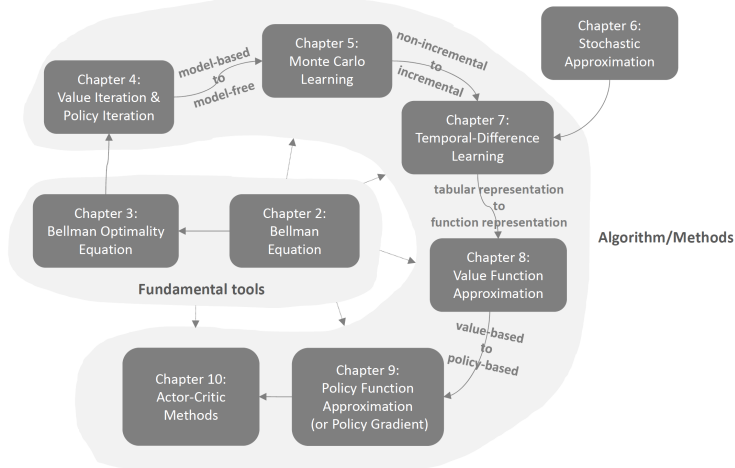


Lecture 5: Monte Carlo Learning

Shiyu Zhao

Outline



- 1 Motivating example
- 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

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Motivating example: Monte Carlo estimation

▷ 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 $\mathbb{E}[X]$.

Motivating example: Monte Carlo estimation

▷ Method 1: Model-based

- 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!!**

Motivating example: Monte Carlo estimation

▷ **Method 2: Model-free**

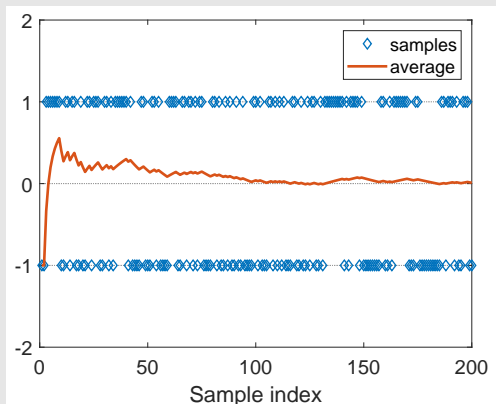
- *Idea:* Flip the coin many times, and then calculate the average of the outcomes.
- Suppose we get a sample sequence: $\{x_1, x_2, \dots, x_N\}$.
Then, the mean can be approximated as

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

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.
 - As N *increases*, the approximation becomes more and more accurate.



Motivating example: Monte Carlo estimation

Law of Large Numbers

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

$$\mathbb{E}[\bar{x}] = \mathbb{E}[X],$$

$$\text{Var}[\bar{x}] = \frac{1}{N} \text{Var}[X].$$

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.

Motivating example: Monte Carlo estimation

▷ 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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Convert policy iteration to be model-free

The key to understand the algorithm is to understand [how to convert the policy iteration algorithm to be model-free](#).

- Should understand policy iteration well.
- Should understand the idea of Monte Carlo mean estimation.

Convert policy iteration to be model-free

Policy iteration has two steps in each iteration:

$$\left\{ \begin{array}{l} \textbf{Policy evaluation: } v_{\pi_k} = r_{\pi_k} + \gamma P_{\pi_k} v_{\pi_k} \\ \textbf{Policy improvement: } \pi_{k+1} = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_{\pi_k}) \end{array} \right.$$

The elementwise form of the **policy improvement step** is:

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

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

Convert policy iteration to be model-free

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 calculate $q_{\pi_k}(s, a)$ based on *data (samples or experiences)*!

Convert policy iteration to be model-free

The procedure of Monte Carlo estimation of action values:

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

The MC Basic algorithm

▷ Description of the algorithm:

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

- **Step 1: policy evaluation.** This step is to obtain $q_{\pi_k}(s, a)$ for all (s, a) . Specifically, for each action-state pair (s, a) , run an infinite number of (or sufficiently many) episodes. The average of their returns is used to approximate $q_{\pi_k}(s, a)$.
- **Step 2: policy improvement.** This step is to solve $\pi_{k+1}(s) = \arg \max_{\pi} \sum_a \pi(a|s) q_{\pi_k}(s, a)$ for all $s \in \mathcal{S}$. The greedy optimal policy is $\pi_{k+1}(a_k^*|s) = 1$ where $a_k^* = \arg \max_a q_{\pi_k}(s, a)$.

