

10-701: Introduction to Machine Learning

Lecture 11: Q-Learning and Policy Gradient RL

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10/04/23

Front Matter

- Announcements
 - HW2 released 9/20, due 10/4 (today!) at 11:59 PM
 - HW3 released 10/4 (today!), due 10/11 at 11:59 PM
 - Project details will be released on 10/13
 - You will have a choice between a more research-based project and a more implementation-focused project
 - You must work on the project in groups of 3 or 4;
you may not work on the project alone.
- Recommended Readings
 - Mitchell, Chapter 13

Two big Q's

1. What can we do if the reward and/or transition functions/distributions are unknown?
2. How can we handle infinite (or just very large) state/action spaces?

Recall: Value Iteration

- Inputs: $R(s, a)$, $p(s' | s, a)$, γ
- Initialize $V^{(0)}(s) = 0 \forall s \in \mathcal{S}$ (or randomly) and set $t = 0$
- While not converged, do:

- For $s \in \mathcal{S}$
 - For $a \in \mathcal{A}$

$$Q(s, a) = \underbrace{R(s, a)} + \gamma \sum_{s' \in \mathcal{S}} \underbrace{p(s' | s, a)V(s')}$$

- $V(s) \leftarrow \max_{a \in \mathcal{A}} Q(s, a)$

- For $s \in \mathcal{S}$

$$\pi^*(s) \leftarrow \operatorname{argmax}_{a \in \mathcal{A}} R(s, a) + \gamma \sum_{s' \in \mathcal{S}} p(s' | s, a)V(s')$$

- Return π^*

$Q^*(s, a)$ w/
deterministic
rewards

- $Q^*(s, a) = \mathbb{E}[\text{total discounted reward of taking action } a \text{ in state } s, \text{ assuming all future actions are optimal}]$

$$= R(s, a) + \gamma \sum_{s' \in \mathcal{S}} p(s' | s, a) V^*(s')$$

~~$V^*(s') \equiv \max_{a' \in \mathcal{A}} Q^*(s', a')$~~ 

$$Q^*(s, a) = R(s, a) + \gamma \sum_{s' \in \mathcal{S}} p(s' | s, a) \left[\max_{a' \in \mathcal{A}} Q^*(s', a') \right]$$

$$\pi^*(s) = \operatorname{argmax}_{a \in \mathcal{A}} Q^*(s, a)$$

- Insight: if we know Q^* , we can compute an optimal policy π^* !

$Q^*(s, a)$ w/
deterministic
rewards and
transitions

- $Q^*(s, a) = \mathbb{E}[\text{total discounted reward of taking action } a \text{ in state } s, \text{ assuming all future actions are optimal}]$

$$= R(s, a) + \gamma V^*(\delta(s, a))$$

- $V^*(\delta(s, a)) = \max_{a' \in \mathcal{A}} Q^*(\delta(s, a), a')$

$$Q^*(s, a) = R(s, a) + \gamma \max_{a' \in \mathcal{A}} Q^*(\delta(s, a), a')$$

$$\pi^*(s) = \operatorname{argmax}_{a \in \mathcal{A}} Q^*(s, a)$$

- Insight: if we know Q^* , we can compute an optimal policy π^* !

Learning $Q^*(s, a)$ w/ deterministic rewards and transitions

Algorithm 1: Online learning (table form)

- Inputs: discount factor γ , an initial state s
- Initialize $Q(s, a) = 0 \forall s \in \mathcal{S}, a \in \mathcal{A}$ (Q is a $|\mathcal{S}| \times |\mathcal{A}|$ array)
- While TRUE, do
 - Take a random action a
 - Receive reward $r = R(s, a)$
 - Update the state: $s \leftarrow s'$ where $s' = \delta(s, a)$
 - Update $Q(s, a)$:

$$Q(s, a) \leftarrow r + \gamma \max_{a'} Q(s', a')$$

Learning $Q^*(s, a)$ w/ deterministic rewards and transitions

Algorithm 2: ϵ -greedy online learning (table form)

- Inputs: discount factor γ , an initial state s , greediness parameter $\epsilon \in [0, 1]$
- Initialize $Q(s, a) = 0 \forall s \in \mathcal{S}, a \in \mathcal{A}$ (Q is a $|\mathcal{S}| \times |\mathcal{A}|$ array)
- While TRUE, do
 - With probability ϵ , take the greedy action
 $\longrightarrow a = \operatorname{argmax}_{a' \in \mathcal{A}} Q(s, a')$
 - \longrightarrow Otherwise, with probability $1 - \epsilon$, take a random action a
 - Receive reward $r = R(s, a)$
 - Update the state: $s \leftarrow s'$ where $s' = \delta(s, a)$
 - Update $Q(s, a)$:
$$Q(s, a) \leftarrow r + \gamma \max_{a'} Q(s', a')$$

Learning $Q^*(s, a)$ w/ deterministic rewards

Algorithm 3: ϵ -greedy online learning (table form)

- Inputs: discount factor γ , an initial state s , greediness parameter $\epsilon \in [0, 1]$, learning rate $\alpha \in [0, 1]$ (“trust parameter”)
- Initialize $Q(s, a) = 0 \forall s \in \mathcal{S}, a \in \mathcal{A}$ (Q is a $|\mathcal{S}| \times |\mathcal{A}|$ array)
- While TRUE, do
 - With probability ϵ , take the greedy action
$$a = \operatorname{argmax}_{a' \in \mathcal{A}} Q(s, a')$$
 - Otherwise, with probability $1 - \epsilon$, take a random action a
 - Receive reward $r = R(s, a)$
 - Update the state: $s \leftarrow s'$ where $s' \sim p(s' | s, a)$
 - Update $Q(s, a)$:

$$\rightarrow Q(s, a) \leftarrow (1 - \alpha) \underbrace{Q(s, a)}_{\text{Current value}} + \alpha \underbrace{\left(r + \gamma \max_{a'} Q(s', a') \right)}_{\text{Update w/ deterministic transitions}}$$

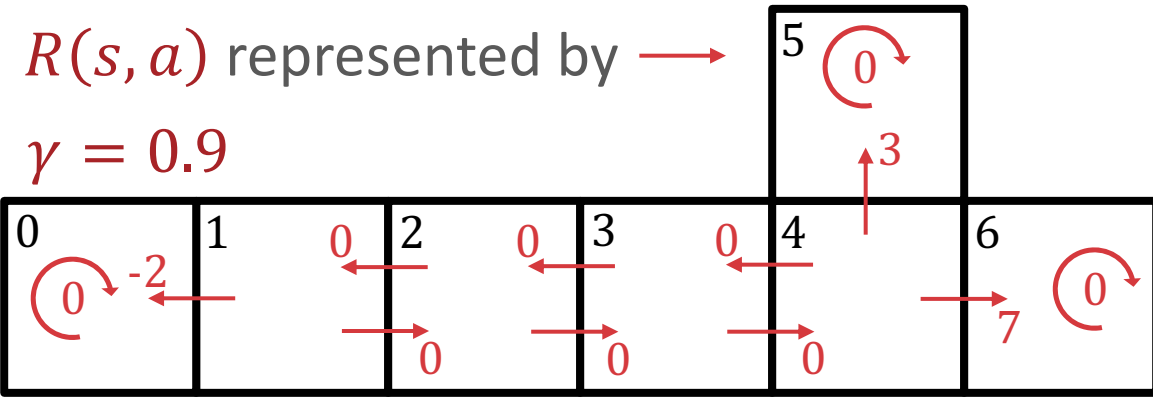
Learning $Q^*(s, a)$ w/ deterministic rewards

