L13: Basic Deep RL Algorithms

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Contents are based on ***Reinforcement Learning: An Introduction*** *from Prof. Richard S. Sutton and Prof. Andrew G. Barto, and* ***COMPM050/COMPGI13*** *taught at UCL by Prof. David Silver.*

Agenda

- Optimal Policy and Optimal Value Function
- Estimating Value Function for a Given Policy
- Q-Learning for Tabular RL
- Deep Q-Learning
- REINFORCE

click to jump to the section.

Optimal Policy and Optimal Value Function

Optimal Value Function

- Due to the Markovian property, the return starting from a state s is independent of its history. Therefore, we can compare the return of all policies starting from s and find the optimal one.
- The optimal state-value function $V^*(s)$ is the maximum value function over all policies
  - $V^*(s) = \max_\pi V_\pi(s)$
- The optimal action-value function $Q_*(s, a)$ is the maximum action-value function over all policies
  - $Q^*(s, a) = \max_\pi Q_\pi(s, a)$
- The optimal value function specifies the best possible performance in the MDP.

Optimal Policy

- Define a partial ordering over policies

$$\pi \geq \pi' \text{ if } V_\pi(s) \geq V_{\pi'}(s), \forall s$$

Theorem: For any Markov Decision Process

- *There exists an optimal policy π_* that is better than, or equal to, all other policies, $\pi_* \geq \pi, \ \forall \pi$*
- *All optimal policies achieve the optimal value function, $V_{\pi^*}(s) = V^*(s)$*
- *All optimal policies achieve the optimal action-value function, $Q_{\pi^*}(s,a) = Q^*(s,a)$*

- An optimal policy can be found by maximizing over $Q^*(s,a)$,

$$\pi^*(a|s) = \begin{cases} 1, & \text{if } \ a = \text{argmax}_{a \in \mathcal{A}} \ Q^*(s,a) \\ 0, & \text{otherwise} \end{cases}$$

Bellman Optimality Equation

- Optimal value functions also satisfy recursive relationships

$$
\begin{aligned}
V^*(s) &= \max_a \mathbb{E}_{\pi_*}[G_t | S_t = s, A_t = a] \\
&= \max_a \mathbb{E}_{\pi_*}[R_{t+1} + \gamma G_{t+1} | S_t = s, A_t = a] \\
&= \max_a \mathbb{E}[R_{t+1} + \gamma V^*(S_{t+1}) | S_t = s, A_t = a]
\end{aligned}
$$

- Similarly, for action-value function, we have

$$
Q^*(s, a) = \mathbb{E}[R_{t+1} + \gamma \max_{a'} Q^*(S_{t+1}, a') | S_t = s, A_t = a]
$$

- They are called **Bellman Optimality Equations**

Solving the Bellman Optimality Equation

- Bellman Optimality Equation is non-linear (because there is the max operation).
- No closed form solution (in general)
- Many iterative solution methods:
  - Value Iteration
  - Policy Iteration
  - Q-learning (we will talk about this later)
  - SARSA

Estimating Value Function for a Given Policy

Goal: Given a policy $\pi(a|s)$, estimate the value of the policy.

Monte-Carlo Policy Evaluation

- Learn V_π from episodes of experience under policy π
  - $S_0, A_0, R_1, S_1, A_1, R_2, \ldots, S_T \sim \pi$
- Recall that the *return* is the total discounted reward:
  - $G_t = R_{t+1} + \gamma R_{t+2} + \ldots + \gamma^{T-t-1} R_T$
- Recall that the value function is the expected return:
  - $V_\pi(s) = \mathbb{E}_\pi[G_t | S_t = s]$

Monte-Carlo Policy Evaluation

- Suppose that we have collected a number of trajectories, Monte-Carlo policy evaluation uses *empirical mean return* instead of *expected return*
  - Every time-step t that state s is visited in an episode
    - Increment state visit counter $N(s) \leftarrow N(s) + 1$
    - Increment total return $S(s) \leftarrow S(s) + G_t$
  - Value is estimated by mean return $V(s) = S(s)/N(s)$
  - By law of large numbers, $V(s) \rightarrow V_\pi(s)$ as $N(s) \rightarrow \infty$

Incremental Monte-Carlo Updates

- We can also update $V(s)$ incrementally after episode $S_0, A_0, R_1, \ldots, S_T$.

