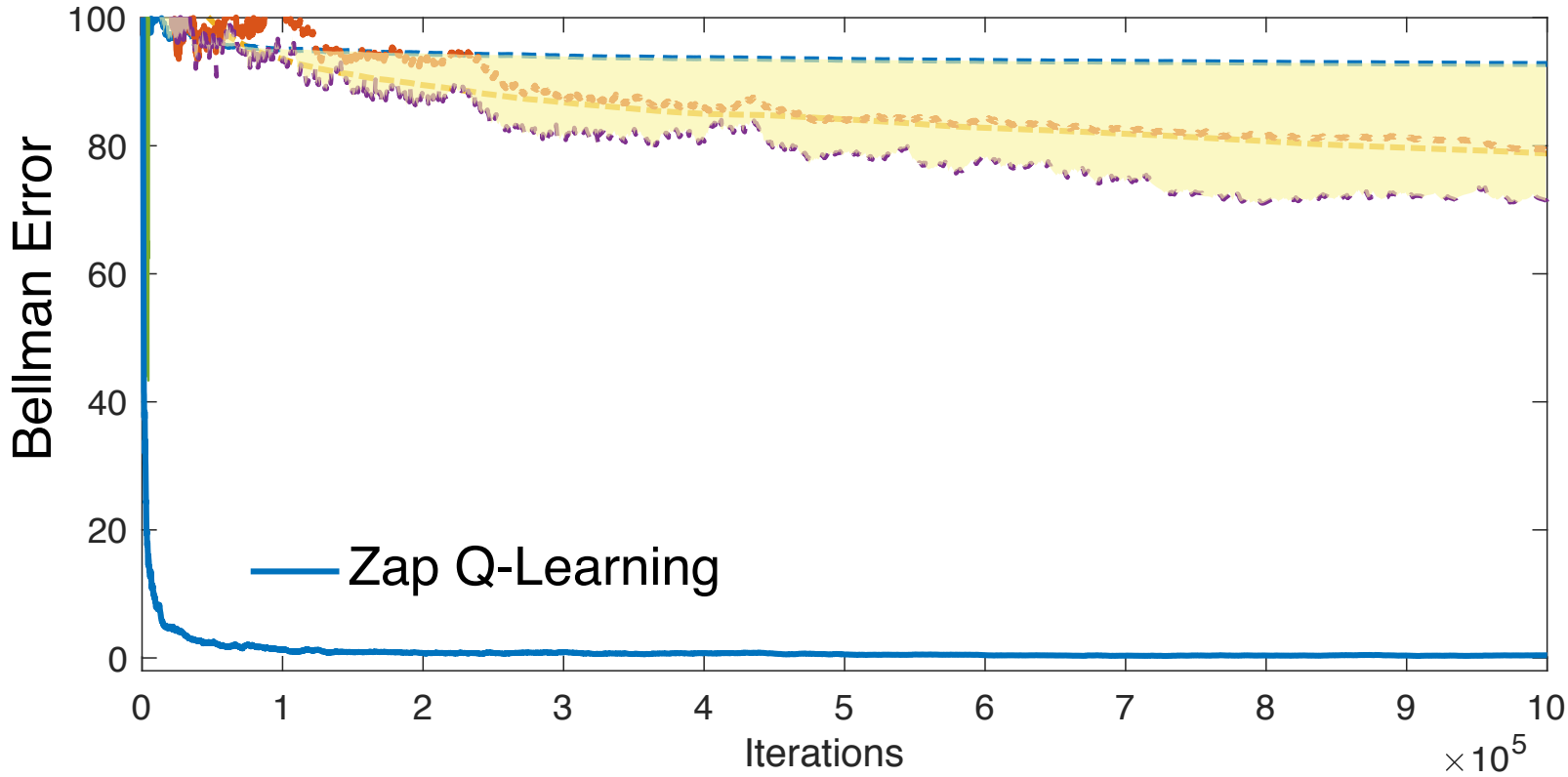
Newton, Polyak, and Nesterov

Outline



Reinforcement Learning and Stochastic Approximation

Stochastic Optimal Control

MDP Model

$\boldsymbol{X}$ is a stationary controlled Markov chain, with input $\boldsymbol{U}$

- For all states x and sets A,

$$\mathsf{P}\{X_{n+1} \in A \mid X_n = x,\ U_n = u, \text{and prior history}\} = P_u(x, A)$$

- $c\colon \mathsf{X} \times \mathsf{U} \to \mathbb{R}$ is a cost function
- $\beta < 1$ a discount factor

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Q-function:

$$Q^*(x,u) = \min_{\boldsymbol{U}} \sum_{n=0}^{\infty} \beta^n \mathsf{E}[c(X_n, U_n) \mid X(0) = x, U(0) = u]$$

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Bellman equation:

$$Q^*(x,u) = c(x,u) + \beta \mathsf{E}\big[\min_{u'} Q^*(X_{n+1}, u') \mid X_n = x,\ U_n = u\big]$$

Q-learning and Galerkin Relaxation

Dynamic programming

Find function Q^* that solves

$$\mathsf{E}\big[c(X_n, U_n) + \beta \underline{Q}^*(X_{n+1}) - Q^*(X_n, U_n) \mid \mathcal{F}_n\big] = 0$$

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Q-learning

Given $\{Q^\theta : \theta \in \mathbb{R}^d\}$, find θ^* that solves

$$\mathsf{E}\big[\big(c(X_n, U_n) + \beta \underline{Q}^{\theta^*}((X_{n+1}) - Q^{\theta^*}((X_n, U_n)\big)\zeta_n\big] = 0$$

The family $\{Q^\theta\}$ and "*eligibility vectors*" $\{\zeta_n\}$ are part of algorithm design.

Q-learning and Stochastic Approximation

Q-learning with linear parameterization:

$Q^\theta(x,u) = \theta^\intercal \psi(x,u) \qquad \theta \in \mathbb{R}^d, \quad \psi : \mathsf{X} \times \mathsf{U} \to \mathbb{R}^d$

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Example: $\zeta_n = \nabla_\theta Q^\theta(X_n,U_n) = \psi(X_n,U_n)$

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Root finding problem: $\bar{f}(\theta^*) = \boldsymbol{A}(\theta^*)\theta^* - \boldsymbol{b} = 0$

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$$\boldsymbol{A}(\theta) = \mathsf{E}\big[\zeta_n\big[\beta\psi(X_{n+1},\phi^\theta(X_{n+1})) - \psi(X_n,U_n)\big]^\intercal\big]$$
$$\boldsymbol{b} := \mathsf{E}\big[\zeta_n c(X_n,U_n)\big]$$
$$\phi^\theta(x) := \arg\min_u Q^\theta(x,u)$$

$$\mathsf{E}[f(\theta, W)]\Big|_{\theta=\theta^*} = 0$$

Stochastic Approximation

What is Stochastic Approximation?

A simple goal: Find the solution θ^* to

$$\bar{f}(\theta^*) := \mathsf{E}[f(\theta, W)]\Big|_{\theta=\theta^*} = 0\,, \qquad \theta \in \mathbb{R}^d\,, \bar{f} : \mathbb{R}^d \to \mathbb{R}^d$$

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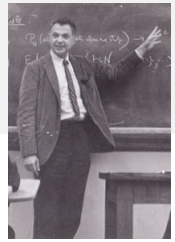
1. The distribution of the random variable W may not be known
2. Computation of the expectation may be expensive: root finding requires multiple evaluations of the expectation for different θ
3. The recursive algorithms we come up with are often slow, and their variance may be **infinite**: typical in Q-learning [Devraj & M 2017]

Algorithm & Convergence

$\bar{f}(\theta^*) = \mathsf{E}[f(\theta^*, W)] = 0$



SA Algorithm:

$$\theta_{n+1} = \theta_n + \alpha_{n+1} f(\theta_n, W_{n+1}) \qquad \text{[Robbins \& Monro 1951]}$$

The step-size satisfies:

- $\sum \alpha_n = \infty \qquad \sum \alpha_n^2 < \infty$
- Usually we take $\alpha_n = 1/n$

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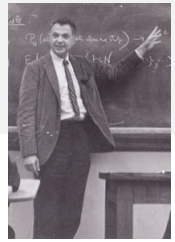

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Analysis: θ^* : *stationary point* of the ODE $\dfrac{d}{dt} x(t) = \bar{f}(x(t))$

SA is a noisy Euler approximation:

$$\theta_{n+1} = \theta_n + \alpha_{n+1}[\bar{f}(\theta_n) + \Delta_{n+1}]$$

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Stability of the ODE $\oplus$ (See Vivek's monograph) $\Longrightarrow$

$$\lim_{n\to\infty} \theta_n = \theta^*$$

Performance Criteria

Error sequence:

$$\tilde{\theta}_n := \theta_n - \theta^*$$

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Two standard approaches to evaluate performance,

