

10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University



Matt Gormley, Henry Chai, Hoda Heidari Lecture 22 Apr. 5, 2024

Reminders

- Homework 7: Deep Learning
 - Out: Thu, Mar. 28
 - Due: Mon, Apr. 8 at 11:59pm
- Schedule Notes
 - Lecture 22: Fri, Apr. 5
 - HW8 Recitation: Mon, Apr. 8
- Homework 8: Deep RL
 - Out: Mon, Apr. 8
 - Due: Fri, Apr. 19 at 11:59pm

Q-LEARNING

What can we do if we don't know the reward function / transition probabilities? $V(s) \leftarrow Max R(s_{19}) + \delta \underset{s'}{=} p(s'|s_{19}) V(s')$

Today's lecture is brought to you by the letter Q



Source: https://en.wikipedia.org/wiki/Avenue Q#/media/File:Image-AvenueQlogo.png

Today's lecture is brought to you by the letter Q



Today's lecture is brought to you by the letter Q



Value Iteration

Algorithm 1 Value Iteration

- 1: **procedure** VALUEITERATION(R(s, a) reward function, $p(\cdot|s, a)$ transition probabilities)
- 2: Initialize value function V(s) = 0 or randomly
- 3: while not converged do
- 4: for $s \in \mathcal{S}$ do
- 5: for $a \in \mathcal{A}$ do

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

- 7: $V(s) = \max_a Q(s, a)$
- 8: Let $\pi(s) = \operatorname{argmax}_a Q(s, a), \ \forall s$
- 9: return π

6:

Variant 1: with Q(s,a) table

Q-Learning Motivation and Q*(s,a) $V^{T}(s)$ Q^T(s,a) the expected discorded follow rewrite of taky active a Q-Learning Motivation is state s and then followy policy TT Q: What if we don't know R(s,a) or p(s' | s, a)? A: Then value iteration and policy iteration don't work!

non-deterministic version

Definition: Let Q*(s,a) be the (true) expected discounted future reward of taking action • a in states and followy optimal policy TX

$$V^{*}(s) = \max_{a} Q^{*}(s, a)$$

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

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

Key insight: if we can learn Q*, we can define π^* without knowing R(s,a) or p(s' | s, a)! ۲

$$TT^{*}(s) = \arg Q^{*}(s,a)$$

 $q \in A$

Q-Learning Motivation and Q*(s,a)

• Q-Learning Motivation

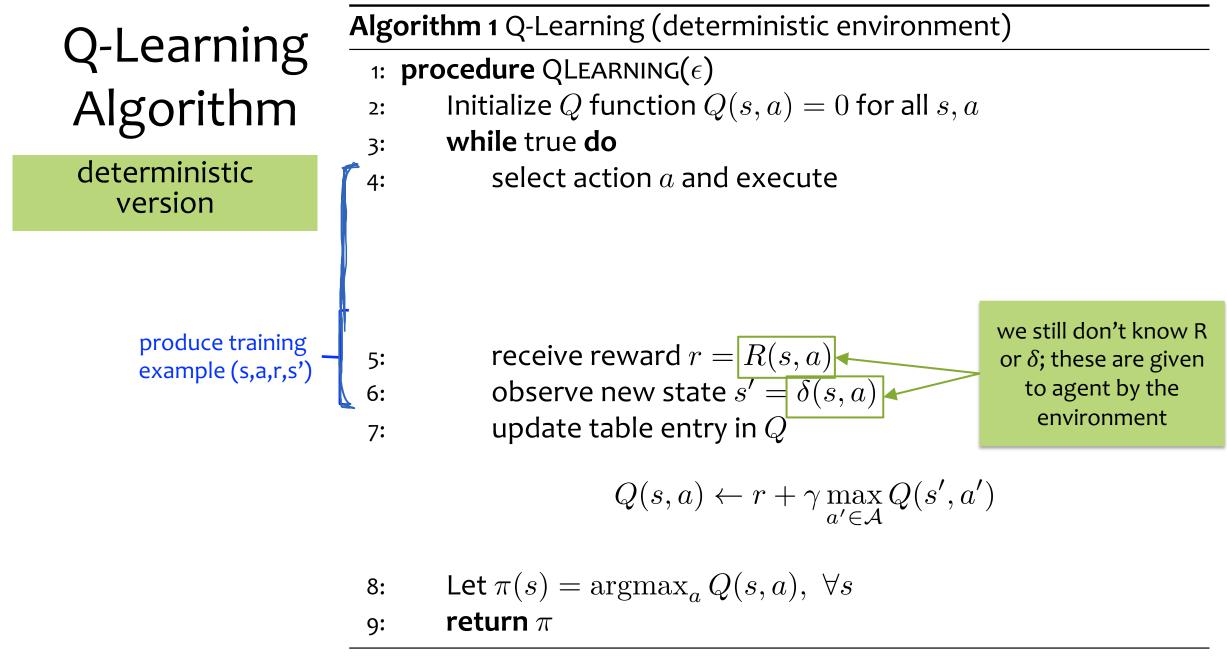
Q: What if we don't know R(s,a) or $\delta(s, a)$? A: Then value iteration and policy iteration don't work!

