Zap Stochastic Approximation and Reinforcement Learning

Reading Group Network Theory
Lincs

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Motivation:
Stochastic Approximation and RL

What is Stochastic Approximation?

Problem

- W random variable, $\theta \in \mathbb{R}^d$ variable.
- $f(\theta, W) \in \mathbb{R}^d$.
- $\bar{f}(\theta) := \mathsf{E}[f(\theta, W)]$.

Goal: find θ^* s.t.

$$\bar{f}(\theta^*) = 0.$$

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Traditional example (with $d = 1$)

- θ: dosage of a medicine (e.g. insulin).
- $f(\theta, W)$: effect (e.g. blood sugar level − ideal blood sugar level).
- θ^*: ideal dosage s.t. $\bar{f}(\theta^*) = 0$.

Robbins-Monro Algorithm

Principle

Initial estimate: θ_0 (arbitrary).
Update rule:

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

where the step-size α_{n+1} is part of the algorithm design.

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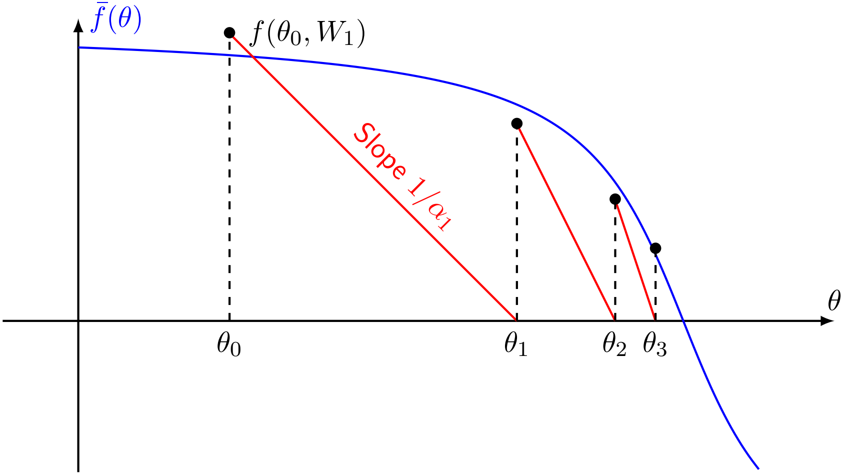
Traditional example (continued)

- Try dosage θ_0 with patient 1.
- This gives effect $f(\theta_0, W_1)$: a noisy version of $\bar{f}(\theta_0)$.
- New estimated dosage $\theta_1 = \theta_0 + \alpha_1 f(\theta_0, W_1)$.
- Etc.

Robbins-Monro Algorithm: Illustration

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



Robbins-Monro Algorithm: Convergence

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

The step-size satisfies:

- $\sum \alpha_n = \infty$,
- $\sum \alpha_n^2 < \infty$.

Usually we take $\alpha_n = 1/n$.

Monte-Carlo Estimation, Seen as an SA Approach

Problem

We want to estimate $\mathsf{E}[W]$, where W is a random variable.

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Conversion to SA problem

Let $f(\theta, W) = W - \theta$. Then $\bar{f}(\theta) = \mathsf{E}[W] - \theta$.
We want to find θ^* s.t. $\bar{f}(\theta^*) = 0$.

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Application of Robbins-Monro Algorithm

$$\begin{aligned}
\theta_{n+1} &= \theta_n + \frac{1}{n+1}(W_{n+1} - \theta_n) \\
&= \frac{n}{n+1}\theta_n + \frac{1}{n+1}W_{n+1} \\
&= \frac{1}{n+1}\sum_{k=1}^{n+1} W_k \qquad \Rightarrow \text{This is Monte-Carlo!}
\end{aligned}$$

Many RL challenges are SA Problems Too

In Monte-Carlo, we want to solve $\mathrm{E}[W - \theta] = 0$.

