Approximate Value Iteration and Variants

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Final Project

Milestone (mid-project report) – due on March 29

- Title, Authors
- Introduction: Introduce the problem and its motivation
- Related works: Related works and how they relate to your project
- Approach: The methods you tried or intend to apply to your problem
- Preliminary Results: Current state of the project and your results so far

Use NeurIPS format

(https://neurips.cc/Conferences/2023/PaperInformation/StyleFiles)

Number of pages ≤ 4

Final Project

In-class presentation

- 4/15, 4/17, 4/22, 4/24
- Four groups each day
- Each group gives a 15-minute presentation

Final report

- A paper that presents the results
- NeurIPS format: ≤ 8 pages of main texts + unbounded pages of appendix

Value Iteration

$$V^{(k)}(s) \leftarrow \max_{\alpha} \left\{ \begin{array}{c} R(s_{i\alpha}) + \gamma \sum_{s'} P(s'|s_{i\alpha}) V^{(k-1)}(s') \\ \\ Q^{(k)}(s_{i\alpha}) \end{array} \right. \xrightarrow{\max_{\alpha} Q^{(k-1)}(s';\alpha')}$$

For
$$k=1, 2, ...$$

$$\forall s, a, \qquad Q^{(k)}(s,a) \leftarrow \boxed{R(s,a)} + \gamma \sum_{s'} \boxed{P(s'|s,a)} \max_{a'} Q^{(k-1)}(s',a')$$
 unknown unknown

Idea: In each iteration, use multiple samples to estimate the right-hand side.

Least-Square Value Iteration (LSVI)

For k = 1, 2, ...

We want these samples to be "exploratory"

Obtain n samples $\mathcal{D}^{(k)} = \{(s_i, a_i, r_i, s_i')\}_{i=1}^n$ where $\mathbb{E}[r_i] = R(s_i, a_i)$, $s_i' \sim P(\cdot | s_i, a_i)$

Perform **regression** on $\mathcal{D}^{(k)}$ to find $Q^{(k)}$ such that

$$Q^{(k)}(s,a) \approx R(s,a) + \gamma \mathbb{E}_{s' \sim P(\cdot \mid s,a)} \left[\max_{a'} Q^{(k-1)}(s',a') \right]$$

Tabular
$$\forall s, a, \qquad Q^{(k)}(s, a) = \frac{\sum_{i=1}^{n} \mathbb{I}\{(s_i, a_i) = (s, a)\}}{\sum_{i=1}^{n} \mathbb{I}\{(s_i, a_i) = (s, a)\}}$$
 $r_i + \gamma \max_{a'} Q^{(k-1)}(s'_i, a')$ $r_i + \gamma \max_{a'} Q^{(k)}(s_i, a')$

General function approximation $\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^n \left(Q_{\theta}(s_i, a_i) - r_i - \gamma \max_{a'} Q_{\theta_{k-1}}(s_i', a') \right)^2$

Linear function approximation
$$\theta_k = \left(\lambda I + \sum_{i=1}^{(n^k)} \phi(s_i, a_i) \phi(s_i, a_i)^{\mathsf{T}}\right)^{-1} \left(\sum_{i=1}^{(n_k)} \phi(s_i, a_i) \left(r_i + \gamma \max_{a'} \phi(s'_i, a')^{\mathsf{T}} \theta_{k-1}\right)\right)$$

Comparison with Contextual Bandits

Exploration

$$p_t(a) \propto e^{\lambda \, \hat{R}(x_t, a)}$$

$$a_t = \underset{a}{\operatorname{argmax}} \left(\hat{R}(x_t, a) + b_t(a) \right)$$
...

Regression

Fit $\hat{R}(x_i, a_i) \approx r_i$

Exploration

$$p_t(a) \propto e^{\lambda Q^{(k)}(s_t, a)}$$

$$a_t = \underset{a}{\operatorname{argmax}} \left(Q^{(k)}(s_t, a) + b_t(a) \right)$$

