Reinforcement Learning

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I. Introduction

Reinforcement learning is a sub-field of machine learning that has a unique setting that sets itself apart from other machine learning fields, such as supervised learning, and unsupervised learning. Unlike these methods, which rely on pre-sampled data, reinforcement learning involves an agent learning to decide the optimal actions by interacting with an environment. The agent explores the environment, receives feedback in the form of rewards, and uses this feedback to learn and improve its sequential decision-making over time. Therefore, the objective of reinforcement learning is for the agent to learn to take actions that maximizes the expected total reward. In this paper, we will discuss in detail of what this means.

II. Markov Decision Process

A Markov decision process (MDP) is a mathematical model of the environment with which an agent interacts. The defining feature of an MDP is the Markov property (Markov chain), which asserts that the future state of the environment depends only on the current state and action, not on the sequence of preceding states. This property enables the formulation of Bellman's optimality and expectation equations, where the value of a state depends solely on the immediate reward and the expected value of the next state. By leveraging Bellman's equations, an agent can iteratively update its value and policy functions without needing complete knowledge of all possible episodes. The following subsections will clarify these concepts in greater detail.

A. Markov Chain

MDP formally describes an environment that an agent interacts with. To understand MDP, we first need to formally define Markov property (chain), which states, "the future is independent of the past given the present."

To understand Markov chain, we first need to briefly understand stochastic process, because Markov chain is stochastic process with a special property. Stochastic process is a collection of random variables indexed by a time set. For example, discrete time stochastic process can be described as

$$S_0, S_1, \ldots, S_t, S_{t+1}, \ldots, \tag{1}$$

where the random variables $S_0, S_1, \ldots$ represent states at different time steps. The specific distribution of each random variable is less important than the fact that they form an ordered sequence over time. Similarly, a continuous time random process can be expressed as

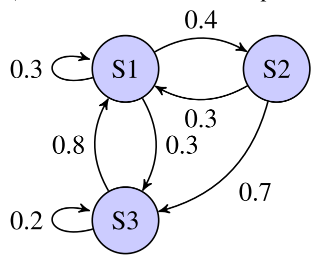
$$\{S_t | t \geq 0\}. \tag{2}$$

Markov chain is stochastic process with a special property; i.e., a stochastic process is Markov chain if it satisfy the following condition:

$$P(S_{t+1} = s_{t+1} | S_t = s_t) = P(S_{t+1} = s_{t+1} | S_t = s_t, \ldots, S_0 = s_0), \tag{3}$$

where $P(S_{t+1} = s_{t+1})$ is the probability that future state S_{t+1} takes the value of s_{t+1}, given that the current state is $S_t = s_t$. This means that the probability of the future state depends only on the current state and not on the sequence of past states. We denote that $P(S_{t+1} = s' | S_t = s)$ is the transition probability from current state s to future state s'. To this end, we can define Markov chain as a tuple (S, P). Here, S represents a set of states, and P represents a transition probability matrix.

1) Markov Chain Example: Consider this example, we have a Markov chain represented by this graph.



This graph can be described by transition matrix expressed as

$$\begin{bmatrix} 0.3 & 0.4 & 0.0 \\ 0.3 & 0.0 & 0.7 \\ 0.8 & 0.0 & 0.2 \end{bmatrix}. \tag{4}$$

Let us look at an example, consider that S_t (current state) is S_2. Given this information, the probability of next state being S_3 is $P(S_{t+1} = S_3 | S_t = S_2) = 0.7$.

B. Markov Decision Process

MDP is very similar to Markov chain but the difference is that it is defined by a tuple (S, A, P, R, γ), where

- S: state space, set of all possible states
- A: action space, set of all possible actions
- P: state transition probability, which gives the probability of transitioning from state s to state s' given action a,
- R: reward function, which gives the immediate reward received after transitioning from state s to state s' under action a,
- γ: discount factor.

