

# Deep Reinforcement Learning



Han Cheol Moon  
School of Computer Science and Engineering  
Nanyang Technological University  
Singapore  
[tabularasa8931@gmail.com](mailto:tabularasa8931@gmail.com)  
[hancheol1001@edu.ntu.edu.sg](mailto:hancheol1001@edu.ntu.edu.sg)

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Introduction . . . . .	1
1.1.1	Sequential Decision Making . . . . .	1
1.1.2	Exploration and Exploitation . . . . .	2
1.2	Markov Chain . . . . .	3
1.3	Multi-Armed Bandits . . . . .	4
1.3.1	Action-value Methods . . . . .	4
1.3.2	Incremental Implementation of The Action-value Methods . . . . .	5
<b>2</b>	<b>Markov Decision Process</b>	<b>6</b>
2.1	Markov Reward Process . . . . .	6
2.2	Markov Decision Process . . . . .	6
2.3	Policies and Value Functions . . . . .	9
2.3.1	The State-Value Functions . . . . .	9
2.3.2	The Action-Value Function . . . . .	10
2.3.3	The Action-Advantage Function . . . . .	12
2.4	Optimality . . . . .	12
<b>3</b>	<b>Dynamic Programming</b>	<b>14</b>
3.1	Policy Evaluation . . . . .	15
3.2	Policy Improvement . . . . .	15
3.3	Value Iteration . . . . .	15
<b>4</b>	<b>Monte Carlo Methods</b>	<b>17</b>

<i>CONTENTS</i>	2
4.1 Monte Carlo Prediction (Evaluation) . . . . .	17
4.1.1 First Visit vs. Every Visit . . . . .	17
4.2 Monte Carlo Control . . . . .	18
4.3 On-Policy vs. Off-Policy . . . . .	19
4.4 Exploration-Exploitation Trade-off . . . . .	20
4.4.1 On Policy . . . . .	20
4.4.2 Off Policy . . . . .	21
4.5 Temporal-Difference Learning . . . . .	22
4.5.1 Q-learning: Off-policy TD Control . . . . .	23
4.5.2 Sarsa: On-policy TD Control . . . . .	23
4.5.3 Double Q-learning . . . . .	23
<b>5 Deep Reinforcement Learning</b>	<b>24</b>
<b>6 Deep Q-Network</b>	<b>25</b>
<b>7 Policy Gradient</b>	<b>26</b>
7.0.1 Causality . . . . .	27
7.1 Natural Policy Gradient . . . . .	27
7.1.1 KL-divergence between perturbed distributions . . . . .	27
7.2 Proximal Policy Optimization . . . . .	29
<b>8 Search Algorithm</b>	<b>31</b>
8.1 Monte Carlo Tree Search . . . . .	31
8.1.1 Tree Traversal . . . . .	32
8.1.2 Expansion . . . . .	32
8.1.3 Rollout (Random Simulation) . . . . .	32
8.1.4 Backpropagation . . . . .	32
8.2 Uniform Cost Search . . . . .	33
8.3 A* Search . . . . .	34

<i>CONTENTS</i>	3
<b>Appendices</b>	<b>39</b>
<b>Appendix</b>	<b>39</b>
A.1 Bellman Equation . . . . .	39
B.2 Importance Sampling . . . . .	41
C.3 Fisher Information . . . . .	42
D.4 Score Function . . . . .	42
E.5 Incremental Monte-Carlo . . . . .	43
F.6 Derivative of Softmax . . . . .	43
G.7 Policy Gradient Theorem . . . . .	44
G.7.1 Proof of Policy Gradient Theorem . . . . .	45

# Chapter 1

## Introduction

### 1.1 Introduction

Reinforcement learning (RL) is a science of decision making. RL is learning what to do so as to maximize a numerical reward signal. The learner is not told which actions to take, but instead must discover which actions yield the most reward by trying them. In the most interesting and challenging cases, actions may affect not only the immediate reward but also the next situation and, through that, all subsequent rewards. There are some differences compared to other machine learning paradigms:

- RL uses training information that *evaluates* the actions taken rather than *instructs* by giving correct actions.
  - Evaluative feedback, not about best or worst.
  - There is no supervisor, only a *reward* signal
- Delayed reward: Feedback is delayed, not instantaneous.
- Time really matters (sequential, non i.i.d. data).
- Agent's action affects the subsequent data it receives. e.g., a robot moves around a room and it receives a different front view.
- The environment is initially unknown. The agent interacts with the environment. The agent improves its policy
  - Trial-and-error search
- Planning: the environment is known.
- Exploitation: the model finds more information about the environment
- Exploration: the model exploits known information

#### 1.1.1 Sequential Decision Making

- Goal: select actions to maximize total future reward

- Actions may have long term consequences (we have to plan ahead)
- Reward may be delayed
- It may be better to sacrifice immediate reward to gain more long-term reward.

Fully observability: agent directly observes environment state. Fully observable environment is one in which the agent can always see the entire state of environment. In case of fully observable environments all relevant portions of the environment are observable.

$$O_t = S_t^a = S_t^w$$

So agent state is equal to environment state and information state. Formally, this is a **Markov decision process** (MDP).

Partially observability: agent indirectly observes environment. For example, a robot with camera vision isn't told its absolute location or a trading agent doesn't tell about a trend and only observes current prices. Now agent state is not equal to the environment state. Formally this is a partially observable Markov decision process (POMDP).

RL agents can be categorized as follows:

- Value based: policy is implicit
- Policy based
- Actor-Critic
- Model-free: Model-free reinforcement learning algorithms are a class of approaches where the agent learns to make decisions without explicit knowledge of the underlying dynamics or transition probabilities of the environment.
- Model-based: Model-based reinforcement learning (MBRL) algorithms are approaches where the agent learns an explicit model of the environment, including transition dynamics and reward structure. Instead of directly interacting with the environment to learn a policy or value function, the agent builds a model and then uses that model for planning and decision-making. The learned model is typically used to simulate possible future trajectories, which the agent can then optimize to make decisions.

### 1.1.2 Exploration and Exploitation

- Reinforcement learning is like a 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
- Exploitation: exploits known information to maximize reward
  - Restaurant selection:
    - \* Exploitation: go to your favorite restaurant
    - \* Exploration: try a new
  - Oil drilling:
    - \* Exploitation: drill at the best location
    - \* Exploration: try a new location

## 1.2 Markov Chain

- Reachable:  $i \rightarrow j$
- Communicate:  $i \leftrightarrow j$
- Irreducible:  $i \leftrightarrow j, \forall i, j$
- Absorbing state: If the only possible transition is to itself. This is also a terminal state.
- Transient state: A state  $s$  is called a transient state, if there is another state  $s'$ , that is reachable from  $s$ , but not vice versa.
- Recurrent state: A state that is not transient.
- Periodic: A state is periodic if all of the paths leaving  $s$  come back after some multiple steps ( $k > 1$ ).
  - Recurrent state is aperiodic if  $k = 1$ .
- Ergodicity if a Markov chain follows:
  - Irreducible
  - Recurrent
  - Aperiodic

## 1.3 Multi-Armed Bandits

Bandit problems are stateless. Each arm has a fixed distribution of rewards. It does not depend on which arms were pulled previously. The goal is to explore the reward distributions of all arms and then keep pulling the best one. We only have a single chance of selecting an action in each episode.

Markov decision processes are a temporal extension of bandit problems: pulling an arm influences the future rewards. Technically, there is a state that changes by pulling an arm. The reward distributions depend on that state.

You can view bandit problems as Markov decision processes where all states are terminal. In that case, all decision sequences have a length of 1 and subsequent pulls don't influence each other.

- When the lever of a slot machine is pulled it gives a random reward coming from a probability distribution specific to that machine.
- Although the machines look identical, their reward probability distributions are different.
- In each turn, gamblers need to decide whether to play the machine that has given the highest average reward so far, or to try another machine.

In our  $k$ -armed bandit problem, each of the  $k$  actions has an expected or mean reward given that that action is selected: let us call this the *value* of that action. We denote the action selected on time step  $t$  as  $A_t$ , and the corresponding reward as  $R_t$ . The value then of an arbitrary action  $a$ , denoted  $q_*(a)$ , is the expected reward given that  $a$  is selected:

$$q_*(a) = \mathbb{E}[R_t | A_t = a].$$

Since we do not know which action is the best, we have to estimate the value of actions  $a$  at time step  $t$ ,  $Q_t(a)$ .

### 1.3.1 Action-value Methods

One natural way to estimate this is by averaging the rewards actually received:  $Q_t(a)$  is sum of rewards when  $a$  taken prior  $t$  over number of times  $a$  taken prior to  $t$ :

$$Q_t(a) = \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbb{1}_{A_i=a}}{\sum_{i=1}^{t-1} \mathbb{1}_{A_i=a}}$$

In other words, the average reward (action value) observed before the  $n$ -th selection of this action is  $Q_n = (R_1 + \dots + R_{n-1}) / (n - 1)$

Then, the simplest action selection rule is to select one of the actions with the highest estimated value, which is a greedy action selection method represented as follows:

$$A_t = \underset{a}{\operatorname{argmax}} Q_t(a).$$

This approach always exploits current knowledge to maximize immediate reward; it spends no time at all sampling apparently inferior actions to see if they might really be better. A simple



alternative is to behave greedily most of the time, but every once in a while, instead select randomly from among all the actions. This near greedy action selection rule is called  $\epsilon$ -greedy method. In the limit as the number of steps increases, every action will be sampled an infinite number of times, which ensures all the  $Q_t(a)$  converge to  $q_*(a)$ .

### 1.3.2 Incremental Implementation of The Action-value Methods

$$\begin{aligned}
 Q_{n+1} &= \frac{1}{n} \sum_{i=1}^n R_i \\
 &= \frac{1}{n} \left( R_n + \sum_{i=1}^{n-1} R_i \right) \\
 &= \frac{1}{n} \left( R_n + (n-1) \frac{1}{n-1} \sum_{i=1}^{n-1} R_i \right) \\
 &= \frac{1}{n} \left( R_n + (n-1) Q_n \right) \\
 &= Q_n + \frac{1}{n} [R_n - Q_n]
 \end{aligned}$$

- $Q_n$ : Old estimate
- $Q_{n+1}$ : New estimate
- $R_n$ : New reward

This is an incremental formulas for updating averages with small, constant computation required to process each new reward. This update rule can be expressed in a general form:

$$\text{NewEstimate} \leftarrow \text{OldEstimate} + \text{StepSize} \underbrace{\left[ \text{Target} - \text{OldEstimate} \right]}_{\text{error}}.$$

The target is presumed to indicate a desirable direction in which to move, though it may be noisy. So, we adjust our current estimate,  $Q_n$ , in the direction of the error that we calculate based on the latest observed reward,  $R_n - Q_n$ , with a step size of  $1/n$  and obtain a new estimate,  $Q_{n+1}$ .

```

1 class GaussianBandit:
2     def __init__(self, mean=0, stdev=1):
3         self.mean = mean
4         self.stdev = stdev
5
6     def pull_lever(self):
7         reward = np.random.normal(self.mean, self.stdev)
8         return np.round(reward, 1)
9
10 slotA = GaussianBandit(5, 3)
11 slotB = GaussianBandit(6, 2)
12 slotC = GaussianBandit(1, 5)
13
14 game = GaussianBanditGame([slotA, slotB, slotC])
15 game.user_play()

```

## Chapter 2

# Markov Decision Process

### 2.1 Markov Reward Process

In reinforcement learning, a MRP arises when you fix a policy for your MDP. Then all the decision making is accounted for, and we have a MRP with the induced transition kernel

$$\begin{aligned} v(s) &= \mathbb{E}[G_t | S_t = s] \\ &= \mathbb{E}\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} | S_t = s\right] \\ &= \sum_{s', r} p(s', r | s) [r + \gamma v(s')] \end{aligned}$$

Bellman equation for MRP. In matrix form,

$$v = PR + \gamma Pv.$$

We can solve this system by

$$v = (I - \gamma P)^{-1} PR$$

An MRP is fully characterized by a  $\langle S, P, R, \gamma \rangle$  tuple, where  $S$  is a set of states,  $P$  is a transition probability matrix,  $R$  is a reward function, and  $\gamma \in [0, 1]$  is a discount factor.

### 2.2 Markov Decision Process

The general framework of MDPs (representing environments as MDPs) allows us to model virtually any complex sequential decision-making problem under uncertainty in a way that RL agents can interact with and learn to solve solely through experience.