- W is new data / sample,
- θ_n is an old estimation,
- θ_{n+1} is the new estimation: $\theta_{n+1} = \theta_n + \alpha_{n+1} *$ *observed difference*.

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Many RL algorithms rely on a temporal difference (TD) term of the same form. For example, for Q-Learning:

- New data / sample $= c(X_n, U_n) + \beta \min_u [Q^n(X_{n+1}, u)]$,
- Old estimation $= Q^n(X_n, U_n)$.
- New estimation $= Q^{n+1}(X_n, U_n)$.

We will develop more on this in the section about Q-Learning.

Zap Stochastic Approximation

Difficulties of Stochastic Approximation

Reminder: we search the solution θ^* to

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

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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.

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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. We will see that it is typically the case for Q-Learning, unfortunately.

Convergence

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

Robbins-Monro Algorithm (reminder): $\theta_{n+1} = \theta_n + \alpha_{n+1} f(\theta_n, W_{n+1})$.

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

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

Performance Criteria

SA recursion:

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

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):

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

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Asymptotic Covariance

$\Sigma = \lim_{n\to\infty} \Sigma_n = \lim_{n\to\infty} n\mathsf{E}\big[\tilde\theta_n \tilde\theta_n^{\mathsf{T}}\big]$

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$\Sigma = \lim_{n\to\infty} \Sigma_n = \lim_{n\to\infty} n\mathsf{E}\big[\tilde\theta_n \tilde\theta_n^{\mathsf{T}}\big]$

Linearized SA recursion for the error sequence $\{\tilde\theta_n\}$:

$$\tilde\theta_{n+1} \approx \tilde\theta_n + \frac{1}{n}\Big\{A\tilde\theta_n + \Delta_{n+1}\Big\}$$

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

Asymptotic Covariance

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

Scaled, linearized SA recursion for the error sequence:

$$\sqrt{n+1}\tilde{\theta}_{n+1} \approx \sqrt{n}\tilde{\theta}_n + \tfrac{1}{n}\Big\{(A + \tfrac{1}{2}I)\sqrt{n}\tilde{\theta}_n\Big\} + \frac{1}{\sqrt{n}}\Delta_{n+1}$$

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

$$\sqrt{n+1} \approx \sqrt{n} + \tfrac{1}{2\sqrt{n}}$$

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 $\{\Sigma_n\}$:

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

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

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

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

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, and linearize:

$$\tilde{\theta}_{n+1} \approx \tilde{\theta}_n + \alpha_{n+1} G \big(A \tilde{\theta}_n + \Delta_{n+1} \big), \qquad A = \frac{d}{d\theta} \bar{f}\,(\theta^*)$$

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Asymptotic Variance Theory

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

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

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

- Resembles Newton-Raphson
- It is optimal: $\Sigma^* = G^* \Sigma_\Delta G^{*\,T} \leq \Sigma^G$ *any other* G

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

Optimal Variance and Stochastic Newton Raphson (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:

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

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

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$$\theta_{n+1} = \theta_n + \alpha_{n+1}(-\widehat{A}_{n+1})^{-1} f(\theta_n, W_{n+1})$$
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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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$$\widehat{A}_{n+1} \approx A(\theta_n) \text{ requires high-gain, } \frac{\gamma_n}{\alpha_n} \to \infty, \qquad n \to \infty$$

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

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

Application to Q-Learning

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:

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

Stochastic Optimal Control Seen As an SA Problem

Problem

Find function Q^* that solves

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

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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*" $\{\zeta_n\}$, $\zeta_n \in \mathbb{R}^d$ are part of algorithm design.