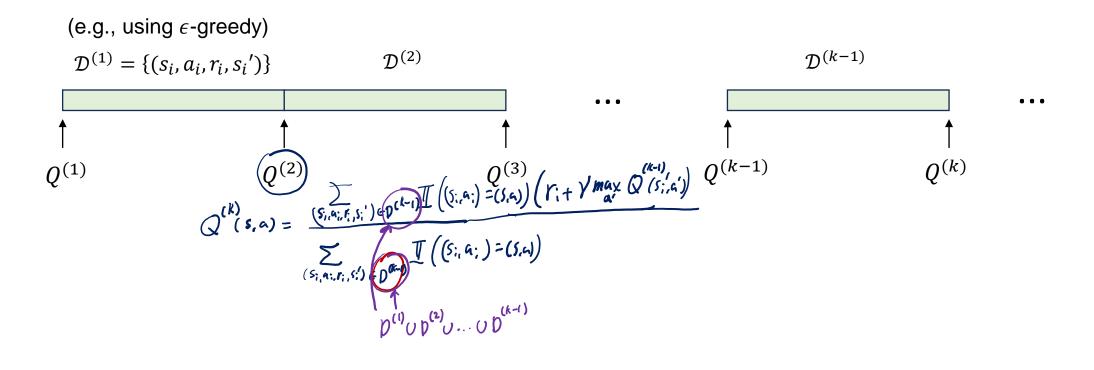
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Value Iteration + Regression

For
$$k = 1, 2, ...$$

Fit
$$Q^{(k)}(s_i, a_i) \approx r_i + \gamma \max_{a'} Q^{(k-1)}(s'_i, a')$$

It is Valid to Reuse Samples



LSVI that Reuses All Previous Samples

For k=1, 2, ...Obtain n samples $\mathcal{D}^{(k)} = \{(s_i, a_i, r_i, s_i')\}_{i=1}^n$ where $\mathbb{E}[r_i] = R(s_i, a_i), s_i' \sim P(\cdot | s_i, a_i)$ Perform **regression** on $\mathcal{D}^{(1)} \cup \mathcal{D}^{(2)} \cup \cdots \cup \mathcal{D}^{(k)}$ to find $Q^{(k)}$ such that $Q^{(k)}(s, a) \approx R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\max_{a'} Q^{(k-1)}(s', a') \right]$

In practice, we reuse "recent" data but not all previous data (discussed later).

Analysis of LSVI under Certain Assumptions

To theoretically show that LSVI converges to the optimal value function, we will make some assumptions to ensure the following holds for all iteration k:

$$Q^{(k)}(s,a) \approx R(s,a) + \gamma \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[\max_{a'} Q^{(k-1)}(s',a') \right]$$

Linear case:

$$\phi(s, a)^{\top} \theta_k \approx R(s, a) + \gamma \, \mathbb{E}_{s' \sim P(\cdot \mid s, a)} \left[\max_{a'} \phi(s', a')^{\top} \theta_{k-1} \right]$$

Analysis of LSVI under Certain Assumptions (5.4) - (5.4) - th entry

$$d = S \cdot A$$

$$\phi(S, a) = \begin{cases} \vdots \\ \vdots \\ \vdots \\ \vdots \end{cases} (S, a) - th \ \text{entry}$$

1. Bellman Completeness Assumption: For any $\theta \in \mathbb{R}^d$, there exists a $\theta' \in \mathbb{R}^d$ \mathbb{R}^d such that

$$\phi(s, a)^{\mathsf{T}} \theta' = R(s, a) + \gamma \, \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\max_{a'} \phi(s', a')^{\mathsf{T}} \theta \right] \qquad \forall s, \alpha$$

This ensures that no matter what θ_{k-1} is, there always exists a θ_k^* such that

$$\psi(s,a)^{\top} \theta_{k}^{\star} = R(s,a) + \gamma \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[\max_{a'} \phi(s',a')^{\top} \theta_{k-1} \right]$$
one-hat at (s,a) entry

This is similar to the linear assumption $\phi(s,a)^{\mathsf{T}}\theta^* = R(s,a)$ in contextual bandits, but is qualitatively stronger because the assumption require "for any θ ".

