Lecture 5: Monte Carlo Learning

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Outline



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- 2 The simplest MC-based RL algorithm
 - Algorithm: MC Basic
- 3 Use data more efficiently
 - Algorithm: MC Exploring Starts
- 4 MC without exploring starts
 - Algorithm: MC ε -Greedy

1 Motivating example

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- How can we estimate something without models?
- The simplest idea: Monte Carlo estimation.

Example: Flip a coin

The result (either head or tail) is denoted as a random variable X

- if the result is head, then X = +1
- if the result is tail, then X = -1

The *aim* is to compute $\mathbb{E}[X]$.

▷ Method 1: with model

• Suppose the probabilistic model is known as

$$p(X = 1) = 0.5, \quad p(X = -1) = 0.5$$

Then by definition

$$\mathbb{E}[X] = \sum_{x} xp(x) = 1 \times 0.5 + (-1) \times 0.5 = 0$$

• Problem: it may be impossible to know the precise distribution!

Method 2: without model or called model-free

- *Idea:* Flip the coin many times, and then calculate the average of the outcomes.
- Suppose we get a sample sequence: $\{x_1, x_2, \dots, x_N\}$. Then, the mean can be approximated as

$$\mathbb{E}[X] \approx \bar{x} = \frac{1}{N} \sum_{j=1}^{N} x_j.$$

This is the idea of Monte Carlo estimation!

Motivating example: Monte Carlo estimation

- > Question: Is the Monte Carlo estimation accurate?
- When N is small, the approximation is inaccurate.
- When N is large, the approximation is more accurate.



Law of Large Numbers

For a random variable X, suppose $\{x_j\}_{j=1}^N$ are some iid samples. Let $\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$ be the average of the samples. Then,

$$\mathbb{E}[\bar{x}] = \mathbb{E}[X],$$
$$\operatorname{Var}[\bar{x}] = \frac{1}{N} \operatorname{Var}[X].$$

As a result, \bar{x} is an unbiased estimate of $\mathbb{E}[X]$ and its variance decreases to zero as N increases to infinity.

The samples must be iid (independent and identically distributed)
 For the proof, see the book.

- ▷ Summary:
- Monte Carlo estimation refers to a broad class of techniques that rely on repeated random sampling to solve approximation problems.
- Why we care about Monte Carlo estimation? Because it does not require the model!
- Why we care about mean estimation? Because state value and action value are defined as expectations of random variables!

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The key idea is to convert the *policy iteration* algorithm to be model-free. It is simple to understand if you

- understand the policy iteration algorithm well, and
- understand the idea of Monte Carlo mean estimation.

Policy iteration has two steps in each iteration:

Policy evaluation:
$$v_{\pi_k} = r_{\pi_k} + \gamma P_{\pi_k} v_{\pi_k}$$

Policy improvement: $\pi_{k+1} = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_{\pi_k})$

The elementwise form of the policy improvement step is:

$$\begin{split} \pi_{k+1}(s) &= \arg\max_{\pi} \sum_{a} \pi(a|s) \left[\sum_{r} p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v_{\pi_k}(s') \right] \\ &= \arg\max_{\pi} \sum_{a} \pi(a|s)q_{\pi_k}(s,a), \quad s \in \mathcal{S} \end{split}$$

The key is to calculate $q_{\pi_k}(s, a)!$

Two expressions of action value:

• Expression 1 requires the model:

$$q_{\pi_k}(s,a) = \sum_{r} p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v_{\pi_k}(s')$$

• Expression 2 does not require the model:

$$q_{\pi_k}(s,a) = \mathbb{E}[G_t | S_t = s, A_t = a]$$

Idea to achieve model-free RL: We can use expression 2 to obtain $q_{\pi_k}(s, a)$ based on *data (samples or experiences)*!

How to obtain $q_{\pi_k}(s, a)$ based on data?

- Starting from (s, a), following policy π_k , generate an episode.
- The return of this episode is g(s, a), which is a sample of G_t in

$$q_{\pi_k}(s,a) = \mathbb{E}[G_t | S_t = s, A_t = a]$$

• Suppose we have a set of episodes and hence $\{g^{(j)}(s,a)\}$. Then,

$$q_{\pi_k}(s,a) = \mathbb{E}[G_t|S_t = s, A_t = a] \approx \frac{1}{N} \sum_{i=1}^N g^{(i)}(s,a).$$

Fundamental idea: When model is unavailable, we can use data.