Components of RL:

- An agent
- A policy

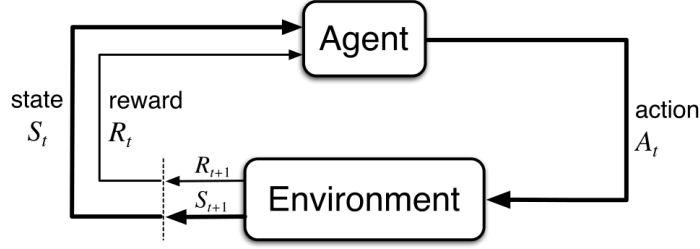


Figure 2.1: The agent-environment interaction in a Markov decision process.

- A reward signal: what is good in an immediate sense.
- A value function: what is good in the long run.
- A model of the environment: This allows inferences to be made about how the environment will behave.

An MDP is fully characterized by a  $\langle SA, P, R, \gamma \rangle$  tuple, where  $S$  is a set of states,  $P$  is a transition probability matrix,  $R$  is a reward function, and  $\gamma \in [0, 1]$  is a discount factor.

**Definition 1 (Markov Property)** A state  $S_t$  is *Markov* if and only if

$$P[S_{t+1}|S_t, A_t] = P[S_{t+1}|S_t, A_t, S_{t-1}, A_{t-1}, \dots]$$

- Actions: a mechanism to influence the environment
- State: specific configurations of the environment

**Definition 2 (Transition Function)**

$$p(s', r|s, a) = P(S_t = s', R_t = r | S_{t-1} = s, A_{t-1} = a)$$

- The way the environment changes as a response to actions is referred to as the state-transition probabilities, or more simply, the transition function, and is denoted by  $T(s, a, s')$ .
- $\sum_{r \in \mathcal{R}} \sum_{s' \in \mathcal{S}} p(s', r|s, a) = 1, \quad \forall s \in \mathcal{S}, \forall a \in \mathcal{A}(s)$
- $p(s'|s, a) = P(S_t = s' | S_{t-1} = s, A_{t-1} = a) = \sum_{r \in \mathcal{R}} p(s', r|s, a)$

**Definition 3 (Reward Hypothesis)** All goals can be described by the maximization of expected cumulative reward.

- That all of what we mean by goals and purposes can be well thought of as the maximization of the expected value of the cumulative sum of a received scalar signal (called reward).

**Definition 4 (Reward Function)**

$$\begin{aligned} r(s, a) &= \mathbb{E}[R_t | S_{t-1} = s, A_{t-1} = a] \\ &= \sum_{r \in \mathcal{R}} r \sum_{s' \in \mathcal{S}} p(s', r|s, a) \end{aligned}$$

- $R_t \in \mathcal{R} \subset \mathbb{R}$ .
  - Note that negative reward is still reward.
- The expected reward function is defined as a function that takes in a state-action pair.
- It is the expectation of reward at time step  $t$ , given the state-action pair in the previous time step.
- The reward function can also be defined as a function that takes a full transition tuple  $s, a, s'$ .

$$\begin{aligned} r(s, a, s') &= \mathbb{E}[R_t | S_{t-1} = s, A_{t-1} = a, S_t = s'] \\ &= \sum_{r \in \mathcal{R}} \frac{p(s', r | s, a)}{p(s' | s, a)} r \end{aligned}$$

**Definition 5 (Discount Factor,  $\gamma$ )**

$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots + \gamma^{T-t} R_T$$

- **The sum of all rewards obtained during the course of an episode** is referred to as the *return*,  $G_t$ .
- Episodic tasks:  $G_t = R_{t+1} + R_{t+2} + \cdots + R_T$ .
  - $G_t = R_{t+1} + \gamma G_{t+1}$
- Continuing tasks:  $G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1}$ .
  - $\gamma = 0$ : myopic evaluation
  - $\gamma = 1$ : far-sighted evaluation
  - Uncertainty about the future that may not be fully observed
  - Mathematically convenient to discount rewards.
  - Avoid infinite returns in cyclic Markov processes.

**A Simple Example:**

- Environment:
  - The grid world has 3 states:  $S1$ ,  $S2$ , and  $S3$ .
  - The agent can take actions  $A = \{left, right\}$ .
  - The rewards are as follows:
    - \*  $R_{left} = 1$ : penalty for moving left
    - \*  $R_{right} = +1$ : reward for moving right
  - The discount factor  $\gamma$ : 0.9.
- Episode:
  1. The agent starts in  $S1$ .
  2. If the agent moves left, it incurs a penalty ( $R_{left} = 1$ ), and the episode ends.

3. If the agent moves right, it receives a reward ( $R_{right} = +1$ ), transitions to  $S2$ , and the episode continues.
  4. In  $S2$ , the agent faces the same choices.
  5. The episode ends when the agent either moves left or reaches  $S3$ .
- Return Calculation:
    - Let's calculate the return for a sample trajectory:  $\{S1, right, S2, right, S3\}$ .
    - $G = R_{right} + \gamma R_{right} + \gamma^2 R_{right} = 2.71$
    - So, the return for this trajectory is 2.71.

## 2.3 Policies and Value Functions

- Policies are universal plans, which provides all possible plans for all states.
  - Plans are not enough to fully describe an environment in stochastic environments.
    - \* What if an agent intends to move right, but ends up going left. Which action does the agent take?
  - Policies are the per-state action descriptions.
  - Policy can be stochastic or deterministic.
  - A policy is a function that prescribes actions to take for a given non-terminal state.

Formally, a policy is a mapping from states to probabilities of selecting each possible action. It can be defined

$$\pi(a|s)$$

### 2.3.1 The State-Value Functions

Almost all reinforcement learning algorithms involve estimating *value functions*, functions of states (or of state-action pairs) that estimate how good it is for the agent to be in a given state (or how good it is to perform a given action in a given state). The notion of “how good” here is defined in terms of future rewards that can be expected, or, to be precise, in terms of **expected return**. Of course, the rewards the agent can expect to receive in the future depend on what actions it will take. Accordingly, value functions are defined with respect to particular ways of action, called policies.

**Definition 6 (The State-Value Function,  $V$ )** *The state-value function  $v(s)$  for policy  $\pi$  of an Markov Reward Process is the expected return starting from state  $s$*

$$\begin{aligned} v_{\pi}(s) &= \mathbb{E}_{\pi}[G_t | S_t = s] \\ &= \mathbb{E}_{\pi} \left[ \sum_{k=0}^{\infty} \gamma^k R_{t+1+k} \middle| S_t = s \right], \quad \forall s \in \mathcal{S} \end{aligned}$$

- The value of a state  $s$  is the expectation over policy  $\pi$ .

- Value function is the expected return.
  - Reward: one-step signal that an agent receives.
  - Return: total discounted rewards, which is the sum of rewards obtained from time  $t$  onward.
- If we are given a policy and the MDP, we should be able to calculate the expected return starting from every single state.

The state-value function satisfies the *Bellman equation*, which expresses the relationship between the value of a state and the values of its successor states:

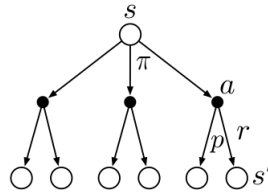
$$v_\pi(s) = \mathbb{E}_\pi[G_t | S_t = s] \quad (2.1)$$

$$= \mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1} | S_t = s] \quad (2.2)$$

$$= \mathbb{E}_\pi[R_{t+1} + \gamma v_\pi(s_{t+1}) | S_t = s] \quad (2.3)$$

$$= \sum_a \pi(a|s) \sum_{s', r} p(s', r | s, a) [r + \gamma v_\pi(s')], \forall s \in \mathcal{S}. \quad (2.4)$$

For better understanding, let's look at the §2.3.1. Starting from state  $s$ , the root node at the top, the agent could take any of some set of actions (three actions are shown in the diagram), based on its policy  $\pi$ . From each of these, the environment could respond with one of several next states,  $s'$  (two states are shown in the figure), along with a reward,  $r$ , depending on its dynamics given by the function  $p$ . The Bellman equation averages over all the possibilities, weighting each by its probability of occurring. **It states that the value of the start state must equal (discounted) the value of the expected next state, plus the reward expected along the way.** The derivation of Eq. (2.4) is given in Appendix A.1. The state-value function is



essential for understanding the value of different states in a Markov Decision Process (MDP) and is often used in various reinforcement learning algorithms, such as value iteration and policy iteration.

### 2.3.2 The Action-Value Function

- Another critical question that we often need to ask is not merely about the value of a state but the value of taking action  $a$  at a state  $s$ .
- Which action is better under each policy?
- The action-value function, also known as  $Q$ -function or  $Q^\pi(s, a)$ , captures precisely this.
  - The expected return if the agent follows policy  $\pi$  after taking action  $a$  in state  $s$ .

**Definition 7 (The Action-Value Function,  $Q$ )** The action-value function  $q_\pi(s, a)$  for policy  $\pi$  is the expected return starting from state  $s$ , tacking action  $a$  under policy  $\pi$

$$q_\pi(s, a) = \mathbb{E}_\pi[G_t | S_t = s, A_t = a] = \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \middle| S_t = s, A_t = a \right]$$

- The Bellman equation for the action-value function is given by

$$\begin{aligned}
q_\pi(s, a) &= \mathbb{E}_\pi[G_t | S_t = s, A_t = a] \\
&= \mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1} | S_t = s, A_t = a] \\
&= \sum_{s', r} p(s', r | s, a) [r + \gamma v_\pi(s')]
\end{aligned}$$

- Notice that we do not weight over actions because we are interested only in a specific action.
- The action-value function is crucial for understanding the value of different state-action pairs in a Markov Decision Process (MDP) and is used in various reinforcement learning algorithms, such as Q-learning and deep Q-networks (DQN).
- The derivation is given in Appendix A.1

The state-value function can be also expressed by using the action-value function as follows:

$$\begin{aligned}
v_\pi(s) &= \mathbb{E}_\pi[G_t | S_t = s] \\
&= \sum_{g_t} g_t \cdot P[G_t | S_t = s] \\
&= \sum_{g_t} g_t \cdot P[G_t, S_t = s] / P[S_t = s] \\
&= \sum_{g_t} g_t \cdot \sum_a P[G_t, S_t = s, A_t = a] / P[S_t = s] \\
&= \sum_{g_t} g_t \cdot \sum_a \left[ P[G_t | S_t = s, A_t = a] P[S_t = s, A_t = a] \right] / P[S_t = s] \\
&= \sum_{g_t} g_t \sum_a P[G_t, A_t = a | S_t = s] P[A_t = a | S_t = s] \\
&= \sum_a \sum_{g_t} g_t P[G_t | S_t = s, A_t = a] P[A_t = a | S_t = s] \\
&= \sum_a q_\pi(s, a) \pi(a | s)
\end{aligned}$$

Note that the expectation is parameterized  $\pi$  as written in  $\mathbb{E}_\pi$ . We can also simply prove it by the *Law of Total Expectation*<sup>1</sup>,

$$\begin{aligned}
v_\pi(s) &= \mathbb{E}_\pi[G_t | S_t = s] \\
&= \mathbb{E}[\mathbb{E}_\pi[G_t | S_t = s, A_t = a]] \\
&= \sum_a \mathbb{E}_\pi[G_t | S_t = s, A_t = a] P(A_t = a | S_t = s) \\
&= \sum_a q_\pi(s, a) \pi(a | s)
\end{aligned}$$

An intuitive explanation of this derivation is that the expectation depends on an action  $a \sim \pi(a | s)$ . We want to estimate the expected total return by the sampled action (this is because the total return is the function of  $a$ , implicitly). Then, we need to introduce an action variable  $a$  and its probability in the expression as the second line of the equation.

---

<sup>1</sup> $\mathbb{E}[\mathbb{E}[X|Y]] = \sum_y \left[ \sum_x x \cdot p(X = x|Y) \right] p(Y = y) = \mathbb{E}[X]$

### 2.3.3 The Action-Advantage Function

**Definition 8 (The Action-Advantage Function,  $A$ )**

$$a_\pi(s, a) = q_\pi(s, a) - v_\pi(s)$$

The advantage function describes how much better it is to take action  $a$  instead of following policy  $\pi$ . In other words, the advantage of choosing action  $a$  over the default action, set by the policy.