Analysis of LSVI under Certain Assumptions

2. Coverage Assumption: The dataset \mathcal{D} collected up to k-th iteration allows us to find θ_k so that for any s, a,

$$\left| \phi(s, a)^{\mathsf{T}} \theta_k - \phi(s, a)^{\mathsf{T}} \theta_k^{\star} \right| \le \epsilon_{\mathsf{stat}}$$

(Similar to linear contextual bandits analysis) With

$$\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^n \left(\phi_i^{\mathsf{T}} \theta - \left(r_i + \gamma \max_{a'} \phi(s_i', a')^{\mathsf{T}} \theta_{k-1} \right) \right)^2 + \lambda \|\theta\|^2$$

$$= \underset{\theta}{\operatorname{Expectation}} = \phi_i^{\mathsf{T}} \theta_k^{\star}$$

we have $|\phi(s,a)^{\mathsf{T}}(\theta_k - \theta_k^{\star})| \lesssim \sqrt{\beta} \|\phi(s,a)\|_{\Lambda^{-1}}$ where $\Lambda = \lambda I + \sum_{i=1}^n \phi_i \phi_i^{\mathsf{T}}$

In linear CB, we did not make such an assumption. What we did there is adding $\sqrt{\beta} \|\phi(s,a)\|_{\Lambda^{-1}}$ as **exploration bonus**, which encourages exploration and aims to make $\sqrt{\beta} \|\phi(s,a)\|_{\Lambda^{-1}}$ small for all s,a.

Analysis of LSVI under Certain Assumptions (Recap)

1. Bellman Completeness (i.e., function approximation is sufficiently expressive)

$$\forall \theta_{k-1}, \exists \theta_k^{\star} \qquad \phi(s, a)^{\top} \theta_k^{\star} = R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot \mid s, a)} \left[\max_{a'} \phi(s', a')^{\top} \theta_{k-1} \right] \quad \forall s, a$$

$$\left[\forall \theta_{k-1}, \exists \theta_k^{\star} \qquad Q_{\theta_k^{\star}}(s, a) = R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot \mid s, a)} \left[\max_{a'} Q_{\theta_{k-1}}(s', a') \right] \quad \forall s, a \right]$$

2. Coverage Assumption (i.e., the collected data is sufficient and explores the stateaction space) Regression over $\mathcal{D}^{(k)}$ allows us to find θ_k such that

$$\left| \phi(s, a)^{\mathsf{T}} \theta_k - \phi(s, a)^{\mathsf{T}} \theta_k^{\star} \right| \le \epsilon_{\mathsf{stat}} \quad \forall s, a$$

$$\left(\left| Q_{\theta_k}(s, a) - Q_{\theta_k^{\star}}(s, a) \right| \le \epsilon_{\text{stat}} \quad \forall s, a \right)$$

The two assumptions jointly imply $Q_{\theta_k}(s, a) \approx R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\max_{a'} Q_{\theta_{k-1}}(s, a) \right]$

Analysis of LSVI under Certain Assumptions

Under Bellman completeness and coverage assumptions, LSVI ensures

$$\left\| Q^{(k)} - Q^* \right\|_{\infty} \le O\left(\gamma^k \left\| Q^{(0)} - Q^* \right\|_{\infty} + \frac{\epsilon_{\text{stat}}}{1 - \gamma} \right)$$

where
$$\|Q^{(k)} - Q^*\|_{\infty} := \max_{s,a} |Q^{(k)}(s,a) - Q^*(s,a)|$$

Also, the greedy policy $\pi^{(k)}(s) = \operatorname{argmax} Q^{(k)}(s, a)$ satisfies for all s,

$$V^{\star}(s) - V^{\pi^{(k)}}(s) \le O\left(\gamma^{k} \|Q^{(0)} - Q^{\star}\|_{\infty} + \frac{\epsilon_{\text{stat}}}{1 - \gamma}\right)$$

Notes on Exploration in MDPs

The Coverage Assumption

$$\left|\phi(s,a)^{\top}\theta_k - \phi(s,a)^{\top}\theta_k^{\star}\right| \leq \epsilon_{\text{stat}} \ \, \forall s,a$$