Given an initial policy π_0 , there are two steps in the *k*th iteration.

- Step 1: policy evaluation. This step aims to estimate q_{πk}(s, a) for all (s, a). Specifically, for each (s, a), run sufficiently many episodes. The average of their returns, denoted as q_k(s, a), is used to approximate q_{πk}(s, a).
 - The first step of the *policy iteration algorithm* calculates $q_{\pi_k}(s, a)$ by firstly solving the state values v_{π_k} from the Bellman equation. This requires the model.
 - The first step of the *MC Basic algorithm* is to directly estimate $q_k(s, a)$ from experiences samples. This does not require the model.
- Step 2: policy improvement. This step aims to solve
 π_{k+1}(s) = arg max_π ∑_a π(a|s)q_k(s, a) for all s ∈ S. The greedy optimal
 policy is π_{k+1}(a^{*}_k|s) = 1 where a^{*}_k = arg max_a q_k(s, a).
 - This step is exactly the same as the second step of the policy iteration algorithm.

The MC Basic algorithm

▷ Description of the algorithm:

Pseudocode: MC Basic algorithm (a model-free variant of policy iteration)

```
Initialization: Initial guess \pi_0.
Aim: Search for an optimal policy.
For the kth iteration (k = 0, 1, 2, ...), do
     For every state s \in \mathcal{S}, do
           For every action a \in \mathcal{A}(s), do
                Collect sufficiently many episodes starting from (s, a) following \pi_k
                Policy evaluation:
                q_{\pi_k}(s,a) \approx q_k(s,a) = average return of all the episodes starting
                from (s, a)
           Policy improvement:
           a_k^*(s) = \arg \max_a q_k(s, a)
           \pi_{k+1}(a|s) = 1 if a = a_k^*, and \pi_{k+1}(a|s) = 0 otherwise
```

- MC Basic is a variant of the policy iteration algorithm.
- The model-free algorithms are built up based on model-based ones. It is, therefore, necessary to understand model-based algorithms first before studying model-free algorithms.
- MC Basic is useful to reveal the core idea of MC-based model-free RL, but not practical due to low efficiency.
- Why does MC Basic estimate action values instead of state values? That is because state values cannot be used to improve policies directly. When models are not available, we should directly estimate action values.
- Since policy iteration is convergent, the *convergence* of MC Basic is also guaranteed to be convergent given sufficient episodes.



Task:

- An initial policy is shown in the figure.
- Use MC Basic to find the optimal policy.
- $r_{\text{boundary}} = -1$, $r_{\text{forbidden}} = -1$, $r_{\text{target}} = 1$, $\gamma = 0.9$.



Outline: given the current policy π_k

- Step 1 policy evaluation: calculate $q_{\pi_k}(s, a)$ How many state-action pairs? 9 states \times 5 actions =45 state-action pairs!
- Step 2 policy improvement: select the greedy action
 a^{*}(s) = arg max_a q_{π_k}(s, a)



- \triangleright Due to space limitation, we only show $q_{\pi_k}(\mathbf{s_1}, a)$
- ▷ Step 1 policy evaluation:
- Since the current policy is deterministic, one episode would be sufficient to get the action value! Otherwise, if the policy or model is stochastic, many episodes are required!

Illustrative example 1: step by step



• Starting from (s_1, a_1) , the episode is $s_1 \xrightarrow{a_1} s_1 \xrightarrow{a_1} s_1 \xrightarrow{a_1} \dots$ Hence, the action value is

$$q_{\pi_0}(s_1, a_1) = -1 + \gamma(-1) + \gamma^2(-1) + \dots$$

• Starting from (s_1, a_2) , the episode is $s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_3} \dots$ Hence, the action value is

$$q_{\pi_0}(s_1, a_2) = 0 + \gamma 0 + \gamma^2 0 + \gamma^3(1) + \gamma^4(1) + \dots$$

• Starting from (s_1, a_3) , the episode is $s_1 \xrightarrow{a_3} s_4 \xrightarrow{a_2} s_5 \xrightarrow{a_3} \dots$ Hence, the action value is

$$q_{\pi_0}(s_1, a_3) = 0 + \gamma 0 + \gamma^2 0 + \gamma^3(1) + \gamma^4(1) + \dots$$