The transition probability is defined as

$$P^a_{ss'} = P(s'|s,a) = P(S_{t+1} = s'|S_t = s, A_t = a), \tag{5}$$

where the future state depends on current state and the action. In reinforcement learning, when the word *environment* appears, it is referring to MDP. Note that when MDP is known, all transition probability of the environment is known. Because it is known, we can use the Bellman's equation to find the optimal policy and value functions based on dynamic programming. However, in many real world problems, MDP is unknown. In this case, we use reinforcement learning to find optimal policy and value functions.

1) Example: Transition Probability with MDP: Consider an environment that is described by MDP shown in Fig. 1. Given s and a, the transition probability getting s' is described by (5). With law of total probability (46), this can be expressed in terms of reward as

$$P^a_{ss'} = P(s'|s,a) = \sum_{r\in\mathcal{R}} P(s', r|s,a), \tag{6}$$

where $\mathcal{R}$ is the set of all possible rewards. Now, conditional joint probability $P(s', r|s, a)$ can be decomposed to $P(s', r|s, a) = P(s'|s, a, r)P(r|a, s)$. For example, transition probability of next state being s' given current state s, and action a would be

$$P(s'|s,a) = \sum_{r\in\mathcal{R}} P(s'|s,a,r)P(r|s,a) = P(s'|s,a,r')P(r'|s,a) + P(s'|s,a,r'')P(r''|s,a) = 0.4 \cdot 0.5 + 0.4 \cdot 0.5 = 0.4. \tag{7}$$

III. Reward and Return

A. Reward

Reward, denoted as R_t, is a scalar feedback indicating how well the agent is making decisions at step t. As mentioned in Sec. I, the underlying objective in reinforcement learning is to find optimal actions that would maximize the expected cumulative rewards. There are two important points to note. First, notice how the goal for the agent is to maximize the *expected* cumulative reward. What does it mean to have an expected reward? We describe this by considering an example depicted by Fig. 1. As

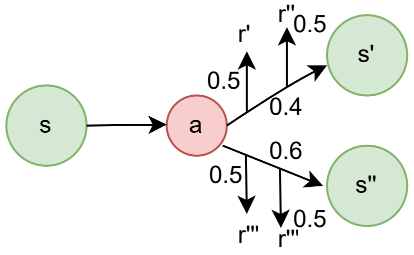


Fig. 1. Simple Markov Decision Process

shown, there are two states s' and s'' that we can transition to by taking action a. For each transition from the action to the states, there are two possible rewards. Therefore, we need to take in the account of all the rewards that we can get from a single state-action pair. This is why the agent is interested in maximizing the *expected* cumulative reward. The expression of expected reward is described as

$$R^a_s = r(s,a) = \mathbb{E}[R_{t+1}|S_t = s, A_t = a] = \sum_{r\in\mathcal{R}} r \sum_{s'\in\mathcal{S}} P(s', r|s,a). \tag{8}$$

Next, we describe the meaning of *cumulative* reward. This means that the agent considers the rewards accumulated over many, or even all, time steps. This accumulated reward is referred to as the return, which will be explained in the next subsection.

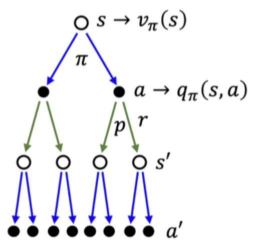


Fig. 2. Backup Diagram for Value Function

B. Return

While reward is the immediate scalar feedback from the environment to the agent after the agent takes one action from a particular state, return is the total *discounted* reward from time step t. This is described as

$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \ldots = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1}, \tag{9}$$

where $\gamma \in [0,1]$ is the discount factor. This awards the immediate actions and compensates the far actions. Most MDPs are discounted because of the following reasons,

- mathematically convenient,
- uncertainty of the future and
- immediate rewards may earn more interest than delayed rewards.