1. Finite-n bound:

$$\mathsf{P}\{\|\tilde{\theta}_n\| \geq \varepsilon\} \leq ?$$

2. Asymptotic covariance (CLT):

$$\Sigma = \lim_{n\to\infty} n\mathsf{E}\left[\tilde{\theta}_n \tilde{\theta}_n^{\mathsf{T}}\right], \qquad \sqrt{n}\tilde{\theta}_n \approx N(0, \Sigma)$$

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Asymptotic Covariance

$$\Sigma = \lim_{n\to\infty} \Sigma_n = \lim_{n\to\infty} n\mathsf{E}\left[\tilde{\theta}_n \tilde{\theta}_n^T\right]$$

Recall the SA recursion:

$$\theta_{n+1} = \theta_n + \alpha_{n+1}[\bar{f}(\theta_n) + \Delta_{n+1}]$$

Asymptotic Covariance

$$\Sigma = \lim_{n\to\infty} \Sigma_n = \lim_{n\to\infty} n\mathsf{E}\big[\tilde{\theta}_n \tilde{\theta}_n^{\intercal}\big]$$

SA recursion for $\{\Sigma_n\}$:

$$\Sigma_{n+1} \approx \Sigma_n + \tfrac{1}{n}\Big\{(A + \tfrac{1}{2}I)\Sigma_n + \Sigma_n(A + \tfrac{1}{2}I)^{\intercal} + \Sigma_\Delta\Big\}$$

$$A = \frac{d}{d\theta}\bar{f}\,(\theta^*)$$

$$\Sigma_\Delta = \mathsf{E}[\Delta_{n+1}\Delta_{n+1}^{\intercal}]$$

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Asymptotic Variance Theory

1. If $\operatorname{Re}\lambda(A) \geq -\frac{1}{2}$ for some eigenvalue then Σ is (typically) infinite
2. If all $\operatorname{Re}\lambda(A) < -\frac{1}{2}$, $\Sigma = \lim_{n\to\infty} \Sigma_n$ solves the Lyapunov equation:

$$\boxed{0 = (A+\tfrac{1}{2}I)\Sigma + \Sigma(A+\tfrac{1}{2}I)^{\intercal} + \Sigma_\Delta}$$

Optimal Asymptotic Covariance

Basis of Ruppert's Stochastic Newton Raphson, and Polyak-Ruppert Averaging

Introduce a $d \times d$ matrix gain sequence $\{G_n\}$:

$$\theta_{n+1} = \theta_n + \alpha_{n+1} G_{n+1} f(\theta_n, W_{n+1})$$

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Assume it converges:

$$\lim_{n \to \infty} G_n = G$$

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Asymptotic Variance Theory

- If $\operatorname{Re}\lambda(GA) \geq -\frac{1}{2}$ for some eigenvalue then Σ^G is (typically) infinite
- If $\operatorname{Re}\lambda(GA) < -\frac{1}{2}$ for all, Σ^G solves the Lyapunov equation:

$$\boxed{0 = (GA + \tfrac{1}{2}I)\Sigma^G + \Sigma^G(GA + \tfrac{1}{2}I)^\intercal + G\Sigma_\Delta G^\intercal}$$

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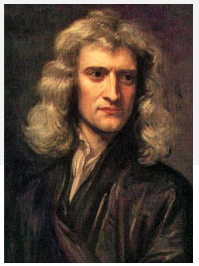
Optimal Matrix Gain: $G^* := -A^{-1}$

- Resembles Newton-Rapshon
- It is optimal: $\Sigma^* = G^* \Sigma_\Delta G^{*\intercal} \le \Sigma^G$ *any other* G

$$0 = (GA + \tfrac{1}{2} I)\Sigma^G + \Sigma^G (GA + \tfrac{1}{2} I)^\intercal + G\Sigma_\Delta G^\intercal$$

Optimal Variance and SNR

$\bar{f}(\theta) = A\theta - b \qquad \frac{\partial}{\partial\theta}(\bar{f}(\theta)) = A$



Stochastic Newton Raphson: Matrix gain algorithm with $G_n \approx G^* = -A^{-1}$:

SNR Algorithm:

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$$G_n^{-1} = -\frac{1}{n+1}\sum_{k=1}^{n+1} A_k \qquad A_{n+1} = \frac{d}{d\theta} f(\theta_n, W_{n+1})$$

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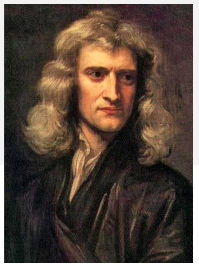

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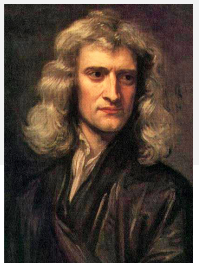

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Example: LSTD(λ), *but this was* **not** *their motivation!*

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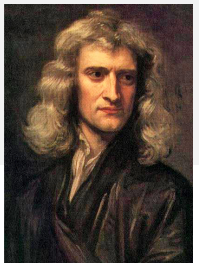

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Yes, TD(λ) can have ***infinite*** *asymptotic variance!*

Optimal Variance and Zap-SNR

$A(\theta) = \frac{\partial}{\partial\theta}\bar{f}(\theta)$ is a function of θ

Zap-SNR (designed to emulate deterministic Newton-Raphson)

$$\text{Requires} \quad \widehat{A}_{n+1} \approx A(\theta_n) := \frac{d}{d\theta}\bar{f}\,(\theta_n)$$

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Always: $\alpha_n = 1/n$. Numerics that follow: $\gamma_n = (1/n)^\rho$, $\rho \in (0.5, 1)$

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ODE for Zap-SNR

$$\frac{d}{dt}x_t = -\big[A(x_t)\big]^{-1}\bar{f}\,(x_t), \qquad A(x) = \frac{d}{dx}\bar{f}\,(x)$$

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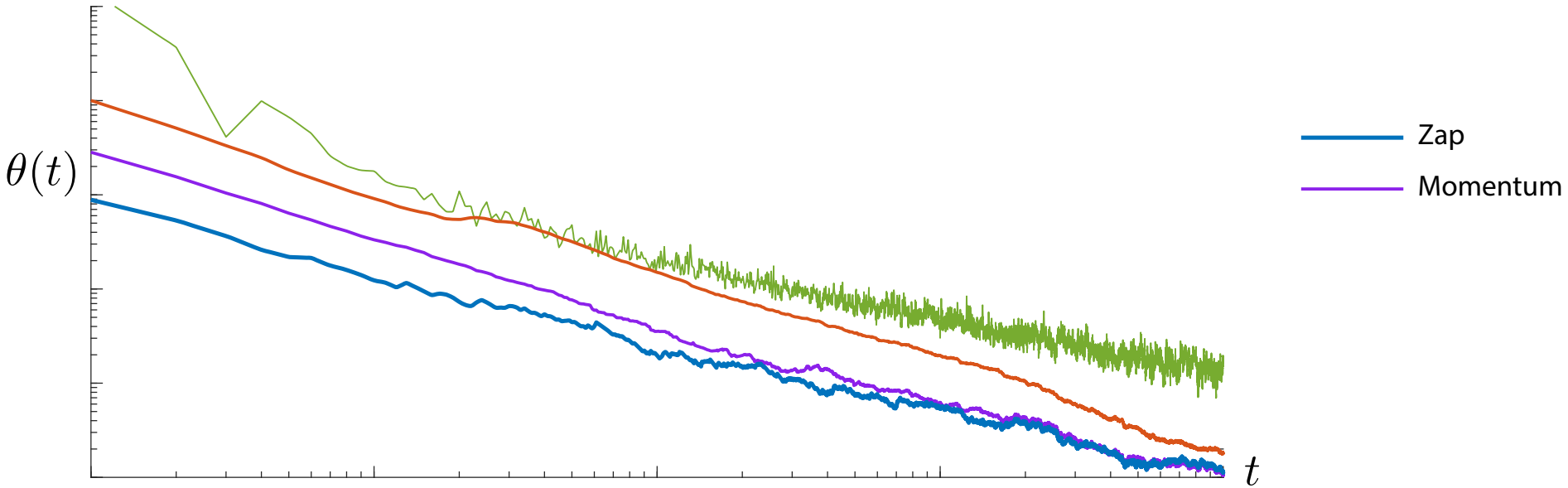
Stability? *Virtually universal*



Optimal Momentum Stochastic Approximation

Momentum based Stochastic Approximation

$\Delta\theta_n := \theta_n - \theta_{n-1}$ $\quad$ $f_{n+1}(\theta) := f(\theta, W_{n+1})$

Matrix Gain Stochastic Approximation:

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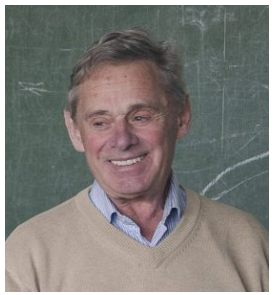

Heavy Ball Stochastic Approximation:

following Polyak, 1964 [12]

$$\Delta\theta_{n+1} = m\Delta\theta_n + \alpha_n f_{n+1}(\theta_n)$$

Momentum based Stochastic Approximation

$\Delta\theta_n := \theta_n - \theta_{n-1}$ $\quad$ $f_{n+1}(\theta) := f(\theta, W_{n+1})$