Exactly the same as the policy iteration algorithm, except

- Estimate $q_{\pi_k}(s, a)$ directly, instead of solving $v_{\pi_k}(s)$.

The MC Basic algorithm

- ▷ Description of the algorithm:

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

Initialization: Initial guess π_0 .

Aim: Search for an optimal policy.

While the value estimate has not converged, for the k th iteration, 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 π_k

MC-based policy evaluation step:

$q_{\pi_k}(s, a) =$ average return of all the episodes starting from (s, a)

Policy improvement step:

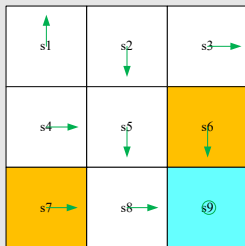
$a_k^*(s) = \arg \max_a q_{\pi_k}(s, a)$

$\pi_{k+1}(a|s) = 1$ if $a = a_k^*$, and $\pi_{k+1}(a|s) = 0$ otherwise

The MC Basic algorithm

- 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.

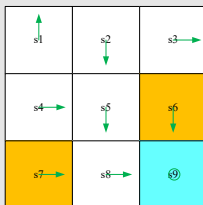
Illustrative example 1: step by step



Task:

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

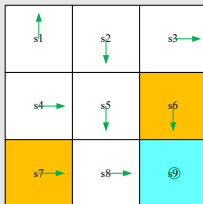
Illustrative example 1: step by step



Outline: given the current policy π_k

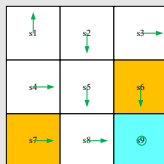
- Step 1 - policy evaluation: calculate $q_{\pi_k}(s, a)$
How many state-action pairs? 9 states \times 5 actions = 45 state-action pairs!
- Step 2 - policy improvement: select the greedy action
$$a^*(s) = \arg \max_{a_i} q_{\pi_k}(s, a)$$

Illustrative example 1: step by step



- ▷ Due to space limitation, we only show $q_{\pi_k}(s_1, a)$
- ▷ **Step 1 - policy evaluation:**
 - Since the current policy is deterministic, one episode would be sufficient to get the action value!
 - If the current policy is stochastic, an infinite number of episodes (or at least many) 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

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

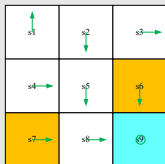
- Starting from (s_1, a_2) , the episode is $s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_3} \dots$. Hence, the action value is

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

- 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

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

Illustrative example 1: step by step



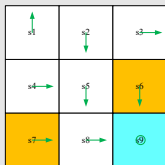
- Starting from (s_1, a_4) , the episode is $s_1 \xrightarrow{a_4} s_1 \xrightarrow{a_1} s_1 \xrightarrow{a_1} \dots$. Hence, the action value is

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

- 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

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

Illustrative example 1: step by step



▷ 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*.

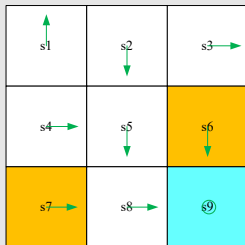
- As a result, the policy can be improved as

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

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

One iteration is sufficient for this simple example!

Illustrative example 1: step by step



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

Illustrative example 2: Episode length

Examine the impact of episode length:

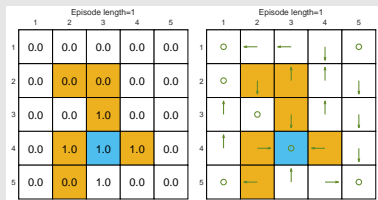
- We need sample episodes, but the length of an episode cannot be infinitely long.
- How long should be the episodes?

Example setup:

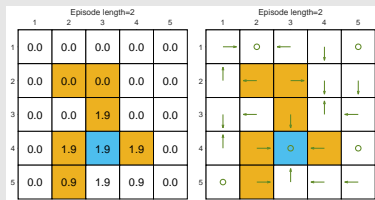
- 5-by-5 grid world
- Reward setting: $r_{\text{boundary}} = -1$, $r_{\text{forbidden}} = -10$, $r_{\text{target}} = 1$, $\gamma = 0.9$

Illustrative example 2: Episode length

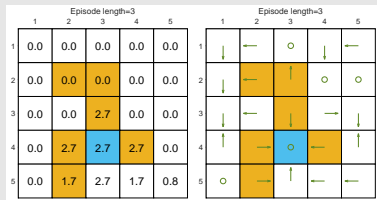
- ▷ Use MC Basic to search optimal policies with different episode lengths.