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

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Watkins' Q-learning ($=$ "Vanilla" Tabular Q-Learning)

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

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

- Linearly parameterized family of functions: $Q^\theta(x,u)=\theta^\intercal\psi(x,u)$
- $\zeta_n:=\psi(X_n,U_n)$
- $\psi_i(x,u):=\mathbb{I}\{x=x^i,u=u^i\}$ (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 $\beta > \frac{1}{2}$:

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

[Devraj & Meyn, 2017]

Watkins' Q-learning (= "Vanilla" Tabular Q-Learning)

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

Watkin's algorithm is Stochastic Approximation

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

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

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

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

[Devraj & Meyn, 2017]

Watkins' Q-learning (= "Vanilla" Tabular Q-Learning)

Big Question: *Can we Zap Q-Learning?*

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

Watkin's algorithm is Stochastic Approximation

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Linear Parametrization of Q-Learning

Definition

$Q^\theta(x,u) = \theta^T \psi(x,u)$, where:

- $\theta \in \mathbb{R}^d$ denotes the parameter vector,
- $\psi(x,u)$ represents the features of (x,u).

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Particular Case: Tabular Q-Learning

- $\psi_i(x,u) = \mathbb{I}(x = x^i, u = u^i)$,
- (x^i, u^i) enumerate all state-action pairs,
- $1 \leq i \leq d$, where $d = |\text{states}| * |\text{actions}|$.

Q(λ) Algorithm

1. $d_{n+1} = c(X_n, U_n) + \beta \underline{Q}^{\theta_n}(X_{n+1}) - Q^{\theta_n}(X_n, U_n)$
2. $\theta_{n+1} = \theta_n + \alpha_{n+1}\zeta_n d_{n+1}$
3. $\zeta_{n+1} = \lambda\beta\zeta_n + \psi(X_{n+1}, U_{n+1})$

Zap-Q(λ) Algorithm

1. $d_{n+1} = c(X_n, U_n) + \beta \underline{Q}^{\theta_n}(X_{n+1}) - Q^{\theta_n}(X_n, U_n)$
2. $A_{n+1} = \zeta_n [\beta \psi(X_{n+1}, \phi_n(X_{n+1})) - \psi(X_n, U_n)]^T$
3. $\widehat{A}_{n+1} = \widehat{A}_n + \gamma_{n+1}[A_{n+1} - \widehat{A}_n]$
4. $\theta_{n+1} = \theta_n + \alpha_{n+1} \widehat{A}_{n+1}^{-1} \zeta_n d_{n+1}$
5. $\zeta_{n+1} = \lambda \beta \zeta_n + \psi(X_{n+1}, U_{n+1})$

Zap-Q(λ) Algorithm: Issues and Possible Solutions

Work in Progress...

Issue 1: $\widehat{A}_{n+1}$ is proven to be eventually invertible, but is generally not invertible during the early stages of the algorithm.

$\Rightarrow$ Use Moore-Penrose pseudoinverse $\widehat{A}_{n+1}^{+}$.

Zap-Q(λ) Algorithm: Issues and Possible Solutions

Work in Progress...

Issue 1: $\widehat{A}_{n+1}$ is proven to be eventually invertible, but is generally not invertible during the early stages of the algorithm.

$\Rightarrow$ Use Moore-Penrose pseudoinverse $\widehat{A}^{+}_{n+1}$.

Issue 2: Computing $\widehat{A}^{-1}_{n+1}$ (or $\widehat{A}^{+}_{n+1}$) is expensive.

$\Rightarrow$ In fact we do not need $\widehat{A}^{+}_{n+1}$ itself but only $\widehat{A}^{+}_{n+1}\zeta_n$. This can be done by solving a least squares problem: find X that minimizes $\|\widehat{A}_{n+1}X - \zeta_n\|_2$. Still expensive...

$\Rightarrow$ Since $\widehat{A}_{n+1}$ is updated by adding a matrix of rank 1 at each step, it can be computed cheaply by Sherman-Morrison-Woodbury formula.

Conclusion

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Take-aways:

- *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.

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Current/future works:

- Implementation in the Stable-Baselines framework.
- Q-learning with function-approximation: obtain conditions for a stable algorithm in a general setting.

This Presentation

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