Matrix Gain Stochastic Approximation:

$$\Delta\theta_{n+1} = \alpha_n G_{n+1} f_{n+1}(\theta_n)$$

Heavy Ball Stochastic Approximation:

following Polyak, 1964 [12]

$$\Delta\theta_{n+1} = m\Delta\theta_n + \alpha_n f_{n+1}(\theta_n)$$

Matrix Heavy Ball Stochastic Approximation:

$$\Delta\theta_{n+1} = M_{n+1}\Delta\theta_n + \alpha_n G_{n+1} f_{n+1}(\theta_n)$$

Matrix Heavy Ball Stochastic Approximation

Optimizing $\{M_{n+1}\}$ and $\{G_{n+1}\}$

Matrix Heavy Ball Stochastic Approximation:

$$\Delta\theta_{n+1} = M_{n+1}\Delta\theta_n + \alpha_{n+1}G_{n+1}f_{n+1}(\theta_n)$$

Heuristic: Assume $\Delta\theta_n \to 0$ much faster than $\theta_n \to \theta^*$

Matrix Heavy Ball Stochastic Approximation

Optimizing $\{M_{n+1}\}$ and $\{G_{n+1}\}$

Matrix Heavy Ball Stochastic Approximation:

$$\Delta\theta_{n+1} = M_{n+1}\Delta\theta_n + \alpha_{n+1}G_{n+1}f_{n+1}(\theta_n)$$

Heuristic: Assume $\Delta\theta_n \to 0$ much faster than $\theta_n \to \theta^*$

$$\Delta\theta_{n+1} \approx M_{n+1}\Delta\theta_{n+1} + \alpha_{n+1}G_{n+1}f_{n+1}(\theta_n)$$

Matrix Heavy Ball Stochastic Approximation

Optimizing $\{M_{n+1}\}$ and $\{G_{n+1}\}$

Matrix Heavy Ball Stochastic Approximation:

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$$\Delta\theta_{n+1} \approx [I - M_{n+1}]^{-1}\alpha_{n+1}G_{n+1}f_{n+1}(\theta_n)$$

Matrix Heavy Ball Stochastic Approximation

Optimizing $\{M_{n+1}\}$ and $\{G_{n+1}\}$

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Try this: $M_{n+1} = I + G_{n+1}\widehat{A}_{n+1}$

Matrix Heavy Ball Stochastic Approximation

Optimizing $\{M_{n+1}\}$ and $\{G_{n+1}\}$

Matrix Heavy Ball Stochastic Approximation:

$$\Delta\theta_{n+1} = M_{n+1}\Delta\theta_n + \alpha_{n+1}G_{n+1}f_{n+1}(\theta_n)$$

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Try this: $M_{n+1} = I + G_{n+1}\widehat{A}_{n+1}$

$$= -\alpha_{n+1}\widehat{A}_{n+1}^{-1}f_{n+1}(\theta_n) \qquad \text{SNR!}$$

Momentum based Stochastic Approximation

$\widehat{A}_{n+1} \approx \frac{d}{d\theta} \bar{f}(\theta_n)$

SNR: $\Delta\theta_{n+1} = -\alpha_{n+1} \widehat{A}_{n+1}^{-1} f_{n+1}(\theta_n)$

Momentum based Stochastic Approximation

$\widehat{A}_{n+1} \approx \frac{d}{d\theta} \bar{f}\,(\theta_n)$

Special case $G_n = \zeta I$

$$\text{SNR:} \quad \Delta\theta_{n+1} = -\alpha_{n+1} \widehat{A}_{n+1}^{-1} f_{n+1}(\theta_n)$$

$$\text{PolSA:} \quad \Delta\theta_{n+1} = [I + \zeta \widehat{A}_{n+1}]\Delta\theta_n + \alpha_{n+1}\zeta f_{n+1}(\theta_n)$$

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NeSA: $\Delta\theta_{n+1} = \Delta\theta_n + \zeta[f_{n+1}(\theta_n) - f_{n+1}(\theta_{n-1})]$
$\qquad + \alpha_{n+1}\zeta f_{n+1}(\theta_n)$

following Nesterov, 1983 [13]

Momentum based Stochastic Approximation

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Coupling of SNR and PolSA: $\|\theta_n^{\text{SNR}} - \theta_n^{\text{PolSA}}\| = O(n^{-1})$

Momentum based Stochastic Approximation

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- $\{\Delta_{n+1}\}$ square-integrable martingale difference sequence
- A Hurwitz *and* eig$(I + \zeta A) \in$ open unit disk

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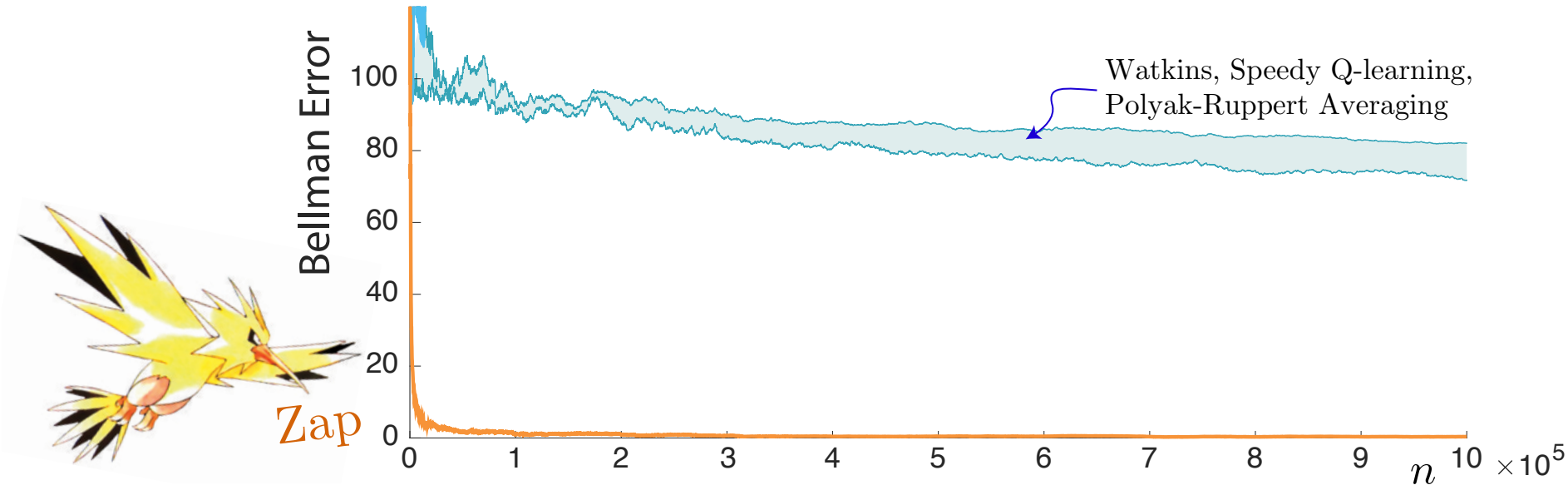
PolSA has optimal asymptotic variance



Zap & Momentum in Reinforcement Learning

Watkins' Q-learning

Goal: *Galerkin relaxation of Bellman equation*

$$0 = \mathsf{E}\Big[\big(c(X_n, U_n) + \beta \underline{Q}^{\theta^*}(X_{n+1}) - Q^{\theta^*}(X_n, U_n)\big)\zeta_n\Big]$$

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Watkin's algorithm is Stochastic Approximation

The family $\{Q^\theta\}$ and *eligibility vectors* $\{\zeta_n\}$ in this design:

- Linearly parameterized family of functions: $Q^\theta(x,u) = \theta^\intercal \psi(x,u)$
- $\zeta_n \equiv \psi(X_n, U_n)$
- $\psi_i(x,u) = \mathbb{I}\{x = x^i, u = u^i\}$ (complete basis)

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Algorithm:

$$\theta_{n+1} = \theta_n + \alpha_{n+1}\big(c(X_n, U_n) + \beta \underline{Q}^{\theta^*}(X_{n+1}) - Q^{\theta^*}(X_n, U_n)\big)\zeta_n$$

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Converges, but has infinite asymptotic variance if $\beta > \frac{1}{2}$:

$$\lambda_{\max}\big(\boldsymbol{A}(\theta^*)\big) > -\tfrac{1}{2}$$

[D & Meyn, 2017]

Watkins' Q-learning

Goal: *Galerkin relaxation of Bellman equation*

$$0 = \mathsf{E}\Big[\big(c(X_n, U_n) + \beta \underline{Q}^{\theta^*}(X_{n+1}) - Q^{\theta^*}(X_n, U_n)\big)\zeta_n\Big]$$

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Convergence rate for $\beta > \frac{1}{2}$:

$$\mathcal{O}(1/n^{1-\beta})$$

[D & Meyn, 2017]

Watkins' Q-learning

Can we *Zap* Q-Learning?