 θ_k : our regression solution

 θ_k^{\star} : ground truth

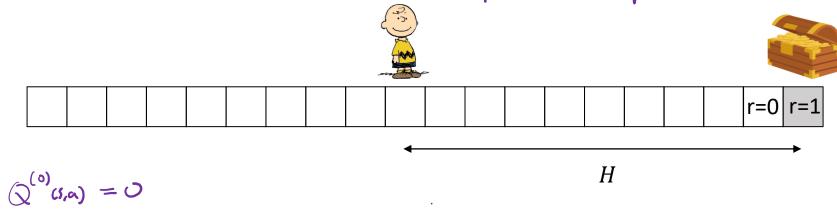
- Requires the state-action space to be explored
 - **Tabular case**: every state-action pair needs to be visited many times
 - **Linear case**: the feature space $\{\phi(s,a)\}_{s,a}$ needs to be explored in all directions
- In bandits, we focus on "action-space" exploration
 - Exploration bonus (UCB, Thompson Sampling) $a_t = argmax \{ R(a) + b_t(a) \}$
 - Randomization (ϵ -greedy, Boltzmann exploration, inverse-gap weighting)

$$P_{t}(y) \propto exp(\lambda \hat{R}(u))$$

• In MDPs, we further need "state-space" exploration

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rud episode has H steps to execute



If we do randomised exploration e.g. $f_t(a) \propto \exp(\lambda Q^{(k)}(s_{t,a}))$ \longrightarrow $f_{rob}(reacting the roll state) <math>\approx \frac{1}{2^H}$ $\approx \frac{1}{2^{1/2}}$ $\approx \frac{1}{2^{1/2}}$ $\approx \frac{1}{2^{1/2}}$ $\approx \frac{1}{2^{1/2}}$

Removing the Coverage Assumption

Use exploration bonus in LSVI:

Tabular Case:
$$\tilde{R}(s,a) = \hat{R}(s,a) + \frac{\text{const}}{\sqrt{n(s,a)}}$$

Linear MDP (a class of MDPs that satisfies linear Bellman completeness):
$$\tilde{R}(s,a) = \phi(s,a)^{\mathsf{T}}\hat{\theta} + \text{const} \|\phi(s,a)\|_{\Lambda^{-1}}$$
 where $\Lambda = I + \sum_{i=1}^{t-1} \phi(s_i,a_i)\phi(s_i,a_i)^{\mathsf{T}}$

UCB in tabular MDP: Minimax regret bounds for reinforcement learning. 2017.

UCB in linear MDP: Provably efficient reinforcement learning with linear function approximation. 2019.

TS in tabular MDP: Near-optimal randomized exploration for tabular Markov decision processes. 2021.

TS in linear MDP: Frequentist regret bounds for randomized least-squares value iteration. 2020.

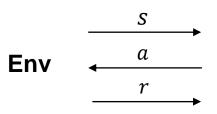
Exploration bonus for general function approximation (deep learning):

Unifying Count-Based Exploration and Intrinsic Motivation

Curiosity-driven Exploration by Self-supervised Prediction

Exploration by Random Network Distillation

Summary for LSVI



 $\mathcal{D}^{(2)}$

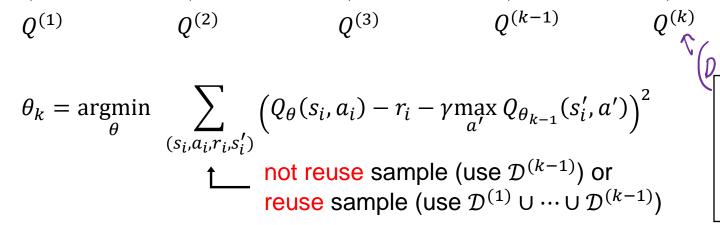
Exploration Mechanism

 $\mathcal{D}^{(k-1)}$

Value Iteration + Regression

Value Iteration + Regression

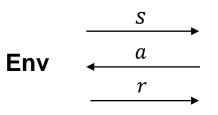
 $\mathcal{D}^{(1)} = \{(s, a, r, s')\}$



cf. Contextual bandits (only regression)

$$\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{(x_i, a_i, r_i)} (R_{\theta}(x_i, a_i) - r_i)^2$$

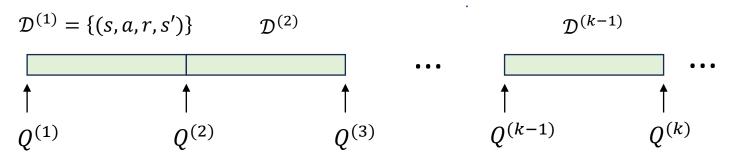
Summary for LSVI



Exploration Mechanism

Value Iteration + Regression

Value Iteration + Regression



Bellman completeness assumption $\Rightarrow \exists \theta_k^{\star}, \forall s, a, Q_{\theta_k^{\star}}(s, a) = R(s, a) + \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\max_{a'} Q_{\theta_{k-1}}(s', a') \right]$ (function expressiveness assumption)