IV. Policy and Value Function

A. Policy

Policy, denoted as π, is a probability distribution over actions for given states. This is expressed as

$$\pi(a|s) = P(A_t = a|S_t = s). \tag{10}$$

We note that this is the case for stochastic policy. Stochastic policy has a probability distribution of actions when given a state, while deterministic policy has a defined action for a given state. Therefore, deterministic policy is described as

$$\pi(s) = a. \tag{11}$$

B. Value Functions

Value function measures the goodness of each state s (or state-action pair (s,a)) when following a policy π in terms of the expectation of returns G_t. Note that we are now computing the *expected* G_t. Reason for this can be explain with Fig. 2. Notice that the tree starts out with a state s. Then, because there are multiple actions you can take from s, with π, it branches out to many possible actions and states. When the sequences of actions terminate, and the agent ends up in a final state, we say that one episode ended. All these episodes end up with returns and we can denote them as G_t^j, where $j = 1, ..., N$, and N is total number of episodes. We have to take into account of all the episodes and the corresponding returns to measure the goodness of one state; therefore, we find the expected return value to define the value function. This can be described as

$$v_\pi(s) = G_t^1 P(G_t^1|s) + G_t^2 P(G_t^2|s) + \cdots + G_t^N P(G_t^N|s) = \mathbb{E}_\pi[G_t|S_t = s], \tag{12}$$

where $P(G_t^j|s)$ is probability of G_t^j happening when state s is given.

There are two types of value function: *state-value* and *action-value*. We will describe them in the following subsections.

C. State-Value Function

There are two types of value functions. First one is state-value function denoted as $v_\pi(s)$. This measures the quality of the state when following π. The function is described as

$$v_\pi(s) = \mathbb{E}_\pi[G_t|S_t = s]. \tag{13}$$

Consider a backup diagram illustrated by Fig. 2. We are given a state and based on the state, the policy π has two actions. Each action transitions to different states with transition probability p with reward r. Then the process continues until the episode ends. Each episode outputs a return and expected value of each episode given a state is the state-value function.

D. *Action-Value Function*

Action-value function for policy π is the expected return starting from state s, taking action a, and following policy π. This is described as

$$q_\pi(s,a) = \mathbb{E}_\pi[G_t|S_t = a, A_t = a]. \tag{14}$$

Only difference between action-value function and state-value function is that action value considers a state-action pair. Therefore, complexity to solve for action-value function is greater than that of state-value function because action-value has to consider all the actions derived from each state. Action-value function is also known as q-function.

We can express state-value function in terms of action-value function as

$$v_\pi(s) = \sum_a \pi(a|s) q_\pi(s,a). \tag{15}$$

Further, we can express action-value function in terms of state-value function as

$$A_\pi(s,a) = q_\pi(s,a) - v_\pi(s). \tag{16}$$

V. Bellman Equation

A. *Bellman Expectation Equation*

Bellman expectation equation is a recursive equation decomposing state-value function $v_\pi(s)$ into immediate reward R_{t+1} and discounted next state-value $\gamma v_\pi(S_{t+1})$. Derivation for this expression is described as follows

$$\begin{aligned}
v_\pi(s) &= \mathbb{E}_\pi[G_t|S_t = s] && (17)\\
&= \sum_a \mathbb{E}_\pi[G_t|S_t = s, A_t = a] \underbrace{P(A_t = a|S_t = s)}_{\pi(a|s)} && (18)\\
&= \sum_a \pi(a|s)\mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1}|S_t = s, A_t = a], && (19)\\
&= \sum_a \pi(a|s) \sum_{s'}\sum_r \mathbb{E}_\pi[R_{t+1} + \gamma G_{t+1}|S_t = s, A_t = a, S_{t+1} = s', R_{t+1} = r] P(s', r|s,a) && (20)\\
&= \sum_a \pi(a|s) \sum_{s'}\sum_r P(s', r|s,a)\big[r + \gamma \underbrace{\mathbb{E}[G_{t+1}|S_{t+1} = s']}_{v_\pi(s')}\big] = \sum_a \pi(a|s)\sum_{s'}\sum_r P(s',r|s,a)\big[r + \gamma v_\pi(s')\big] && (21)\\
&= \sum_a P(a|s)\Big[\sum_{s'}\sum_r r P(s',r|s,a) + \sum_{s'}\sum_r \gamma v_\pi(s') P(s',r|s,a)\Big] && (22)\\
&= \sum_a P(a|s)\Big[\sum_r r P(r|s,a) + \sum_{s'} \gamma v_\pi(s') P(s'|s,a)\Big] && (23)\\
&= \sum_a P(a|s)\big[\mathbb{E}[R_{t+1}|S_t = s, A_t = a] + \mathbb{E}[\gamma v_\pi(s')|S_t = s, A_t = a]\big] && (24)\\
&= \sum_a P(a|s)\big[\mathbb{E}[R_{t+1} + \gamma v_\pi(s')|S_t = s, A_t = a]\big] && (25)\\
&= \mathbb{E}_\pi[R_{t+1} + \gamma v_\pi(s')|S_t = s]. && (26)
\end{aligned}$$