Watkin's algorithm is Stochastic Approximation

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Zap Q-learning

Zap Q-Learning ≡ Zap-SNR for Q-Learning

Algorithm:

$$\theta_{n+1} = \theta_n + \alpha_n \widehat{A}_{n+1}^{-1} \big(c(X_n, U_n) + \beta \underline{Q}^{\theta_n}(X_{n+1}) - Q^{\theta_n}(X_n, U_n) \big) \zeta_n$$

Zap Q-learning

Zap Q-Learning ≡ Zap-SNR for Q-Learning

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$$\theta_{n+1} = \theta_n + \alpha_n \widehat{A}_{n+1}^{-1} \big(c(X_n, U_n) + \beta \underline{Q}^{\theta_n}(X_{n+1}) - Q^{\theta_n}(X_n, U_n) \big) \zeta_n$$

$$\widehat{A}_{n+1} \approx A(\theta_n)$$

Zap Q-learning

Zap Q-Learning ≡ Zap-SNR for Q-Learning

Algorithm:

$$\theta_{n+1} = \theta_n + \alpha_n \widehat{A}_{n+1}^{-1} \big(c(X_n, U_n) + \beta \underline{Q}^{\theta_n}(X_{n+1}) - Q^{\theta_n}(X_n, U_n) \big) \zeta_n$$

ODE Analysis: change of variables $q = \mathcal{Q}^*(\varsigma)$

Functional $\mathcal{Q}^*$ maps cost functions to Q-functions:

$$q(x,u) = \varsigma(x,u) + \beta \sum_{x'} P_u(x,x') \min_{u'} q(x',u')$$

Zap Q-learning

Zap Q-Learning ≡ Zap-SNR for Q-Learning

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Functional $\mathcal{Q}^*$ maps cost functions to Q-functions:

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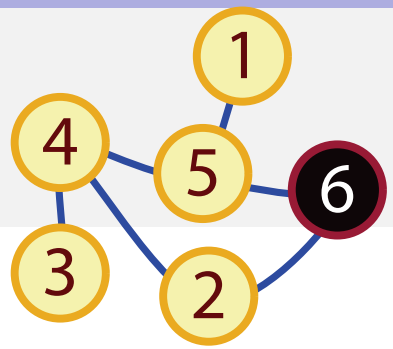
ODE for Zap-Q:

$$q_t = \mathcal{Q}^*(\varsigma_t), \qquad \frac{d}{dt}\varsigma_t = -\varsigma_t + c$$

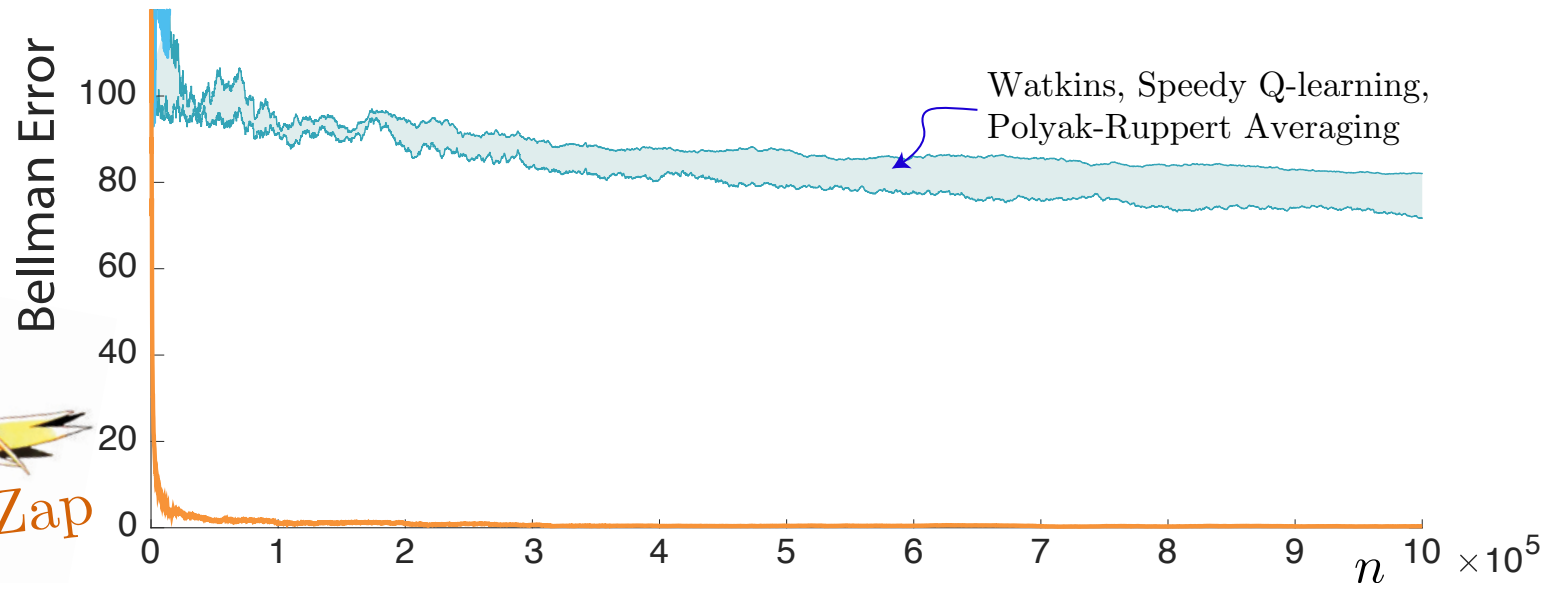
$\Rightarrow$ convergence, optimal covariance, ...