Coverage assumption $\Rightarrow \forall s, a, \quad \left| Q_{\theta_k}(s, a) - Q_{\theta_k^{\star}}(s, a) \right| \leq \epsilon_{\text{stat}}$ (exploration assumption)

Summary for LSVI



Exploration Mechanism

- 1. Randomized policies (ϵ -Greedy, Boltzmann exploration, inverse-gap weighting)
 - perform local exploration
- 2. Exploration bonus (UCB) / Randomized values (TS)
 - can give rigorous regret bounds for tabular MDPs and MDPs with linear Bellman completeness
 - perform wider state space exploration

Other names for LSVI: Fitted Q Iteration, Least-square Q Iteration

Q-Learning

Q-Learning (Watkins, 1992)

For
$$i = 1, 2, ...$$
Obtain sample (s_i, a_i, r_i, s_i')

$$Q^{(i)}(s_i, a_i) \leftarrow (1 - \alpha_i)Q^{(i-1)}(s_i, a_i) + \alpha_i \left(r_i + \gamma \max_a Q^{(i-1)}(s_i', a)\right)$$

$$Q^{(i)}(s, a) \leftarrow Q^{(i-1)}(s, a) \quad \forall (s, a) \neq (s_i, a_i)$$

cf. LSVI:

$$\forall s, a, \qquad Q^{(k)}(s, a) \leftarrow \frac{\sum_{i=1}^{n_k} \mathbb{I}\{(s_i, a_i) = (s, a)\} \left(r_i + \gamma \max_{a'} Q^{(k-1)}(s_i', a')\right)}{\sum_{i=1}^{n_k} \mathbb{I}\{(s_i, a_i) = (s, a)\}}$$

Q-Learning (Watkins, 1992)

Q-Learning (Watkins, 1992)

Suppose that $\alpha_i = \frac{1}{i^{\beta}}$ for some $\frac{1}{2} < \beta \le 1$, and every state-action pair is visited infinitely often. Then

$$Q^{(i)}(s,a) \to Q^*(s,a) \quad \forall s,a.$$

Gen Li, Yuting Wei, Yuejie Chi, Yuantao Gu, Yuxin Chen. <u>Sample Complexity of Asynchronous Q-Learning: Sharper Analysis and Variance Reduction</u>. 2020.

Watkin's Q-Learning + Linear Function Approximation

For i = 1, 2, ...

Obtain sample (s_i, a_i, r_i, s'_i)

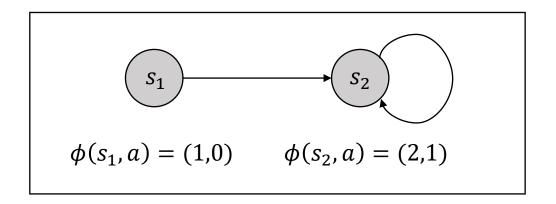
$$\theta_{i} \leftarrow \theta_{i-1} - \alpha \nabla_{\theta} \left(\phi(s_{i}, a_{i})^{\mathsf{T}} \theta - r_{i} - \gamma \max_{a} \phi(s'_{i}, a)^{\mathsf{T}} \theta_{i-1} \right)^{2} \bigg|_{\theta = \theta_{i-1}}$$

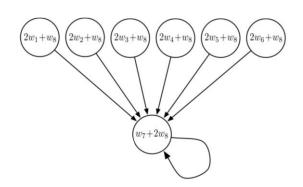
$$= \theta_{i-1} - 2\alpha \left(\phi(s_{i}, a_{i})^{\mathsf{T}} \theta_{i-1} - r_{i} - \gamma \max_{a} \phi(s'_{i}, a)^{\mathsf{T}} \theta_{i-1} \right) \phi(s_{i}, a_{i})$$

c.f. LSVI:
$$\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{n_k} \left(\phi(s_i, a_i)^{\top} \theta - r_i - \gamma \max_{a'} \phi(s'_i, a')^{\top} \theta_{k-1} \right)^2$$

Watkin's Q-Learning + LFA Does Not Converge

Even when Bellman completeness and coverage assumptions hold





Simplified from the "Baird's counterexample" (see Sutton and Barto Section 11.2)

