10-301/601: Introduction to Machine Learning Lecture 22: Q-learning and Deep RL

Matt Gormley & Henry Chai

11/13/24

### Front Matter

- Announcements
	- HW7 released 11/7, due 11/17 at 11:59 PM
		- Please be mindful of your grace day usage (see [the course syllabus](https://www.cs.cmu.edu/~hchai2/courses/10601/#Syllabus) for the policy)
	- Exam 2 viewings happening this week on Tuesday, Wednesday and Thursday, after our regularly scheduled OH
		- Please check [the OH calendar](https://www.cs.cmu.edu/~mgormley/courses/10601/officehours.html) for exact times and locations

Q: How can I get one of those sweet hoodies you're wearing?

- Applications are due by Wednesday, November 20<sup>th</sup> (1 week from today)
- For more information and the application, see [https://www.ml.cmu.edu](https://www.ml.cmu.edu/academics/ta.html) /academics/ta.html



## Recall: Synchronous vs. Asynchronous Value Iteration

Algorithm 1 Asynchronous Value Iteration

- 1: **procedure** ASYNCHRONOUSVALUEITERATION $(R(s, a), p(\cdot | s, a))$
- Initialize value function  $V(s) = 0$  or randomly  $2:$
- while not converged do  $\overline{3}$ :

$$
\mathsf{for} s \in S/\mathsf{do}
$$

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

Let  $\pi(s) = \arg\max_a R(s, a) + \gamma \sum_{s' \in S} p(s'|s, a)V(s')$ ,  $\forall s$  $6:$ 

return  $\pi$  $7:$ 

4:  $5:$ 

Algorithm 1 Synchronous Value Iteration 1: **procedure** SYNCHRONOUSVALUE TERATION( $R(s, a)$ ,  $p(\cdot|s, a)$ ) Initialize value function  $V(s)^{(0)} = 0$  or randomly  $2:$  $t=0$  $\ddot{ }$ while not converged do  $4:$ for  $s \in \mathcal{S}$  do  $5:$  $V(s)^{(t+1)} = \max_{a} R(s,a) + \gamma \sum_{s' \in \mathcal{S}} p(s'|s,a)V(s')^{(t)}$ 6:  $t=t+1$  $7:$ Let  $\pi(s) = \argmax_a R(s, a) + \gamma \sum_{s' \in S} p(s'|s, a)V(s')$ ,  $\forall s$ 8: return  $\pi$ 9:

asynchronous updates: compute and update  $V(s)$  for each state one at a time

synchronous updates: compute all the fresh values of  $V(s)$  from all the stale values of  $V(s)$ , then update  $V(s)$  with fresh values

#### Recall:

## Value Iteration **Theory**

**Theorem 1**: Value function convergence

V will converge to  $V^*$  if each state is "visited"

infinitely often (Bertsekas, 1989)

 **Theorem 2**: Convergence criterion if max  $s \in \mathcal{S}$  $|V^{(t+1)}(s) - V^{(t)}(s)| < \epsilon,$ then max  $s \in \mathcal{S}$  $|V^{(t+1)}(s) - V^*(s)| <$  $2\epsilon\gamma$  $1-\gamma$ (Williams & Baird, 1993) **Theorem 3**: Policy convergence The "greedy" policy,  $\pi(s) = \argmax\,Q(s,a)$ , converges to the  $a \in \mathcal{A}$ optimal  $\pi^*$  in a finite number of iterations, often before the value function has converged! (Bertsekas, 1987)

Q: What happens when the rewards are stochastic? **Theorem 1**: Value function convergence

V will converge to  $V^*$  if each state is "visited"

infinitely often (Bertsekas, 1989)

 **Theorem 2**: Convergence criterion if max  $s \in \mathcal{S}$  $|V^{(t+1)}(s) - V^{(t)}(s)| < \epsilon,$ then max  $s \in \mathcal{S}$  $|V^{(t+1)}(s) - V^*(s)| <$  $2\epsilon\gamma$  $1-\gamma$ (Williams & Baird, 1993) **Theorem 3**: Policy convergence

The "greedy" policy,  $\pi(s) = \argmax\,Q(s,a)$ , converges to the  $a \in \mathcal{A}$ optimal  $\pi^*$  in a finite number of iterations, often before

the value function has converged! (Bertsekas, 1987)

## **Stochastic** Rewards

• Insight: one way of representing stochastic rewards is with *deterministic* rewards that depend on the next state,  $s_{t+1}$ , assuming transitions are stochastic



### **Stochastic** Rewards

• Insight: one way of representing stochastic rewards is with *deterministic* rewards that depend on the next state,  $s_{t+1}$ , assuming transitions are stochastic

This optimal value function can be represented recursively as:

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

If  $R(s, a, s') = R(s, a)$  (deterministic reward), then we have the form:

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

## **Stochastic** Rewards

• Insight: one way of representing stochastic rewards is with *deterministic* rewards that depend on the next state,  $s_{t+1}$ , assuming transitions are stochastic

Algorithm 1 Value Iteration (stochastic transitions, stochastic rewards)

- 1: **procedure** VALUEITERATION( $R(s, a, s')$  reward function,  $p(\cdot|s, a)$  transition probabilities)
- Initialize value function  $V(s) = 0$  or randomly  $2:$
- while not converged do  $3:$

4: **for** 
$$
s \in S
$$
 **do**  
\n5:  $V(s) = \max_{a} \sum_{s' \in S} p(s'|s, a) (R(s, a, s') + \gamma V(s'))$   
\n6: Let  $\pi(s) = \operatorname{argmax}_{a} \sum_{s' \in S} p(s'|s, a) (R(s, a, s') + \gamma V(s'))$ ,  $\forall s$   
\n**return**  $\pi$ 

Q: If the thing we care about learning is the policy, why don't we just learn that directly?

• Insight: one way of representing stochastic rewards is with *deterministic* rewards that depend on the next state,  $s_{t+1}$ , assuming transitions are stochastic

Algorithm 1 Value Iteration (stochastic transitions, stochastic rewards)

- 1: **procedure** VALUEITERATION( $R(s, a, s')$  reward function,  $p(\cdot|s, a)$  transition probabilities)
- Initialize value function  $V(s) = 0$  or randomly  $2:$
- while not converged do  $3:$

4: **for** 
$$
s \in S
$$
 **do**  
\n5:  $V(s) = \max_{a} \sum_{s' \in S} p(s'|s, a) (R(s, a, s') + \gamma V(s'))$   
\n6: Let  $\pi(s) = \operatorname{argmax}_{a} \sum_{s' \in S} p(s'|s, a) (R(s, a, s') + \gamma V(s'))$ ,  $\forall s$   
\n**return**  $\pi$ 

Policy Iteration

- $\cdot$  Inputs:  $R(s, a)$ ,  $p(s' | s, a)$
- $\cdot$  Initialize  $\pi$  randomly
- While not converged, do:

• Solve the Bellman equations defined by policy  $\pi$ 

$$
\begin{aligned}\n\mathbf{\nabla}_{S} & V^{\pi}(s) = R(s, \pi(s)) + \gamma \sum_{s' \in S} p(s' \mid s, \pi(s)) V^{\pi}(s') \\
&\cdot \text{Update } \pi \\
\mathbf{\nabla}_{S} & \pi(s) \leftarrow \operatorname*{argmax}_{a \in \mathcal{A}} \left[ R(s, a) + \gamma \sum_{s' \in S} p(s' \mid s, a) V^{\pi}(s') \right] \\
&\cdot \text{Return } \pi\n\end{aligned}
$$

Policy Iteration **Theory** 

- $\cdot$  In policy iteration, the policy improves in each iteration.
- Given finite state and action spaces, there are finitely many possible policies
- Thus, the number of iterations needed to converge is bounded!
- Value iteration takes  $O(|\mathcal{S}|^2|\mathcal{A}|)$  time / iteration
- Policy iteration takes  $O(|S|^2|\mathcal{A}| + |S|^3)$  time / iteration
	- However, empirically policy iteration requires fewer iterations to converge

MDP and Value/Policy Iteration Learning **Objectives** 

You should be able to…

- Compare reinforcement learning to other learning paradigms
- Cast a real-world problem as a Markov Decision Process
- Depict the exploration vs. exploitation tradeoff via MDP examples
- Explain how to solve a system of equations using fixed point iteration
- Define the Bellman Equations
- Show how to compute the optimal policy in terms of the optimal value function
- Explain the relationship between a value function mapping states to expected rewards and a value function mapping state-action pairs to expected rewards
- **· Implement value iteration and policy iteration**
- Contrast the computational complexity and empirical convergence of value iteration vs. policy iteration
- Identify the conditions under which the value iteration algorithm will converge to the true value function
- <sup>11/13/24</sup> **Describe properties of the policy iteration algorithm** 13



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?