• Starting from (s_1, a_4) , the episode is $s_1 \xrightarrow{a_4} s_1 \xrightarrow{a_1} s_1 \xrightarrow{a_1} \dots$ Hence, the action value is

$$q_{\pi_0}(s_1, a_4) = -1 + \gamma(-1) + \gamma^2(-1) + \dots$$

• Starting from (s_1, a_5) , the episode is $s_1 \xrightarrow{a_5} s_1 \xrightarrow{a_1} s_1 \xrightarrow{a_1} \dots$ Hence, the action value is

$$q_{\pi_0}(s_1, a_5) = 0 + \gamma(-1) + \gamma^2(-1) + \dots$$



- **Step 2 policy improvement:**
- By observing the action values, we see that

$$q_{\pi_0}(s_1, a_2) = q_{\pi_0}(s_1, a_3)$$

are the maximum.

• As a result, the policy can be improved as

$$\pi_1(a_2|s_1) = 1$$
 or $\pi_1(a_3|s_1) = 1$.

In either way, the new policy for s_1 becomes optimal.

One iteration is sufficient for this simple example!

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Exercise: now update the policy for s_3 using MC Basic!

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The MC Basic algorithm:

- Advantage: reveal the core idea clearly!
- Disadvantage: too simple to be practical.

However, MC Basic can be extended to be more efficient.

 \triangleright Consider a grid-world example, following a policy $\pi,$ we can get an episode such as

$$s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_4} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots$$

 \triangleright **Visit:** every time a state-action pair appears in the episode, it is called a *visit* of that state-action pair.

> Methods to use the data: Initial-visit method

- Just calculate the return and approximate $q_{\pi}(s_1, a_2)$.
- This is what the MC Basic algorithm does.
- Disadvantage: Not fully utilize the data.

 \triangleright The episode also visits other state-action pairs.

Can estimate $q_{\pi}(s_1, a_2)$, $q_{\pi}(s_2, a_4)$, $q_{\pi}(s_2, a_3)$, $q_{\pi}(s_5, a_1)$,...

Data-efficient methods:

- first-visit method
- every-visit method

 \triangleright Another aspect in MC-based RL is when to update the policy. There are two methods.

- The first method is, in the policy evaluation step, to collect all the episodes starting from a state-action pair and then use the average return to approximate the action value.
 - This is the one adopted by the MC Basic algorithm.
 - The problem of this method is that the agent has to wait until all episodes have been collected.
- The second method uses the return of a single episode to approximate the action value.
 - In this way, we can improve the policy episode-by-episode.

▷ Will the second method cause problems?

- One may say that the return of a single episode cannot accurately approximate the corresponding action value.
- In fact, we have done that in the truncated policy iteration algorithm introduced in the last chapter!
- **>** Generalized policy iteration:
- Not a specific algorithm.
- It refers to the general idea or framework of switching between policy-evaluation and policy-improvement processes.
- Many RL algorithms fall into this framework.

 \triangleright If we use data and update estimate more efficiently, we get a new algorithm called MC Exploring Starts:

```
Algorithm: MC Exploring Starts (an efficient variant of MC Basic)
Initialization: Initial policy \pi_0(a|s) and initial value q(s, a) for all (s, a). Returns(s, a) = 0 and
\operatorname{Num}(s, a) = 0 for all (s, a).
Goal: Search for an optimal policy.
For each episode, do
     Episode generation: Select a starting state-action pair (s_0, a_0) and ensure that all pairs can be possibly
     selected (this is the exploring-starts condition). Following the current policy, generate an episode of
     length T: s_0, a_0, r_1, \ldots, s_{T-1}, a_{T-1}, r_T.
     Initialization for each episode: q \leftarrow 0
     For each step of the episode, t = T - 1, T - 2, \ldots, 0, do
          g \leftarrow \gamma g + r_{t+1}
          \mathsf{Returns}(s_t, a_t) \leftarrow \mathsf{Returns}(s_t, a_t) + a
          Num(s_t, a_t) \leftarrow Num(s_t, a_t) + 1
          Policy evaluation:
          q(s_t, a_t) \leftarrow \mathsf{Returns}(s_t, a_t) / \mathsf{Num}(s_t, a_t)
          Policy improvement:
          \pi(a|s_t) = 1 if a = \arg \max_a q(s_t, a) and \pi(a|s_t) = 0 otherwise
```

MC Exploring Starts

What is exploring starts?