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- Consider a general problem of computing the mean for stream data
  - The mean $\mu_1, \mu_2, \ldots$ of a sequence of general vectors $x_1, x_2, \ldots$ can be computed incrementally,
  - $\mu_k = \mu_{k-1} + \frac{1}{k}(x_k - \mu_{k-1})$

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- For each state S_t with return G_t
  - $N(S_t) \leftarrow N(S_t) + 1$
  - $V(S_t) \leftarrow V(S_t) + \frac{1}{N(S_t)}(G_t - V(S_t))$
  - It can be proved that $V(s) \rightarrow V_\pi(s)$.

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  - It can be proved that $V(s) \rightarrow V_\pi(s)$.
- In non-stationary problems, it can be useful to track a running mean, i.e. forget old episodes.
  - $V(S_t) \leftarrow V(S_t) + \alpha(G_t - V(S_t))$
  - You may regard the α as the learning rate in supervised learning
  - May **not** converge for stationary problems. For small α, good enough.

Monte-Carlo Methods

- Quick facts:
  - MC methods learn directly from episodes of experience
  - MC is model-free: no knowledge of MDP transitions / rewards
  - MC uses the simplest possible idea: **value = mean return**
- Caveat: can only apply MC to episodic MDPs
  - All episodes must terminate

Temporal-Difference Learning

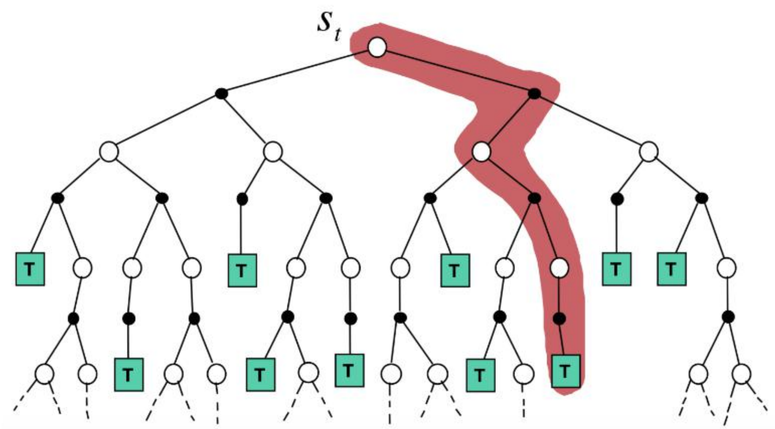
- Learn V_π online from experience under policy π
  - $S_1, A_1, R_2, S_2, A_2, R_3, \ldots, S_T \sim \pi$
- Recall: Incremental Monte-Carlo
  - Update value $V(S_t)$ toward actual return G_t
  - $V(S_t) \leftarrow V(S_t) + \alpha(G_t - V(S_t))$
- Simplest temporal-difference learning algorithm: TD(0)
  - Update value $V(S_t)$ toward estimated return $R_{t+1} + \gamma V(S_{t+1})$
  - $V(S_t) \leftarrow V(S_t) + \alpha(R_{t+1} + \gamma V(S_{t+1}) - V(S_t))$
  - $R_{t+1} + \gamma V(S_{t+1})$ is called the *TD target*
  - $\delta_t = R_{t+1} + \gamma V(S_{t+1}) - V(S_t)$ is called the *TD error*
- If we expand one step further, we got TD(1)
  - $V(S_t) \leftarrow V(S_t) + \alpha(R_{t+1} + \gamma R_{t+1} + \gamma^2 V(S_{t+2}) - V(S_t))$
  - Similarly, we can have TD(2), TD(3), ...

Temporal-Difference Learning

- Quick facts:
  - TD methods learn directly from episodes of experience
  - TD is model-free: no knowledge of MDP transitions / rewards
  - TD learns from incomplete episodes, by **bootstrapping**
  - TD updates a guess towards a guess

Visualizations for MC and TD

$$V(S_t) \leftarrow V(S_t) + \alpha\left(G_t - V(S_t)\right)$$



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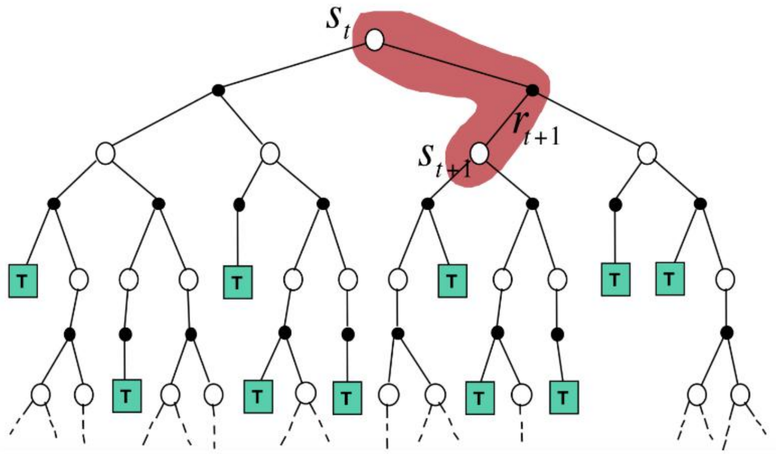