(Asynchronous) Value Iteration

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

$$
\bigtimes V(s) \leftarrow \max_{a \in \mathcal{A}} R(s, a) + \gamma \sum_{s' \in \mathcal{S}} p(s' \mid s, a) V(s')
$$

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

(Asynchronous) Value Iteration Revisited

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

 $\cdot$  For  $a \in \mathcal{A}$ 

$$
Q(s, a) = R(s, a) + \gamma \sum_{s' \in S} p(s' \mid s, a)V(s')
$$
  
•  $V(s) \leftarrow \max_{a \in \mathcal{A}} Q(s, a)$ 

 $\cdot$  For  $s \in S$  $\pi^*(s) \leftarrow \text{argmax}$  $a \in \mathcal{A}$  $R(s, a) + \gamma$  $s' \in \mathcal{S}$  $p(s' \mid s, a)V(s')$ • Return  $\pi^*$ 

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

•  $Q^*(s, a) =$  F [total discounted reward of taking action a in state s, assuming all future actions are optimal]  $= R(s, a) + \gamma$  $s' \in \mathcal{S}$  $p(s' \mid s, a)V^*(s')$  $V^*(s') = \max$  $a^{\prime} \in \mathcal{A}$  $Q^*(s', a')$  $Q^*(s, a) = R(s, a) + \gamma$  $s' \in \mathcal{S}$  $p(s'\mid s,a) \big\vert$  max  $a^{\dagger} \in \mathcal{A}$  $Q^*(s', a')$  $\pi^*(s) = \text{argmax } Q^*(s, a)$  $a \in \mathcal{A}$ 

• Insight: if we know  $Q^*$ , we can compute an optimal policy  $\pi^*!$ 

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

•  $Q^*(s, a) =$  E[total discounted reward of taking action  $a$  in state  $s$ , assuming all future actions are optimal]

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

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

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

• Insight: if we know  $Q^*$ , we can compute an optimal policy  $\pi^*!$ 

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 $\rightarrow$   $s' = \mathcal{S}(s,a)$ 

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

Algorithm 1: Online learning (table form)

 $\cdot$  Inputs: discount factor  $\gamma$ , an initial state s

 $\cdot$  Initialize  $Q(s, a) = 0 \forall s \in S, a \in \mathcal{A}$  (Q is a  $|S| \times |A|$  array)

- While TRUE, do
	- $\cdot$  Take a random action  $a$

- Receive reward  $r = R(s, a)$
- Update the state:  $s \leftarrow s'$  where  $s' = \delta(s, a)$

 $\cdot$  Update  $Q(s, a)$ :

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

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

Algorithm 2:  $\epsilon$ -greedy online learning (table form)

 $\cdot$  Inputs: discount factor  $\gamma$ , an initial state  $s$ , greediness parameter  $\epsilon \in [0,1]$ 

 $\cdot$  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  $\epsilon$ , take the greedy action

 $a = \argmax$  $a^{\mathsf{T}} \in \mathcal{A}$  $Q(s, a^{\prime})$ 

Otherwise, with probability  $1 - \epsilon$ , take a random action a

- Receive reward  $r = R(s, a)$
- Update the state:  $s \leftarrow s'$  where  $s' = \delta(s, a)$

 $\cdot$  Update  $Q(s, a)$ :

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

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

Algorithm 3: -greedy online learning (table form)

 $\cdot$  Inputs: discount factor  $\gamma$ , an initial state  $s$ , greediness parameter  $\epsilon \in [0, 1]$ , learning rate  $\alpha \in [0,1]$  ("trust parameter")

 $\cdot$  Initialize  $Q(s, a) = 0 \forall s \in S, a \in \mathcal{A}$  (Q is a  $|S| \times |A|$  array)

- While TRUE, do
	- With probability  $\epsilon$ , take the greedy action

 $a = \argmax Q(s, a')$  $a^{\bar{I}} \in A$ 

Otherwise, with probability  $1 - \epsilon$ , take a random action a

- Receive reward  $r = R(s, a)$
- Update the state:  $s \leftarrow s'$  where  $s' \sim p(s' | s, a)$

 $\cdot$  Update  $Q(s, a)$ :  $Q(s, a) \leftarrow (1 - \alpha)Q(s, a) + \alpha (r + \gamma)$  max  $\overline{a'}$  $Q(s', a')$ Current value Update w/ deterministic transitions

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

Algorithm 3:  $\epsilon$ -greedy online learning (table form)

 $\cdot$  Inputs: discount factor  $\gamma$ , an initial state  $s$ , greediness parameter  $\epsilon \in [0, 1]$ , learning rate  $\alpha \in [0,1]$  ("trust parameter")

 $\cdot$  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  $\epsilon$ , take the greedy action

 $a = \argmax Q(s, a')$  $a' \in A$ 

Otherwise, with probability  $1 - \epsilon$ , take a random action a

- Receive reward  $r = R(s, a)$
- Update the state:  $s \leftarrow s'$  where  $s' \sim p(s' | s, a)$  Temporal  $\cdot$  Update  $Q(s, a)$ :

difference

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

$$
\gamma = 0.9
$$
\n
$$
\begin{bmatrix}\n0 & 1 & 2 \\
0 & 2 & 3\n\end{bmatrix}
$$
\n
$$
\begin{bmatrix}\n5 & 3 & 3 \\
4 & 6 & 7\n\end{bmatrix}
$$

$$
R(s,a) = \left\{\n \begin{array}{c}\n \vdots \\
 \vdots \\
 \vdots \\
 \vdots\n \end{array}\n \right.
$$

 $\sqrt{-2}$  if entering state 0 (safety) 3 if entering state 5 (field goal) 7 if entering state 6 (touch down) 0 otherwise



Poll Question 1:

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



Poll Question 1:

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





















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  $\alpha_t$  follows some "schedule" s.t.