• **Definition**: Let Q*(s,a) be the (true) expected discounted future reward of taking action a in state s

$$V^{*}(s) = \max_{a} Q^{*}(s, a)$$
$$Q^{*}(s, a) = R(s, a) + \gamma V^{*}(\delta(s, a))$$
$$\bigvee_{a'} (\varsigma_{a'}) = R(s, a) + \gamma \left[\max_{a'} Q^{*}(\delta(s, a), a')\right]$$

• **Key insight:** if we can learn Q*, we can define π^* without knowing R(s,a) or $\delta(s, a)$!

deterministic version



Q-Learning	Algorithm 1 Q-Learning (deterministic env., ϵ -greedy variant)
	1: procedure QLEARNING(e) Initialize 5
Algorithm	2: Initialize Q function $Q(s, a) = 0$ for all s, a
J	3: while true do
deterministic version	4: select action a and execute
VCISION	with prob. $(1 - \epsilon)$: select $a = \max_{a' \in \mathcal{A}} Q(s, a')$
	with prob. ϵ : select $a \in \mathcal{A}$ randomly $4 - explore$
produce training example (s,a,r,s')	5:receive reward $r = R(s, a)$ we still don't know R6:observe new state $s' = \delta(s, a)$ or δ ; these are given to agent by the environment7:update table entry in Q
	$Q(s, a) \leftarrow r + \gamma \max_{a' \in \mathcal{A}} Q(s', a')$
	7.5 $S = S'$ 8: $\int \text{Let } \pi(s) = \operatorname{argmax}_a Q(s, a), \ \forall s$
	8: \bigvee Let $\pi(s) = \operatorname{argmax}_a Q(s, a), \forall s$
	9: return π

Q-Learning Algorithm

non-deterministic version

 $\alpha_n = \frac{1}{1 + \text{visits}(s, a, n)}$ visits(s, a, n) = # of visits to (s, a) up to and including step n

Algorithm 1 Q-Learning (non-deterministic env., ϵ -greedy variant) 1: procedure QLEARNING Initialize Q function Q(s, a) = 0 for all s, a2: while true do 3: select action a and execute 4: with prob. $(1 - \epsilon)$: select $a = \max_{a' \in \mathcal{A}} Q(s, a')$ with prob. ϵ : select $a \in \mathcal{A}$ randomly receive reward r = R(s, a)observe new state $s' = \delta(s, a) p(s'|s, a)$ update table entry in Q

$$Q(s, a) \leftarrow (1 - \alpha_n)Q(s, a) + \alpha_n(r + \gamma \max_{a' \in \mathcal{A}} Q(s', a'))$$

Let $\pi(s) = \operatorname{argmax}_a Q(s, a), \forall s$
Ceturn π
Q-learning update
from deterministic
version

Q-Learning Algorithm

non-deterministic version

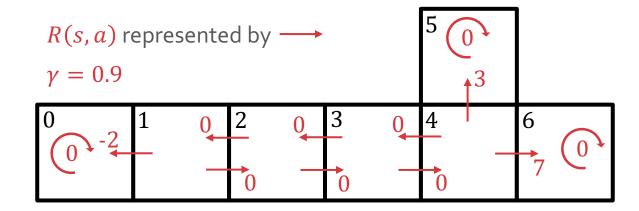
$$\alpha_n = \frac{1}{1 + \text{visits}(s, a, n)}$$

visits $(s, a, n) = \text{# of visits to}$
 (s, a) up to and including step r

Algorithm 1 Q-Learning (non-deterministic env., ϵ -greedy variant) 1: procedure QLEARNING Initialize Q function Q(s, a) = 0 for all s, a2: while true do 3: select action a and execute 4: with prob. $(1 - \epsilon)$: select $a = \max_{a' \in \mathcal{A}} Q(s, a')$ with prob. ϵ : select $a \in \mathcal{A}$ randomly receive reward r = R(s, a)observe new state $s' = \delta(s, a)$ temporal difference update table entry in Q $Q(s,a) \leftarrow Q(s,a) + \alpha_n(r + \gamma \max_{a' \in \mathcal{A}} Q(s',a') - Q(s,a))$ Let $\pi(s) = \operatorname{argmax}_{a} Q(s, a), \ \forall s$ temporal difference return π target in the table