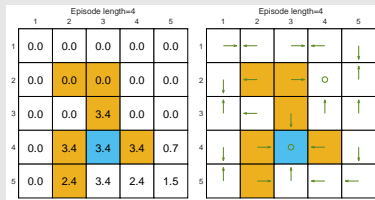
Estimated state value and policy with episode length=1



Estimated state value and policy with episode length=2

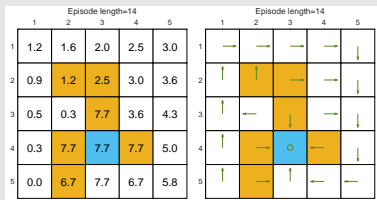


Estimated state value and policy with episode length=3

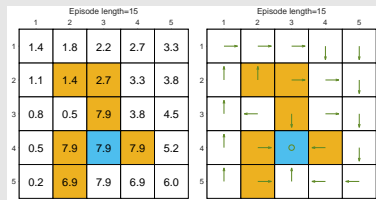


Estimated state value and policy with episode length=4

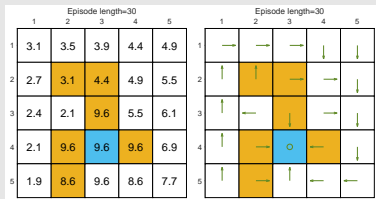
Illustrative example 2: Episode length



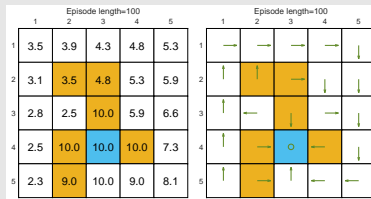
Estimated state value and policy with episode length=14



Estimated state value and policy with episode length=15

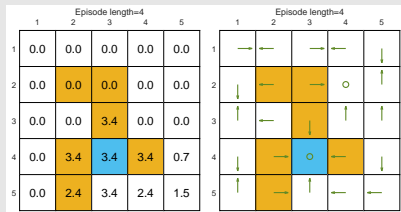


Estimated state value and policy with episode length=30



Estimated state value and policy with episode length=100

Illustrative example 2: Episode length



► Findings:

- When the episode length is short, only the states that are close to the target have nonzero state values.
- As the episode length increases, the states that are closer to the target have nonzero values earlier than those farther away.
- The episode length should be sufficiently long.
- The episode length does not have to be infinitely long.

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Use data more efficiently

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.

Use data more efficiently

- ▷ Consider a grid-world example, following a policy π , we can get an episode such as

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

- ▷ **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.

Use data more efficiently

- ▷ The episode also visits other state-action pairs.

$s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_4} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots$ [original episode]

$s_2 \xrightarrow{a_4} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots$ [episode starting from (s_2, a_4)]

$s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots$ [episode starting from (s_1, a_2)]

$s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots$ [episode starting from (s_2, a_3)]

$s_5 \xrightarrow{a_1} \dots$ [episode starting from (s_5, a_1)]

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

Data-efficient methods:

- first-visit method
- every-visit method

Update value estimate more efficiently

- ▷ 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.

Update value estimate more efficiently

- ▷ 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 model-based and model-free RL algorithms fall into this framework.

MC Exploring Starts

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

Pseudocode: MC Exploring Starts (a sample-efficient variant of MC Basic)

Initialization: Initial guess π_0 .

Aim: Search for an optimal policy.

For each episode, do

Episode generation: Randomly select a starting state-action pair (s_0, a_0) and ensure that all pairs can be possibly selected. Following the current policy, generate an episode of length T : $s_0, a_0, r_1, \dots, s_{T-1}, a_{T-1}, r_T$.