## 2.4 Optimality

Solving a reinforcement learning task means, roughly, finding a policy that achieves a lot of reward over the long run. For finite MDPs, we can precisely define an optimal policy in the following way. Value functions define a partial ordering over policies. A policy  $\pi$  is defined to be better than or equal to a policy  $\pi'$  if its expected return is greater than or equal to that of  $\pi'$  for all states. In other words,  $\pi \geq \pi'$  if and only if  $v_\pi(s) \geq v_{\pi'}(s)$  for all  $s \in \mathcal{S}$ . There is always at least one policy that is better than or equal to all other policies. This is an *optimal policy*. The optimal state-value function, denoted  $v_*$  can be defined as

**Definition 9 (Optimal State-Value Function)** *The optimal state-value function  $v_*(s)$  is the maximum value over all policies*

$$v_*(s) = \max_{\pi} v_\pi(s), \quad \forall s \in \mathcal{S}.$$

- The optimal state-value function can be obtained as follows:

$$\begin{aligned} v_*(s) &= \max_{a \in \mathcal{A}(s)} q_{\pi_*}(s, a) \\ &= \max_a \mathbb{E}_{\pi_*}[G_t | S_t = s, A_t = a] \\ &= \max_a \mathbb{E}_{\pi_*}[R_{t+1} + \gamma G_{t+1} | S_t = s, A_t = a] \\ &= \max_a \mathbb{E}_{\pi_*}[R_{t+1} + \gamma v_*(S_{t+1}) | S_t = s, A_t = a] \\ &= \max_a \sum_{r, s'} p(s', r | s, a) [r + \gamma v_*(s')] \end{aligned}$$

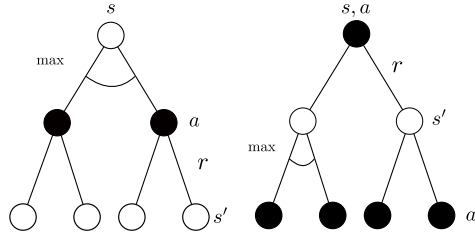
**Definition 10 (Optimal Action-Value Function)** *The optimal action-value function  $q_*(s, a)$  is the maximum value over all policies*

$$q_*(s, a) = \max_{\pi} q_\pi(s, a), \quad \forall s \in \mathcal{S} \text{ and } a \in \mathcal{A}.$$

- The optimal action-value function can be obtained as follows:

$$\begin{aligned} q_*(s, a) &= \mathbb{E}[R_{t+1} + \gamma v_*(S_{t+1}) | S_t = s, A_t = a] \\ &= \sum_{s', r} p(s', r | s, a) [r + \gamma \max_a q_*(s', a')] \end{aligned}$$





- The optimal value function specifies the best possible performance in the MDP.
- The MDP is solved when we know the optimal value function

### Theorem 1 (Optimal Policy Theorem)

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

For any Markov Decision Process:

- There exists an optimal policy  $\pi_*$  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  $q_*(s, a)$ ,

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

- There is always a deterministic optimal policy for any MDP
- If we know  $q_*(s, a)$ , we immediately have the optimal policy
  - Q-learning: learns Q values first
  - Policy gradient: learns optimal policy without learning Q values

## Chapter 3

# Dynamic Programming

The term dynamic programming (DP) refers to a collection of algorithms that can be used to compute optimal policies given a perfect model of the environment as a Markov decision process (MDP). Classical DP algorithms are of limited utility in reinforcement learning both because of their assumption of a perfect model and because of their great computational expense, but they are still important theoretically. The key idea of DP, and of reinforcement learning generally, is the use of value functions to organize and structure the search for good policies.

Let  $\pi$  and  $\pi'$  be any pair of deterministic policies such that, for all  $s \in \mathcal{S}$ ,

$$q_\pi(s, \pi'(s)) \geq v_\pi(s).$$

Then, the policy  $\pi'$  must be as good as, or better than  $\pi$ . Equivalently, it must obtain the following inequality for all states  $s \in \mathcal{S}$ :

$$v'_\pi(s) \geq v_\pi(s).$$

**Theorem 2 (Policy Improvement Theorem)**  $q_\pi(s, \pi'(s)) \geq v_\pi(s)$ , then  $v'_\pi(s) \geq v_\pi(s)$ .

Proof.

$$\begin{aligned} v_\pi(s) &\leq q_\pi(s, \pi'(s)) \\ &= \mathbb{E}[R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s, A_t = \pi'(s)] \\ &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s] \\ &\leq \mathbb{E}_{\pi'}[R_{t+1} + \gamma q_\pi(S_{t+1}, \pi'(S_{t+1})) | S_t = s] \\ &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma \mathbb{E}_{\pi'}[R_{t+2} + \gamma v_\pi(S_{t+2}) | S_{t+1}, A_{t+1} = \pi'(S_{t+1})] | S_t = s] \\ &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma R_{t+2} + \gamma^2 v_\pi(S_{t+2}) | S_t = s] \\ &\leq \mathbb{E}_{\pi'}[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \gamma^3 v_\pi(S_{t+3}) | S_t = s] \\ &\vdots \\ &\leq \mathbb{E}_{\pi'}[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \gamma^3 R_{t+4} + \dots | S_t = s] \\ &= \mathbb{E}_{\pi'}[G_t | S_t = s] \\ &= v_{\pi'}(s). \end{aligned}$$

### 3.1 Policy Evaluation

- Prediction problem: refers to the problem of **evaluating policies** (simply, rating policies), of estimating value functions given a policy (learning to predict returns).
- Control problem: problem of **finding optimal policies**. Usually solved by the pattern of generalized policy iteration (GPI), where the competing processes of policy evaluation and policy improvement progressively move policies towards optimality.
- Policy evaluation: refers to algorithms that solve the prediction problem.
  - Iterative policy evaluation:

$$v_{k+1}(s) = \sum_a \pi(a|s) \sum_{s',r} p(s',r|s,a)[r + \gamma v_k(s')].$$

1. Init  $v_0(s)$  for all  $s$  arbitrarily and to 0 if  $s$  is terminal.
2. Bootstrapping:  $v_1(s) \rightarrow v_2(s) \rightarrow \dots \rightarrow v_N(s)$

A single round of updates,  $k$ , involves updating all the state values. The algorithm stops until the changes in state values are sufficiently small in successive iterations.

### 3.2 Policy Improvement

Our reason for computing the value function for a policy is to help find better policies. The goal of policy improvement is to modify the policy to make it better with respect to the value function. This is done by selecting actions that are known to be better, according to the current value estimates.

- The key is the action-value function,  $q_\pi(s, a)$ . We can select the action that maximizes the action-value function in a greedy way:

$$\begin{aligned} \pi'(s) &= \operatorname{argmax}_a q_\pi(s, a) \\ &= \operatorname{argmax}_a \sum_{s',r} p(s',r|s,a)[r + \gamma v_\pi(s')]. \end{aligned}$$

- The greedy policy takes the action that looks best in the short term according to  $v_\pi$ .

The process of policy evaluation and improvement is often repeated iteratively until the policy converges to an optimal policy that maximizes the expected return in the given environment. This iterative process is the basis for algorithms like *policy iteration* and *value iteration* in reinforcement learning.

### 3.3 Value Iteration

One drawback to policy iteration is that each of its iterations involves policy evaluation, which may itself be a protracted iterative computation requiring multiple sweeps through the state set.

In fact, the policy evaluation step of policy iteration can be truncated in several ways without losing the convergence guarantees of policy iteration.

$$v_{k+1}(s) = \max_a \sum_{s',r} p(s',r|s,a)[r + \gamma v_k(s')], \forall s \in \mathcal{S}. \quad (3.1)$$

For arbitrary  $v_0$ , the sequence  $v_k$  can be shown to converge to  $v_*$  under the same conditions that guarantee the existence of  $v_*$ .

# Chapter 4

## Monte Carlo Methods

Monte Carlo methods are a class of computational algorithms that rely on random sampling to obtain numerical results. In the context of reinforcement learning (RL), Monte Carlo methods are often used to estimate the value of states or state-action pairs in a Markov Decision Process (MDP).

### 4.1 Monte Carlo Prediction (Evaluation)

Recall that the value of a state is the expected return starting from that state. An obvious way to estimate it from experience, then, is simply to average the returns observed after visits to that state. As more returns are observed, the average should converge to the expected value. This idea is the core of Monte Carlo methods.

#### 4.1.1 First Visit vs. Every Visit

Suppose we wish to estimate  $v_\pi(s)$ , the value of a state  $s$  under policy  $\pi$ , given a set of episodes obtained by following  $\pi$  and passing through  $s$ . Each occurrence of state  $s$  in an episode is called a visit to  $s$ .

**The first-visit MC** method estimates  $v_\pi(s)$  as the average of the returns following first visits to  $s$ , whereas *the every-visit MC* method averages the returns following all visits to  $s$ .

- First visit MC treats each trajectory as an i.i.d., sample of  $v(s)$ .
- For instance, we have two example episodes,
  - $A, 3 \rightarrow A, 2 \rightarrow B, -4 \rightarrow A, 4 \rightarrow B, -3$ .
  - $B, -2 \rightarrow A, 3 \rightarrow B, -3$ .
- Each number next to the states are reward. Let's say discount factor is 1 and we want to compute  $V(A)$ , then the first visit MC computes a return by summing all the rewards ( $G \leftarrow \gamma G + R_{t+1}$ ) coming after the first visit to the state  $A$ . Therefore, we can't have more than one summation term for each episode for a state. In sum,

- For the first episode:  $3 + 2 - 4 + 4 - 3 = 2$ .
- For the second episode:  $3 - 3 = 0$ .
- Thus,  $V(A) = (2 + 0)/2 = 1$ .
- It must be noted that if an episode doesn't have an occurrence of 'A', it won't be considered in the average. Hence if a 3rd episode is given like  $B, 3 \rightarrow B, 3 \rightarrow \text{terminate}$  existed, still  $V(A) = 1$ .

**First-visit MC prediction, for estimating  $V \approx v_\pi$**

Input: a policy  $\pi$  to be evaluated

Initialize:

- $V(s) \in \mathbb{R}$ , arbitrarily, for all  $s \in \mathcal{S}$
- $Returns(s) \leftarrow$  an empty list, for all  $s \in \mathcal{S}$

Loop forever (for each episode):

- Generate an episode following  $\pi$ :  $S_0, A_0, R_1, S_1, A_1, R_2, \dots, S_{T-1}, A_{T-1}, R_T$
- $G \leftarrow 0$
- Loop for each step of episode,  $t = T-1, T-2, \dots, 0$ :
  - $G \leftarrow \gamma G + R_{t+1}$
  - Unless  $S_t$  appears in  $S_0, S_1, \dots, S_{t-1}$ :
    - Append  $G$  to  $Returns(S_t)$
    - $V(S_t) \leftarrow \text{average}(Returns(S_t))$

Figure 4.1: First-visit MC prediction algorithm.

**Every visit MC** method averages the returns following **all visits** to  $s$ .

- Here, we would be creating a new summation term adding all rewards coming after every occurrence of 'A'(including that of A as well).
  - From 1st episode:  $(3 + 2 - 4 + 4 - 3) + (2 - 4 + 4 - 3) + (4 - 3) = 2 - 1 + 1$
  - From 2nd episode:  $(3 - 3) = 0$
  - As we got 4 summation terms, we will be averaging using  $N = 4$  i.e.,
  - $V(A) = (2 - 1 + 1 + 0)/4 = 0.5$

## 4.2 Monte Carlo Control

$$\pi_0 \xrightarrow{E} q_{\pi_0} \xrightarrow{I} \pi_0 \xrightarrow{E} q_{\pi_0} \xrightarrow{I} \dots \xrightarrow{I} \pi_* \xrightarrow{E} q_{\pi_*},$$

- $\pi_0$ : arbitrary policy.
- Policy improvement is done by making the policy greedy with respect to the current value function (action-value function).
- For any action-value function  $q$ , the corresponding greedy policy is the one that, for each  $s \in \mathcal{S}$ , deterministically chooses an action with maximal action-value:

$$\pi(S) = \operatorname{argmax}_a q(s, a).$$

- Policy improvement then can be done by constructing each  $\pi_{k+1}$  as the greedy policy with respect to  $q_{\pi_k}$ .
- By Theorem 2, each  $\pi_{k+1}$  is uniformly better than  $\pi_k$  or just as good as  $\pi_k$ .