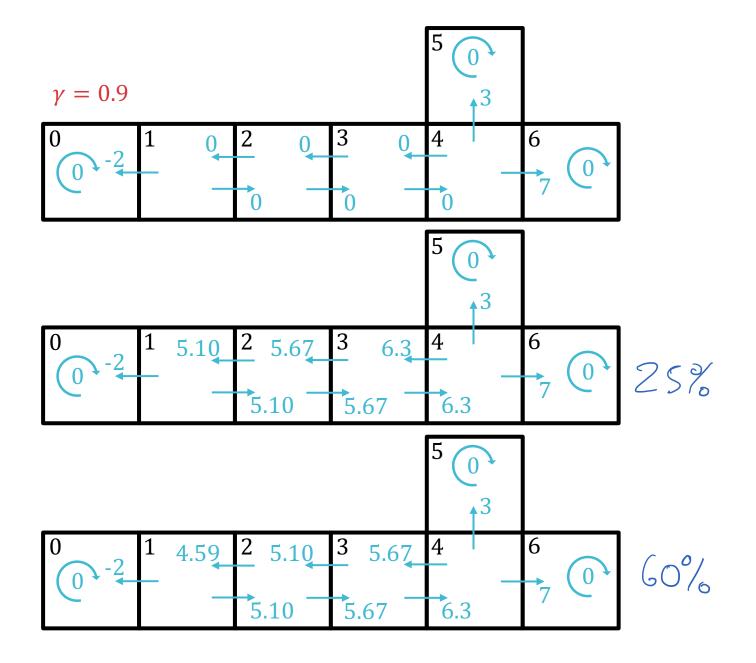
$\gamma = 0.$	9			5 3	
0 -2	1	2	3	4	6 7

	-2 if entering state 0 (safety)
$R(s,a) = \langle$	3 if entering state 5 (field goal)
$\pi(s, u) = \gamma$	7 if entering state 6 (touch down)
	<mark>0</mark> otherwise

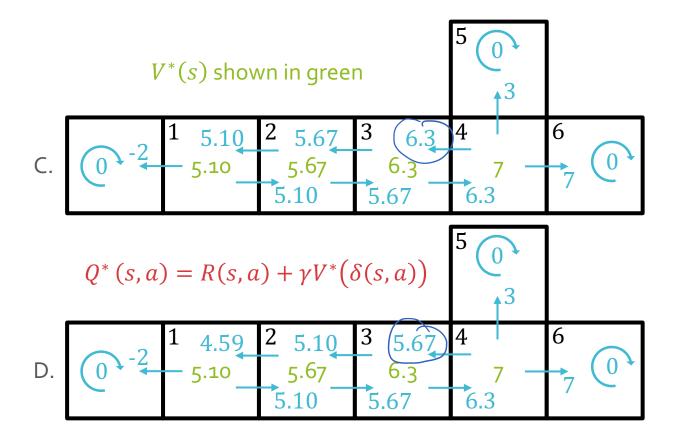


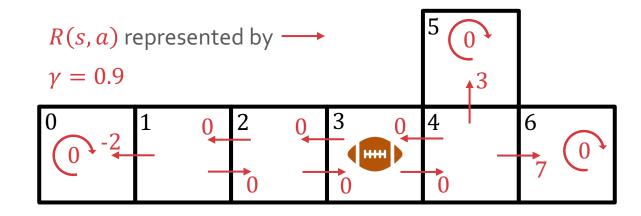
Q1

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

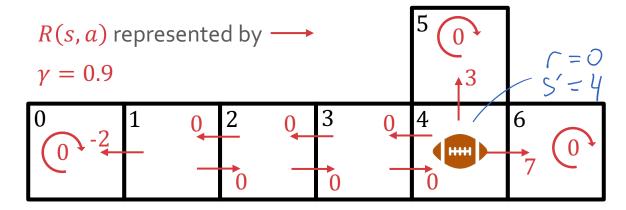


Poll: Which set of blue arrows corresponds to $Q^*(s, a)$?