Note that (21) can also be expressed as $\sum_a \pi(a|s)[R_s^a + \gamma \sum_{s'} P_{ss'}^a v_\pi(s')]$. Now with (26), we have expressed the state-value function in terms of immediate reward and value-function of next state. This means that we do not have to wait until we get all possible episodes to end in order to find the value-function as expressed in (17).

Similarly, we can express the action-function in a same way. This is expressed as

$$\begin{aligned}
q_\pi(s,a) &= \mathbb{E}_\pi[G_t|S_t = s, A_t = a] && (27)\\
&= \sum_{s'}\sum_r P(s',r|s,a)[r + \gamma \sum_{a'} \pi(a'|s') q_\pi(s',a')] && (28)\\
&= \mathbb{E}_\pi[R_{t+1} + \gamma q_\pi(S_{t+1}, A_{t+1})|S_t = s, A_t = a]. && (29)
\end{aligned}$$

B. *Bellman Optimality Equation*

Before we describe the optimality equation, we first explain the optimal value function and policy. The optimal value function yields maximum value compared to all other value function. The goal of MDP is to find this optimal value function described as

$$v_*(s) = \max_\pi v_\pi(s). \tag{30}$$

Similarly, optimal action-value function is expressed as

$$q_*(s,a) = \max_\pi q_\pi(s,a). \tag{31}$$

We define a partial ordering policy that says $\pi' \geq \pi$ if $v_{\pi'} \geq v_\pi(s)$ for all s. This means that to say a policy π' is greater than or equal to π, the state-value function of π' must be greater than or equal to π for all s.

Fundamental theorem of MDP states that any MDP satisfies the following:

- there exists an *optimal policy* $\pi_* \geq \pi, \forall \pi$,
- all optimal policies achieve optimal state-value function $v_{\pi_*} = v_*(s)$,
- all optimal policies achieve optimal action-value function $q_{\pi_*}(s,a) = q_*(s,a)$.

Then, most important question narrows down to how we find this optimal policy. This is found by maximizing over $q_*(s,a)$. That is,

$$\pi_*(a|s) = \begin{cases} 1 & \text{if } a = \arg\max_a q_*(s,a), \\ 0 & \text{otherwise.} \end{cases} \tag{32}$$

Note that since $v_\pi(s) = \sum_a \pi(a|s) q_\pi(s,a)$, then, the optimal state-value function is $v_{\pi_*} = \sum_a \pi_*(a|s) q_{\pi_*}(s,a)$. We noted that $v_{\pi_*} = v_*(s)$ and $q_{\pi_*}(s,a) = q_*(s,a)$. Therefore,

$$v_{\pi_*}(s) = \sum_a \pi_*(a|s) q_{\pi_*}(s,a) \tag{33}$$

$$= v_*(s) = \sum_a \pi_*(a|s) q_*(s,a), \tag{34}$$

where optimal policy $\pi_*(a|s)$ will deterministically only take action that yields maximum action-value. Therefore, optimal state-value function is the maximum action-value function, which is described as

$$v_*(s) = \max_a q_*(s,a). \tag{35}$$

We can see from (35), that if we know the optimal action-function, we can immediately find (35). The optimal action-function is described as

$$q_*(s,a) = r(s,a) + \gamma \sum_{s'} P(s'|s,a) v_*(s'), \tag{36}$$

where $r(s,a)$ is described by (8). We can see that from (36), optimal action-value is found if we know optimal state-value for the next state, but only under the condition that transition probability $P(s'|s,a)$ is known. Therefore, if the MDP is known, we can solve for optimal state and action functions based on the known transition probabilities. This can be efficiently solved by dynamic programming. However, if the transition probabilities are not known, we use random sampling to approximate the optimal action-value. This method is solved with reinforcement learning.