### 4.3 On-Policy vs. Off-Policy

**On-policy** learns about the optimal policy by executing the policy and evaluating and improving it.

- Learning to be great by itself.
- The agent learns from the experiences it gathers while following its current policy.
- The policy is typically denoted by  $\pi$ .
- The learning process is directly tied to the policy being used for action selection.
- Examples of on-policy algorithms include REINFORCE (Monte Carlo Policy Gradient) and Proximal Policy Optimization (PPO).

**Off-policy** learns about the optimal policy by using data generated by another policy.

- Learning from others.
- The agent can learn from historical data, which may have been generated by an older policy.
- The policy used for learning is not necessarily the one used for action selection.
- The data collected can be more efficiently reused for learning new policies.
- Examples of off-policy algorithms include Q-learning, Deep Q Networks (DQN), and Actor-Critic methods.

#### Exploration-Exploitation Trade-off

- On-policy algorithms often struggle with exploration because they are committed to following their current policy, which may not explore the state space efficiently.
- Off-policy algorithms can be more sample-efficient in exploration as they can learn from a mixture of data from different policies.

#### Data Efficiency

- Off-policy algorithms can potentially be more data-efficient since they can reuse past experiences collected by any policy.
- On-policy algorithms typically require more samples to update the policy effectively.

## Stability and Convergence

- On-policy algorithms can be more stable because they are directly optimizing the policy they are following.
- Off-policy algorithms might face challenges related to the stability of learning, especially when dealing with function approximation, as is often the case with deep learning.

Both on-policy and off-policy algorithms have their strengths and weaknesses, and the choice between them depends on the specific requirements and characteristics of the problem at hand.

## 4.4 Exploration-Exploitation Trade-off

The more episodes are collected, the better, but there is a problem. If the algorithm for policy improvement always updates the policy greedily, meaning it takes only actions leading to immediate reward, actions and states not on the greedy path will not be sampled sufficiently, and potentially better rewards would stay hidden from the learning process.

Essentially, we are forced to make a choice between making the best decision given the current information or start exploring and finding more information. This is also known as the Exploration vs. Exploitation Dilemma.

We are looking for something like a middle ground between those. Full-on exploration would mean that we would need a lot of time to collect the needed information, and full-on exploitation would make the agent stuck into a local reward maximum. There are two approaches to ensure all actions are sampled sufficiently called on-policy and off-policy methods.

### 4.4.1 On Policy

On-policy methods solve the exploration vs exploitation dilemma by including randomness in the form of a policy that is soft, meaning that non-greedy actions are selected with some probability. These policies are called  $\epsilon$ -greedy policies as they select random actions with an  $\epsilon$  probability and follow the optimal action with  $1 - \epsilon$  probability

Since the probability of selecting from the action space randomly is  $\epsilon$ , the probability of selecting any particular non-optimal (non-greedy) action is  $\epsilon/|\mathcal{A}(s)|$ . The probability of following the optimal action will always be slightly higher, however, because we have a  $1 - \epsilon$  probability of selecting it outright and  $\epsilon/|\mathcal{A}(s)|$  probability of selecting it from sampling the action space <sup>1</sup>

$$P(a_t^*) = 1 - \epsilon + \epsilon/|\mathcal{A}(s)|.$$

It is also worth noting that because the optimal action will be sampled more often than the others making on-policy algorithms will generally converge faster but they also have the risk of trapping the agent into a local optimum of the function.

---

<sup>1</sup>Since the greedy (or optimal) action can be selected by either  $1-\epsilon$  or  $\epsilon/|\mathcal{A}(s)|$ ,  $a_1 = \epsilon/|\mathcal{A}(s)|$ ,  $a_2 = \epsilon/|\mathcal{A}(s)|$ ,  $\dots$ ,  $a_{best} = 1 - \epsilon + \epsilon/|\mathcal{A}(s)|$ ,  $a_n = \epsilon/|\mathcal{A}(s)|$



### 4.4.2 Off Policy

All learning control methods face a dilemma: They seek to learn action values conditional on subsequent *optimal* behavior, but they need to behave non-optimally in order to explore all actions (to find the optimal actions). How can they learn about the optimal policy while behaving according to an exploratory policy? The on-policy approach in the preceding section is actually a compromise. It learns action values not for the optimal policy, but for a near-optimal policy that still explores. A more straightforward approach is to **leverage two policies**, one that is learned about and that becomes the optimal policy, and one that is more exploratory and is used to generate behavior. The policy being learned about is called the *target policy*, and the policy used to generate behavior is called the *behavior policy*. In this case we say that learning is from data “off” the target policy, and the overall process is termed *off-policy learning*.

Suppose we wish to estimate  $v_\pi$  or  $q_\pi$ , but all we have are episodes following another policy  $b$ , where  $b \neq \pi$ . In this case,  $\pi$  is the target policy,  $b$  is the behavior policy, and both policies are considered fixed and given.

In order to use episodes from  $b$  to estimate values for  $\pi$ , we require that every action taken under  $\pi$  is also taken, at least occasionally, under  $b$ . That is, we require that  $\pi(a|s) > 0$  implies  $b(a|s) > 0$ . This is called the assumption of *coverage*. It follows from coverage that  $b$  must be stochastic in states where it is not identical to  $\pi$ . The target policy  $\pi$ , on the other hand, may be deterministic, and, in fact, this is a case of particular interest in control applications. In control, the target policy is typically the deterministic greedy policy with respect to the current estimate of the action-value function. This policy becomes a deterministic optimal policy while the behavior policy remains stochastic and more exploratory, for example, an  $\epsilon$ -greedy policy.

Almost all off-policy methods utilize *importance sampling*, a general technique for **estimating expected values under one distribution given samples from another**. We apply importance sampling to off-policy learning by weighting returns according to the relative probability of their trajectories occurring under the target and behavior policies, called the *importance-sampling ratio*. Given a starting state  $S_t$ , the probability of the subsequent state-action trajectory,  $A_t, S_{t+1}, A_{t+1}, \dots, S_T$ , occurring under any policy  $\pi$  is

$$\begin{aligned} P(A_t, S_{t+1}, A_{t+1}, \dots, S_T) &= \pi(A_t|S_t)p(S_{t+1}|S_t, A_t)\pi(A_{t+1}|S_{t+1}) \cdots (S_T|S_{T-1}, A_{T-1}) \\ &= \prod_{k=t}^{T-1} \pi(A_k|S_k)p(S_{k+1}|S_k, A_k), \end{aligned}$$

where  $p$  here is the state-transition probability function. Thus, the relative probability  $\rho$  of the trajectory under the target ( $\pi$ ) and behavior policies ( $b$ ) is

$$\begin{aligned} \rho_{t:T-1} &= \frac{\prod_{k=t}^{T-1} \pi(A_k|S_k)p(S_{k+1}|S_k, A_k)}{\prod_{k=t}^{T-1} b(A_k|S_k)p(S_{k+1}|S_k, A_k)} \\ &= \prod_{k=t}^{T-1} \frac{\pi(A_k|S_k)}{b(A_k|S_k)}. \end{aligned}$$

The importance sampling ratio ends up depending only on the two policies and the sequence, not on the MDP’s state-transition probability.

Recall that we wish to estimate the expected returns under the target policy, but all we have are returns  $G_t$  from the behavior policy, which results in

$$\mathbb{E}[G_t|S_t = s] = v_b(s).$$

So, the ratio  $\rho_{t:T-1}$  transforms the returns

$$\mathbb{E}[\rho_{t:T-1}G_t|S_t = s] = v_\pi(s).$$

## 4.5 Temporal-Difference Learning

One of the central ideas of reinforcement learning is temporal-difference (TD) learning. TD learning is a combination of Monte Carlo ideas and dynamic programming (DP) ideas. Like Monte Carlo methods, TD methods can learn directly from raw experience without a model of the environment's dynamics. Like DP, TD methods update estimates based in part on other learned estimates, without waiting for a final outcome (they bootstrap).

One of the main drawbacks of MC methods is the fact that the agent has to wait until the end of an episode when it can obtain the actual  $G_t$ . Then, it uses that return as a target for  $V(S_t)$ .

The core of TD learning is the Temporal Difference (TD) error, denoted as  $\delta_t$ , which represents the difference between the estimated value of a state at time  $t$  and the estimated value at time  $t + 1$ . It is calculated as the difference between the reward at time  $t + 1$  and the discounted estimate of the value function at time  $t$ .

Constant- $\alpha$  MC:

$$V(S_t) \leftarrow V(S_t) + \alpha [G_t - V(S_t)]$$

One-step TD (or TD(0)):

$$V(S_t) \leftarrow V(S_t) + \alpha \underbrace{[R_{t+1} + \gamma V(S_{t+1}) - V(S_t)]}_{\text{TD error, } \delta}$$

To clarify the difference, let's consider a simple example of a grid-world navigation task.

**MC Method** The agent explores the grid-world and reaches a target goal ( $S_9$ ). The episode ends, and the agent receives a reward of +1. At the end of the episode, the agent updates the value of each visited state based on the observed return. If the trajectory is  $S_1 \rightarrow S_2 \rightarrow \dots \rightarrow S_9$ , then the value update for each visited state would be based on the return of +1.

**TD Learning** The agent starts at  $S_1$ , moves to  $S_2$ , and receives a reward of 0.1 for the movement. The agent updates the value of  $S_1$  based on the observed TD error, which is the immediate reward plus the discounted estimate of the next state. If the agent moves right from  $S_1$  to  $S_2$ , the update for  $S_1$  would be based on  $R_{move} + \gamma V(S_2)$ .

- Monte Carlo:
  - Pros: Unbiased estimate of value functions.
  - Cons: Requires complete episodes, might be computationally expensive.
- Temporal Difference:
  - Pros: Updates at each time step, more sample-efficient.

- Cons: Potential bias due to bootstrapping.

In summary, in the grid-world example, Monte Carlo methods would update values based on complete episodes, whereas TD learning would update values at each time step. The choice depends on the nature of the task, the availability of information, and the computational resources.

#### 4.5.1 Q-learning: Off-policy TD Control

$$Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \alpha \left[ R_{t+1} + \gamma \max_a Q(S_{t+1}, a) - Q(S_t, A_t) \right]$$

- Off-policy. For instance, we can sample an action  $A_t$  from a  $\epsilon$ -greedy policy.
- Update  $Q$  for each step.
- Maximization bias in  $Q$ -learning

#### 4.5.2 Sarsa: On-policy TD Control

$$Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \alpha \left[ R_{t+1} + \gamma Q(S_{t+1}, A_{t+1}) - Q(S_t, A_t) \right]$$

- On-policy algorithm, unlike  $Q$ -learning, we sample both  $A_t$  and  $A_{t+1}$  from another policy like  $\epsilon$ -greedy policy.

#### 4.5.3 Double Q-learning

Randomly select  $Q_1$  or  $Q_2$ .

$$Q_1(S_t, A_t) \leftarrow Q_1(S_t, A_t) + \alpha \left[ R_{t+1} + \gamma \max_a Q_2(S_{t+1}, a^*) - Q_1(S_t, A_t) \right],$$

where  $a^*$  is

$$a^* = \operatorname{argmax}_a Q_1(s', a).$$

$$Q_2(S_t, A_t) \leftarrow Q_2(S_t, A_t) + \alpha \left[ R_{t+1} + \gamma \max_a Q_1(S_{t+1}, a^*) - Q_2(S_t, A_t) \right],$$

where  $a^*$  is

$$a^* = \operatorname{argmax}_a Q_2(s', a).$$

## Chapter 5

# Deep Reinforcement Learning

Three challenges in DRL:

- Sequential feedback
- Evaluative feedback
- Sampled feedback

Select:

1. A value function to approximate.
2. A neural network architecture
  - e.g., value (single output node) or action (multiple output nodes)
3. What to optimize
4. Policy evaluation algorithm
5. Exploration strategy
6. A loss function
7. Optimization method

Some considerations:

- Non-stationary target
- Data correlated with time
  - Samples in a batch are correlated, given that most of these samples come from the same trajectory and policy. It breaks the i.i.d. assumptions.

## Chapter 6

# Deep Q-Network

Q-learning is a popular model-free reinforcement learning algorithm that is used to find an optimal action-selection policy for a given finite Markov decision process (MDP). It's a form of temporal difference learning, where the agent learns from the consequences of its actions in the environment.

The main goal of  $Q$ -learning is to learn a policy, represented by the action-value function  $Q(s, a)$ , which estimates the expected cumulative future rewards of taking action  $a$  in state  $s$ .