- Exploring starts means we need to generate sufficiently many episodes
 starting from every state-action pair.
- For example, we need episodes starting from $\{(s_1, a_j)\}_{j=1}^5$, $\{(s_2, a_j)\}_{j=1}^5$, ..., $\{(s_9, a_j)\}_{j=1}^5$.

Otherwise, if there are no episodes starting from (s_i, a_j) , then (s_i, a_j) may not be visited by any episodes, and hence $q_{\pi}(s_i, a_j)$ cannot be estimated.



• Both MC Basic and MC Exploring Starts need this assumption.

> Why do we need to consider exploring starts?

- In theory, only if every action value for every state is well explored, can we select the optimal actions correctly.
 Otherwise, if an action is not explored, this action may happen to be the optimal one and hence be missed.
- In practice, exploring starts is difficult to achieve. For many applications, especially those involving physical interactions with environments, it is difficult to collect episodes starting from every state-action pair.

Can we remove the requirement of exploring starts? We next show that we can do that by using soft policies.

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▷ What is a soft policy?

- A policy is *soft* if the probability to take any action is positive.
 - Deterministic policy: for example, greedy policy
 - Stochastic policy: for example, soft policy
- ▷ Why introducing soft policies?
- With a soft policy, a few episodes that are sufficiently long can visit every state-action pair.
- Then, we do not need to have a large number of episodes starting from every state-action pair. Hence, the requirement of exploring starts can be removed.
▷ What soft policies will we use? Answer: ε -greedy policies ▷ What is the ε -greedy policy?

$$\pi(a|s) = \begin{cases} 1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1), & \text{for the greedy action,} \\ \frac{\varepsilon}{|\mathcal{A}(s)|}, & \text{for the other } |\mathcal{A}(s)| - 1 \text{ actions.} \end{cases}$$

where $\varepsilon \in [0,1]$ and $|\mathcal{A}(s)|$ is the number of actions for s.

• Example: if $\epsilon = 0.2$, then

$$\frac{\varepsilon}{|\mathcal{A}(s)|} = \frac{0.2}{5} = 0.04, \qquad 1 - \frac{\varepsilon}{|\mathcal{A}(s)|}(|\mathcal{A}(s)| - 1) = 1 - 0.04 \times 4 = 0.84$$

• The chance to choose the greedy action is always greater than other actions, because

$$1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1) = 1 - \varepsilon + \frac{\varepsilon}{|\mathcal{A}(s)|} \ge \frac{\varepsilon}{|\mathcal{A}(s)|}$$

 ε -greedy policies can balance exploitation and exploration.

• When $\varepsilon \to 0$, it becomes greedy!

$$\pi(a|s) = \begin{cases} 1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1) = 1, & \text{for the greedy action,} \\ \frac{\varepsilon}{|\mathcal{A}(s)|} = 0, & \text{for the other } |\mathcal{A}(s)| - 1 \text{ actions.} \end{cases}$$

More exploitation but less exploration.

• When $\varepsilon \to 1,$ it becomes a uniform distribution.

$$\pi(a|s) = \begin{cases} 1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1) = \frac{1}{|\mathcal{A}(s)|}, & \text{for the greedy action,} \\ \frac{\varepsilon}{|\mathcal{A}(s)|} = \frac{1}{|\mathcal{A}(s)|}, & \text{for the other } |\mathcal{A}(s)| - 1 \text{ actions.} \end{cases}$$

More exploration but less exploitation.

> Can a single episode visit all state-action pairs?

When $\varepsilon=1,$ the policy (uniform distribution) has the strongest exploration ability.



Click here to play a video (the video is only on my computer)

> Can a single episode visit all state-action pairs?

When ε is small, the exploration ability of the policy is also small.



\triangleright How to embed ε -greedy into the MC-based RL algorithms?

Originally, the policy improvement step in MC Basic and MC Exploring Starts is to solve

$$\pi_{k+1}(s) = \arg\max_{\pi\in\Pi}\sum_{a} \pi(a|s)q_{\pi_k}(s,a).$$

where Π denotes the set of all possible policies. The optimal policy here is

$$\pi_{k+1}(a|s) = \begin{cases} 1, & a = a_k^*, \\ 0, & a \neq a_k^*, \end{cases}$$

where $a_k^* = \arg \max_a q_{\pi_k}(s, a)$.