We now describe Bellman optimality equation that is used to find the optimal value-function and action-function which then gets used to find the optimal policy. First, we describe the optimal value-function as

$$v_*(s) = \max_{a \in \mathcal{A}(s)} q*(s,a) = \max_a \mathbb{E}_{\pi_*}[G_t | S_t = s, A_t = a] \tag{37}$$

$$= \max_a \mathbb{E}_{\pi_*}[R_{t+1} + \gamma G_{t+1} | S_t = s, A_t = a] \tag{38}$$

$$= \max_a \mathbb{E}_{\pi_*}[R_{t+1} + \gamma v_*(S_{t+1}) | S_t = s, A_t = a] \tag{39}$$

$$= \max_a \sum_{s'} \sum_r P(s', r|s,a)[r + \gamma v_*(s')]. \tag{40}$$

Similarly, optimal action-function is described as

$$q_*(s,a) = \mathbb{E}[R_{t+1} + \gamma \max_{a'} q_*(S_{t+1}, a') | S_t = s, A_t = a] \tag{41}$$

$$= \sum_{s'} \sum_r P(s', r|s,a)[r + \gamma \max_{a'} q_*(s', a')]. \tag{42}$$

VI. Optimal Policy With Dynamic Programming

A. Value Iteration

Value iteration computes the following expression until convergence

$$V_{k+1}(s) \leftarrow \max_a \sum_{s', r} P(s', r|s,a)[r + \gamma V_k(s')]. \tag{43}$$

B. Policy Iteration

Algorithm 1 Value Iteration

```
1: Hyperparameter: Small threshold $\epsilon > 0$ for the convergence check.
2: Initialize $V(s)$ arbitrarily for all $s \in \mathcal{S}$, except $V(\text{terminal}) = 0$.
3: repeat
4:     $\Delta \leftarrow 0$
5:     for each state $s \in \mathcal{S}$ do
6:         $v \leftarrow V(s)$
7:         $V(s) \leftarrow \max_{a\in\mathcal{A}} \sum_{s'} P(s'|s,a)[R(s,a,s') + \gamma V(s')]$
8:         $\Delta \leftarrow \max(\Delta, |v - V(s)|)$
9:     end for
10: until $\Delta < \epsilon$
```

Appendix A
Appendix A: Law of Total Probability

We have a sample space S, it consists of n disjoint events $B_1, B_2, \cdots, B_n$ which makes up the sample space S. We also have an event A, in the sample space, which is made up of parts in $B_1, B_2, \cdots, B_n$. Then, event A can be described as

$$A = (A \cap B_1) \cup (A \cap B_2) \cup \cdots \cup (A \cap B_n). \tag{44}$$

The probability of event A happening then is expressed as

$$P(A) = P(A \cap B_1) + P(A \cap B_2) + \cdots + P(A \cap B_n), \tag{45}$$

where we use sum rule of probability to sum the probabilities because $B_1, B_2, \cdots, B_n$ are disjoint. Then, using the conditional probability, we can express $P(A \cap B) = P(A|B)P(B)$. Therefore, (45) can be expressed as

$$P(A) = \sum_n P(A|B_n)P(B_n). \tag{46}$$

Now, this can be applied to expected value where expected value of random variable X can be expressed in Y as

$$\mathbb{E}[X] = \sum_y \mathbb{E}[X|Y = y]P(Y = y), \tag{47}$$

where $\mathbb{E}[X] = \sum_x xP(X = x)$. This can be extended to conditional expected value, where it is expressed as

$$\mathbb{E}[X|Z = z] = \sum_y \mathbb{E}[X|Y = y, Z = z]P(Y = y|Z = z). \tag{48}$$