Pros and Cons of MC vs. TD

- TD can learn *before* knowing the final outcome
  - TD can learn online after every step
  - MC must wait until end of episode before return is known
- TD can learn *without* the final outcome
  - TD can learn from incomplete sequences
  - MC can only learn from complete sequences
  - TD works in continuing (non-terminating) environments
  - MC only works for episodic (terminating) environments

Bias/Variance Trade-Off

- Return $G_t = R_{t+1} + \gamma R_{t+2} + \ldots + \gamma^{T-t-1} R_T$ is always an unbiased estimate of $V_\pi(S_t)$
- True TD target $R_{t+1} + \gamma V_\pi(S_{t+1})$ is an unbiased estimate of $V_\pi(S_t)$
- However, if we will update π along the learning process, the TD target $R_{t+1} + \gamma V(S_{t+1})$ is a biased estimate of $V_\pi(S_t)$
  - Note that $V(S_{t+1})$ is an estimation from previous π instead of the true value
- When π is being updated slowly (e.g., through some sort of gradient descent), TD target has much lower variance than the return:
  - Return depends on many random actions, transitions, rewards
  - TD target depends on *one* random action, transition, reward

Pros and Cons of MC vs. TD (2)

- MC has high variance, zero bias
  - Good convergence properties(even with function approximation)
  - Not very sensitive to initial value
  - Very simple to understand and use
- TD has low variance, some bias
  - Usually more efficient than MC
  - TD(0) converges to $V_\pi(s)$ (but not always with function approximation)
  - More sensitive to initial value

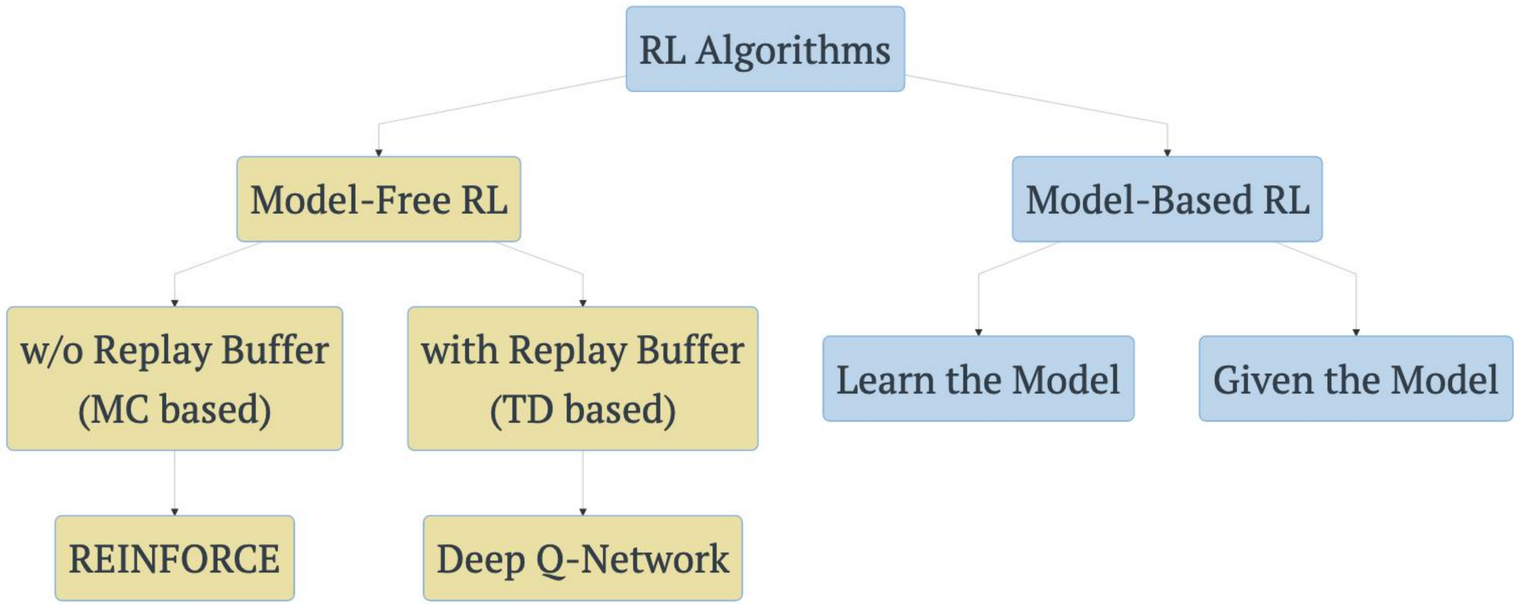
MC-based RL vs TD-based RL

- Monte-Carlo and TD are two fundamental ideas of value estimation for policies.
- Each has its Pros and Cons.
- Based on them, there are two families of model-free RL algorithms, both well developed. Some algorithms leverage both.
- Fundamentally, it is about the balance between bias and variance (sample complexity).