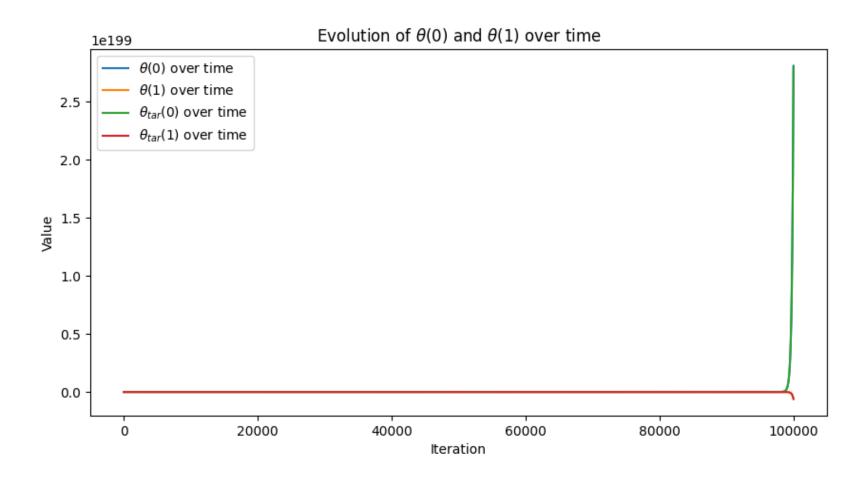
The Effect of Fixing the Target

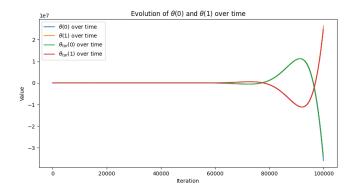
For
$$k=1,\ 2,\dots$$

$$\theta_{k-1} \leftarrow \theta$$
 For $i=1,\dots,n$:
$$\theta \leftarrow \theta - \alpha \sum_{s \in \{s_1,s_2\}} \left(\phi(s,a)^{\mathsf{T}}\theta - r - \gamma \phi(s',a)^{\mathsf{T}}\theta_{k-1} \right) \phi(s,a)$$

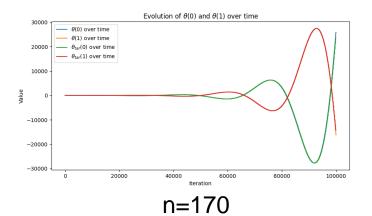
$$\theta_k \leftarrow \theta$$

The Effect of Fixing the Target



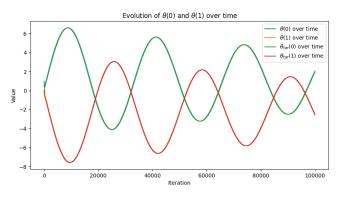


n=150

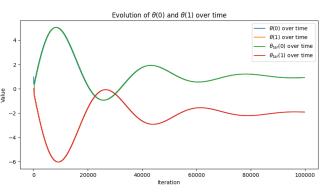


Evolution of $\theta(0)$ and $\theta(1)$ over time $\theta(0) \text{ over time} \\ \theta(1) \text{ over time} \\ \theta_{13r}(0) \text{ over time}$ $\theta_{13r}(1) \text{ over time}$ 100 -100 -200 0 20000 40000Reration 80000 100000

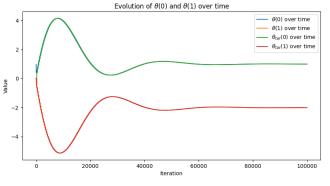
n=190



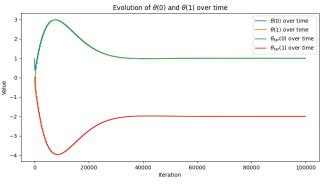
n=210



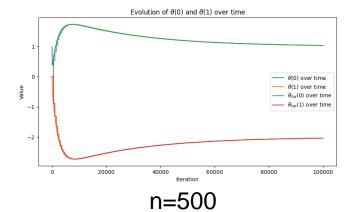
n=230



n=250

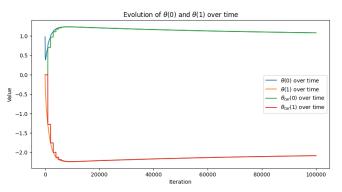


n=300

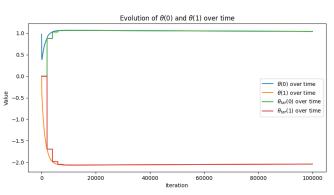


Evolution of $\theta(0)$ and $\theta(1)$ over time 1.5 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 0 20000 40000 60000 80000 100000