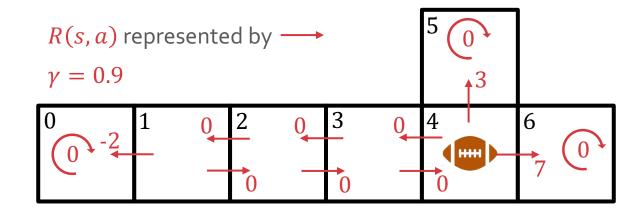


Q(s,a)	\rightarrow	←	1	U
Ο	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

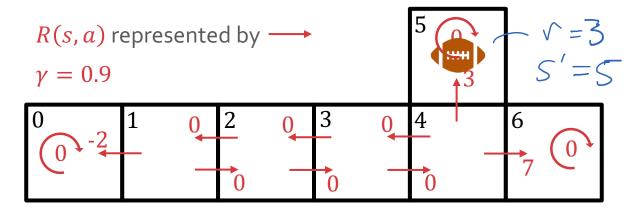


 $Q(3,\rightarrow) \leftarrow 0 + (0.9) \max_{a' \in \{\rightarrow,\leftarrow,\uparrow,\circlearrowright\}} Q(4,a') = 0$

Q(s,a)	\rightarrow	←	1	U
Ο	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	ο	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0

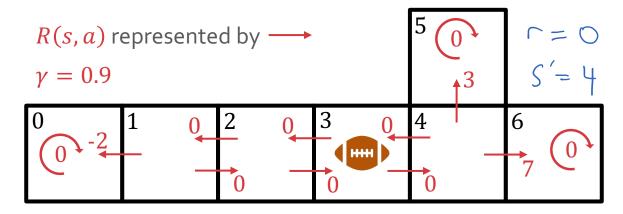


Q(s,a)	\rightarrow	←	1	U
Ο	0	0	0	0
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0



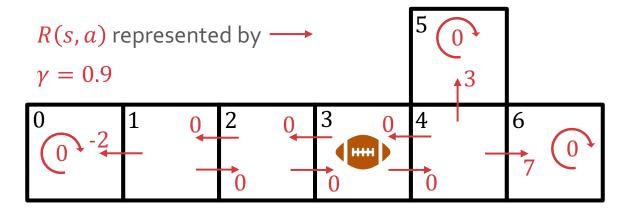
 $Q(4,\uparrow) \leftarrow 3 + (0.9) \max_{a' \in \{\rightarrow,\leftarrow,\uparrow,\cup\}} Q(5,a') = 3$

Q(s,a)	\rightarrow	←	1	U
Ο	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



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

Q(s,a)	\rightarrow	←	1	U
Ο	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



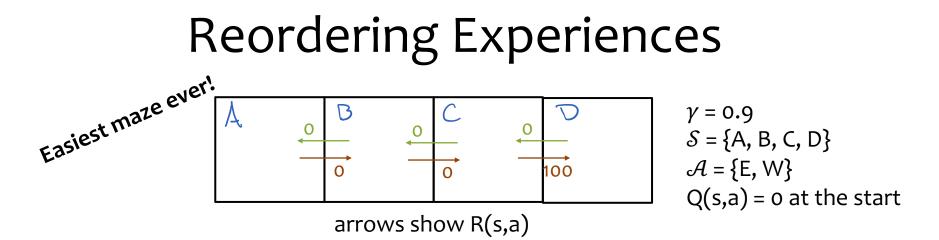
 $Q(3, \rightarrow) \leftarrow 0 + (0.9) \max_{a' \in \{\rightarrow, \leftarrow, \uparrow, \bigcup\}} Q(4, a') = 2.7$

Q(s,a)	\rightarrow	←	1	U
Ο	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

Q-Learning Convergence

Remarks

- **Q** converges to **Q*** with probability 1.0, assuming...
 - 1. each <s, a> is visited infinitely often
 - $2. \quad 0 \leq Y < 1$
 - 3. rewards are bounded $|R(s,a)| < \beta$, for all <s,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 $\sum_{t=0}^{\infty} \alpha_t^2 = 0$, e.g., $\alpha_t = 1/t+1$
- Q-Learning is exploration insensitive
 ⇒ visiting the states in any order will work assuming point 1 is satisfied
- May take many iterations to converge in practice



1. Suppose we visit states as below

i	S	а	r	s'
1	А	E	0	В
2	В	E	0	C
3	С	E	100	D

Q(A, E) = 0 Q(B, E) = 0 Q(C, E) = 100

2. Suppose we visit states in reverse

i	S	а	r	s'
1	С	E	100	D
2	В	E	0	C
3	А	E	0	В

Q(C, E) = 100Q(B, E) = 90Q(A, E) = 81

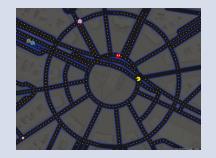
Designing State Spaces

- **Q:** Do we have to retrain our RL agent every time we change our state space?
- A: Yes. But whether your state space changes from one setting to another is determined by your design of the state representation. 74