We start from REINFORCE and Deep Q-Learning

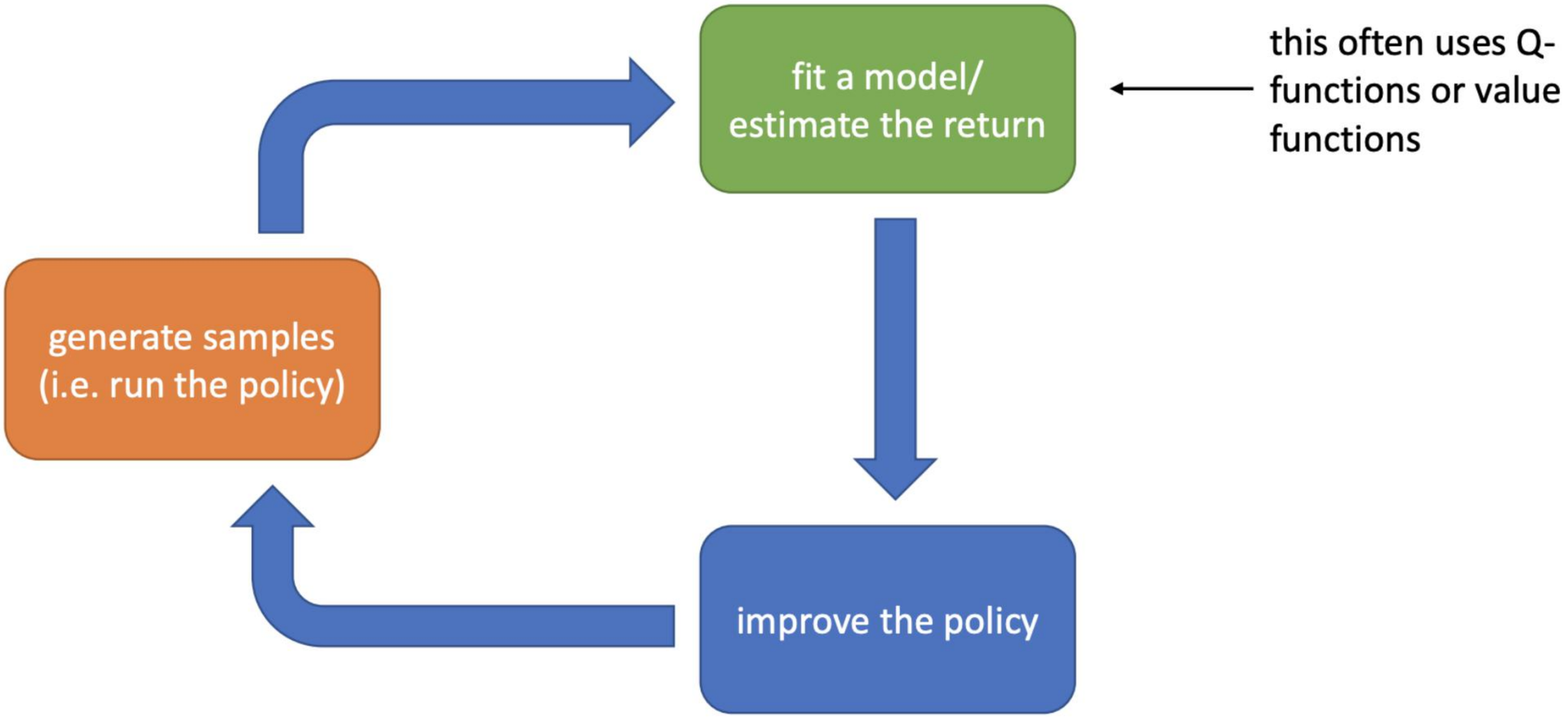
- Reason I:
  - REINFORCE is MC-based
  - Deep Q-Learning (DQN) is TD-based
- Reason II:
  - REINFORCE only has a **policy network**
  - DQN only has a **value network**

A Taxonomy of RL Algorithms and Examples



Q-Learning for Tabular RL

The Anatomy of an RL algorithm



CS285 *taught at UC Berkeley by Prof. Sergey Levine.*

- Suppose we are going to learn the Q-function. Let us follow the previous flow chart and answer three questions:
  1. Given transitions $\{(s, a, s', r)\}$ from some trajectories, how to improve the current Q-function?