 \triangleright How to embed ε -greedy into the MC-based RL algorithms? Now, the policy improvement step is changed to solve

$$\pi_{k+1}(s) = \arg\max_{\pi\in\Pi_{\varepsilon}}\sum_{a}\pi(a|s)q_{\pi_k}(s,a),$$

where Π_{ε} denotes the set of all ε -greedy policies with a fixed value of ε . The optimal policy here is

$$\pi_{k+1}(a|s) = \begin{cases} 1 - \frac{|\mathcal{A}(s)| - 1}{|\mathcal{A}(s)|}\varepsilon, & a = a_k^*, \\ \frac{1}{|\mathcal{A}(s)|}\varepsilon, & a \neq a_k^*. \end{cases}$$

Summary:

- MC ε-Greedy is the same as that of MC Exploring Starts except that the former uses ε-greedy policies.
- It does not require exploring starts, but still requires to visit all state-action pairs in a different form.

Algorithm: MC *e*-Greedy (a variant of MC Exploring Starts)

```
Initialization: Initial policy \pi_0(a|s) and initial value q(s, a) for all (s, a). Returns(s, a) = 0 and
\operatorname{Num}(s, a) = 0 for all (s, a). \epsilon \in (0, 1]
Goal: Search for an optimal policy.
For each episode, do
      Episode generation: Select a starting state-action pair (s_0, a_0) (the exploring starts con-
      dition is not required). Following the current policy, generate an episode of length T:
      s_0, a_0, r_1, \ldots, s_{T-1}, a_{T-1}, r_T.
      Initialization for each episode: a \leftarrow 0
      For each step of the episode, t = T - 1, T - 2, \ldots, 0, do
            g \leftarrow \gamma g + r_{t+1}
            \mathsf{Returns}(s_t, a_t) \leftarrow \mathsf{Returns}(s_t, a_t) + q
            Num(s_t, a_t) \leftarrow Num(s_t, a_t) + 1
            Policy evaluation:
            q(s_t, a_t) \leftarrow \mathsf{Returns}(s_t, a_t) / \mathsf{Num}(s_t, a_t)
            Policy improvement:
            Let a^* = \arg \max_a q(s_t, a) and
                                  \pi(a|s_t) = \begin{cases} 1 - \frac{|\mathcal{A}(s_t)| - 1}{|\mathcal{A}(s_t)|} \epsilon, & a = a^* \\ \frac{1}{|\mathcal{A}(s_t)|} \epsilon, & a \neq a^* \end{cases}
```

Example

 \triangleright Demonstrate the MC ε -Greedy algorithm.

In every iteration, do the following:

- In the episode generation step, use the previous policy generates a single episode of 1 million steps!
- In the rest steps, use the single episode to update the policy.
- Two iterations can lead to the optimal ε -greedy policy.

Here, $r_{\text{boundary}} = -1$, $r_{\text{forbidden}} = -10$, $r_{\text{target}} = 1$, $\gamma = 0.9$.



- Compared to greedy policies,
- The advantage of ε -greedy policies is that they have strong exploration ability when ε is large.
 - Then, the exploring starts condition is not required.
- The disadvantage is that ε -greedy polices are not optimal in general.
 - It is only optimal in the set Π_{ε} of all $\varepsilon\text{-greedy policies.}$
 - ε cannot be too large. We can also use a decaying $\varepsilon.$

 \triangleright Next, we use examples to demonstrate. The setup is $r_{\rm boundary}=-1$, $r_{\rm forbidden}=-10,~r_{\rm target}=1,~\gamma=0.9$

Optimality

\triangleright Given an ε -greedy policy, what is its state value?



 $\varepsilon = 0$





 \triangleright When ε increases, the optimality of the policy becomes worse!

> Why is the state value of the target state negative?

Consistency

 \triangleright Find the optimal ε -greedy policies and their state values?



 $\varepsilon = 0$





 \triangleright The optimal ε -greedy policies are not *consistent* with the greedy optimal one! Why is that? Consider the target for example. Key points:

- Mean estimation by the Monte Carlo methods
- Three algorithms:
 - MC Basic
 - MC Exploring Starts
 - MC ε -Greedy
- Relationship among the three algorithms
- Optimality vs exploration of $\varepsilon\text{-greedy policies}$