## Chapter 7

# Policy Gradient

We will use a gradient ascent algorithm:

$$\begin{aligned} J(\theta) &= \mathbb{E}_{\tau \sim \pi_{\theta}(\tau)}[r(\tau)] \\ &= \int \pi_{\theta}(\tau) r(\tau) \end{aligned}$$

It is a expected reward under the policy  $\pi_{\theta}$ .

$$\theta \leftarrow \theta + \eta \nabla_{\theta} J(\theta)$$

Note that by using REINFORCE algorithm which can be expressed as follows:

$$\nabla_{\theta} \pi_{\theta}(\tau) = \pi_{\theta} \frac{\nabla_{\theta} \pi_{\theta}(\tau)}{\pi_{\theta}(\tau)} = \pi_{\theta} \nabla_{\theta} \log \pi_{\theta}(\tau)$$

We can express  $J(\theta)$  as follows:

$$\begin{aligned} \nabla_{\theta} J(\theta) &= \int \nabla_{\theta} \pi_{\theta}(\tau) r(\tau) = \int \pi_{\theta} \nabla_{\theta} \log \pi_{\theta}(\tau) r(\tau) \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}(\tau)}[\nabla_{\theta} \log \pi_{\theta}(\tau) r(\tau)] \end{aligned}$$

Note that  $\nabla_{\theta} \log \pi_{\theta}(\tau)$  is the maximum loglikelihood of trajectory, because gradient is the maximum direction of the function. This expectation can be estimated by Monte-Carlo method.

We just sample trajectories using current policy and adjust the likelihood of trajectories by episodic rewards.

$$\pi_{\theta}(\tau) = p_{\theta}(s_1, a_1, s_2, a_2, \dots, s_T, a_T) = p(s_1) \prod_{t=1}^T \pi_{\theta}(a_t | s_t) p(s_{t+1} | s_t, a_t)$$

Note that the product term looks causing gradient explosion or vanishing problems for a long sequence problem, but it turns into a multiplication as below by the log-derivative trick, so it can avoid the issues.

In general, the agent has no access to  $p(s_1)$  and  $p(s_{t+1}|s_t, a_t)$  (we don't know transition probability.).

$$\begin{aligned}\nabla_{\theta} \log \pi_{\theta}(\tau) &= \nabla_{\theta} \left[ \log p(s_1) + \sum_{t=1}^T (\log \pi_{\theta}(a_t|s_t) + \log p(s_{t+1}|s_t, a_t)) \right] \\ &= \sum_{t=1}^T \nabla_{\theta} \log \pi_{\theta}(a_t|s_t) \\ r(\tau) &= \sum_{t=1}^T r(s_t, a_t)\end{aligned}$$

By using the above equations, we can re-express the gradient of the cost function as

$$\begin{aligned}\nabla_{\theta} J(\theta) &= \int \nabla_{\theta} \pi_{\theta}(\tau) r(\tau) = \int \pi_{\theta} \nabla_{\theta} \log \pi_{\theta}(\tau) r(\tau) \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}(\tau)} [\nabla_{\theta} \log \pi_{\theta}(\tau) r(\tau)] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}(\tau)} \left[ \left( \sum_{t=1}^T \nabla_{\theta} \log \pi_{\theta}(a_t|s_t) \right) \left( \sum_{t=1}^T r(s_t, a_t) \right) \right]\end{aligned}$$

By using Monte-Carlo method, we can replace the expectation by sampling multiple trajectories in practice:

$$\nabla_{\theta} J(\theta) \approx \frac{1}{N} \sum_{i=1}^N \left[ \left( \sum_{t=1}^T \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_{i,t} | \mathbf{s}_{i,t}) \right) \left( \sum_{t=1}^T r(\mathbf{s}_{i,t}, \mathbf{a}_{i,t}) \right) \right]$$

### 7.0.1 Causality

$$\begin{aligned}\nabla_{\theta} J(\theta) &\approx \frac{1}{N} \sum_{i=1}^N \left[ \sum_{t=1}^T \nabla_{\theta} \log \pi_{\theta}(a_{i,t} | s_{i,t}) \sum_{t=1}^T r(s_{i,t}, a_{i,t}) \right] \\ &= \frac{1}{N} \sum_{i=1}^N \sum_{t=1}^T \left[ \nabla_{\theta} \log \pi_{\theta}(a_{i,t} | s_{i,t}) \sum_{t'=1}^T r(s_{i,t'}, a_{i,t'}) \right] \\ &= \frac{1}{N} \sum_{i=1}^N \sum_{t=1}^T \left[ \nabla_{\theta} \log \pi_{\theta}(a_{i,t} | s_{i,t}) \sum_{t'=t}^T r(s_{i,t'}, a_{i,t'}) \right] \quad \text{by causality}\end{aligned}$$

## 7.1 Natural Policy Gradient

reference: Nathan Ratliff, Information Geometry and Natural Gradients.

### 7.1.1 KL-divergence between perturbed distributions

Let  $p(x; \theta)$  be some family of probability distributions over  $x$  parameterized by a vector of real numbers  $\theta$ . We're interested in knowing how much the distribution changes when we perturb

the parameter vector from a fixed  $\theta_t$  to some new value  $\theta_t + \delta\theta$ . As a measure of change in probability distribution, we can use the KL-divergence measure. Specifically, we want to measure  $D_{KL}(p(x; \theta_t) || p(x; \theta_t + \delta\theta))$ , but we want to write it in a form amenable to the gradient-based update formulation. We can do this by taking it's second-order Taylor expansion around  $\theta_t$ . During the derivation, we'll find that a lot of terms in the expansion disappear leaving us with a very simple expression that's perfect for our purposes.

Looking first at the full KL-divergence, we see that the term we want to

$$\begin{aligned} D_{KL}(p(x; \theta_t) || p(x; \theta_t + \delta\theta)) &= \int p(x; \theta_t) \log \frac{p(x; \theta_t)}{p(x; \theta_t + \delta\theta)} dx \\ &= \int p(x; \theta_t) \log p(x; \theta_t) dx - \int p(x; \theta_t) \log p(x; \theta_t + \delta\theta) dx \end{aligned}$$

Note that the second-order Taylor series expansion is

$$f(\theta) \approx f(\theta_t) + \nabla f(\theta_t)^T \delta\theta + \frac{1}{2} \delta\theta^T \nabla^2 f(\theta_t) \delta\theta,$$

where  $\theta = \theta_t + \delta\theta$ , or equivalently  $\delta\theta = \theta - \theta_t$ . Applying that expansion to the pertinent term in the KL-divergence expression, we get

$$\log p(x; \theta_t + \delta\theta) \approx \log p(x; \theta_t) + \left( \frac{\nabla p(x; \theta_t)}{p(x; \theta_t)} \right)^T \delta\theta + \frac{1}{2} \delta\theta^T (\nabla^2 \log p(x; \theta_t)) \delta\theta.$$

Plugging this second-order Taylor expansion back into the above expression for the  $D_{KL}$  gives

$$\begin{aligned} D_{KL}(p(x; \theta_t) || p(x; \theta_t + \delta\theta)) &= \int p(x; \theta_t) \log p(x; \theta_t) dx - \int p(x; \theta_t) \log p(x; \theta_t + \delta\theta) dx \\ &\approx \int p(x; \theta_t) \log p(x; \theta_t) dx \\ &\quad - \int p(x; \theta_t) \left( \log p(x; \theta_t) + \left( \frac{\nabla p(x; \theta_t)}{p(x; \theta_t)} \right)^T \delta\theta + \frac{1}{2} \delta\theta^T (\nabla^2 \log p(x; \theta_t)) \delta\theta \right) dx \\ &= \int p(x; \theta_t) \log \frac{p(x; \theta_t)}{p(x; \theta_t)} dx - \underbrace{\int p(x; \theta_t) \left( \frac{\nabla p(x; \theta_t)}{p(x; \theta_t)} \right)^T dx}_{=0} - \frac{1}{2} \delta\theta^T \left( \int p(x; \theta_t) \nabla^2 \log p(x; \theta_t) dx \right) \delta\theta \\ &= -\frac{1}{2} \delta\theta^T \left( \int p(x; \theta_t) \nabla^2 \log p(x; \theta_t) dx \right) \delta\theta. \end{aligned}$$

$\int \nabla p(x; \theta_t)$  is zero since

$$\int \nabla p(x; \theta_t) = \nabla \int p(x; \theta_t) = \nabla 1 = 0$$



The Hessian can be computed as follows:

$$\begin{aligned}
\frac{\partial^2}{\partial \theta_t^i \partial \theta_t^j} [\log p(x; \theta_t)] &= \frac{\partial}{\partial \theta_t^i} \left( \frac{\frac{\partial}{\partial \theta_t^j} p(x; \theta_t)}{p(x; \theta_t)} \right) \\
&= \frac{p(x; \theta_t) \frac{\partial^2}{\partial \theta_t^i \partial \theta_t^j} p(x; \theta_t) - \frac{\partial}{\partial \theta_t^i} p(x; \theta_t) \frac{\partial}{\partial \theta_t^j} p(x; \theta_t)}{p(x; \theta_t)^2} \\
&= \frac{1}{p(x; \theta_t)} \frac{\partial^2}{\partial \theta_t^i \partial \theta_t^j} p(x; \theta_t) - \left( \frac{\frac{\partial}{\partial \theta_t^i} p(x; \theta_t)}{p(x; \theta_t)} \right) \left( \frac{\frac{\partial}{\partial \theta_t^j} p(x; \theta_t)}{p(x; \theta_t)} \right).
\end{aligned}$$

The second term is an element of the outer product between  $\nabla \log p(x; \theta_t)$  and itself. In matrix form, this becomes

$$\nabla^2 \log p(x; \theta_t) = \frac{1}{p(x; \theta_t)} \nabla^2 p(x; \theta_t) - \nabla \log p(x; \theta_t) \nabla \log p(x; \theta_t)^T.$$

Finally, we get

$$\begin{aligned}
D_{KL}(p(x; \theta_t) || p(x; \theta_t + \delta \theta)) &\approx -\frac{1}{2} \delta \theta^T \int p(x; \theta_t) \nabla^2 \log p(x; \theta_t) dx \delta \theta \\
&= \frac{1}{2} \delta \theta^T \left( \int \nabla^2 \log p(x; \theta_t) dx \right) \delta \theta \\
&\quad + \frac{1}{2} \delta \theta^T \left( \int p(x; \theta_t) [\nabla \log p(x; \theta_t) \nabla \log p(x; \theta_t)^T] dx \right) \delta \theta \\
&= \frac{1}{2} \delta \theta^T \underbrace{\left( \int p(x; \theta_t) [\nabla \log p(x; \theta_t) \nabla \log p(x; \theta_t)^T] dx \right)}_{G(\theta_t)} \delta \theta.
\end{aligned}$$

The central matrix here  $G(\theta_t)$  is known as the **Fisher Information matrix** and can has been thoroughly studied within the field of Information Geometry as the natural Riemannian structure on a manifold of probability distributions. As such it defines a natural norm on perturbations to probability distributions, which was our original motivation for examining the second-order Taylor expansion of the KL-divergence in the first place.

$$\theta_{t+1} = \theta_t - \eta_t G(\theta_t)^{-1} \nabla f(\theta_t).$$

## 7.2 Proximal Policy Optimization

PPO objective is

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \mathbb{E}_{s, a \sim \pi_{\theta_k}} [L(s, a, \theta_k, \theta)],$$

where  $L$  is given by

$$L(s, a, \theta_k, \theta) = \min \left( \frac{\pi_{\theta}(a|s)}{\pi_{\theta_k}(a|s)} A^{\pi_{\theta_k}}(s, a), \operatorname{Clip} \left( \frac{\pi_{\theta}(a|s)}{\pi_{\theta_k}(a|s)}, 1 - \varepsilon, 1 + \varepsilon \right) A^{\pi_{\theta_k}}(s, a) \right).$$

Roughly,  $\varepsilon$  is a hyperparameter which says how far away the new policy is allowed to go from the old one. A simpler expression of the above expression is

$$L(s, a, \theta_k, \theta) = \min \left( \frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A^{\pi_{\theta_k}}(s, a), g(\varepsilon, A^{\pi_{\theta_k}}(s, a)) \right), \quad (7.1)$$

where

$$g(\varepsilon, A) = \begin{cases} (1 + \varepsilon)A & A \geq 0 \\ (1 - \varepsilon)A & A < 0. \end{cases} \quad (7.2)$$

**Positive Advantage:** Suppose the advantage for that state-action pair is positive, in which case its contribution to the objective reduces to

$$L(s, a, \theta_k, \theta) = \min \left( \frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)}, 1 + \varepsilon \right) A^{\pi_{\theta_k}}(s, a). \quad (7.3)$$

Because the advantage is positive, the objective will increase if the action becomes more likely—that is, if  $\pi_\theta(a|s)$  increases. But the min in this term puts a limit to how much the objective can increase. Once  $\pi_\theta(a|s) > (1 + \varepsilon)\pi_{\theta_k}(a|s)$ , the min kicks in and this term hits a ceiling of  $(1 + \varepsilon)A^{\pi_{\theta_k}}(s, a)$ . Thus, the new policy does not benefit by going far away from the old policy.