Algorithm 3: ϵ -greedy online learning (table form)

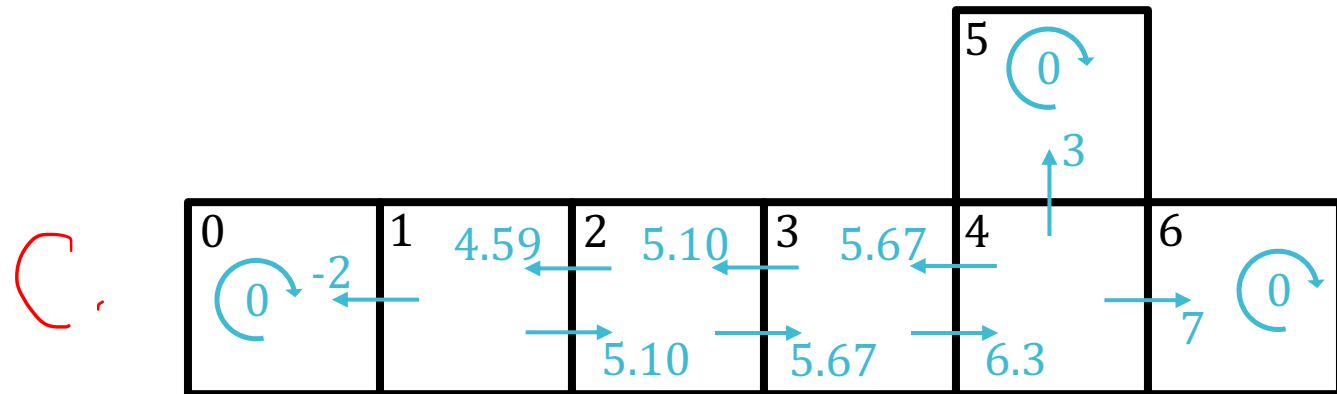
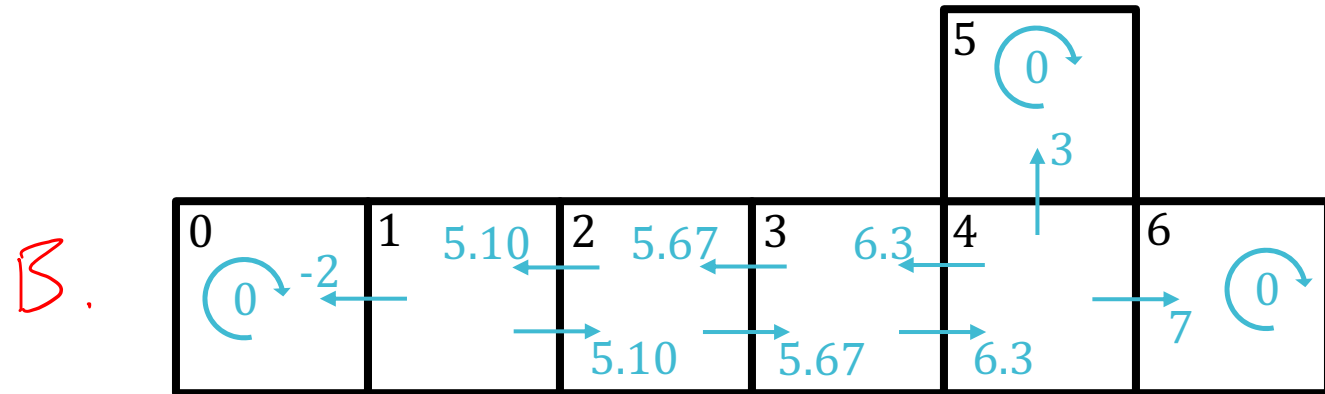
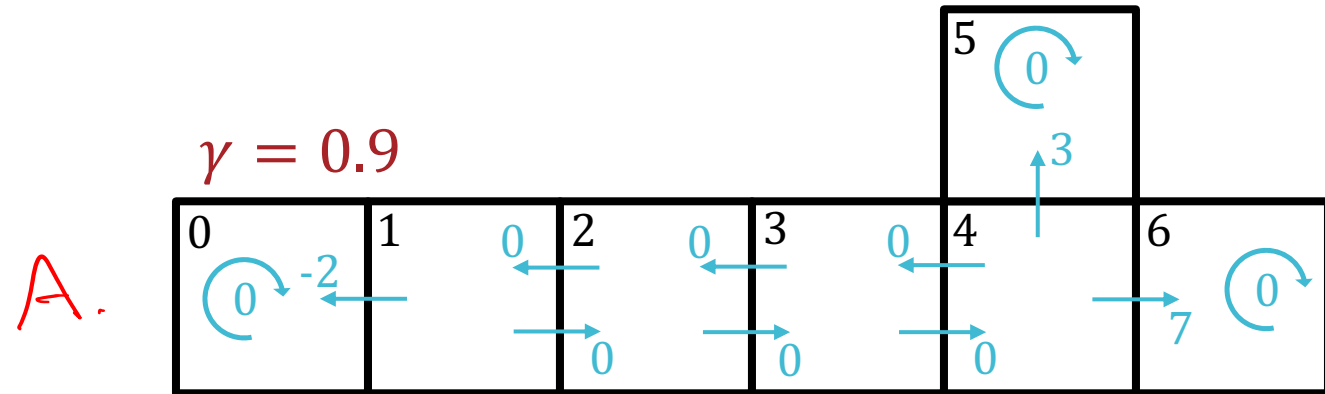
- Inputs: discount factor γ , an initial state s , greediness parameter $\epsilon \in [0, 1]$, learning rate $\alpha \in [0, 1]$ (“trust parameter”)
- Initialize $Q(s, a) = 0 \forall s \in \mathcal{S}, a \in \mathcal{A}$ (Q is a $|\mathcal{S}| \times |\mathcal{A}|$ array)
- While TRUE, do
 - With probability ϵ , take the greedy action
$$a = \operatorname{argmax}_{a' \in \mathcal{A}} Q(s, a')$$
 - Otherwise, with probability $1 - \epsilon$, take a random action a
 - Receive reward $r = R(s, a)$
 - Update the state: $s \leftarrow s'$ where $s' \sim p(s' | s, a)$
 - Update $Q(s, a)$: Temporal difference

$$Q(s, a) \leftarrow \underbrace{Q(s, a)}_{\text{Current value}} + \alpha \left(\underbrace{r + \gamma \max_{a'} Q(s', a')}_{\text{Temporal difference target}} - Q(s, a) \right)$$