Policy evaluation and policy improvement:

Initialization: $g \leftarrow 0$

For each step of the episode, $t = T - 1, T - 2, \dots, 0$, do

$g \leftarrow \gamma g + r_{t+1}$

Use the first-visit method:

If (s_t, a_t) does not appear in $(s_0, a_0, s_1, a_1, \dots, s_{t-1}, a_{t-1})$, then

$Returns(s_t, a_t) \leftarrow Returns(s_t, a_t) + g$

$q(s_t, a_t) = \text{average}(Returns(s_t, a_t))$

$\pi(a|s_t) = 1$ if $a = \arg \max_a q(s_t, a)$

▷ What is exploring starts?

- Exploring starts means we need to generate sufficiently many episodes starting from *every* state-action pair.
- 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.

On the contrary, 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.

Therefore, there is a gap between theory and practice.

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

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- ▷ A policy is called *soft* if the probability to take any action is positive.
- ▷ Why introduce soft policies?
 - With a soft policy, a few episodes that are sufficiently long can visit every state-action pair for sufficiently many times.
 - 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 thus be removed.

ε -greedy policies

▷ What soft policies will we use? Answer: ε -greedy policies

- **What is an 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 .

- The chance to choose the greedy action is always greater than other actions, because $1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1) = 1 - \varepsilon + \frac{\varepsilon}{|\mathcal{A}(s)|} \geq \frac{\varepsilon}{|\mathcal{A}(s)|}$.
- **Why use ε -greedy?** Balance between **exploitation and exploration**
 - When $\varepsilon = 0$, it becomes greedy! Less exploration but more exploitation!
 - When $\varepsilon = 1$, it becomes a uniform distribution. More exploration but less exploitation.

MC ε -Greedy algorithm

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

MC ε -Greedy algorithm

▷ **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

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

- 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.

MC ϵ -Greedy algorithm

Pseudocode: MC ϵ -Greedy (a variant of MC Exploring Starts)

Initialization: Initial guess π_0 and the value of $\epsilon \in [0, 1]$

Aim: Search for an optimal policy.

For each episode, do

Episode generation: Randomly select a starting state-action pair (s_0, a_0) . Following the current policy, generate an episode of length T : $s_0, a_0, r_1, \dots, s_{T-1}, a_{T-1}, r_T$.

Policy evaluation and policy improvement:

Initialization: $g \leftarrow 0$

For each step of the episode, $t = T - 1, T - 2, \dots, 0$, do

$g \leftarrow \gamma g + r_{t+1}$

Use the every-visit method:

If (s_t, a_t) does not appear in $(s_0, a_0, s_1, a_1, \dots, s_{t-1}, a_{t-1})$, then

$Returns(s_t, a_t) \leftarrow Returns(s_t, a_t) + g$

$q(s_t, a_t) = \text{average}(Returns(s_t, a_t))$

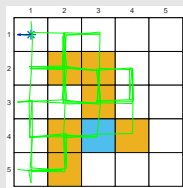
Let $a^* = \arg \max_a q(s_t, a)$ and

$$\pi(a|s_t) = \begin{cases} 1 - \frac{|\mathcal{A}(s_t)|-1}{|\mathcal{A}(s_t)|} \epsilon, & a = a^* \\ \frac{1}{|\mathcal{A}(s_t)|} \epsilon, & a \neq a^* \end{cases}$$

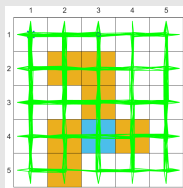
Exploration ability

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

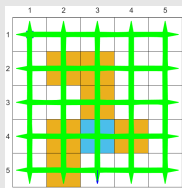
When $\varepsilon = 1$, the policy (uniform distribution) has the strongest exploration ability.



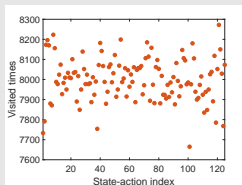
(a) 100 steps



(b) 1000 steps



(c) 10000 steps



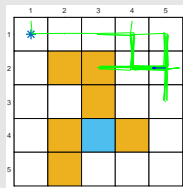
(d)

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

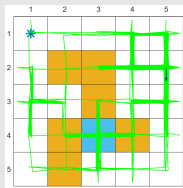
Exploration ability

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

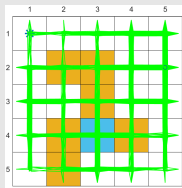
When ε is small, the exploration ability of the policy is also small.