**Negative Advantage:** Suppose the advantage for that state-action pair is negative, in which case its contribution to the objective reduces to

$$L(s, a, \theta_k, \theta) = \min \left( \frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)}, 1 - \varepsilon \right) A^{\pi_{\theta_k}}(s, a). \quad (7.4)$$

Because the advantage is negative, the objective will increase if the action becomes less likely—that is, if  $\pi_\theta(a|s)$  decreases. But the max in this term puts a limit to how much the objective can increase. Once  $\pi_\theta(a|s) < (1 - \varepsilon)\pi_{\theta_k}(a|s)$ , the max kicks in and this term hits a ceiling of  $(1 - \varepsilon)A^{\pi_{\theta_k}}(s, a)$ . Thus, again, the new policy does not benefit by going far away from the old policy.

What we have seen so far is that clipping serves as a regularizer by removing incentives for the policy to change dramatically, and the hyperparameter  $\varepsilon$  corresponds to how far away the new policy can go from the old while still profiting the objective.

# Chapter 8

## Search Algorithm

Reference: John Levine

### 8.1 Monte Carlo Tree Search

Monte Carlo Tree Search (MCTS) is a search technique in the field of Artificial Intelligence (AI). It is a probabilistic and heuristic driven search algorithm that combines the classic tree search implementations alongside machine learning principles of reinforcement learning.

It consists of four phases:

- Tree traversal
- Node expansion
- Rollout
- Backpropagation

In tree search, there's always the possibility that the current best action is actually not the most optimal action. In such cases, MCTS algorithm becomes useful as it continues to evaluate other alternatives periodically during the learning phase by executing them, instead of the current perceived optimal strategy. This is known as the “exploration-exploitation trade-off”. It exploits the actions and strategies that is found to be the best till now but also must continue to explore the local space of alternative decisions and find out if they could replace the current best.

Exploration helps in exploring and discovering the unexplored parts of the tree, which could result in finding a more optimal path. In other words, we can say that exploration expands the tree's breadth more than its depth. Exploration can be useful to ensure that MCTS is not overlooking any potentially better paths. But it quickly becomes inefficient in situations with large number of steps or repetitions. In order to avoid that, it is balanced out by exploitation. Exploitation sticks to a single path that has the greatest estimated value. This is a greedy approach and this will extend the tree's depth more than its breadth. In simple words, UCB formula applied to trees helps to balance the exploration-exploitation trade-off by periodically exploring relatively unexplored nodes of the tree and discovering potentially more optimal paths than the one it is currently exploiting.

For this characteristic, MCTS becomes particularly useful in making optimal decisions in Artificial Intelligence (AI) problems.

### 8.1.1 Tree Traversal

In this process, the MCTS algorithm traverses the current tree from the root node using a specific strategy. The strategy uses an evaluation function to optimally select nodes with the highest estimated value. MCTS uses the Upper Confidence Bound (UCB) formula applied to trees as the strategy in the selection process to traverse the tree. It balances the exploration-exploitation trade-off. During tree traversal, a node is selected based on some parameters that return the maximum value. The parameters are characterized by the formula that is typically used for this purpose is given below:

$$\text{UCB1}(S_i) = \underbrace{\bar{V}_i}_{\text{Exploitation}} + C \underbrace{\sqrt{\frac{\ln N}{n_i}}}_{\text{Exploration}},$$

- $C$  is a balancing factor between exploitation and exploration.
- $N$  the number of visit of parent node
- $n_k$  the number of visit of node  $k$

Let's say there are two successor nodes. One is visited more times than another one. Then, it means it is exploited more times than the other one. Thus, exploration term of the less exploited one would be higher than the highly visited one. By computing the UCB1 score, the agent chooses a successor node with higher UCB1 score.

### 8.1.2 Expansion

Expand successor node

### 8.1.3 Rollout (Random Simulation)

Simulation is completely random. In other words, we don't know how an agent reacts to an environment, so each successor state, the agent randomly decides which action to do till the termination.

### 8.1.4 Backpropagation

Backpropagate rewards (value), and the number of visit at a node.

- $t$ : total score
- $n_k := n_k + 1$

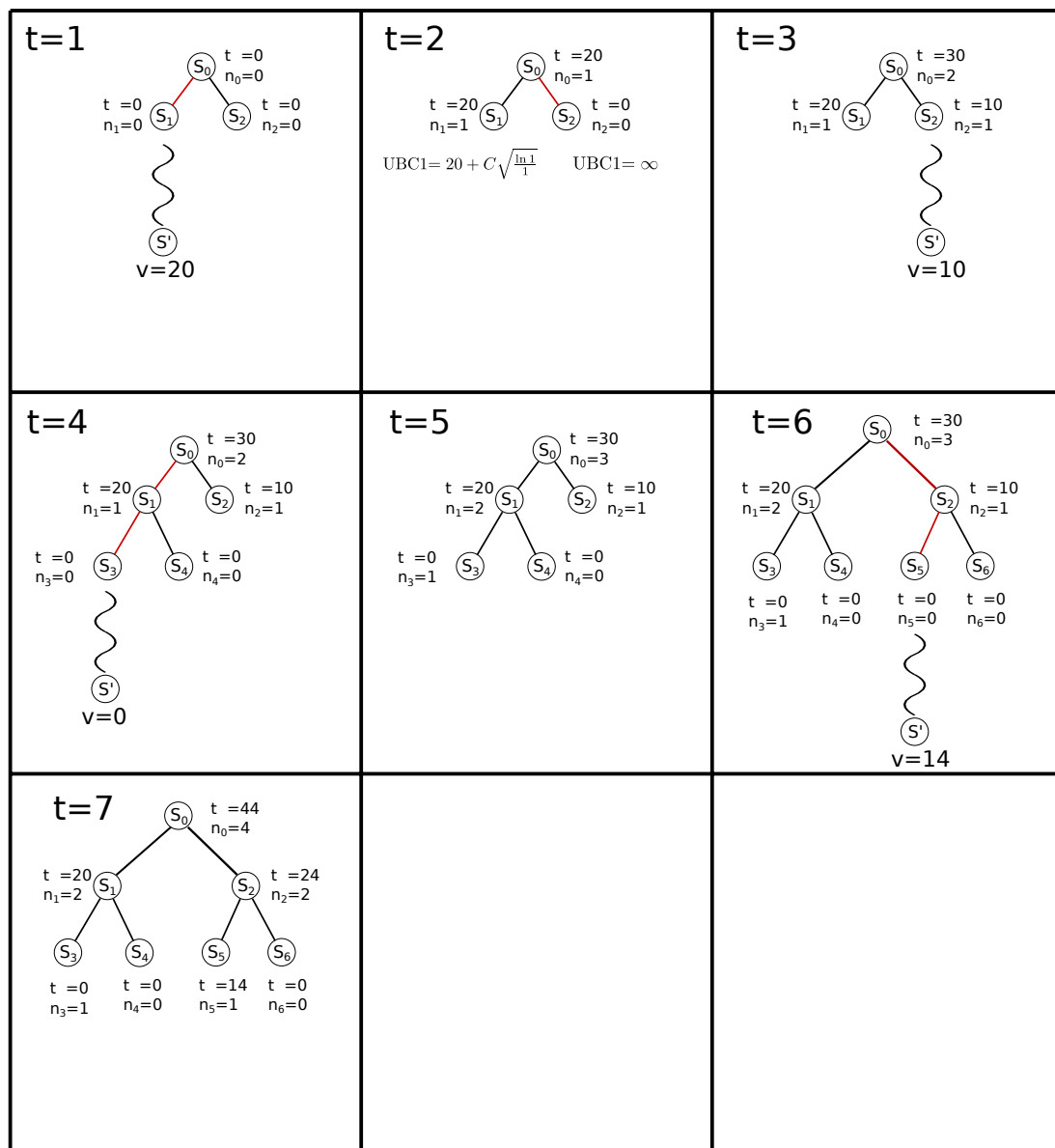
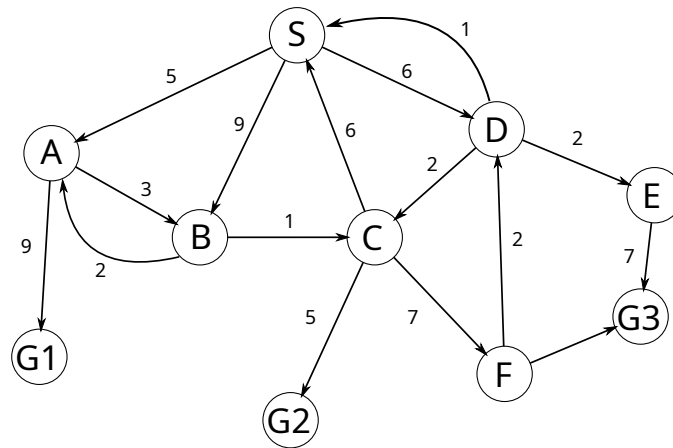


Figure 8.1: MCTS example

## 8.2 Uniform Cost Search

You have three goal states,  $G_1, G_2, G_3$ . Your goal is to reach one of them. UCS is cheapest first search algorithm.



### 8.3 $A^*$ Search

$A^*$  search algorithms is a variant of Dijkstra's algorithm, which incorporate additional *heuristic* information about a graph. Unlike the Dijkstra's algorithm, you can specify a target node that you are interested in so that you don't have to compute all paths.

In addition, the  $A^*$  algorithm is often preferred over Dijkstra's algorithm in scenarios where the cost of reaching a goal from a particular node is not only determined by the actual distance traveled but also influenced by a heuristic estimation of the remaining distance to the goal.

As I said, it exploits heuristics (or estimates). For instance, if we want to get a shortest path to a certain location in a map, then a very reasonable choice is to measure a distance roughly by using Euclidean distance. In Fig. 8.2, we first initialize each node in the graph with our estimates.

Then, we can explore as shown in §8.3. For each visit, take a shortest path.

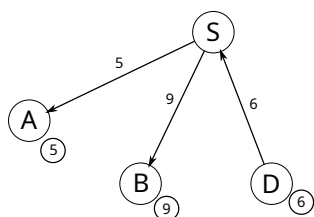
Each number next to the nodes is called  $A^*$  score, which is an estimate of cost to get to one of states.

Note that  $A^*$  algorithm is typically explained with open set and closed sets, which are just sets for nodes to be evaluated and visited.

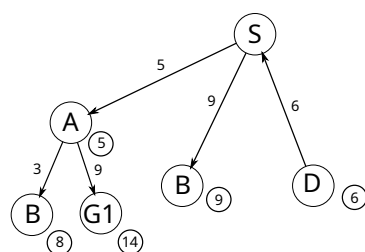
Open Set and Closed Set:

- Open set contains nodes that need to be evaluated,
- Closed set contains nodes that have already been evaluated.