Two examples:

- State Space A: <x,y> position on map e.g. s_t = <74, 152>
- State Space B: window of pixel colors centered at current Pac Man location



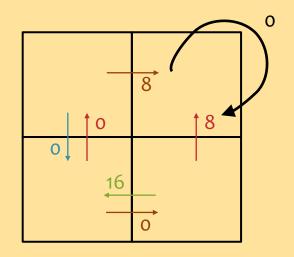


WZ: Skip

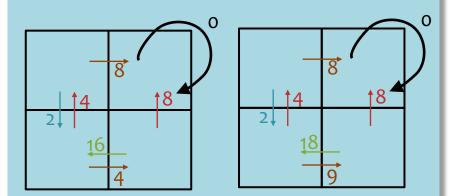
Poll: Q-Learning

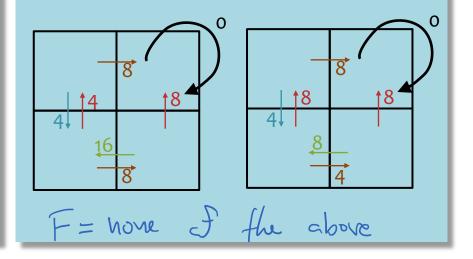
Question:

For the R(s,a) values shown on the arrows below, which are the corresponding Q*(s,a) values? Assume discount factor = 0.5.



Answer:





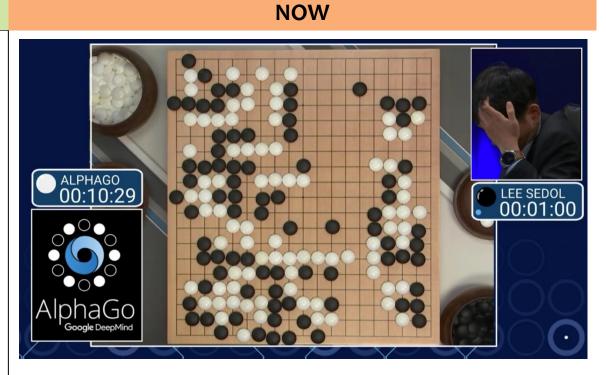
DEEP RL FOR GAME OF GO

TD Gammon \rightarrow Alpha Go

Learning to beat the masters at board games

THEN

"...the world's top computer program for backgammon, TD-GAMMON (Tesauro, 1992, 1995), learned its strategy by playing over one million practice games against itself..."



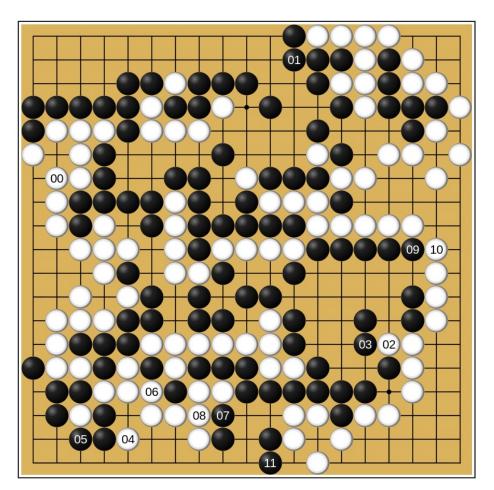
(Mitchell, 1997)

Alpha Go

Game of Go (圍棋)

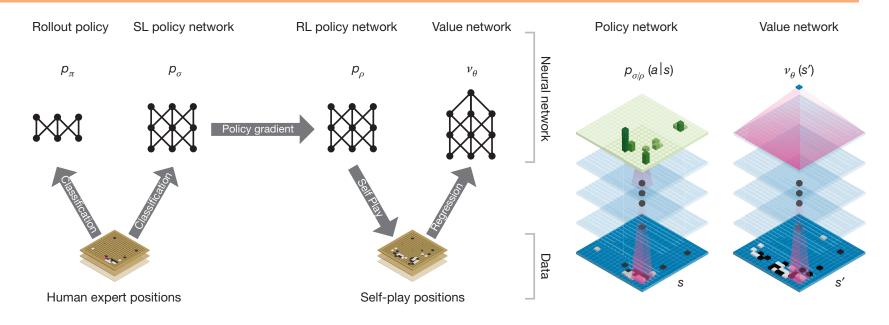
- 19x19 **board**
- Players alternately play black/white stones
- **Goal** is to fully encircle the largest region on the board
- Simple rules, but extremely complex game play