Learning $Q^*(s, a)$: Example

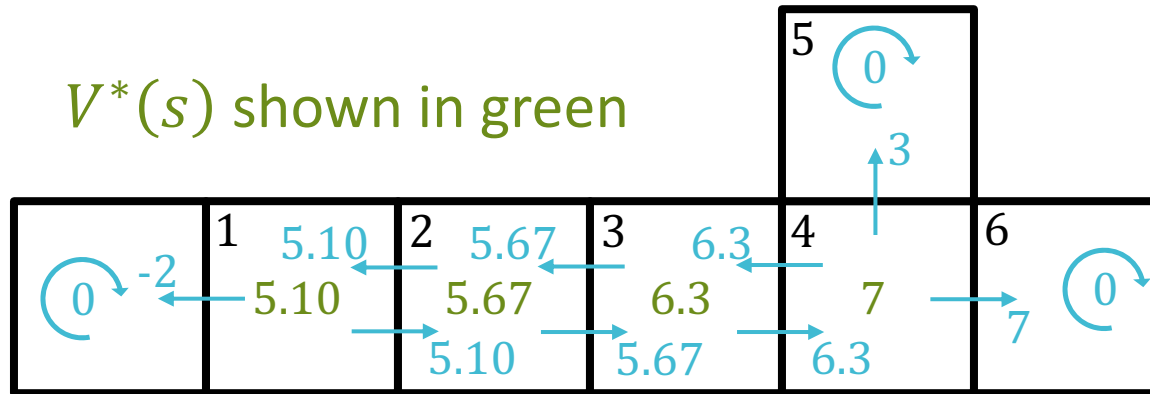


Which set of blue arrows (roughly) corresponds to $Q^*(s, a)$?

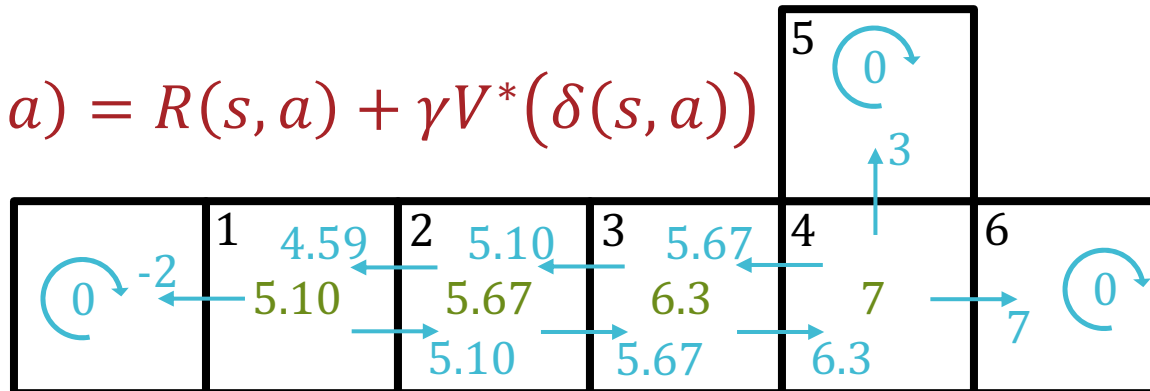


Which set of blue arrows (roughly) corresponds to $Q^*(s, a)$?

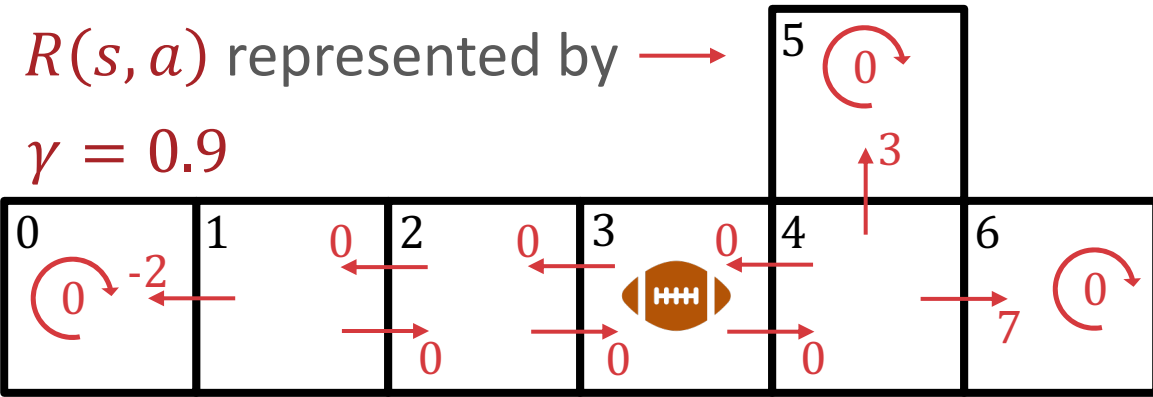
$V^*(s)$ shown in green



$$Q^*(s, a) = R(s, a) + \gamma V^*(\delta(s, a))$$

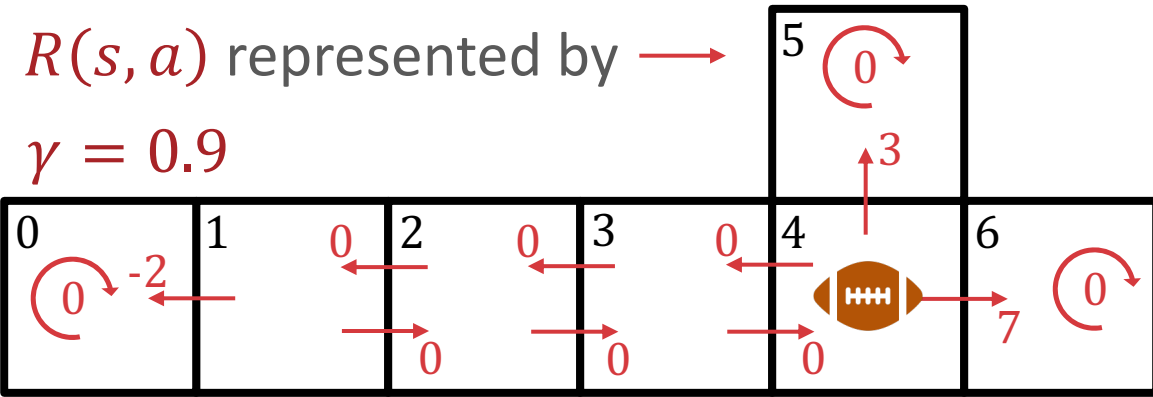


Learning $Q^*(s, a)$: Example



$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\updownarrow
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

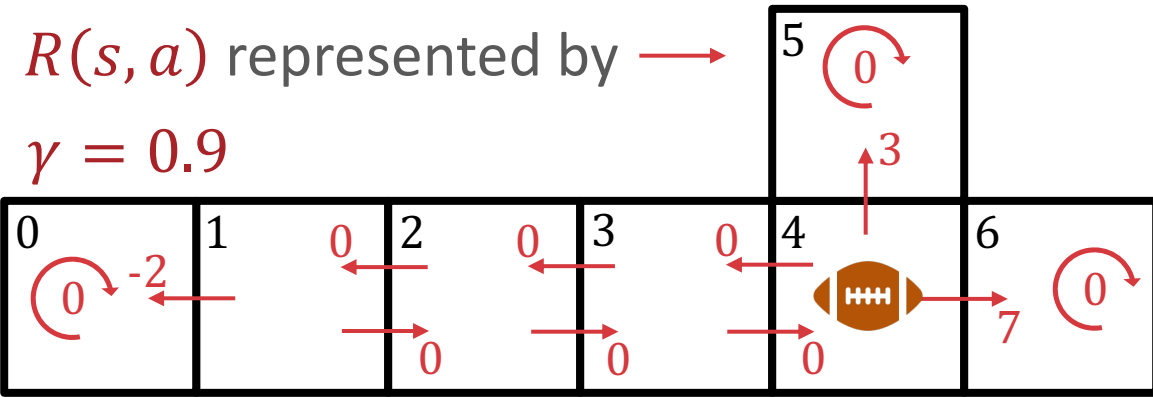
Learning $Q^*(s, a)$: Example



$$Q(3, \rightarrow) \leftarrow 0 + (0.9) \max_{a' \in \{\rightarrow, \leftarrow, \uparrow, \cup\}} Q(4, a') = 0$$