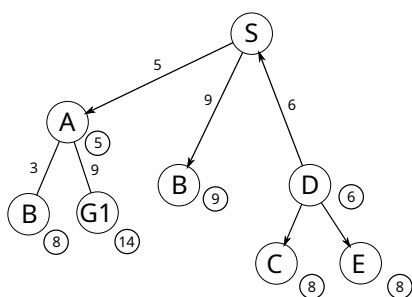
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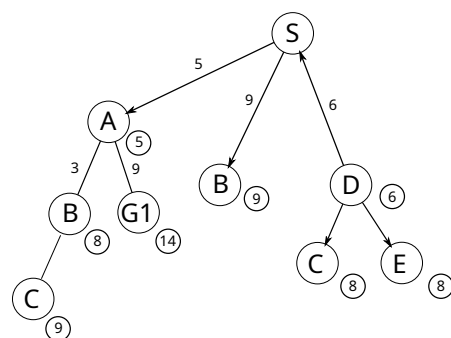
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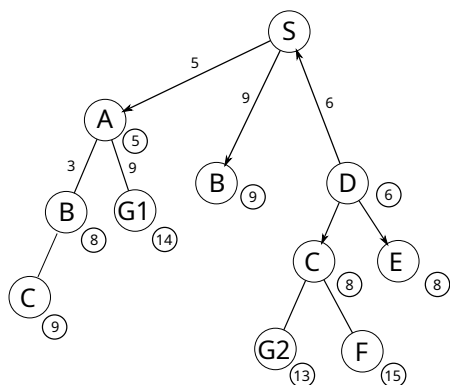
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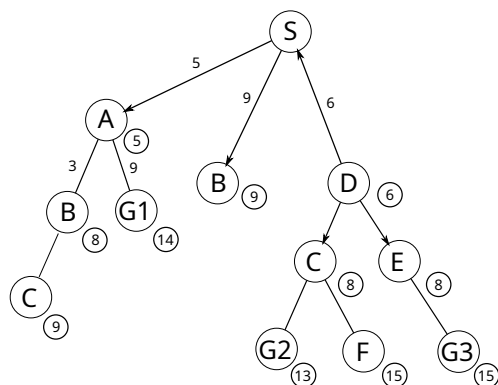
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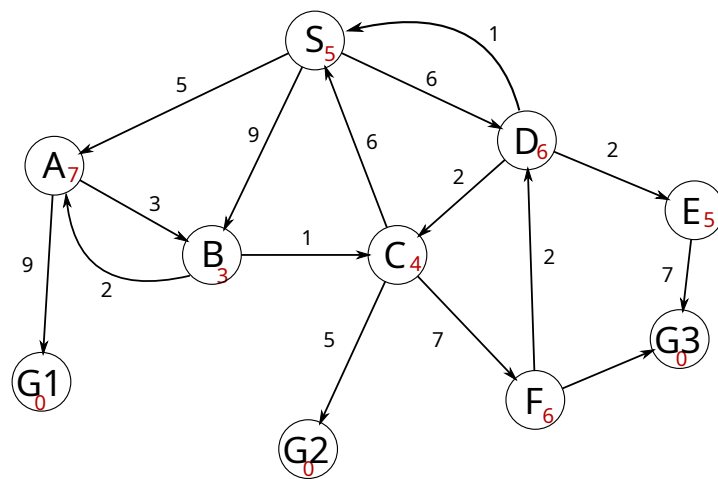


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Visited  
S, A, D, B, C, E

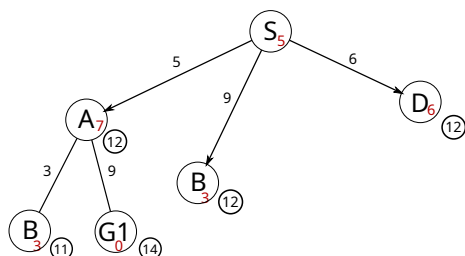


Figure 8.2: Initialize  $A^*$  search algorithm with heuristics.



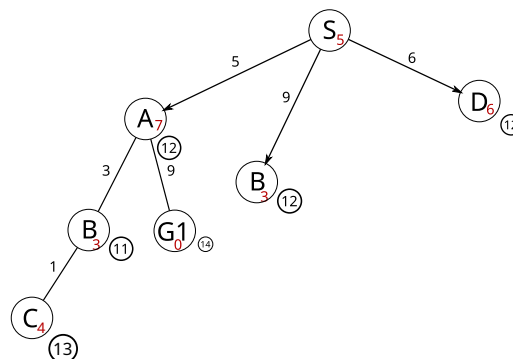
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S(5), A(12)



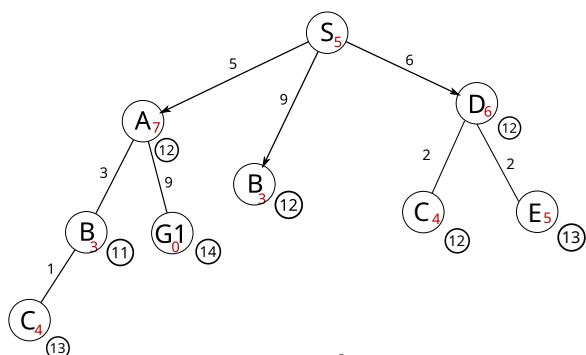
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S(5), A(12), B(11)

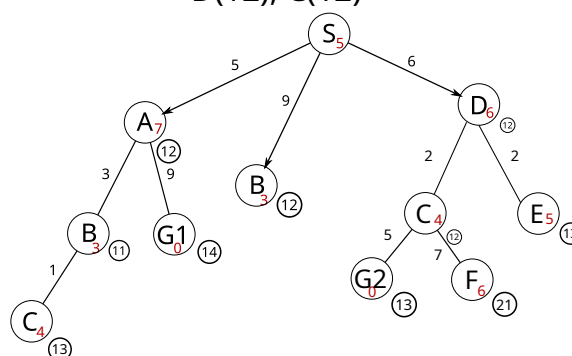


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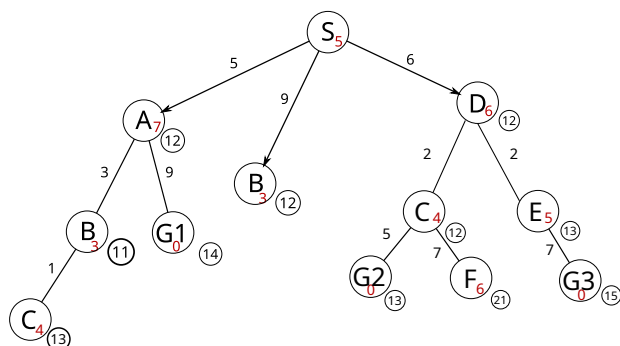
S(5), A(12), B(11), D(12)



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S(5), A(12), B(11),  
D(12), C(12)

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S(5), A(12), B(11),  
D(12), C(12)

# Bibliography

# Appendix

## A.1 Bellman Equation

*Bellman equation* can be derived as follows:

$$\begin{aligned}
v_\pi(s) &= \mathbb{E}_\pi[G_t | S_t = s] \\
&= \mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1} | S_t = s] \\
&= \mathbb{E}_\pi[R_{t+1} | S_t = s] + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s], \quad \text{By Linearity of Expectation.} \\
&= \sum_{r_{t+1}} r_{t+1} P(R_{t+1} | S_t = s) + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s] \\
&= \sum_{r_{t+1}} r_{t+1} \sum_a P(R_{t+1} | S_t = s, A_t = a) P(A_t = a | S_t = s) + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s] \\
&= \sum_a \sum_{r_{t+1}} r_{t+1} \sum_{s'} P(R_{t+1}, S_{t+1} = s' | S_t = s, A_t = a) P(A_t = a | S_t = s) + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s] \\
&= \sum_a \sum_r r \sum_{s'} P(s', r | s, a) \pi(a | s) + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s] \\
&= \sum_a \sum_{s'} \sum_r r P(s', r | s, a) \pi(a | s) + \mathbb{E}_\pi[\gamma G_{t+1} | S_t = s] \\
&= \sum_a \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a \pi(a | s) + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s] \\
&= \sum_a \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a \pi(a | s) + \gamma \sum_a \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a] P(A_t | S_t) \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a] \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{g_{t+1}} g_{t+1} P(G_{t+1} | S_t = s, A_t = a) \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{g_{t+1}} g_{t+1} \frac{P(G_{t+1}, S_t = s, A_t = a)}{P(S_t = s, A_t = a)} \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{g_{t+1}} g_{t+1} \frac{\sum_{s'} P(G_{t+1}, S_t = s, S_{t+1} = s', A_t = a)}{P(S_t = s, A_t = a)} \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{g_{t+1}} g_{t+1} \frac{\sum_{s'} P(G_{t+1} | s, s', a) P(s, s', a)}{P(s, a)} \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{g_{t+1}} g_{t+1} \sum_{s'} P(G_{t+1} | s, s', a) P(s' | s, a) \right] \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{s'} P(s' | s, a) \sum_{g_{t+1}} g_{t+1} P(G_{t+1} | s') \right] \quad \text{by Markov Property} \\
&= \sum_a \pi(a | s) \left[ \sum_{s'} \mathcal{P}_{ss'}^a \mathcal{R}_{ss'}^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a v_\pi(s') \right] \\
&= \sum_a \pi(a | s) \sum_{s'} \mathcal{P}_{ss'}^a \left[ \mathcal{R}_{ss'}^a + \gamma v_\pi(s') \right] \\
&= \sum_a \pi(a | s) \sum_{r, s'} p(s', r | s, a) \left[ r + \gamma v_\pi(s') \right]
\end{aligned}$$

Or simply,

$$\begin{aligned} v_\pi(s) &= \sum_a \pi(a|s) q(s, a) \\ &= \sum_a \pi(a|s) \sum_{r, s'} p(s', r|s, a) [r + \gamma v_\pi(s')] \end{aligned}$$

Reference

Similarly,

$$\begin{aligned} q_\pi(s, a) &= \mathbb{E}_\pi[G_t | S_t = s, A_t = a] \\ &= \mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1} | S_t = s, A_t = a] \\ &= \mathbb{E}_\pi[R_{t+1} | S_t = s, A_t = a] + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a] \\ &= \sum_r r p(r|s, a) + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a] \\ &= \sum_r r \sum_{s'} p(s', r|s, a) + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a] \\ &= \sum_{s', r} r p(s', r|s, a) + \gamma \mathbb{E}[\mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a, R_{t+1}, S_{t+1}]] \quad \text{By Law of Total Expectation.} \\ &= \sum_{s', r} r p(s', r|s, a) + \gamma \sum_{s', r} \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a, R_{t+1} = r, S_{t+1} = s'] p(s', r|s, a) \\ &= \sum_{s', r} p(s', r|s, a) [r + \gamma \mathbb{E}_\pi[G_{t+1} | S_t = s, A_t = a, R_{t+1} = r, S_{t+1} = s']] \\ &= \sum_{s', r} p(s', r|s, a) [r + \gamma \mathbb{E}_\pi[G_{t+1} | S_{t+1} = s']] \quad \text{By Markov Property.} \\ &= \sum_{s', r} p(s', r|s, a) [r + \gamma v_\pi(s')] \end{aligned}$$

## B.2 Importance Sampling

You have two distributions,  $P(A)$  and  $P(B)$ , and you have a sequence sampled from  $A$ . You can estimate an expectation of  $A$ ,

$$\mathbb{E}[A] = \sum p(a) h(a).$$

Can we use the above equation for estimating an expectation of  $B$ ? Yes.

$$\mathbb{E}[B] = \sum \frac{p(b)}{p(a)} h(a).$$

The ratio  $\frac{p(b)}{p(a)}$  tells us how likely to observe some results under  $p(b)$  compared to  $p(a)$ .

Useful factorization of conditional probability:

$$P[A, B|C] = \frac{P[A, B, C]}{P[C]} \quad (1)$$

$$= \frac{P[A, B, C]}{P[C]} \frac{P[B, C]}{P[B, C]} \quad (2)$$

$$= \frac{P[A, B, C]}{P[B, C]} \frac{P[B, C]}{P[C]} \quad (3)$$

$$= P[A|B, C]P[B|C] \quad (4)$$

### C.3 Fisher Information

Suppose we have a model parameterized by parameter vector  $\theta$  that models a distribution  $p(x; \theta)$ . In frequentist statistics, the way we learn  $\theta$  is to maximize the likelihood of  $p(x; \theta)$ . To assess the goodness of our estimate of  $\theta$  we define a **score function** as follows:

$$f(\theta) = \nabla_{\theta} \log p(x; \theta).$$

The expected value of score function is zero.

$$\begin{aligned} \mathbb{E}_{p(x; \theta)}[f(\theta)] &= \mathbb{E}_{p(x; \theta)}[\nabla_{\theta} \log p(x; \theta)] \\ &= \int p(x; \theta) \nabla_{\theta} \log p(x; \theta) dx \\ &= \int p(x; \theta) \frac{\nabla_{\theta} p(x; \theta)}{p(x; \theta)} dx \\ &= 0 \end{aligned}$$

The covariance of the score function is given by

$$\text{Cov}[f(\theta), f(\theta)] = \mathbb{E}_{p(x; \theta)}[(f(\theta) - 0)(f(\theta) - 0)^T] = \text{Var}[f(\theta), f(\theta)].$$

This the definition of Fisher information and it can be written

$$F = \mathbb{E}_{p(x; \theta)}[\nabla \log p(x; \theta) \nabla \log p(x; \theta)^T].$$

Empirically,

$$F = \frac{1}{N} \sum_{i=1}^N \nabla \log p(x; \theta) \nabla \log p(x; \theta)^T.$$

### D.4 Score Function

In statistics, *the score (or informant) is the gradient of the log-likelihood function with respect to the parameter vector.*

- Evaluated at a particular point of the parameter vector, the score indicates the **steepness of the log-likelihood function and thereby the sensitivity to infinitesimal changes to the parameter values.**

- If the log-likelihood function is continuous over the parameter space, the score will **vanish at a local maximum or minimum**; this fact is used in maximum likelihood estimation to find the parameter values that maximize the likelihood function.