  2. Given Q, how to improve policy?

  3. Given π, how to generate trajectories?

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     - By Temporal Difference learning, the update target for $Q(S, A)$ is
       - $R + \gamma \max_a Q(S', a)$
     - Take a small step towards the target
       - $Q(S, A) \leftarrow Q(S, A) + \alpha[R + \gamma \max_a Q(S', a) - Q(S, A)]$
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     - Take the greedy policy based on the current Q
       - $\pi(s) = \text{argmax}_a Q(s, a)$
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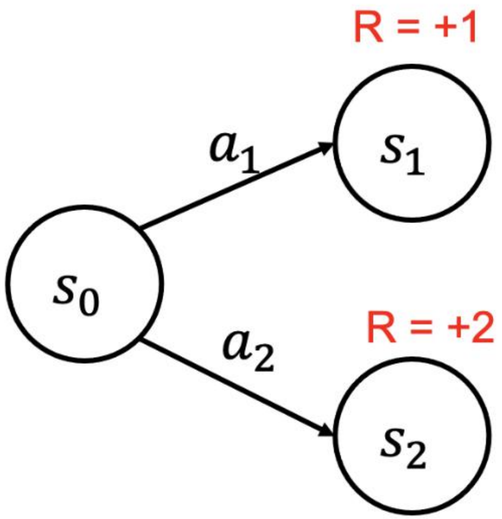
     - Take the greedy policy based on the current Q
       - $\pi(s) = \text{argmax}_a Q(s, a)$
  3. Given π, how to generate trajectories?
     - Simply run the greedy policy in the environment.
     - Any issues?

Failure Example

- Initialize Q
  - $Q(s_0, a_1) = 0, Q(s_0, a_2) = 0$
  - $\pi(s_0) = a_1$
- Iteration 1: take a_1 and update Q
  - $Q(s_0, a_1) = 1, Q(s_0, a_2) = 0$
  - $\pi(s_0) = a_1$
- Iteration 2: take a_1 and update Q
  - $Q(s_0, a_1) = 1, Q(s_0, a_2) = 0$
  - $\pi(s_0) = a_1$
- ...
- **Q stops to improve because the agent is too greedy!**



ϵ-Greedy Exploration

- The simplest and most effective idea for ensuring continual exploration
- With probability $1 - \epsilon$ choose the greedy action
- With probability ϵ choose an action at random
- All m actions should be tried with non-zero probability
- Formally,

$$\pi_*(a|s) = \begin{cases} \epsilon/m + 1 - \epsilon, & \text{if } a = \text{argmax}_{a \in \mathcal{A}} Q(s,a) \\ \epsilon/m, & \text{otherwise} \end{cases}$$