AlphaGo (Black) vs. Lee Sedol (White) - Game 2 Final position (AlphaGo wins in 211 moves)



Alpha Go

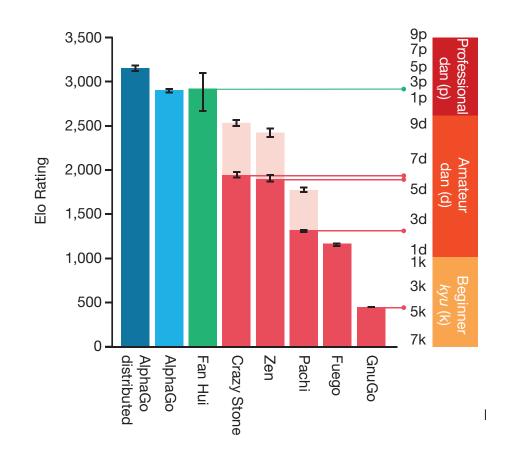
- State space is too large to represent explicitly since # of sequences of moves is O(b^d)
 - Go: b=250 and d=150
 - Chess: b=35 and d=80
- Key idea:
 - Define a neural network to approximate the value function
 - Train by policy gradient



Alpha Go

- Results of a tournament
- From Silver et

 al. (2016): "a
 230 point gap
 corresponds to
 a 79%
 probability of
 winning"



DEEP Q-LEARNING

Deep Q-Learning

Question: What if our state space S is too large to represent with a table?

Examples:

- s_t = pixels of a video game
- s_t = continuous values of a sensors in a manufacturing robot
- s_t = sensor output from a self-driving car

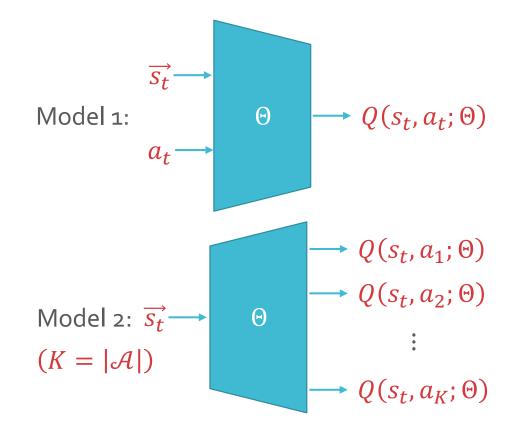
Answer: Use a parametric function to approximate the table entries

Key Idea:

- 1. Use a neural network $Q(s,a; \theta)$ to approximate $Q^*(s,a)$
- 2. Learn the parameters θ via SGD with training examples < s_t, a_t, r_t, s_{t+1} >

Deep Q-learning: Model

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



Deep Q-learning: Model

- Represent states using some feature vector $\vec{s_t} \in \mathbb{R}^M$ e.g., $\vec{s_t} = [1, 0, 0, ..., 1]^T$
- Define a neural network a bunch of linear regressors (technically still neural networks...), one for each action (let $K = |\mathcal{A}|$)

$$Q(\vec{s}, a_k; \Theta) = \overrightarrow{\theta_k}^T \vec{s} \text{ where } \Theta = \begin{bmatrix} \overrightarrow{\theta_1} \\ \overrightarrow{\theta_2} \\ \vdots \\ \overrightarrow{\theta_K} \end{bmatrix} \in \mathbb{R}^{K \times M}$$

• Goal: $K \times M \ll |S| \rightarrow$ computational tractability!

• Gradients are easy:
$$\nabla_{\overrightarrow{\theta_j}} Q(\overrightarrow{s}, a_k; \Theta) = \begin{cases} \overrightarrow{0} & \text{if } j \neq k \\ \overrightarrow{s} & \text{if } j = k \end{cases}$$

Deep Q-learning: Model

- Represent states using some feature vector $\vec{s_t} \in \mathbb{R}^M$ e.g., $\vec{s_t} = [1, 0, 0, ..., 1]^T$
- Define a neural network a bunch of linear regressors (technically still neural networks...), one for each action (let $K = |\mathcal{A}|$)

$$Q(\vec{s}, a_k; \Theta) = \overrightarrow{\theta_k}^T \vec{s} \text{ where } \Theta = \begin{bmatrix} \overrightarrow{\theta_1} \\ \overrightarrow{\theta_2} \\ \vdots \\ \overrightarrow{\theta_K} \end{bmatrix} \in \mathbb{R}^{K \times M}$$

• Goal: $K \times M \ll |S| \rightarrow$ computational tractability!