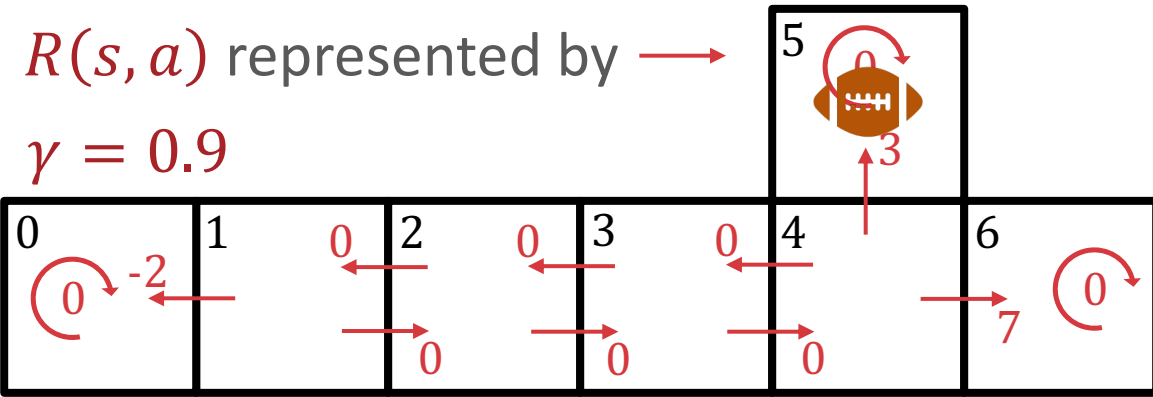
$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\cup
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

Learning $Q^*(s, a)$: Example



$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\updownarrow
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

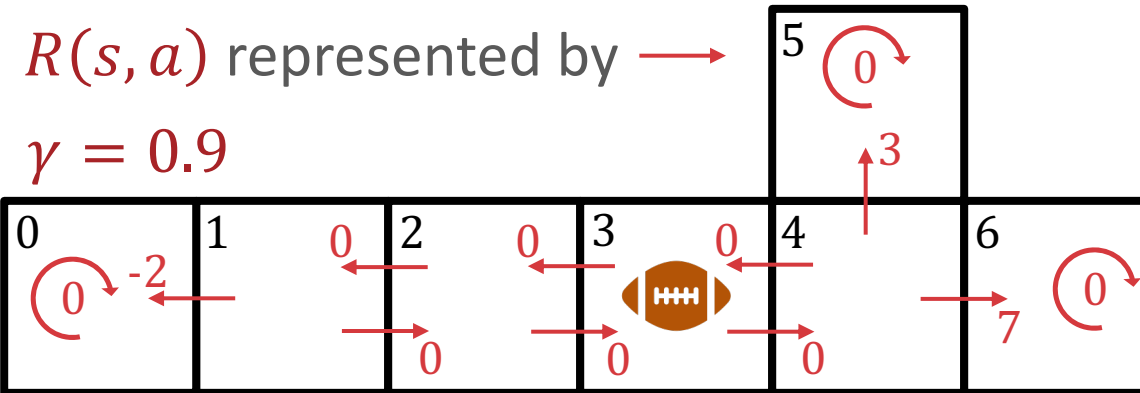
Learning $Q^*(s, a)$: Example



$$Q(4, \uparrow) \leftarrow 3 + (0.9) \max_{a' \in \{\rightarrow, \leftarrow, \uparrow, \cup\}} Q(5, a') = 3$$

$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\cup
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

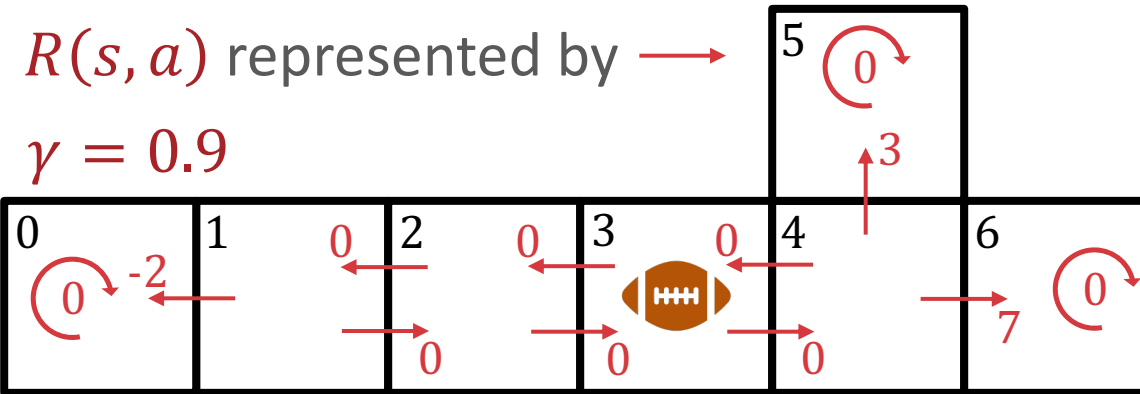
Learning $Q^*(s, a)$: Example



$$Q(3, \rightarrow) \leftarrow 0 + (0.9) \max_{a' \in \{\rightarrow, \leftarrow, \uparrow, \cup\}} Q(4, a') = 2.7$$

$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\cup
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	3	0
5	0	0	0	0
6	0	0	0	0

Learning $Q^*(s, a)$: Example



$$Q(3, \rightarrow) \leftarrow 0 + (0.9) \max_{a' \in \{\rightarrow, \leftarrow, \uparrow, \cup\}} Q(4, a') = 2.7$$

$Q(s, a)$	\rightarrow	\leftarrow	\uparrow	\cup
0	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	2.7	0	0	0
4	0	0	3	0
5	0	0	0	0
6	0	0	0	0

Learning $Q^*(s, a)$: Convergence

- For Algorithms 1 & 2 (deterministic transitions), Q converges to Q^* if
 1. Every valid state-action pair is visited infinitely often
 - Q-learning is exploration-insensitive: any visitation strategy that satisfies this property will work!
 2. $0 \leq \gamma < 1$
 3. $\exists \beta$ s.t. $|R(s, a)| < \beta \forall s \in \mathcal{S}, a \in \mathcal{A}$
 4. Initial Q values are finite