Since the score is a function of the observations that are subject to sampling error, it lends itself to a test statistic known as score test in which the parameter is held at a particular value. Further, the ratio of two likelihood functions evaluated at two distinct parameter values can be understood as a definite integral of the score function.[2]

## E.5 Incremental Monte-Carlo

Incremental Mean:

$$\mu_k = \frac{1}{k} \sum_{j=1}^k x_j \quad (5)$$

$$= \frac{1}{k} \left( x_k + (k-1) \frac{1}{(k-1)} \sum_{j=1}^{k-1} x_j \right) \quad (6)$$

$$= \frac{1}{k} \left( x_k + (k-1) \mu_{k-1} \right) \quad (7)$$

$$= \mu_{k-1} + \frac{1}{k} (x_k - \mu_{k-1}) \quad (8)$$

Incremental MC:

- $N_{n+1}(S_t^n) = N_n(S_t^n) + 1$  for rest  $N_{n+1}(s) = N_n(s)$
- $V_{n+1}(S_t) = V_n(S_t) + \frac{G_{t:T}^n - V_n(S_t)}{N_n(S_t)}$  for rest  $V_{n+1}(s) = V_n(s)$
- $V_{n+1}(S_t) = V_n(S_t) + \alpha(G_{t:T}^n - V_n(S_t))$  for rest  $V_{n+1}(s) = V_n(s)$

## F.6 Derivative of Softmax

Softmax function is given by

$$S(x_i) = \frac{e^{x_i}}{\sum_{k=1}^K e^{x_k}} \quad \text{for } i = 1, \dots, K$$

The derivative of softmax function is

$$\frac{\partial S_i}{\partial x_j} = \begin{cases} S_i(1 - S_j) & \text{if } i = j \\ -S_j S_i & \text{if } i \neq j \end{cases}$$

- Diagonal elements:  $S_i(1 - S_j)$
- Off-diagonal elements:  $-S_j S_i$ :

The Jacobian matrix ( $j \times i$ ) for softmax is

$$\frac{\partial S}{\partial x} = \begin{bmatrix} \frac{\partial S_1}{\partial x_1} & \frac{\partial S_1}{\partial x_2} & \cdots & \frac{\partial S_1}{\partial x_K} \\ \frac{\partial S_2}{\partial x_1} & \frac{\partial S_2}{\partial x_2} & \cdots & \frac{\partial S_2}{\partial x_K} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial S_K}{\partial x_1} & \frac{\partial S_K}{\partial x_2} & \cdots & \frac{\partial S_K}{\partial x_K} \end{bmatrix}$$

The matrix can be expressed as follows:

$$\begin{bmatrix} S(x_1) - S(x_1)S(x_1) & \cdots & 0 - S(x_1)S(x_N) \\ \cdots & S(x_j) - S(x_j)S(x_i) & \cdots \\ 0 - S(x_N)S(x_1) & \cdots & 0 - S(x_N)S(x_N) \end{bmatrix} = \begin{bmatrix} S(x_1) & \cdots & 0 \\ \cdots & S(x_j) & \cdots \\ 0 & \cdots & S(x_N) \end{bmatrix} - \begin{bmatrix} S(x_1)S(x_1) & \cdots & S(x_1)S(x_N) \\ \cdots & S(x_j)S(x_i) & \cdots \\ S(x_N)S(x_1) & \cdots & S(x_N)S(x_N) \end{bmatrix}$$

This can be

```
1 np.diag(S) - np.outer(S, S)
```

## G.7 Policy Gradient Theorem

Function approximation is essential to reinforcement learning, but the standard approach of approximating a value function and determining a policy from it has so far proven theoretically intractable. In this paper we explore an alternative approach in which the policy is explicitly represented by its own function approximator, independent of the value function, and is updated according to the gradient of expected reward with respect to the policy parameters. Williams's REINFORCE method and actor-critic methods are examples of this approach.

We consider the standard reinforcement learning framework, in which a learning agent interacts with a Markov decision process (MDP).

- The state, action, and reward at each time  $t \in \{0, 1, 2, \dots\}$  are denoted  $s_t \in \mathcal{S}$ ,  $a_t \in \mathcal{A}$ , and  $r_t \in \mathbb{R}$ .
- The environment's dynamics are characterized by state transition probabilities and expected rewards:

$$\begin{aligned} \mathcal{P}_{ss'}^a &= P(s_{t+1} = s' | s_t = s, a_t = a) \\ \mathcal{R}_s^a &= \mathbb{E}(r_{t+1} | s_t = s, a_t = a), \forall s, s' \in \mathcal{S}, a \in \mathcal{A} \end{aligned}$$

With function approximation, two ways of formulating the agent's objective are useful: One is the average reward formulation, in which policies are ranked according to their long-term expected reward per-step,  $\rho(\pi)$ :

$$\rho(\pi) = \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E}[r_1 + r_2, \dots, + r_n | \pi] = \sum_s d^\pi(s) \sum_a \pi(a|s) \mathcal{R}_s^a,$$



where  $d^\pi(s) = \lim_{t \rightarrow \infty} P(s_t = s | s_0, \pi)$  is the stationary distribution of states under  $\pi$ , which we assume exists and is independent of  $s_0$  for all policies. Imagine that you can travel along the Markov chain's states forever, and eventually, as the time progresses, the probability of you ending up with one state becomes unchanged. This is the stationary probability that the  $s_t = s$  when starting from  $s_0$  and following policy  $\pi_\theta$  for  $t$  steps. With the average reward formulation, the state-action value function is defined as

$$Q^\pi(s, a) = \sum_{t=1}^{\infty} \mathbb{E}[r_t - \rho(\pi) | s_0 = s, a_0 = a, \pi], \forall s \in \mathcal{S}, a \in \mathcal{A}.$$

### G.7.1 Proof of Policy Gradient Theorem

$$\begin{aligned} J(\theta) &= \sum_{s \in \mathcal{S}} d^\pi(s) V^\pi(s) \\ &= \sum_{s \in \mathcal{S}} d^\pi(s) \sum_{a \in \mathcal{A}} \pi_\theta(a|s) Q^\pi(s, a), \end{aligned}$$

where  $d_\pi(s)$  is the stationary distribution of Markov chain for  $\pi_\theta$  (on-policy state distribution under  $\pi$ ). Imagine that you can travel along the Markov chain's states forever, and eventually, as the time progresses, the probability of you ending up with one state becomes unchanged, this is the stationary probability for  $\pi_\theta$ .

$$\begin{aligned} \nabla_\theta V^\pi(s) &= \nabla_\theta \sum_{a \in \mathcal{A}} \pi_\theta(a|s) Q^\pi(s, a) \\ &= \sum_{a \in \mathcal{A}} \nabla_\theta \pi_\theta(a|s) Q^\pi(s, a) + \pi_\theta(a|s) \nabla_\theta Q^\pi(s, a) \\ &= \sum_{a \in \mathcal{A}} \nabla_\theta \pi_\theta(a|s) Q^\pi(s, a) + \pi_\theta(a|s) \nabla_\theta \sum_{s', r} P(s', r | s, a) (r + V^\pi(s')) \\ &= \sum_{a \in \mathcal{A}} \nabla_\theta \pi_\theta(a|s) Q^\pi(s, a) + \pi_\theta(a|s) \sum_{s', r} P(s', r | s, a) \nabla_\theta V^\pi(s') \quad P(s', r | s, a) \text{ and } r \text{ is not a function of } \theta \\ &= \sum_{a \in \mathcal{A}} \nabla_\theta \pi_\theta(a|s) Q^\pi(s, a) + \pi_\theta(a|s) \sum_{s'} P(s' | s, a) \nabla_\theta V^\pi(s') \end{aligned}$$

This equation has a recursive form. Let's consider a visitation sequence and transition probability from state  $s$  to state  $x$  with policy  $\pi_\theta$  after  $k$  steps as:

$$\rho^\pi(s \rightarrow x, k)$$

- This is a state transition probability with a policy  $\pi_\theta$
- When  $k = 0$ ,  $\rho^\pi(s \rightarrow s, k = 0) = 1$
- When  $k = 1$ ,  $\rho^\pi(s \rightarrow s', k = 1) = \sum_a \pi_\theta(a|s) P(s' | s, a)$
- $\rho^\pi(s \rightarrow x, k + 1) = \sum_{s'} \rho^\pi(s \rightarrow s', k) \rho^\pi(s' \rightarrow x, 1)$ , where  $s'$  is the step right behind the state  $x$  (intermediate step).

$$\begin{aligned}
\nabla_{\theta} V^{\pi}(s) &= \underbrace{\sum_{a \in \mathcal{A}} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s, a) + \pi_{\theta}(a|s) \sum_{s'} P(s'|s, a) \nabla_{\theta} V^{\pi}(s')}_{\doteq \phi(s)} \\
&= \phi(s) + \sum_a \pi_{\theta}(a|s) \sum_{s'} P(s'|s, a) \nabla_{\theta} V^{\pi}(s') \\
&= \phi(s) + \sum_{s'} \sum_a \pi_{\theta}(a|s) P(s'|s, a) \nabla_{\theta} V^{\pi}(s') \\
&= \phi(s) + \sum_{s'} \rho^{\pi}(s \rightarrow s', k=1) \nabla_{\theta} V^{\pi}(s') \\
&= \phi(s) + \sum_{s'} \rho^{\pi}(s \rightarrow s', k=1) \left[ \phi(s') + \sum_{s''} \rho^{\pi}(s' \rightarrow s'', k=1) \nabla_{\theta} V^{\pi}(s'') \right] \\
&= \phi(s) + \sum_{s'} \rho^{\pi}(s \rightarrow s', 1) \phi(s') + \sum_{s''} \sum_{s'} \rho^{\pi}(s \rightarrow s', 1) \rho^{\pi}(s' \rightarrow s'', k=1) \nabla_{\theta} V^{\pi}(s'') \\
&= \phi(s) + \sum_{s'} \rho^{\pi}(s \rightarrow s', 1) \phi(s') + \sum_{s''} \rho^{\pi}(s \rightarrow s'', 2) \nabla_{\theta} V^{\pi}(s'') \\
&\vdots \\
&= \sum_{x \in \mathcal{S}} \sum_{k=0}^{\infty} \rho^{\pi}(s \rightarrow x, k) \phi(x)
\end{aligned}$$

We can rewrite the above equation as

$$\begin{aligned}
\nabla_{\theta} J(\theta) &= \nabla_{\theta} V^{\pi}(s) \\
&= \sum_{x \in \mathcal{S}} \underbrace{\sum_{k=0}^{\infty} \rho^{\pi}(s_0 \rightarrow s, k) \phi(x)}_{\doteq \eta(s)} \\
&= \sum_s \eta(s) \phi(s) \\
&= \underbrace{\sum_s \eta(s)}_{\text{Constant}} \underbrace{\sum_s \frac{\eta(s)}{\sum_s \eta(s)}}_{\text{Normalization}} \phi(s) \\
&\propto \sum_s \frac{\eta(s)}{\sum_s \eta(s)} \phi(s) \\
&= \sum_s d^{\pi}(s) \sum_{a \in \mathcal{A}} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s, a) \\
&= \mathbb{E}_{\pi}[\nabla_{\theta} \ln \pi_{\theta}(a|s) Q^{\pi}(s, a)]
\end{aligned}$$