• Gradients are easy:
$$\nabla_{\Theta} Q(\vec{s}, a_k; \Theta) = \begin{bmatrix} \vec{0} \\ \vec{0} \\ \vdots \\ \vec{s} \\ \vdots \end{bmatrix} \leftarrow \text{Row } k$$

[IJ

Q-Learning (-ish) Update Rule

• Why don't we just do an update akin to what we do in regular Q-Learning?

K

Given
$$(s_{1a}, r_{1s}')$$
:
 $Q(s_{1a}; \Theta) \leftarrow r + 8 \max_{a' \in A} Q(s', a') \Theta$

Deep Q-learning: Loss Function 2. Don't know Q^* • "True" loss $\ell(\Theta) = \sum_{s \in S} \sum_{a \in A} (Q^*(s, a) - Q(s, a; \Theta))^2$

1. 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 Θ^(t) the (temporal difference) target is

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

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

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

Deep Q-learning

- Algorithm: Online learning of Q^* (parametric form)
 - Inputs: discount factor γ,

an initial state s₀,

learning rate α

- Initialize parameters $\Theta^{(0)}$
- For t = 0, 1, 2, ...
 - Gather training sample (s_t, a_t, r_t, s_{t+1})
 - Update Θ^(t) by taking a step opposite the gradient
 - $\Theta^{(const)} \leftarrow \Theta^{(t)}$ $\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \alpha \nabla_{\Theta^{(t)}} \ell(\Theta^{(const)}, \Theta^{(t)})$

where

$$\nabla_{\Theta} \ell(\Theta^{(const)}, \Theta^{(t)}) = 2\left(y - Q(s, a; \Theta^{(t)})\right) \nabla_{\Theta^{(t)}} Q(s, a; \Theta^{(t)})$$
$$= 2\left(r + \gamma \max_{a'} Q(s', a'; \Theta^{(const)}) - Q(s, a; \Theta^{(t)})\right) \nabla_{\Theta^{(t)}} Q(s, a; \Theta^{(t)})$$

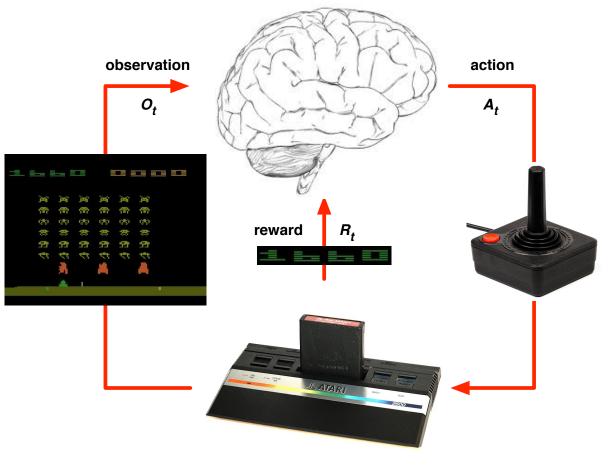
Experience Replay

- **Problems** with online updates for Deep Q-learning:
 - not i.i.d. as SGD would assume
 - quickly forget rare experiences that might later be useful to learn from
- Uniform Experience Replay (Lin, 1992):
 - Keep a replay memory D = {e₁, e₂, ..., e_N} of N most recent experiences $e_t = \langle s_t, a_t, r_t, s_{t+1} \rangle$
 - Alternate two steps:
 - 1. Repeat T times: randomly sample e_i from D and apply a Q-Learning update to e_i
 - 2. Agent selects an action using epsilon greedy policy to receive new experience that is added to D
- Prioritized Experience Replay (Schaul et al, 2016)
 - similar to Uniform ER, but sample so as to prioritize experiences with high error

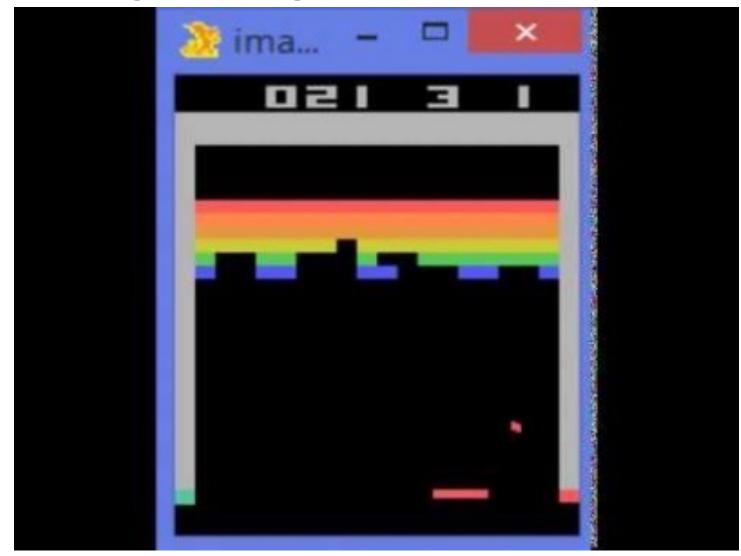
DEEP RL FOR ATARI GAMES

Playing Atari with Deep RL

- Setup: RL system observes the pixels on the screen
- It receives rewards as the game score
- Actions decide how to move the joystick / buttons