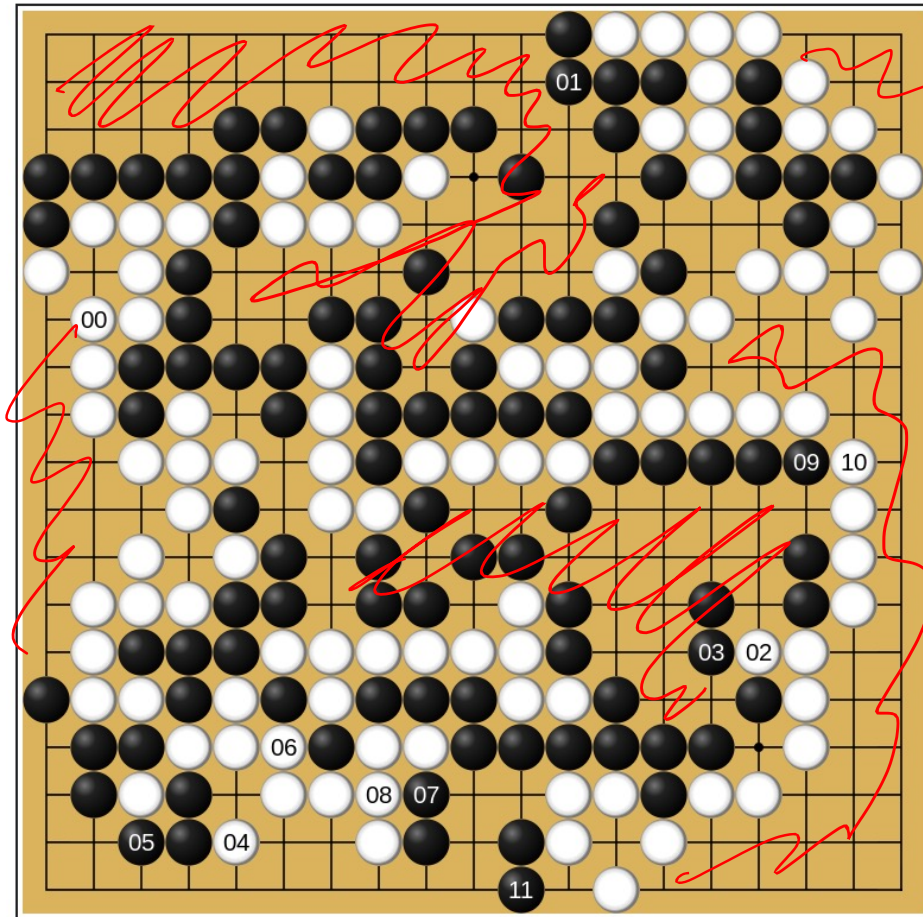
Learning $Q^*(s, a)$: Convergence

- For Algorithm 3 (temporal difference learning), Q converges to Q^* if
 1. Every valid state-action pair is visited infinitely often
 - Q-learning is exploration-insensitive: any visitation strategy that satisfies this property will work!
 2. $0 \leq \gamma < 1$
 3. $\exists \beta$ s.t. $|R(s, a)| < \beta \forall s \in \mathcal{S}, a \in \mathcal{A}$
 4. Initial Q values are finite
 5. Learning rate α_t follows some “schedule” s.t.
 $\sum_{t=0}^{\infty} \alpha_t = \infty$ and $\sum_{t=0}^{\infty} \alpha_t^2 < \infty$ e.g., $\alpha_t = 1/t+1$

Two big Q's

1. What can we do if the reward and/or transition functions/distributions are unknown?
 - Use online learning to gather data and learn $Q^*(s, a)$
2. How can we handle infinite (or just very large) state/action spaces?

AlphaGo (Black) vs. Lee Sedol (White) Game 2 final position (AlphaGo wins)

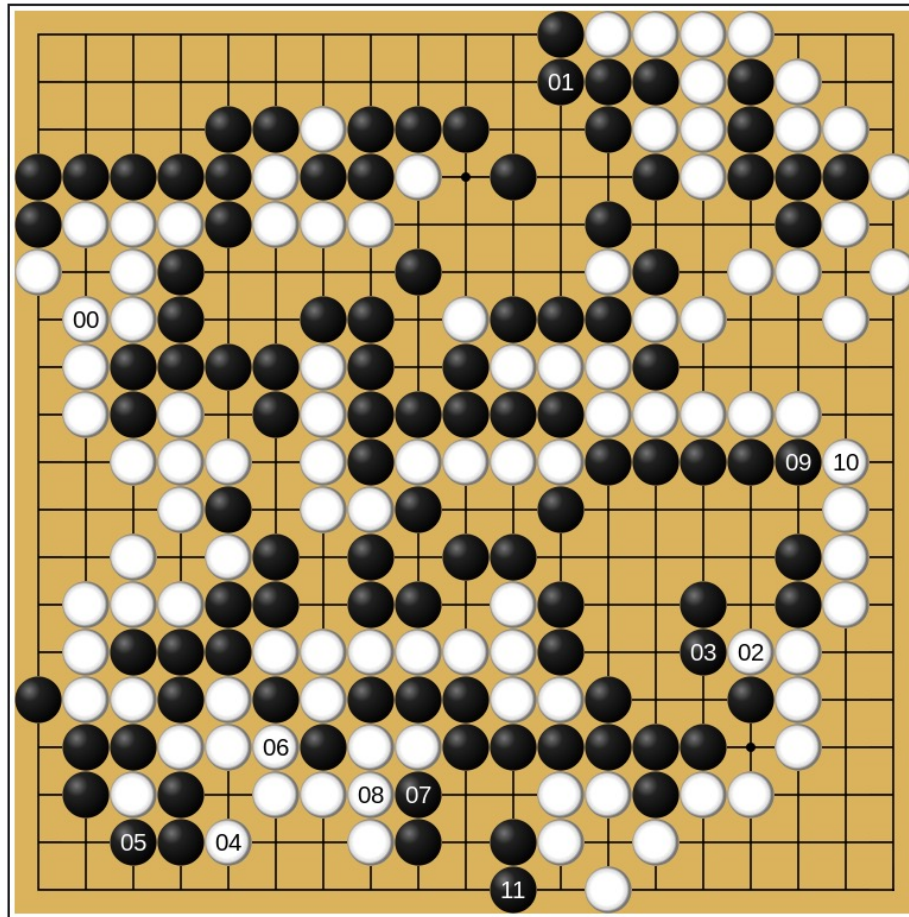


Playing Go

- 19-by-19 board
- Players alternate placing black and white stones
- The goal is claim more territory than the opponent
- How many legal Go board states are there?

of stars in universe $\approx 10^{23}$

AlphaGo (Black) vs. Lee Sedol (White) Game 2 final position (AlphaGo wins)



Playing Go

- 19-by-19 board
- Players alternate placing black and white stones
- The goal is claim more territory than the opponent
- There are $\sim 10^{170}$ legal Go board states!