 $\sum_{t=0}^{\infty}\alpha_t = \infty$  and  $\sum_{t=0}^{\infty}\alpha_t^2 < \infty$  e.g.,  $\alpha_t = \frac{1}{n}$  $t+1$ 

# Two big Q's

- 1. What can we do if the reward and/or transition functions/distributions are unknown?
	- A: 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



Poll Question 2: Which is the best approximation to the number of legal board states in Go?

- A. 42 **(TOXIC)**
- B. The number of stars in the universe ~  $10^{24}$
- C. The number of atoms in the universe ~ 1080
- $\overline{D}$ . A googol =  $10^{100}$
- E. The number of possible *games* of chess ∼ 10<sup>120</sup>
- F. A googolplex  $= 10^{g \text{o o gol}}$

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
- $\cdot$  There are  $^{\sim}10^{170}$ legal Go board states!

# Two big Q's

- 1. What can we do if the reward and/or transition functions/distributions are unknown?
	- A: Use online learning to gather data and learn  $Q^*(s, a)$
- 2. How can we handle infinite (or just very large) state/action spaces?
	- A: 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 SGD
	- Training data  $(s_t, a_t, r_t, s_{t+1})$  gathered online by the agent/learning algorithm

Deep Q-learning: Model

- Represent states using some feature vector  $s_t \in \mathbb{R}^M$ e.g. for Go,  $\bm{s}_{t}=[1, 0, -1, ..., 1]^{T}$
- Define a neural network



Deep Q-learning: Loss Function • "True" loss  $\ell(\Theta) = \sum_{n=1}^{\infty} \binom{Q^*(s, a) - Q(s, a; \Theta)}{n}$  $s \in \mathcal{S}$   $a \in \mathcal{A}$ 2 1.  $S$  too big to compute this sum 2. Don't know  $Q^*$ 

- 
- 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  $\overline{a'}$  $Q(s', a'; \Theta^{(t)}) \coloneqq y$ 

• Set the parameters in the next iteration  $\Theta^{(t+1)}$  such that  $Q\big(s,a;\Theta^{(t+1)}\big)\approx y$  $\ell(\Theta^{(t)}, \Theta) = (y - Q(s, a; \Theta))$ 2

### Deep Q-learning

Algorithm 4: Online learning (parametric form)

 $\cdot$  Inputs: discount factor  $\gamma$ , an initial state  $s_0$ , learning rate  $\alpha$ • Initialize parameters  $\Theta^{(0)}$ 

• For  $t = 0, 1, 2, ...$ 

- Gather training sample  $(s_t, a_t, r_t, s_{t+1})$
- Update  $\Theta^{(t)}$  by taking a step opposite the gradient

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

where

$$
\nabla_{\Theta} \ell(\Theta^{(t)}, \Theta) = 2(y - Q(s, a; \Theta)) \nabla_{\Theta} Q(s, a; \Theta)
$$

Deep Q-learning: **Experience** Replay

• SGD assumes iid training samples but in RL, samples are *highly* correlated

• Idea: maintain a "replay buffer"  $\mathcal{D} = \{e_1, e_2, ..., e_N\}$  of the  $N$  most recent experiences  $e_t = (\mathbf{s}_t, \mathbf{a}_t, r_t, \mathbf{s}_{t+1})$  (Lin, 1992)

- Keeps the agent from "forgetting" recent experiences
- $\cdot$  In each iteration, we:
	- 1. Sample some experience  $e_i$  (or a mini-batch of experiences  $E = \{e_1, ..., e_T\}$ ) uniformly at random from  $D$  and apply the Q-learning update
	- 2. Add a new experience to  $D$
- $\cdot$  Can also sample experiences from  $\mathcal D$  according to some distribution that prioritizes experiences with high error  $11/13/24$  (Schaul et al., 2016)

Q-learning and Deep RL **Learning Objectives** 

You should be able to…

- Apply Q-Learning to a real-world environment
- Implement Q-learning
- Identify the conditions under which the Q-learning algorithm will converge to the true value function
- Adapt Q-learning to Deep Q-learning by employing a neural network approximation to the Q function
- Describe the connection between Deep Q-Learning and regression