Playing Atari games with Deep RL



Playing Atari games with Deep RL



Figure 1: Screen shots from five Atari 2600 Games: (*Left-to-right*) Pong, Breakout, Space Invaders, Seaquest, Beam Rider

	B. Rider	Breakout	Enduro	Pong	Q*bert	Seaquest	S. Invaders
Random	354	1.2	0	-20.4	157	110	179
Sarsa [3]	996	5.2	129	-19	614	665	271
Contingency [4]	1743	6	159	-17	960	723	268
DQN	4092	168	470	20	1952	1705	581
Human	7456	31	368	-3	18900	28010	3690
HNeat Best [8]	3616	52	106	19	1800	920	1720
HNeat Pixel [8]	1332	4	91	-16	1325	800	1145
DQN Best	5184	225	661	21	4500	1740	1075

Table 1: The upper table compares average total reward for various learning methods by running an ϵ -greedy policy with $\epsilon = 0.05$ for a fixed number of steps. The lower table reports results of the single best performing episode for HNeat and DQN. HNeat produces deterministic policies that always get the same score while DQN used an ϵ -greedy policy with $\epsilon = 0.05$.

Learning Objectives

Reinforcement Learning: Q-Learning

You should be able to...

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

BIG PICTURE

ML Big Picture

Learning Paradigms:

What data is available and when? What form of prediction?

- supervised learning
- unsupervised learning
- semi-supervised learning
- reinforcement learning
- active learning
- imitation learning
- domain adaptation
- online learning
- density estimation
- recommender systems
- feature learning
- manifold learning
- dimensionality reduction
- ensemble learning
- distant supervision
- hyperparameter optimization

Theoretical Foundations:

What principles guide learning?

- probabilistic
- information theoretic
- evolutionary search
- ML as optimization

Problem Formulation: What is the structure of our output prediction?					
boolean	Binary Classification				
categorical	Multiclass Classification				
ordinal	Ordinal Classification				
real	Regression				
ordering	Ranking				
multiple discrete	Structured Prediction				
multiple continuous (e.g. dynamical systems)					
both discrete &	(e.g. mixed graphical models)				
cont.					

Facets of Building ML Systems:

How to build systems that are robust, efficient, adaptive, effective?

- Data prep
- Model selection 2.
- Training (optimization / 3. search)
- Hyperparameter tuning on 4. validation data
- (Blind) Assessment on test 5. data

Big Ideas in ML:

Which are the ideas driving development of the field?

- inductive bias .
- generalization / overfitting
- bias-variance decomposition

Application Areas

Key challenges?

Medicine,

Robotics

Vision, Search

omputer

S

Z

- generative vs. discriminative
- deep nets, graphical models .
- PAC learning •
- distant rewards

Learning Paradigms

Paradigm	Data				
Supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N \qquad \mathbf{x} \sim p^*(\cdot) \text{ and } y = c^*(\cdot)$				
\hookrightarrow Regression	$y^{(i)} \in \mathbb{R}$				
\hookrightarrow Classification	$y^{(i)} \in \{1, \dots, K\}$				
\hookrightarrow Binary classification	$y^{(i)} \in \{+1, -1\}$				
\hookrightarrow Structured Prediction	$\mathbf{y}^{(i)}$ is a vector				
Unsupervised	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N \qquad \mathbf{x} \sim p^*(\cdot)$				
Semi-supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N_1} \cup \{\mathbf{x}^{(j)}\}_{j=1}^{N_2}$				
Online	$\mathcal{D} = \{ (\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), (\mathbf{x}^{(3)}, y^{(3)}), \ldots \}$				
Active Learning	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ and can query $y^{(i)} = c^*(\cdot)$ at a cost				
Imitation Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}), (s^{(2)}, a^{(2)}), \ldots\}$				
Reinforcement Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}, r^{(1)}), (s^{(2)}, a^{(2)}, r^{(2)}), \ldots\}$				