Exploration vs. Exploitation

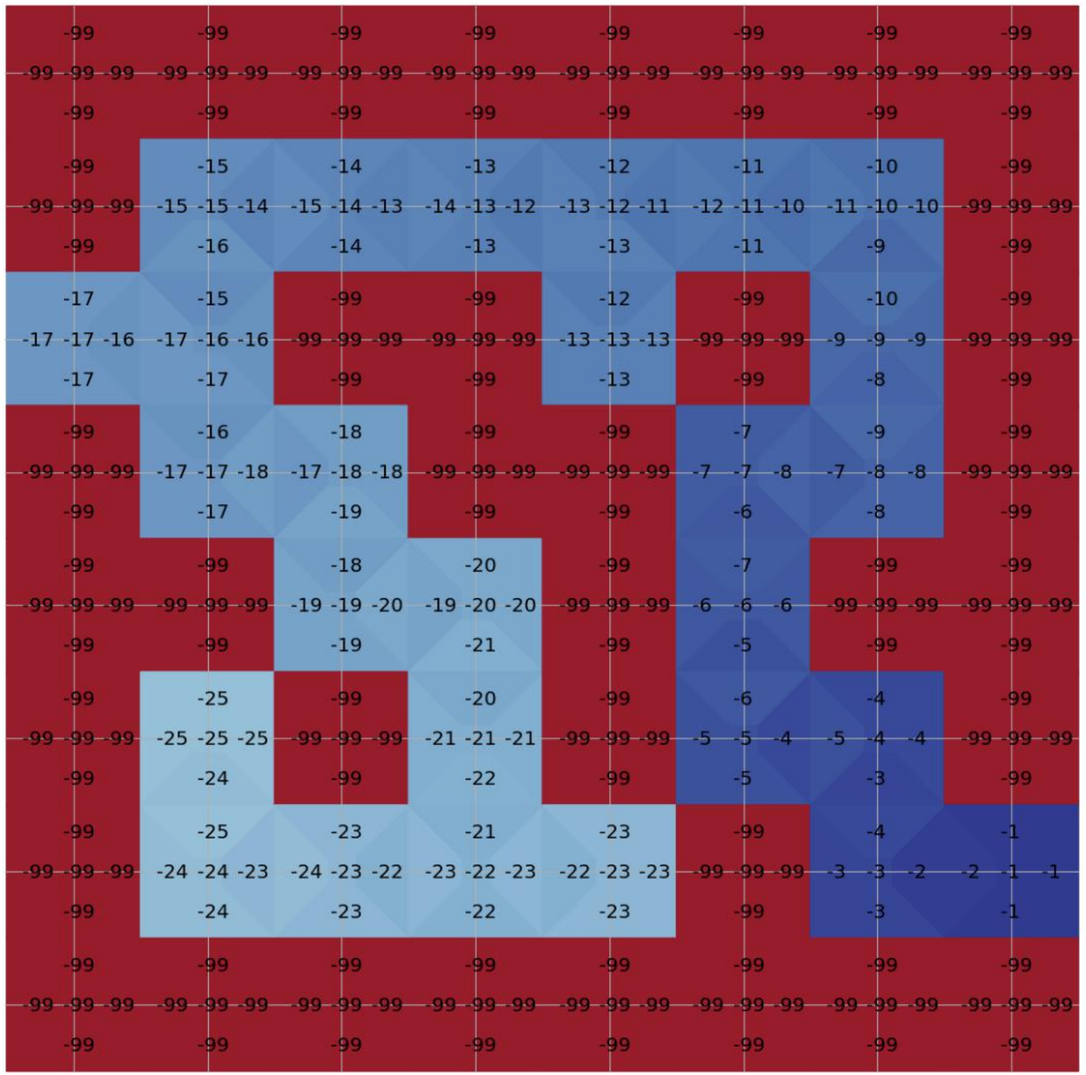
- Two fundamental behaviours of RL agents
  - Reinforcement learning is like trial-and-error learning
  - The agent should discover a good policy
  - From its experiences of the environment
  - Without losing too much reward along the way
- Exploration
  - finds more information about the environment
  - may waste some time
- Exploitation
  - exploits known information to maximize reward
  - may miss potential better policy
- Balancing exploration and exploitation is a key problem of RL. We use will spend a lecture to discuss advanced exploration strategies.

Q-Learning

Q-learning (off-policy TD control) for estimating $\pi \approx \pi_*$

Algorithm parameters: step size $\alpha \in (0, 1]$, small $\varepsilon > 0$
Initialize $Q(s, a)$, for all $s \in \mathcal{S}^+, a \in \mathcal{A}(s)$, arbitrarily except that $Q(terminal, \cdot) = 0$

Loop for each episode:
  Initialize S
  Loop for each step of episode:
    Choose A from S using policy derived from Q (e.g., ε-greedy)
    Take action A, observe R, S'
    $Q(S, A) \leftarrow Q(S, A) + \alpha\big[R + \gamma \max_a Q(S', a) - Q(S, A)\big]$
    $S \leftarrow S'$
  until S is terminal



Running Q-learning on Maze

Plot with the tools in ***an awesome playground for value-based RL*** *from Justin Fu*

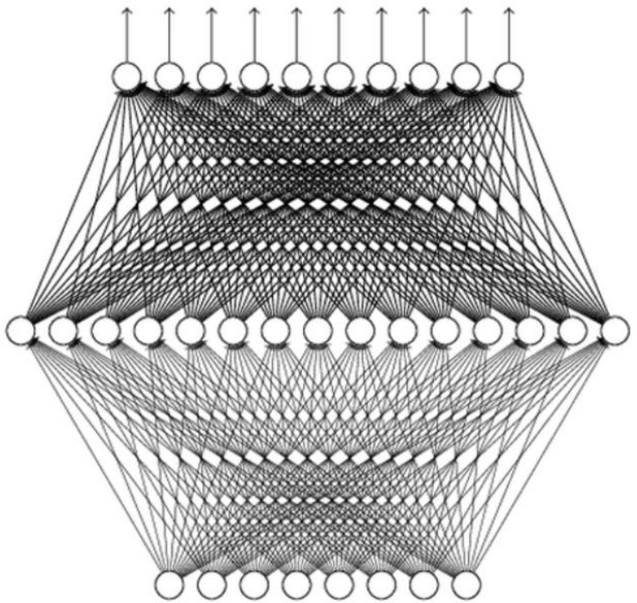
Deep Q-Learning

Challenge of Representing Q

- How do we represent $Q(s, a)$?
- Maze has a discrete and small *state space* that we can deal with by an array.
- However, for many cases the state space is continuous, or discrete but huge, array does not work.