of games of chess $\approx 10^{120}$

Two big Q's

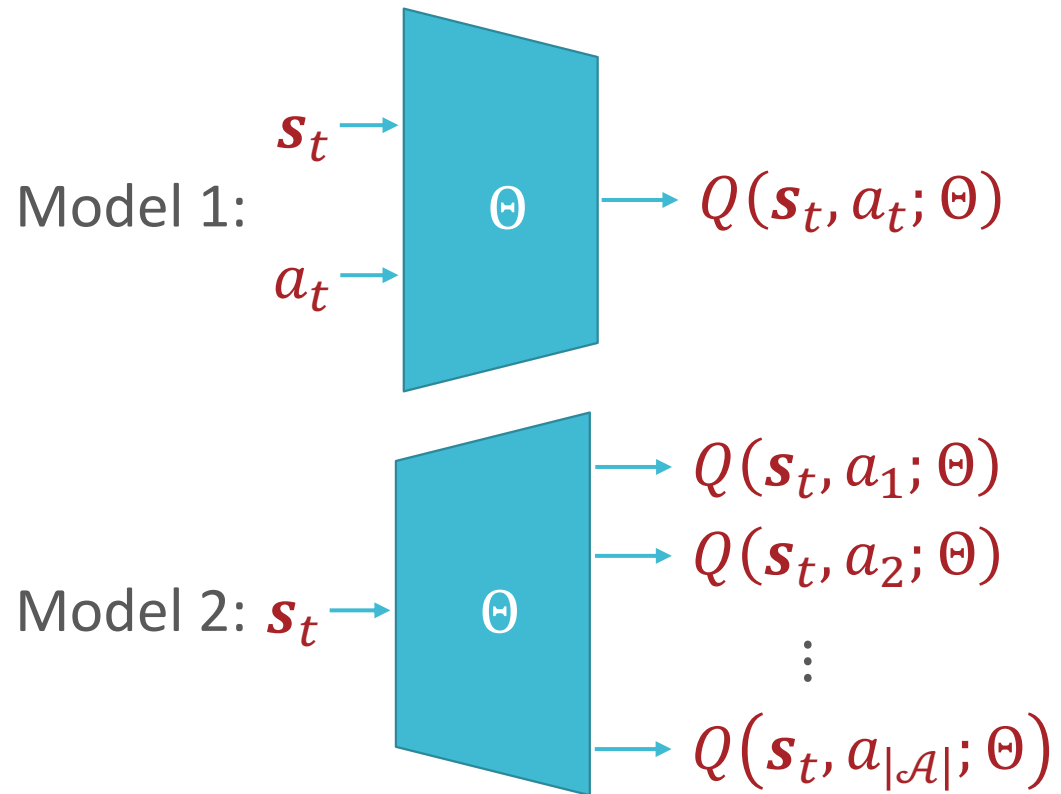
1. What can we do if the reward and/or transition functions/distributions are unknown?
 - Use online learning to gather data and learn $Q^*(s, a)$
2. How can we handle infinite (or just very large) state/action spaces?
 - Throw a neural network at it!

Deep Q-learning

- Use a parametric function, $Q(s, a; \Theta)$, to approximate $Q^*(s, a)$
 - Learn the parameters using *stochastic* gradient descent (SGD)
 - Training data $(\mathbf{s}_t, a_t, r_t, \mathbf{s}_{t+1})$ gathered online by the agent/learning algorithm

Deep Q-learning: Model

- Represent states using some feature vector $\mathbf{s}_t \in \mathbb{R}^M$
e.g. for Go, $\mathbf{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that approximates Q



Deep Q-learning: Loss Function

- “True” loss

$$\ell(\Theta) = \sum_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} \underbrace{(Q^*(s, a) - Q(s, a; \Theta))}_{\text{2. Don't know } Q^*}^2$$

1. \mathcal{S} too big to compute this sum

1. Use stochastic gradient descent: just consider one state-action pair in each iteration

2. Use temporal difference learning:

- Given current parameters $\Theta^{(t)}$ the temporal difference target is

$$Q^*(s, a) \approx r + \gamma \max_{a'} Q(s', a'; \Theta^{(t)}) := y$$

- Set the parameters in the next iteration $\Theta^{(t+1)}$ such that $Q(s, a; \Theta^{(t+1)}) \approx y$

$$\rightarrow \ell(\Theta^{(t)}, \Theta^{(t+1)}) = \left(y - Q(s, a; \Theta^{(t+1)}) \right)^2$$

Deep Q-learning

Algorithm 4: Online learning (parametric form)

- Inputs: discount factor γ , an initial state s_0 , learning rate α
- Initialize parameters $\Theta^{(0)}$
- For $t = 0, 1, 2, \dots$
 - Gather training sample (s_t, a_t, r_t, s_{t+1})
 - Update $\Theta^{(t)}$ by taking a step opposite the gradient

$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \alpha \nabla_{\Theta} \ell(\Theta^{(t)}, \Theta^{(t)})$$

where

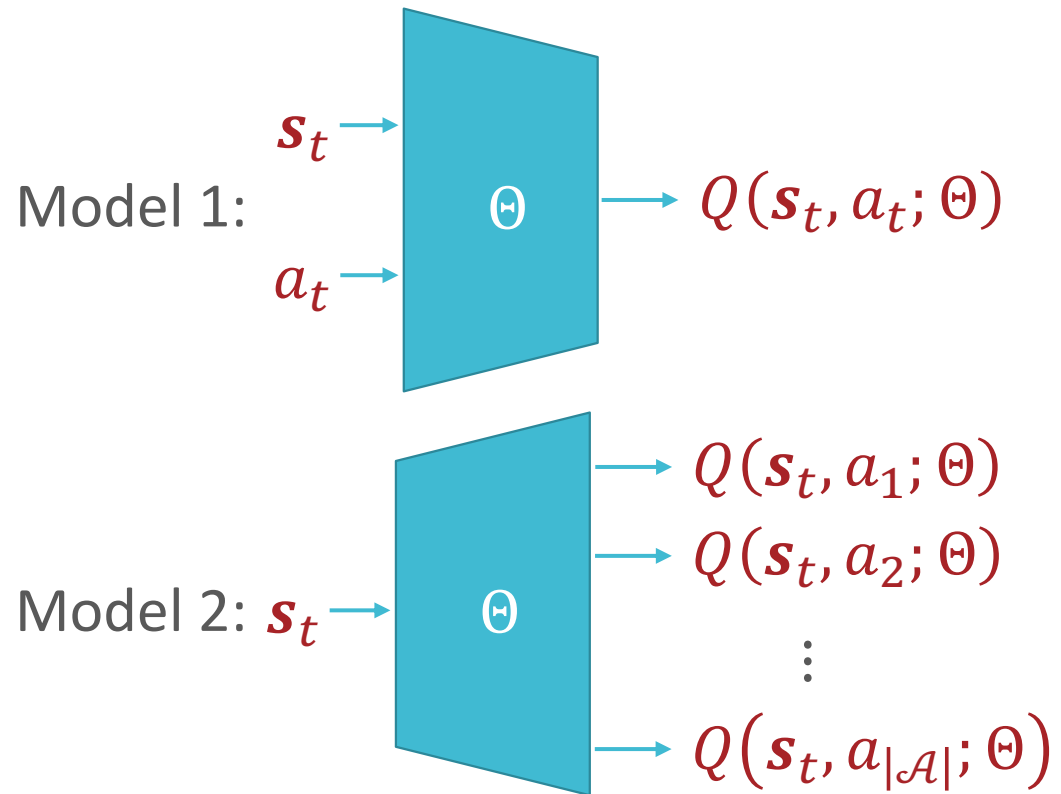
$$\begin{aligned} & \nabla_{\Theta} \ell(\Theta^{(t)}, \Theta^{(t)}) \\ &= 2 \left(\gamma^{(t)} Q(s, a; \Theta^{(t)}) \right) \nabla_{\Theta} Q(s, a; \Theta^{(t)}) \end{aligned}$$