Zap Q-learning

Example: Stochastic Shortest Path



Convergence with Zap gain $\gamma_n = n^{-0.85}$

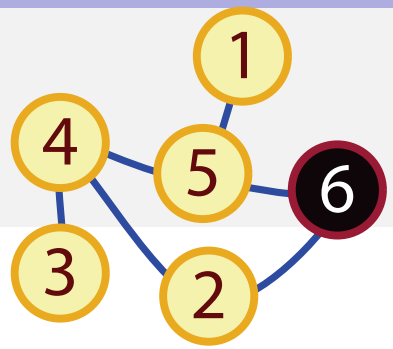


Convergence of Zap-Q Learning

Discount factor: $\beta = 0.99$

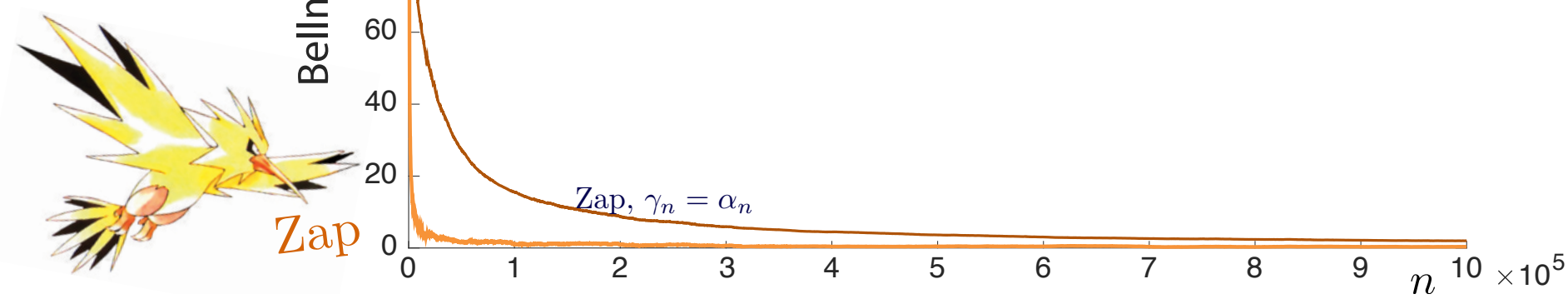
Zap Q-learning

Example: Stochastic Shortest Path



Convergence with Zap gain $\gamma_n = n^{-0.85}$

Watkins' algorithm has infinite asymptotic covariance with $\alpha_n = 1/n$



Convergence of Zap-Q Learning

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Zap Q-learning

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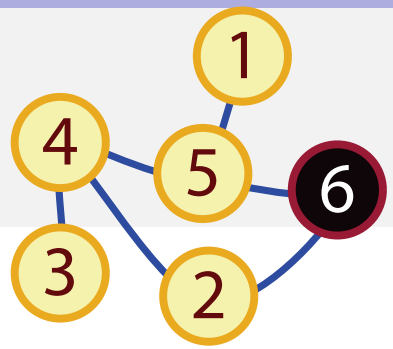
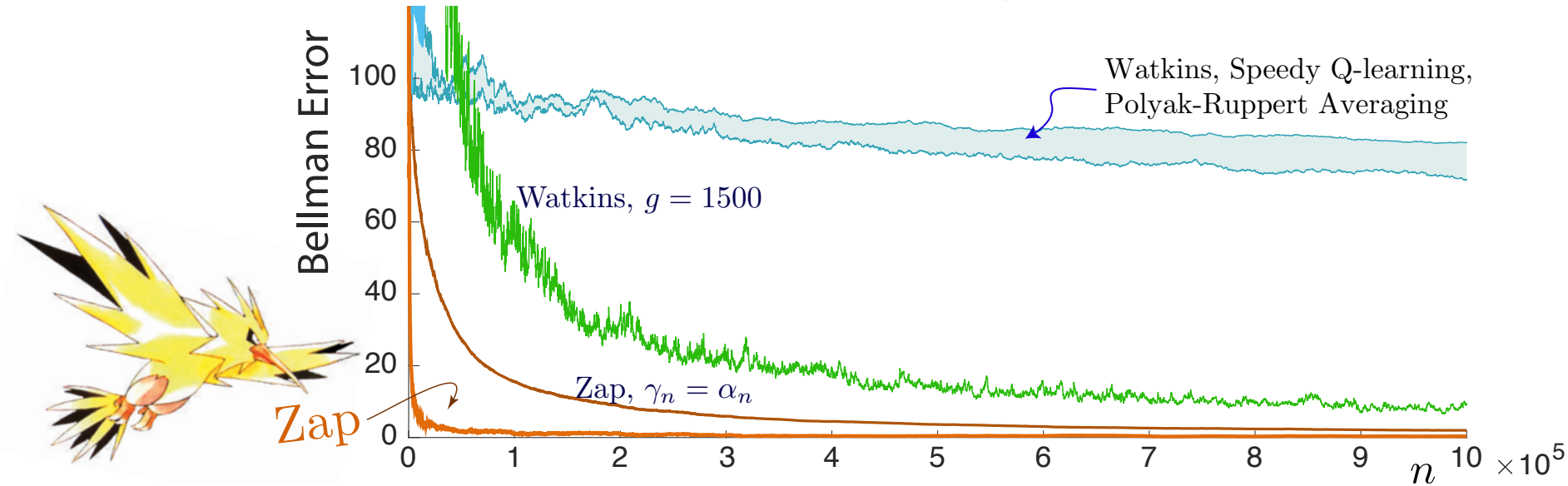


Convergence with Zap gain $\gamma_n = n^{-0.85}$

Watkins' algorithm has infinite asymptotic covariance with $\alpha_n = 1/n$

Optimal scalar gain is approximately $\alpha_n = 1500/n$

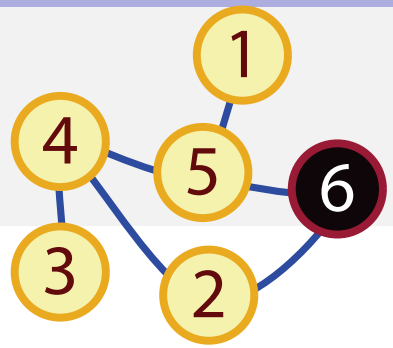


Convergence of Zap-Q Learning

Discount factor: $\beta = 0.99$

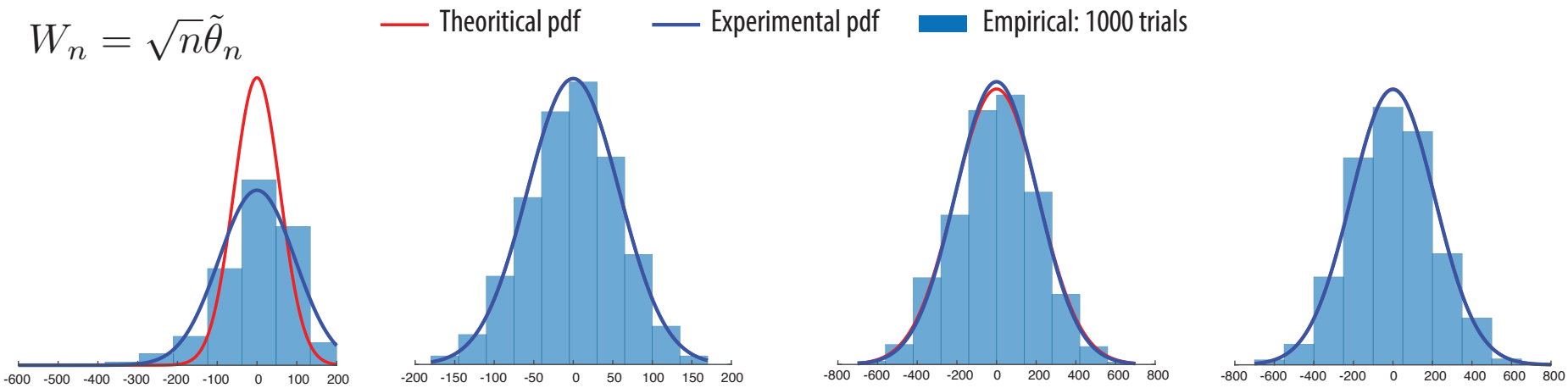
Zap Q-Learning

Optimize Walk to Cafe



Convergence with Zap gain $\gamma_n = n^{-0.85}$

$W_n = \sqrt{n}\tilde{\theta}_n$



Entry #18: $n = 10^4$ $n = 10^6$

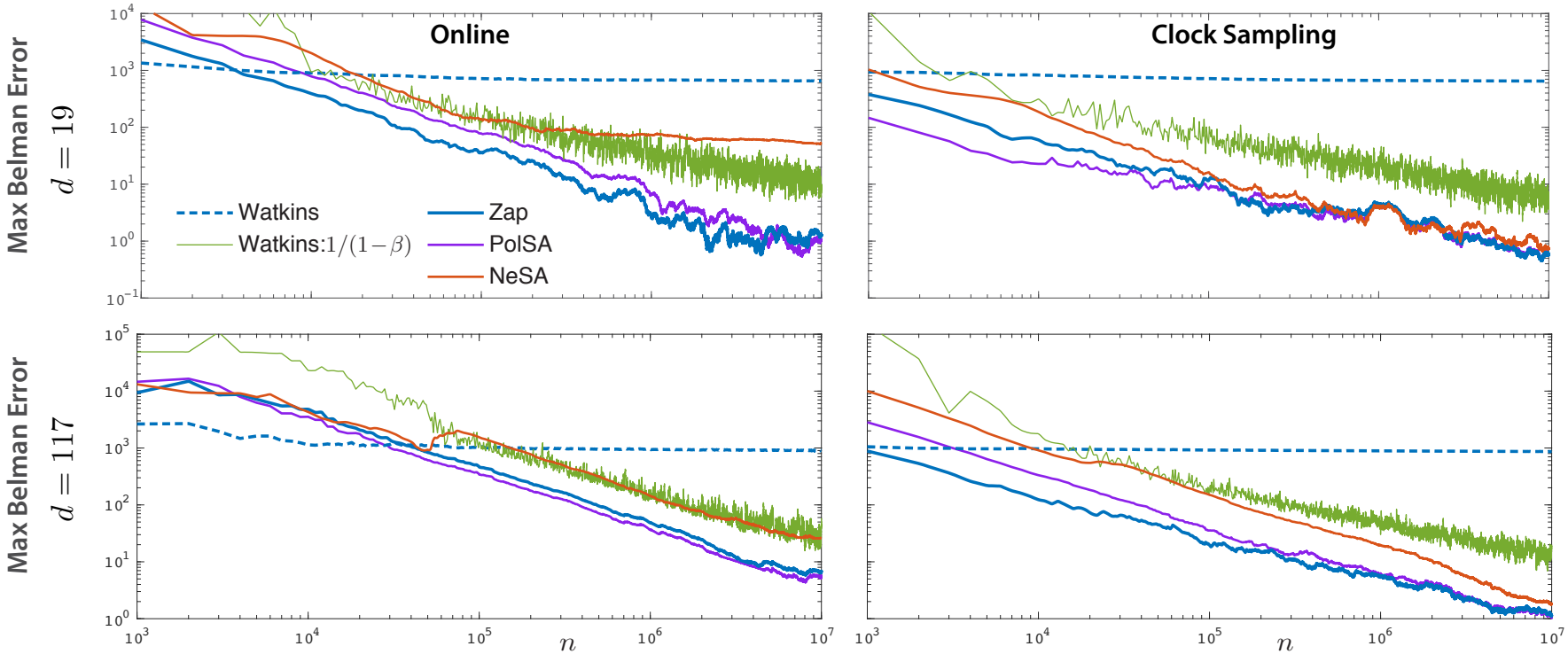
Entry #10: $n = 10^4$ $n = 10^6$

CLT gives good prediction of finite-n performance

Discount factor: $\beta = 0.99$

Zap Q-learning and Momentum

Coupling and convergence for larger models:



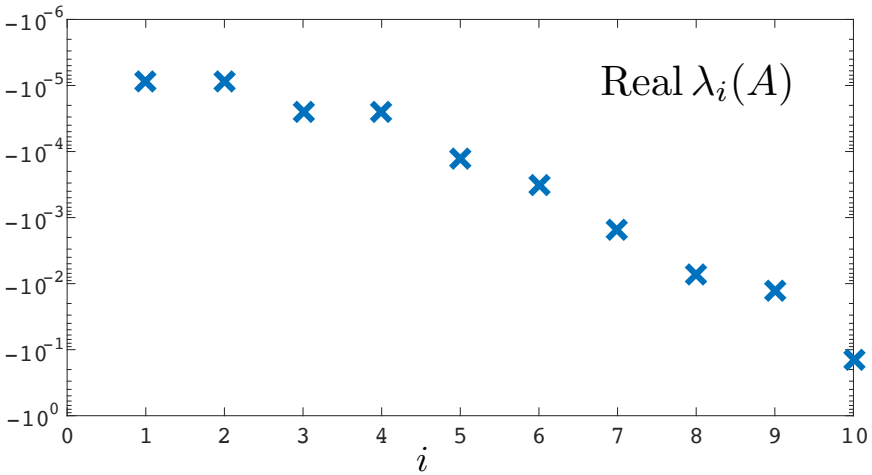
Coupling is amazing

Zap Q-Learning

Model of Tsitsiklis and Van Roy: **Optimal Stopping Time in Finance**

State space: $\mathbb{R}^{100}$

Parameterized Q-function: Q^θ with $\theta \in \mathbb{R}^{10}$



$\mathrm{Real}\,\lambda > -\frac{1}{2}$ for every eigenvalue λ

Asymptotic covariance is infinite

Zap Q-Learning

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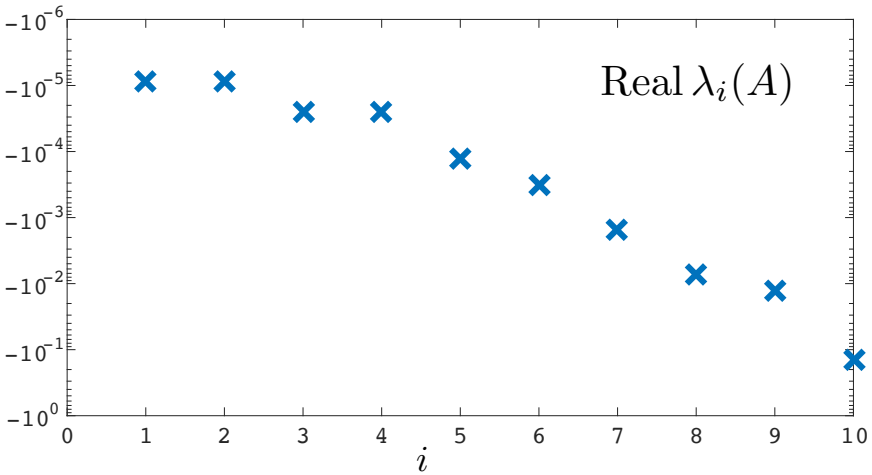

$\mathrm{Real}\,\lambda > -\frac{1}{2}$ for every eigenvalue λ

Asymptotic covariance is infinite

Authors observed slow convergence
Proposed a matrix gain sequence

$\{G_n\}$ (see refs for details)

Zap Q-Learning

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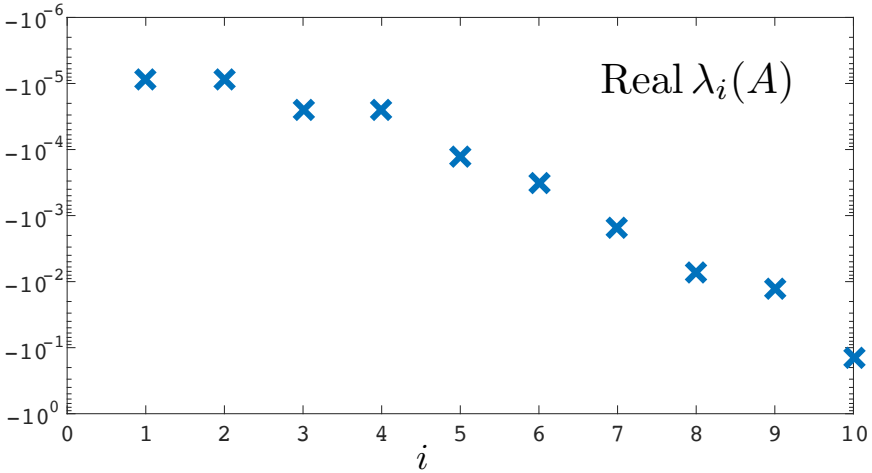

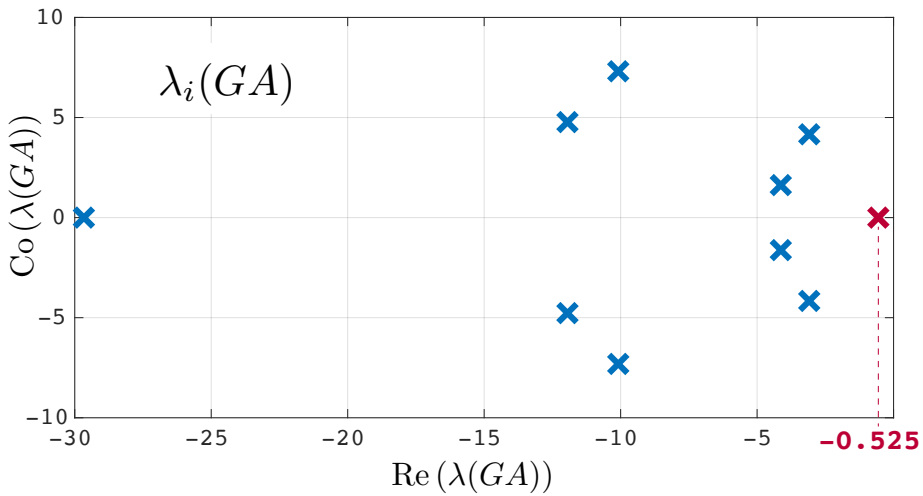

Eigenvalues of A and GA for the finance example

Favorite choice of gain in [25] barely meets the criterion $\text{Re}(\lambda(GA)) < -\frac{1}{2}$

Zap Q-learning

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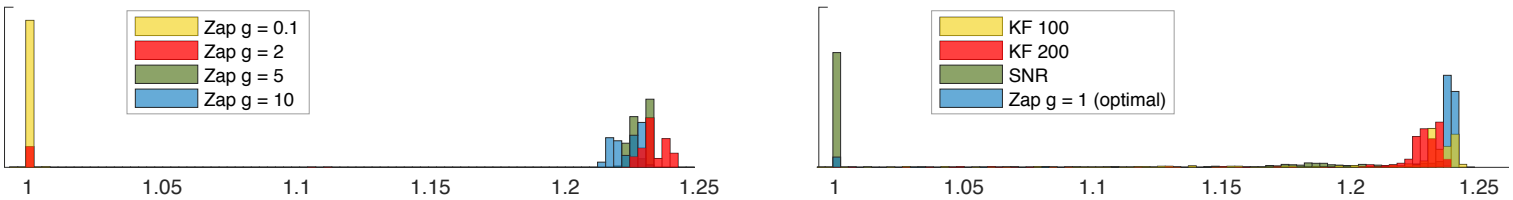
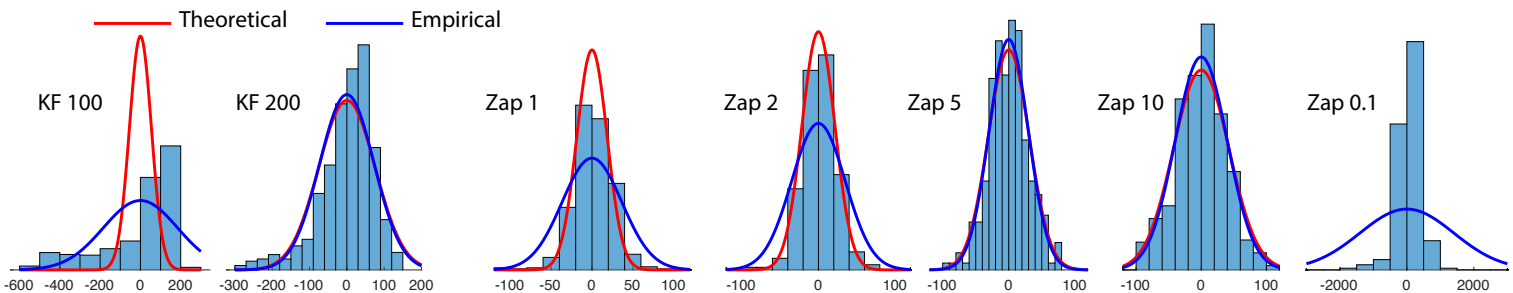
State space: $\mathbb{R}^{100}$

Parameterized Q-function: Q^θ with $\theta \in \mathbb{R}^{10}$

Histograms of the average reward obtained using the different algorithms:



Asymptotic variance for of the algorithms:



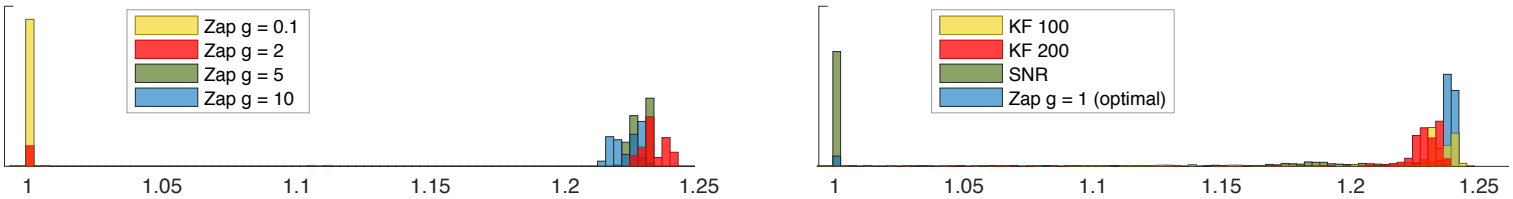
Zap Q-learning

Model of Tsitsiklis and Van Roy: **Optimal Stopping Time in Finance**

State space: $\mathbb{R}^{100}$

Parameterized Q-function: Q^θ with $\theta \in \mathbb{R}^{10}$

Histograms of the average reward obtained using the different algorithms:



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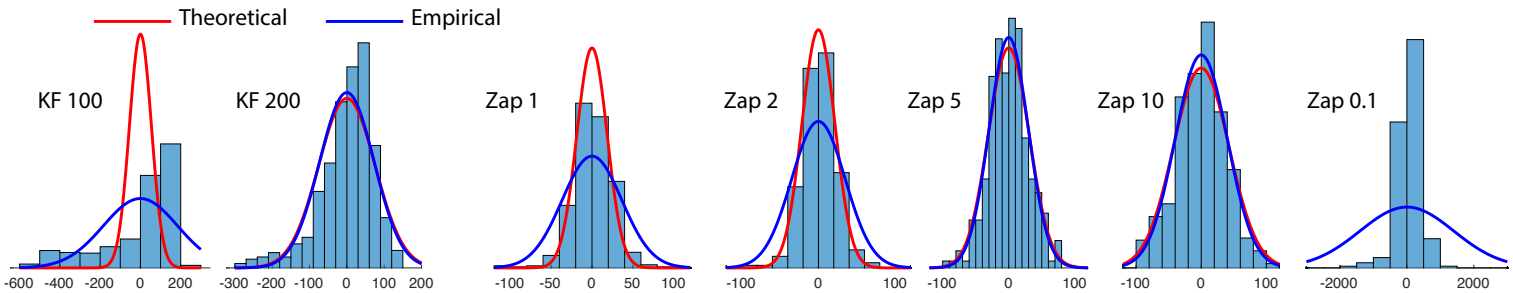

Zap-Q $\gg$ KF

Conclusions & Future Work

Conclusions:

- *Reinforcement Learning is not just cursed by dimension, but also by variance!*
- RL algorithms in their raw form are NO GOOD without careful gain selection
- *We need a richer set of tools for algorithm design*

Conclusions & Future Work

Future work:

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- Q-learning with function-approximation
  - *Obtain conditions for a stable algorithm in a general setting*

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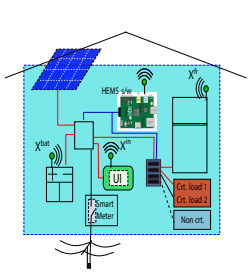

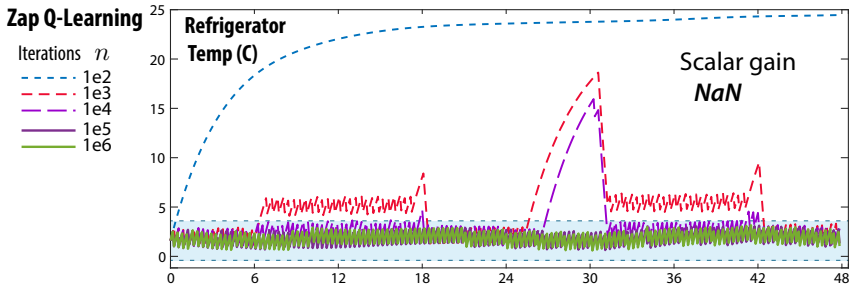

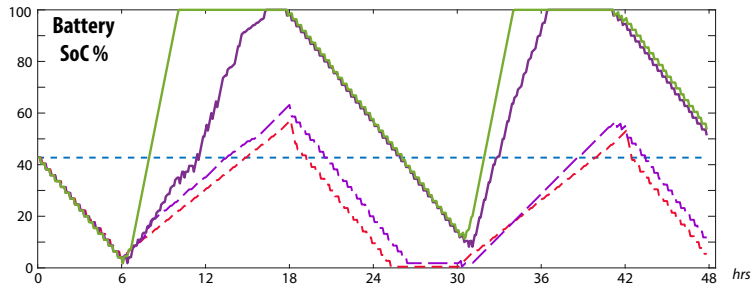

Update in 2019: *stability resolved using second order methods!*

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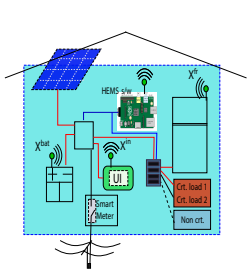

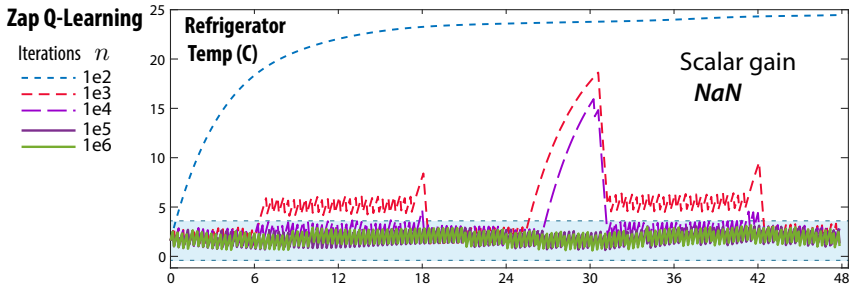

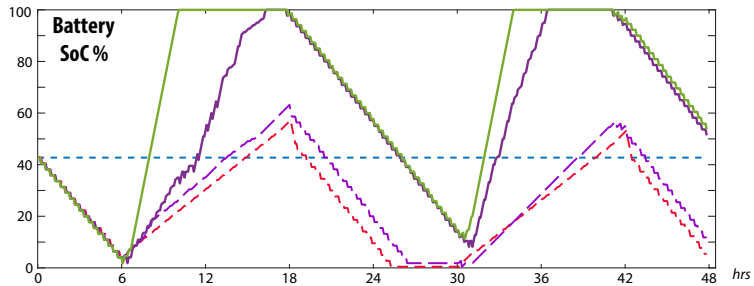

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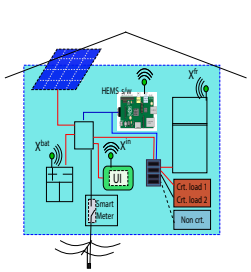

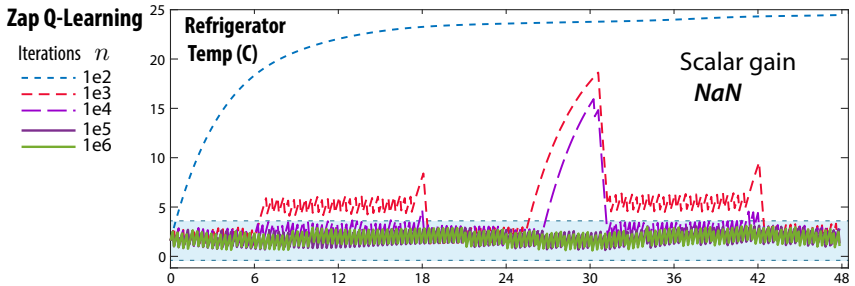

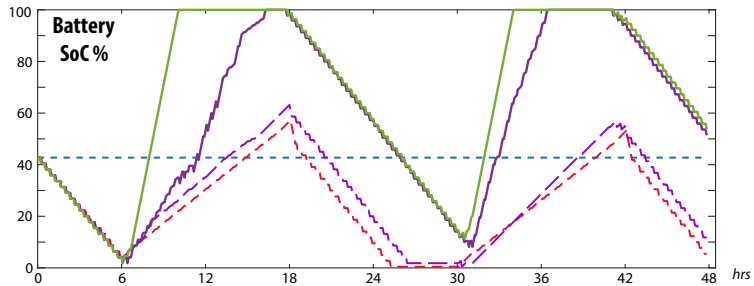

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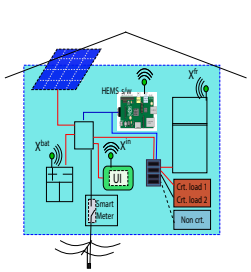