Deep Value Network

- Use a neural network to parameterize Q:
  - Input: state $s \in \mathbb{R}^n$
  - Output: each dimension for the value of an action $Q(s, a; \theta)$



Training Deep Q Network

- Last lecture, we explained tabular TD learning:
  - TD error: $\delta_t = R_{t+1} + \gamma V(S_{t+1}) - V(S_t)$
  - TD update: $V(S_t) \leftarrow V(S_t) + \alpha(G_t - V(S_t))$
- Temporal Difference can also be plugged in an optimization objective to derive the update of the Q network

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- Temporal Difference can also be plugged in an optimization objective to derive the update of the Q network
- Recall the Bellman optimality equation for action-value function:

$$Q^*(s,a) = \mathbb{E}[R_{t+1} + \gamma \max_{a'} Q^*(S_{t+1}, a') | S_t = s, A_t = a]$$

- We create a least-square regression problem accordingly:

$$\sum_{s \in \mathcal{S}, a \in \mathcal{A}} \| Q_\theta(s,a) - \mathbb{E}_{s' \sim P(s'|s,a)}[R(s,a,s') + \gamma \max_{a'} Q_\theta(s', a')] \|^2, \quad \text{where } R_{t+1} = R(s,a,s')$$

Optimization Formulation of TD Learning

- However, the objective is still intractable

$$\sum_{s\in\mathcal{S},a\in\mathcal{A}} \|Q_\theta(s,a) - \mathbb{E}_{s'\sim P(s'|s,a)}[R_{t+1} + \gamma \max_{a'} Q_\theta(s',a')]\|^2$$

- It is natural to build a *new optimization problem* that approximates the above:

$$L(\theta) = \mathbb{E}_{(s,a,s')\sim Env}[TD_\theta(s,a,s')] \qquad \text{(TD loss)}$$

  where $TD_\theta(s,a,s') = \|Q_\theta(s,a) - [R(s,a,s') + \gamma \max_{a'} Q_\theta(s',a')]\|^2$.
- Note: How to obtain the Env distribution has many options!
  - It does not necessarily sample from the optimal policy.
  - A suboptimal, or even bad policy (e.g., random policy), may allow us to learn a good Q.
  - It is a cutting-edge research topic of showing suboptimality bound for non-optimal Env distribution.

Replay Buffer

- As in the previous Q-learning, we consider a routine that we take turns to
  - Sample certain transitions using the current Q_θ
  - Update Q_θ by minimizing the TD loss
- **Exploration:**
  - We use ϵ-greedy strategy to sample transitions, and add (s, a, s', r) in a **replay buffer** (e.g., maintained by FIFO).
- **Exploitation:**
  - We sample a batch of transitions and train the network by gradient descent:

$$\nabla_\theta L(\theta) = \mathbb{E}_{(s,a,s')\sim \text{ReplayBuffer}}[\nabla_\theta TD_\theta(s, a, s')]$$

Deep Q-Learning Algorithm

- Initialize replay buffer D and Q network Q_θ.
- For every episode:
  - Sample the initial state $s_0 \sim P(s_0)$
  - Repeat until the episode is over
    - Let s be the current state
    - With prob. ϵ sample a random action a. Otherwise select $a = \arg\max_a Q_\theta(s, a)$
    - Execute a in the environment, and receive the reward r and the next state s'
    - Add transitions (s, a, s') in D
    - Sample a random batch from D and build the batch TD loss
    - Perform one or a few gradient descent steps on the TD loss

Something More about Q-Learning

- Behavior/Target Network: Recall that $TD_\theta(s,a,s') = \|Q_\theta(s,a) - [R(s,a,s') + \gamma \max_{a'} Q_\theta(s',a')]\|^2$. We keep two Q networks in practice. We only update the blue network by gradient descent and use it to sample new trajectories. Every few episodes we replace the red one by the blue one. The reason is that the blue one changes too fast. The red one is called *target network* (to build target), and the blue one is called *behavior network* (to sample actions).
- Value overestimation: Note that the TD loss takes the maximal a for each $Q(s,\cdot)$. Since TD loss is not unbiased, the max operator will cause the Q-value to be overestimated! There are methods to mitigate (e.g., double Q-learning) or work around (e.g., advantage function) the issue.
- Uncertainty of Q estimation: Obviously, the Q value at some (s,a) are estimated from more samples, and should be more trustable. Those high Q value with low confidence are quite detrimental to performance. Distributional Q-Learning quantifies the confidence of Q and leverages the confidence to recalibrate target values and conduct exploration.
- Theoretically, Q-learning (more precisely, a variation of it) is an **optimal online learning algorithm** for tabular RL.