Deep Q-learning: Experience Replay

- SGD assumes i.i.d. training samples but in RL, samples are *highly* correlated
- Idea: keep a “replay memory” $\mathcal{D} = \{e_1, e_2, \dots, e_N\}$ of the N most recent experiences $e_t = (s_t, a_t, r_t, s_{t+1})$ (Lin, 1992)
 - Also keeps the agent from “forgetting” about recent experiences
- Alternate between:
 1. Sampling some e_i uniformly at random from \mathcal{D} and applying a Q-learning update (repeat T times)
 2. Adding a new experience to \mathcal{D}
- Can also sample experiences from \mathcal{D} according to some distribution that prioritizes experiences with high error (Schaul et al., 2016)

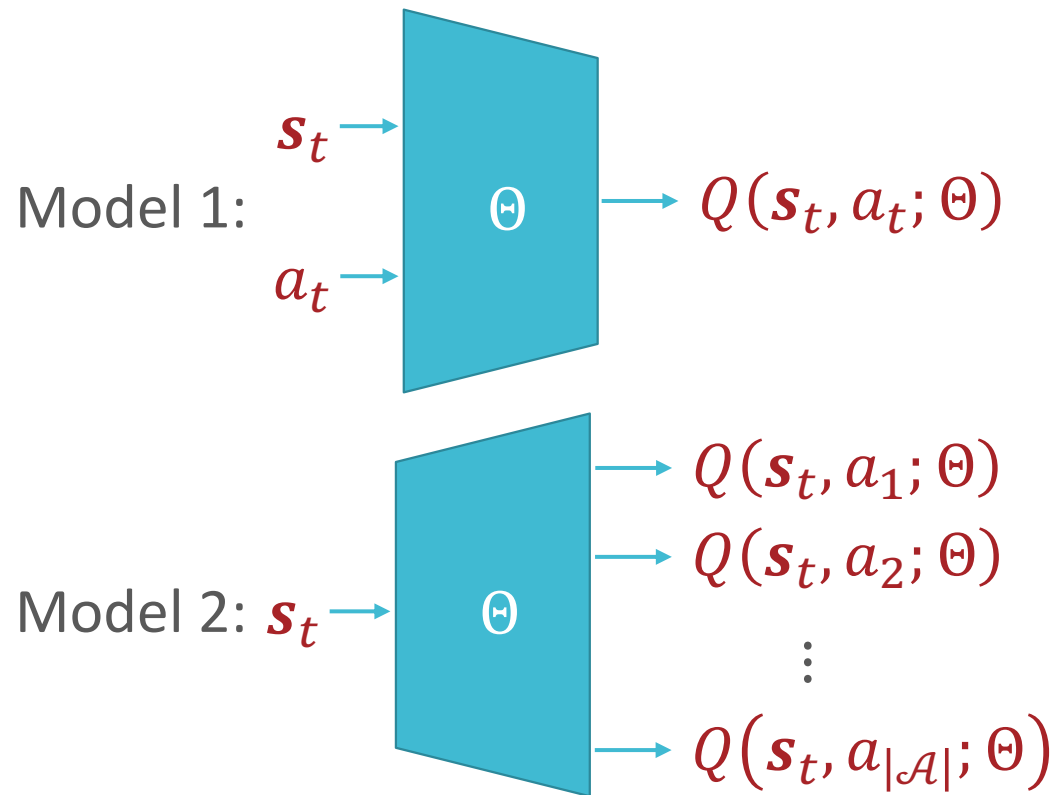
Deep Q-learning: Model

- Represent states using some feature vector $\mathbf{s}_t \in \mathbb{R}^M$
e.g. for Go, $\mathbf{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that approximates Q



What if instead of optimizing the Q-function, we could optimize the policy directly?

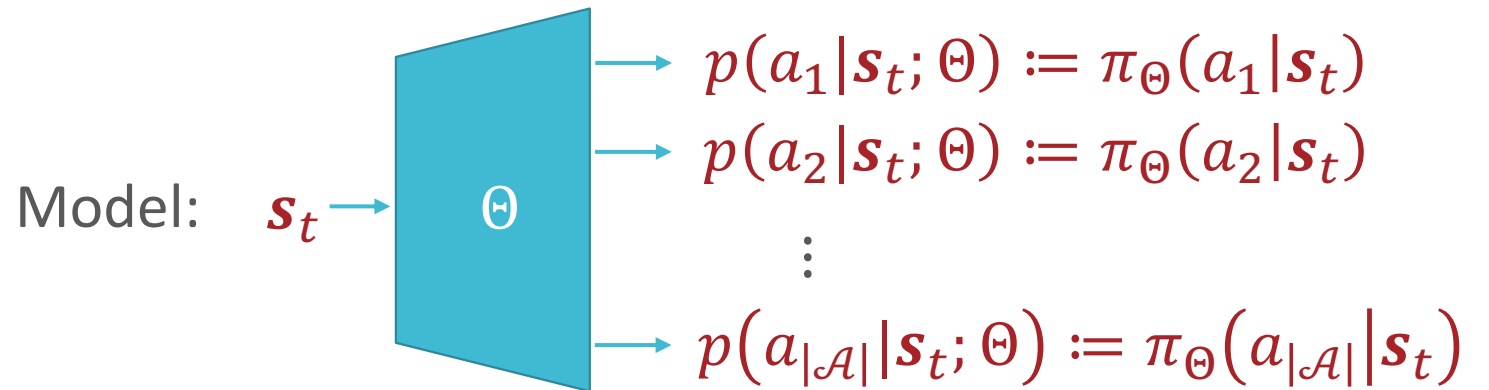
- Represent states using some feature vector $\mathbf{s}_t \in \mathbb{R}^M$ e.g. for Go, $\mathbf{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that approximates Q



Parametrized Stochastic Policies

- Represent states using some feature vector $\mathbf{s}_t \in \mathbb{R}^M$
e.g. for Go, $\mathbf{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that specifies a *stochastic* policy π_{Θ}
- Minimize the negative expected total reward w.r.t. Θ

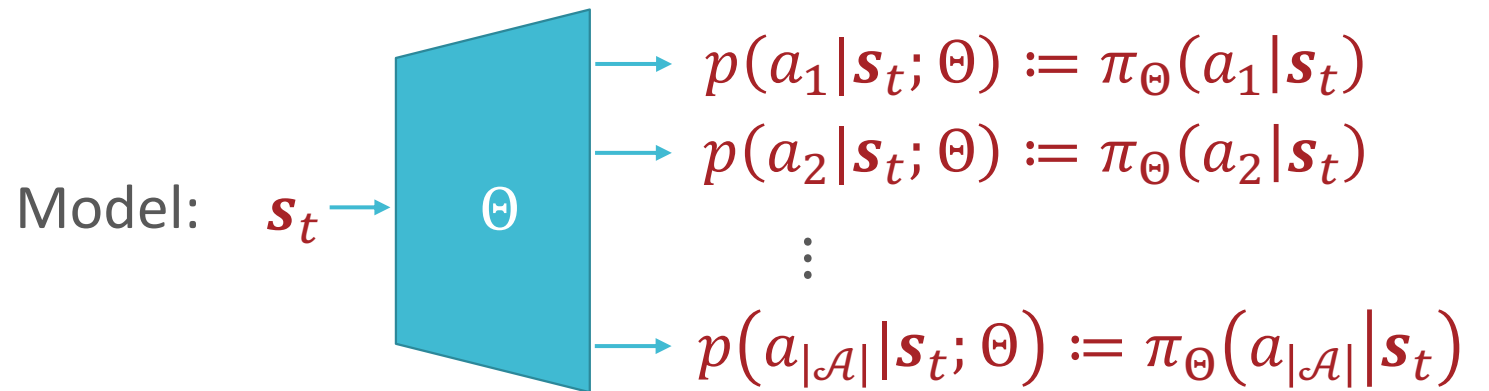
$$\ell(\Theta) = -\mathbb{E}_{\pi_{\Theta}} \left[\sum_{t=0}^{\infty} \gamma^t r_t \right]$$



Okay... but
how on earth
do we
compute the
gradient of this
thing?