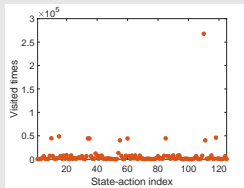
(a) 100 steps



(b) 1000 steps



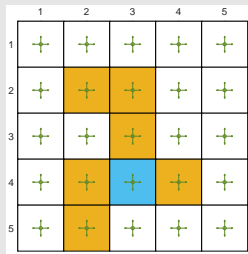
(c) 10000 steps



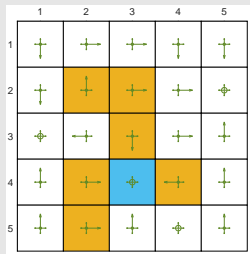
(d)

Estimate based on one episode

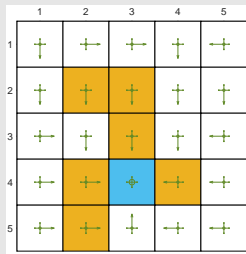
- ▷ Run the MC ϵ -Greedy algorithm as follows. In every iteration:
 - In the episode generation step, use the previous policy generates an episode of 1 million steps!
 - In the rest steps, use the single episode to update the policy.
 - Two iterations can lead to the optimal ϵ -greedy policy.



(a) Initial policy



(b) After the first iteration



(c) After the second iteration

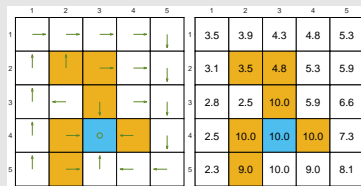
Here, $r_{\text{boundary}} = -1$, $r_{\text{forbidden}} = -10$, $r_{\text{target}} = 1$, $\gamma = 0.9$

Optimality vs exploration

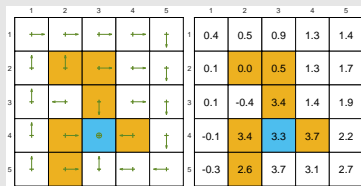
- ▷ Compared to greedy policies,
 - The **advantage** of ε -greedy policies is that they have stronger exploration ability so that the exploring starts condition is not required.
 - The **disadvantage** is that ε -greedy policies are **not optimal** in general (we can only show that there always exist greedy policies that are optimal).
 - The final policy given by the MC ε -Greedy algorithm is only optimal in the set Π_ε of all ε -greedy policies.
 - ε cannot be too large.
- ▷ Next, we use examples to demonstrate. The setup is $r_{\text{boundary}} = -1$, $r_{\text{forbidden}} = -10$, $r_{\text{target}} = 1$, $\gamma = 0.9$

Optimality

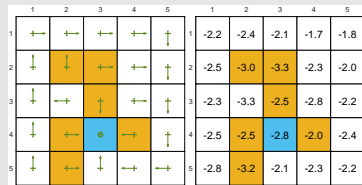
▷ Given an ε -greedy policy, what is its state value?



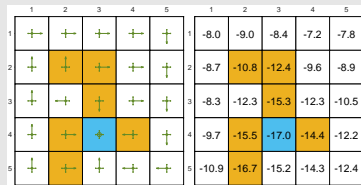
$\varepsilon = 0$



$\varepsilon = 0.1$



$\varepsilon = 0.2$



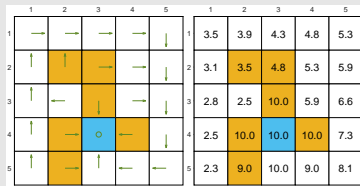
$\varepsilon = 0.5$

▷ When ε increases, the optimality of the policy becomes worse!

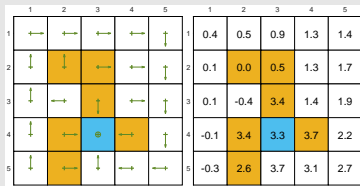
▷ Why is the state value of the target state negative?

Consistency

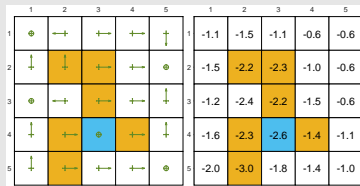
▷ Find the optimal ϵ -greedy policies and their state values?



$\epsilon = 0$



$\epsilon = 0.1$



$\epsilon = 0.2$



$\epsilon = 0.5$

▷ The optimal ϵ -greedy policies are not *consistent* with the greedy optimal one! Why is that? Consider the target for example.

Summary

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 ϵ -greedy policies