REINFORCE

Key Idea

- Unlike Q-learning, REINFORCE method does not need to maintain the value function of states or state-action pairs!
- It uses a neural network to parameterize the policy.
- We update the policy network by applying stochastic gradient descent of the return.

Policy Gradient

- The return of a policy π_θ parameterized by a neural network is:

$$J(\theta) = \mathbb{E}_{\tau \sim P(\pi_\theta}[R(\tau)] = \int_\tau P(\tau) R(\tau) \mathrm{d}\tau$$

- Its gradient is

$$\nabla_\theta J(\theta) = \nabla_\theta \int_\tau R(\tau) \mathrm{P}(\tau|\theta) \mathrm{d}\tau = \int_\tau R(\tau) \nabla_\theta \mathrm{P}(\tau|\theta) \mathrm{d}\tau$$

Policy Gradient

- Note that

$$\nabla_\theta f(\theta) = \frac{\nabla f(\theta)}{f(\theta)} \Rightarrow \nabla f(\theta) = f(\theta) \nabla \log f(\theta)$$

- Therefore,

$$\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \int_\tau R(\tau) \mathrm{P}(\tau|\theta) \mathrm{d}\tau = \int_\tau R(\tau) \nabla_\theta \mathrm{P}(\tau|\theta) \mathrm{d}\tau \\
&= \int_\tau \mathrm{P}(\tau|\theta) R(\tau) \nabla_\theta \log \mathrm{P}(\tau|\theta) \mathrm{d}\tau \\
&\approx \frac{1}{n} \sum_k R(\tau_k) \nabla_\theta \log \mathrm{P}(\tau_k|\theta)
\end{aligned}$$

- We can estimate the gradient of $J(\theta)$ by empirical mean!

Policy Gradient

- Note that

$$\mathrm{P}(\tau|\theta) = \log \mathrm{P}(s_0) + \sum_i \log \pi_\theta(a_i|s_i) + \log \mathrm{P}(s_{i+1}|s_i, a_i)$$

- The environment model does not depend on θ. Therefore, the gradient of the return is

$$\boxed{\nabla_\theta J(\theta) \approx \frac{1}{n} \sum_k R(\tau_k) \sum_i \nabla_\theta \log \pi_\theta(a_i|s_i)}$$

Intuitive Explanation

$$\nabla_\theta J(\theta) \approx \frac{1}{n} \sum_k R(\tau_k) \sum_i \nabla_\theta \log \pi_\theta(a_i|s_i)$$

- Weighted sum of (log) policy gradients for all the trajectories.
- Higher weights for trajectories with higher rewards.

Implementing Policy Gradient

- For discrete actions, π_θ is a soft-max function.
- For continuous actions, π_θ is a Gaussian distribution. We use the policy network to predict the mean and variance.

Policy Gradient Algorithm

- Initialize a policy network π_θ.
- Repeat
  - Sample trajectories $\{\tau_{1:T}^k\}_{k \leq n}$
  - Compute the gradient ∇J by policy gradient

$$\nabla_\theta J(\theta) \approx \frac{1}{n} \sum_k R(\tau_k) \sum_i \nabla_\theta \log \pi_\theta(a_i | s_i)$$

  - Update

$$\theta \leftarrow \theta + \alpha \nabla J(\theta)$$

Some Comments on Policy Gradient Algorithm

- We will introduce improved version of policy gradient in subsequent lectures.
- As an MC-based method, the gradient estimation is unbiased.
- However, its estimate of gradient has a large variance. Therefore, stabilizing the update of π_θ is the key.
- As a high-variance method, it is not quite efficient (even its improved version, e.g, TRPO/PPO). But since it is unbiased, for some hard tasks, it may outperform seemingly more sample-efficient Q-learning methods.

Convergence of Reinforcement Learning Algorithms

We state the facts without proof:

- Q-Learning:
  - Tabular setup: Guaranteed convergence to the optimal solution. A simple proof (using contraction mapping).
  - Value network setup: No convergence guarantee due to the approximation nature of networks.
- Policy Gradient: Next lecture.