- Represent states using some feature vector $\mathbf{s}_t \in \mathbb{R}^M$
e.g. for Go, $\mathbf{s}_t = [1, 0, -1, \dots, 1]^T$
- Define a *differentiable* function that specifies a stochastic policy π_{Θ}
- Minimize the negative expected total reward w.r.t. Θ

$$\ell(\Theta) = -\mathbb{E}_{\pi_{\Theta}} \left[\mathbb{E}_{p(s'|s, a)} \left[\sum_{t=0}^{\infty} \gamma^t r_t \right] \right]$$



Trajectories

- A trajectory $\mathbf{T} = \{\mathbf{s}_0, a_0, \mathbf{s}_1, a_1, \dots, \mathbf{s}_T\}$ is one run of an agent through an MDP ending in a terminal state, \mathbf{s}_T
- Our stochastic policy and the transition distribution induce a distribution over trajectories

$$\begin{aligned} \mathbb{P}_{\Theta}(\mathbf{T}) &= \mathbb{P}(\{s_0, a_0, s_1, a_1, \dots, s_T\}) \\ &= \mathbb{P}(s_0) \prod_{t=0}^{T-1} \underbrace{\pi_{\Theta}(a_t | s_t)}_{\text{distribution over initial states}} p(s_{t+1} | s_t, a_t) \end{aligned}$$

- If all runs end at a terminal state, then we can rewrite the negative expected total reward as

$$\ell(\Theta) = -\mathbb{E}_{\mathbb{P}_{\Theta}(\mathbf{T}=\{s_0, a_0, \dots, s_T\})} \left[\sum_{t=0}^{T-1} \gamma^t R(\mathbf{s}_t, a_t) \right] := -\mathbb{E}_{\mathbb{P}_{\Theta}(\mathbf{T})} [\underline{R(\mathbf{T})}]$$

Likelihood
Ratio
Method
a.k.a.
REINFORCE
(Williams,
1992)

$$\begin{aligned}\nabla_{\Theta} \ell(\Theta) &= \nabla_{\Theta} (-\mathbb{E}_{p_{\Theta}(T)}[R(T)]) = \nabla_{\Theta} \left(-\int R(T) p_{\Theta}(T) dT \right) \\ &= -\int R(T) \nabla_{\Theta} p_{\Theta}(T) dT \\ &= -\int R(T) \nabla_{\Theta} \left(p(\mathbf{s}_0) \prod_{t=0}^{T-1} p(s_{t+1} | s_t, a_t) \pi_{\Theta}(a_t | \mathbf{s}_t) \right) dT\end{aligned}$$

- Issues:
 - The transition probabilities $p(s_{t+1} | s_t, a_t)$ are unknown a priori
 - Computing $\nabla_{\Theta} p_{\Theta}(T)$ involves taking the gradient of a product

Likelihood
Ratio
Method
a.k.a.
REINFORCE
(Williams,
1992)

$$\begin{aligned}\nabla_{\Theta} \ell(\Theta) &= \nabla_{\Theta} (-\mathbb{E}_{p_{\Theta}(T)}[R(T)]) = \nabla_{\Theta} \left(-\int R(T) p_{\Theta}(T) dT \right) \\ &= -\int R(T) \nabla_{\Theta} p_{\Theta}(T) dT \\ &= -\int R(T) \nabla_{\Theta} \left(p(\mathbf{s}_0) \prod_{t=0}^{T-1} p(s_{t+1} | s_t, a_t) \pi_{\Theta}(a_t | s_t) \right) dT\end{aligned}$$

- Insight:

$$\nabla_{\Theta} p_{\Theta}(T) = \frac{p_{\Theta}(T)}{p_{\Theta}(T)} \nabla_{\Theta} p_{\Theta}(T) = p_{\Theta}(T) \nabla_{\Theta} \log p_{\Theta}(T)$$

$$\log p_{\Theta}(T) = \log p(s_0) + \sum_{t=0}^{T-1} \log p(s_{t+1} | s_t, a_t) + \log \pi_{\Theta}(a_t | s_t)$$

$$\nabla_{\Theta} \log p_{\Theta}(T) = \sum_{t=0}^{T-1} \nabla_{\Theta} \log \pi_{\Theta}(a_t | s_t)$$

Likelihood
Ratio
Method
a.k.a.
REINFORCE
(Williams,
1992)

$$\begin{aligned}\nabla_{\Theta} \ell(\Theta) &= \nabla_{\Theta} (-\mathbb{E}_{p_{\Theta}(T)}[R(T)]) = \nabla_{\Theta} \left(-\int R(T) p_{\Theta}(T) dT \right) \\ &= -\int R(T) \nabla_{\Theta} p_{\Theta}(T) dT = -\int R(T) \nabla_{\Theta} (\log p_{\Theta}(T)) p_{\Theta}(T) dT \\ &= -\mathbb{E}_{p_{\Theta}(T)} [R(T) \nabla_{\Theta} (\log p_{\Theta}(T))] \end{aligned}$$

$$\rightarrow \approx -\frac{1}{N} \sum_{n=1}^N R(T^{(n)}) \nabla_{\Theta} (\log p_{\Theta}(T^{(n)}))$$

(where $T^{(n)} = \{\mathbf{s}_0^{(n)}, a_0^{(n)}, \mathbf{s}_1^{(n)}, a_1^{(n)}, \dots, \mathbf{s}_{T^{(n)}}^{(n)}\}$ is a sampled trajectory)

$$= -\frac{1}{N} \sum_{n=1}^N \left(\sum_{t=0}^{T^{(n)}-1} \gamma^t R(\mathbf{s}_t^{(n)}, a_t^{(n)}) \right) \left(\sum_{t=0}^{T^{(n)}-1} \nabla_{\Theta} \log \pi_{\Theta}(a_t^{(n)} | \mathbf{s}_t^{(n)}) \right)$$

Likelihood Ratio Method a.k.a. REINFORCE (Williams, 1992)

- Practical considerations:
 - Sampled trajectories/rewards can be highly variable, which leads to unstable estimates of the expectation
 - Can compare sampled rewards against a *baseline* by subtracting some constant value from $R(T)$ (Peters and Schaal, 2008)
 - Policy gradient methods are *on-policy*: they require using the current (potentially bad) policy to sample (a lot of) trajectories...
 - Can use a surrogate policy and adjust gradient computation via *importance sampling*
 - Not compatible with deterministic policies (would require knowledge of the transition probabilities)

Key Takeaways

- We can use (deep) Q-learning when the reward/transition functions are unknown and/or when the state/action spaces are too large to be modelled directly
 - Also guaranteed to converge under certain assumptions
 - Experience replay can help address non-i.i.d. samples
- If our policy is parametrized, we can directly optimize the parameters using the policy gradient
 - The gradient can be expressed in a tractable way via the likelihood ratio method
 - We can approximate the gradient by sampling trajectories