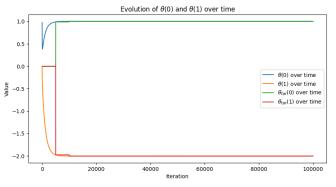




n=1000



n=2000



n=5000

Q-Learning vs. LSVI

Under coverage assumption (i.e., the data $\{(s_i, a_i, r_i, s_i')\}$ sufficiently cover every state-action pair / feature space)

	LSVI	Q-Learning
Convergence in the tabular case	$Q^{(k)} \to Q^*$	$Q^{(k)} \to Q^*$
Convergence under function approximation	$Q^{(k)} \rightarrow Q^*$ under BC	Diverges even with BC
Update style	Two time-scale	Single time-scale

Techniques for Function Approximation (Deep Q-Learning)

Use LSVI Updates

For k = 1, 2, ...

Collect samples $\mathcal{D}^{(k)}$ (consisting of (s, a, r, s') tuples) using some exploratory policy

Perform regression over dataset $\mathcal{D}^{(1)} \cup \mathcal{D}^{(2)} \cup \cdots \cup \mathcal{D}^{(k)}$:

$$\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{(s, a, r, s') \in \mathcal{D}} \left(Q_{\theta}(s, a) - r + \gamma \max_{a'} Q_{\theta_{k-1}}(s', a') \right)^2$$

Regression

Implement Regression with SGD

For k = 1, 2, ...

Collect samples $\mathcal{D}^{(k)}$ (consisting of (s, a, r, s') tuples) using some exploratory policy

$$\theta_{k-1} \leftarrow \theta$$

For i = 1, 2, ..., n:

Randomly draw a minibatch $\{(s_i, a_i, r_i, s_i')\}_{i=1}^b$ from $\mathcal{D}^{(1)} \cup \mathcal{D}^{(2)} \cup \cdots \cup \mathcal{D}^{(k)}$

$$\theta \leftarrow \theta - \alpha \sum_{i=1}^{b} \nabla_{\theta} \left(Q_{\theta}(s_i, a_i) - r_i + \gamma \max_{a'} Q_{\theta_{k-1}}(s'_i, a') \right)^2$$

Standard Implementation of Deep Q-Learning

Interleaving data collection and SGD

For i = 1, 2, ...

Obtain a new sample (s, a, r, s') and insert it to a **replay buffer** \mathcal{B} Randomly draw a minibatch $\{(s_i, a_i, r_i, s_i')\}_{i=1}^b$ from \mathcal{B} and perform

$$\theta \leftarrow \theta - \alpha \sum_{i=1}^{b} \nabla_{\theta} \left(Q_{\theta}(s_i, a_i) - r_i + \gamma \max_{a'} Q_{\theta_{tar}}(s'_i, a') \right)^2$$

// Option 1

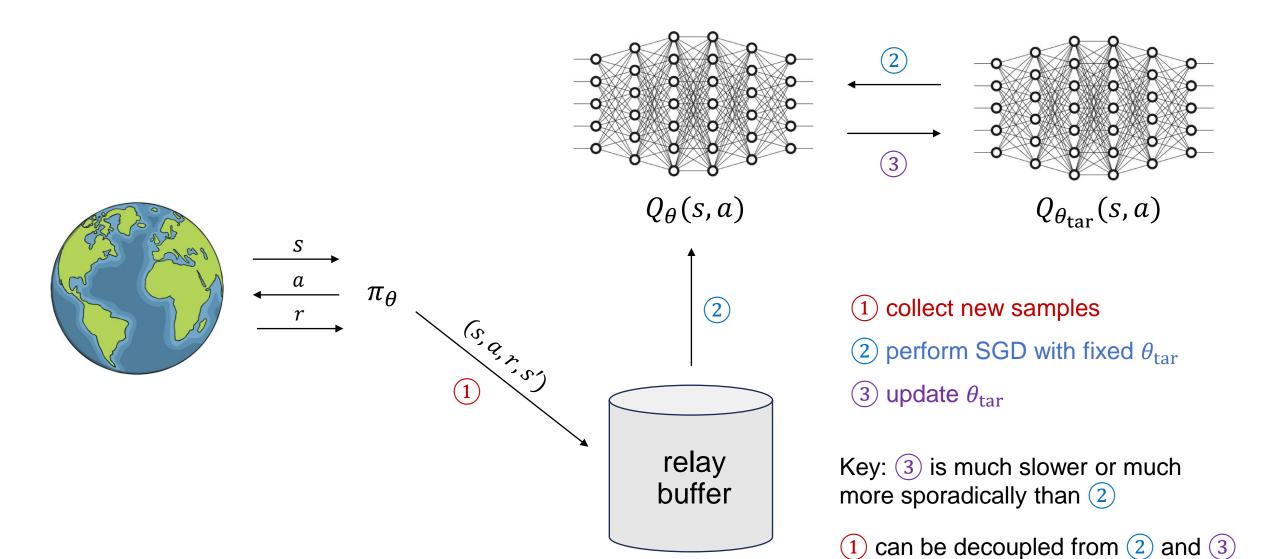
If $i \mod n = 0$:

$$\theta_{\text{tar}} \leftarrow \theta$$

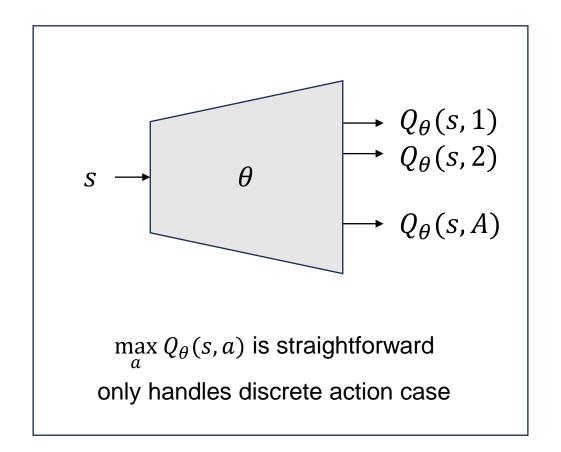
// Option 2

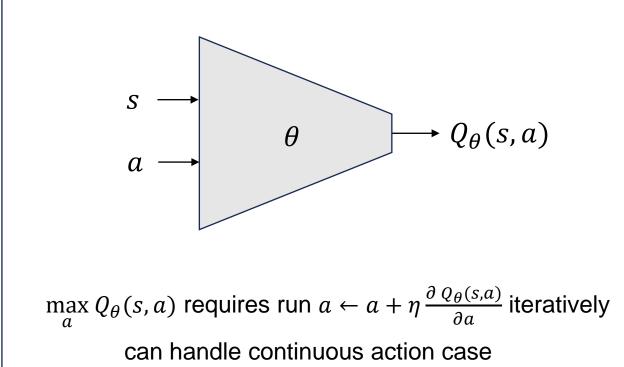
$$\theta_{\text{tar}} \leftarrow \tau \theta_{\text{tar}} + (1 - \tau)\theta$$

Target Network and Replay Buffer



Q-Network Design





Deep Q-Network

Deep Deterministic Policy Gradient (covered later in the semester)

Replay Buffer and Sampling

Standard implementation: First-in-first-out queue + Uniform sampling

- The data collected from π_{θ} is not i.i.d.
- Uniform sampling from a large pool makes the data more similar to i.i.d. the convergence of SGD requires samples to be i.i.d.

Prioritized replay: priority queue + prioritized sampling + importance weight

- Priority queue with priority proportional to $|\delta_i|$, where $\delta_i = Q_{\theta}(s_i, a_i) r_i \gamma \max_{a'} Q_{\theta_{tar}}(s_i', a')$
- Sample from the buffer with probability $P_i \propto |\delta_i|^{\alpha}$
- Perform SGD with importance weight $w_i = \left(\frac{P_i}{\max_j P_j}\right)^{\beta}$, i.e.,

$$\theta \leftarrow \theta - \alpha w_i \nabla_{\theta} \left(Q_{\theta}(s_i, a_i) - r_i + \gamma \max_{a'} Q_{\theta_{tar}}(s'_i, a') \right)^2$$

Schaul, Quan, Antonoglou, Silver. Prioritized Experience Replay. 2015.