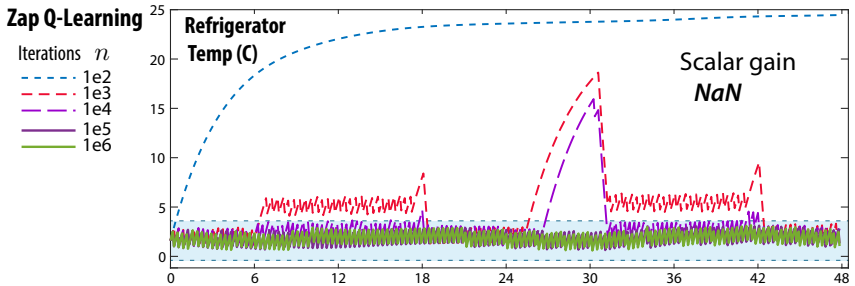

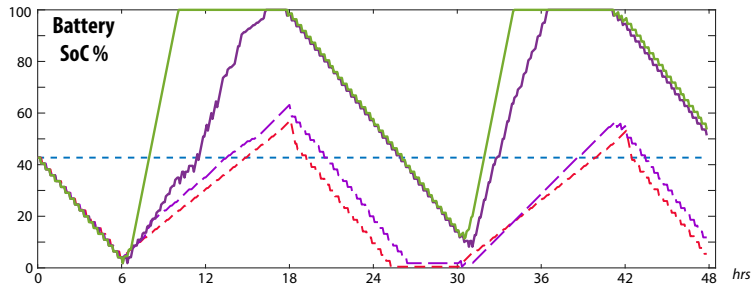

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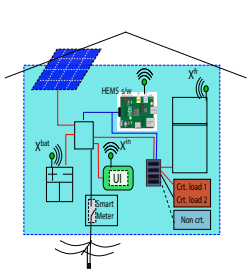

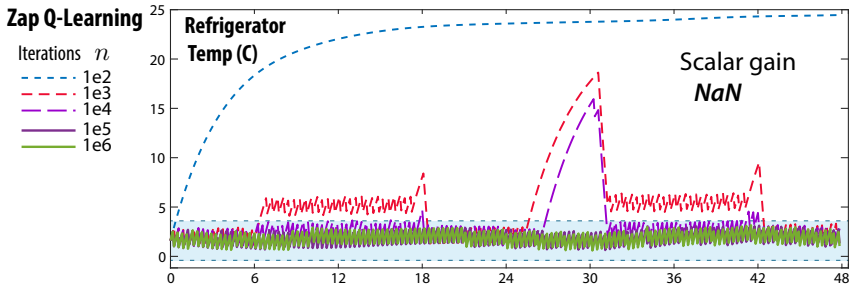

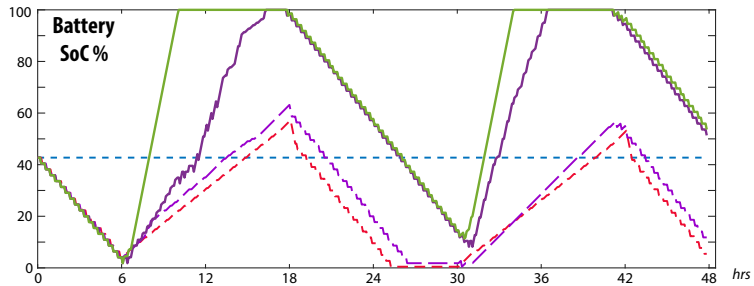

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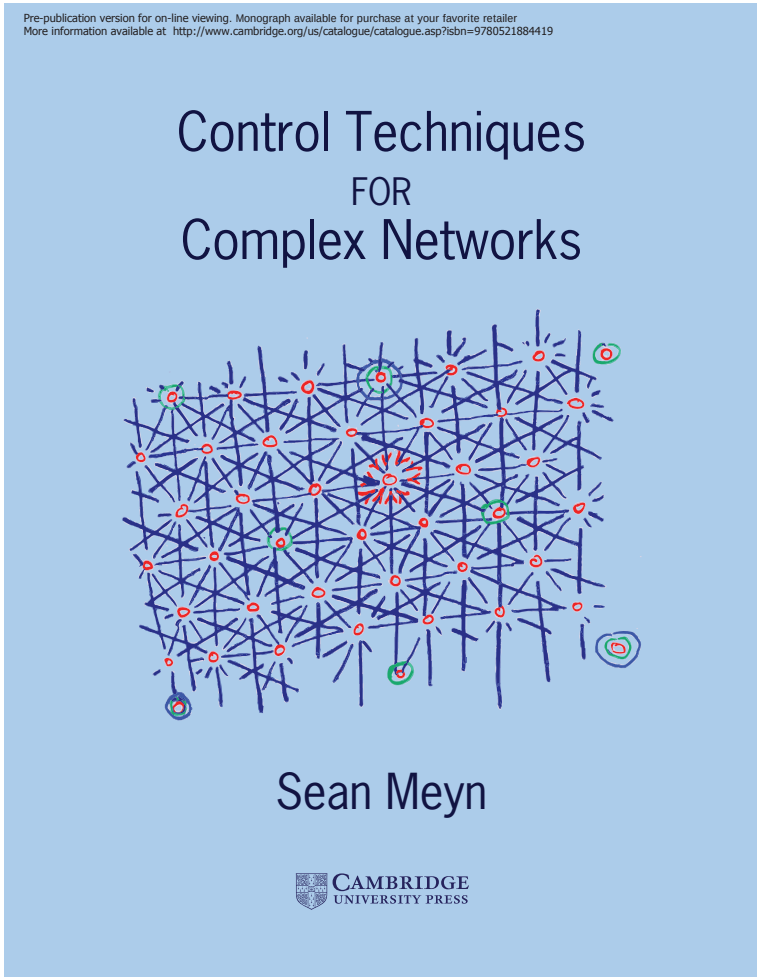
- Applications in Stochastic Optimization

This Presentation

- A. M. Devraj and S. P. Meyn, *Zap Q-learning. Advances in Neural Information Processing Systems (NIPS).* Dec. 2017.
- A. M. Devraj and S. P. Meyn, *Fastest convergence for Q-learning.* Available on *ArXiv*. Jul. 2017.
- A. M. Devraj, A. Bušić, and S. Meyn. *Optimal Matrix Momentum Stochastic Approximation and Applications to Q-learning*. *ArXiv e-prints*, Feb. 2019.
- S. Chen, A. M. Devraj, A. Bušić, and S. Meyn. *Zap Q-learning for Optimal Stopping Time Problems*. *ArXiv e-prints*, Apr. 2019.


Thank you!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Complex Networks
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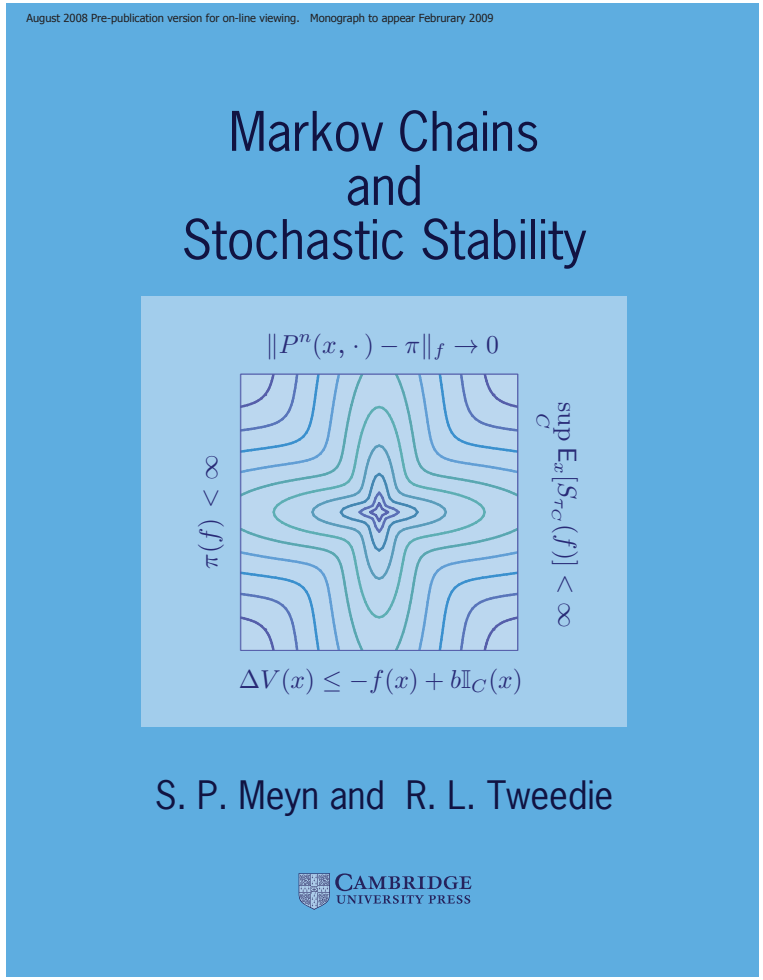
August 2008 Pre-publication version for on-line viewing. Monograph to appear Februrary 2009
Markov Chains
and
Stochastic Stability
$\|P^n(x,\cdot) - \pi\|_f \to 0$
$\pi(f) < \infty$
$\sup_C \mathsf{E}_x[S_{\tau_C}(f)] < \infty$
$\Delta V(x) \le -f(x) + b\mathbb{I}_C(x)$
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