

# 概念

state: 状态

state transition: 状态改变, 可以是确定性的, 也可以是不确定性的

s1	s2	s3
s4	s5	s6
s7	s8	s9

Tabular representation: We can use a table to describe the state transition:

	$a_1$ (upwards)	$a_2$ (rightwards)	$a_3$ (downwards)	$a_4$ (leftwards)	$a_5$ (unchanged)
$s_1$	$s_1$	$s_2$	$s_4$	$s_1$	$s_1$
$s_2$	$s_2$	$s_3$	$s_5$	$s_1$	$s_2$
$s_3$	$s_3$	$s_3$	$s_6$	$s_2$	$s_3$
$s_4$	$s_1$	$s_5$	$s_7$	$s_4$	$s_4$
$s_5$	$s_2$	$s_6$	$s_8$	$s_4$	$s_5$
$s_6$	$s_3$	$s_6$	$s_9$	$s_5$	$s_6$
$s_7$	$s_4$	$s_8$	$s_7$	$s_7$	$s_7$
$s_8$	$s_5$	$s_9$	$s_8$	$s_7$	$s_8$
$s_9$	$s_6$	$s_9$	$s_9$	$s_8$	$s_9$

$$p(s_2 | s_1, a_2) = 1$$
$$p(s_i | s_1, a_2) = 0 \quad \forall i \neq 2$$

action: 某状态采取的动作, 可以用条件概率表示

policy:  $\pi$ :策略

确定性概率:

$$\pi(a_1 | s_1) = 0$$
$$\pi(a_2 | s_1) = 1$$
$$\pi(a_3 | s_1) = 0$$
$$\pi(a_4 | s_1) = 0$$
$$\pi(a_5 | s_1) = 0$$

不确定性: 同样是概率

reward: 当前状态采取动作对应的奖励/惩罚

s1	s2	s3
s4	s5	s6
s7	s8	s9

**Tabular representation of *reward transition*:** how to use the table?

	$a_1$ (upwards)	$a_2$ (rightwards)	$a_3$ (downwards)	$a_4$ (leftwards)	$a_5$ (unchanged)
$s_1$	$r_{\text{bound}}$	0	0	$r_{\text{bound}}$	0
$s_2$	$r_{\text{bound}}$	0	0	0	0
$s_3$	$r_{\text{bound}}$	$r_{\text{bound}}$	$r_{\text{forbid}}$	0	0
$s_4$	0	0	$r_{\text{forbid}}$	$r_{\text{bound}}$	0
$s_5$	0	$r_{\text{forbid}}$	0	0	0
$s_6$	0	$r_{\text{bound}}$	$r_{\text{target}}$	0	$r_{\text{forbid}}$
$s_7$	0	0	$r_{\text{bound}}$	$r_{\text{bound}}$	$r_{\text{forbid}}$
$s_8$	0	$r_{\text{target}}$	$r_{\text{bound}}$	$r_{\text{forbid}}$	0
$s_9$	$r_{\text{forbid}}$	$r_{\text{bound}}$	$r_{\text{bound}}$	0	$r_{\text{target}}$

return: 评价策略好坏, reward总和

discounted return:

1. 防止未来return发散,  $1+1+1+1+1+1\dots$
2. 平衡现在和未来得到的reward
3. 关于 $\gamma$ : 折扣率,  $\in [0,1)$
4. 接近1, 远视; 接近0, 近视

episode: 有限步的一次trial, 存在terminal state

continuing tasks: 没有terminal state, 一直交互

统一方法: 将episode转化为continuing,

- 无论什么action都会回到当前状态, 或者只有留在原地的action, reward=0
- 设置成普通的状态, reward>0/ <0后续可能会跳出来, 更一般

## MDP

马尔可夫决策过程

马尔可夫性质: 和历史无关, 状态转移概率和奖励概率都和历史无关

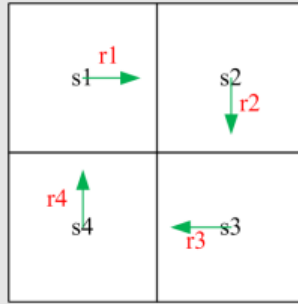
## 贝尔曼公式

state value

贝尔曼公式

## examples

While return is important, how to calculate it?



$$v_1 = r_1 + \gamma(r_2 + \gamma r_3 + \dots) = r_1 + \gamma v_2$$

$$v_2 = r_2 + \gamma(r_3 + \gamma r_4 + \dots) = r_2 + \gamma v_3$$

$$v_3 = r_3 + \gamma(r_4 + \gamma r_1 + \dots) = r_3 + \gamma v_4$$

$$v_4 = r_4 + \gamma(r_1 + \gamma r_2 + \dots) = r_4 + \gamma v_1$$

$v_i$ 表示从某个状态开始计算的return

**The returns rely on each other. Bootstrapping!**

$$\underbrace{\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}}_{\mathbf{v}} = \underbrace{\begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}}_{\mathbf{r}} + \underbrace{\begin{bmatrix} \gamma v_2 \\ \gamma v_3 \\ \gamma v_4 \\ \gamma v_1 \end{bmatrix}}_{\gamma \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}}_{\mathbf{P}} \underbrace{\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}}_{\mathbf{v}}$$

$$\mathbf{v} = \mathbf{r} + \gamma \mathbf{P} \mathbf{v}$$

This is the Bellman equation (for this specific deterministic problem)!!

- Though simple, it demonstrates the core idea: **the value of one state relies on the values of other states.**
- A matrix-vector form is more clear to see how to solve the **state values**

## state value

Consider the following single-step process:

$$S_t \xrightarrow{A_t} R_{t+1}, S_{t+1}$$

- $t, t + 1$ : discrete time instances
- $S_t$ : state at time  $t$
- $A_t$ : the action taken at state  $S_t$
- $R_{t+1}$ : the reward obtained after taking  $A_t$
- $S_{t+1}$ : the state transited to after taking  $A_t$

Note that  $S_t, A_t, R_{t+1}$  are all *random variables*.

This step is governed by the following probability distributions:

- $S_t \rightarrow A_t$  is governed by  $\pi(A_t = a | S_t = s)$
- $S_t, A_t \rightarrow R_{t+1}$  is governed by  $p(R_{t+1} = r | S_t = s, A_t = a)$
- $S_t, A_t \rightarrow S_{t+1}$  is governed by  $p(S_{t+1} = s' | S_t = s, A_t = a)$

At this moment, we assume we know the model (i.e., the probability distributions)!

discounted return is

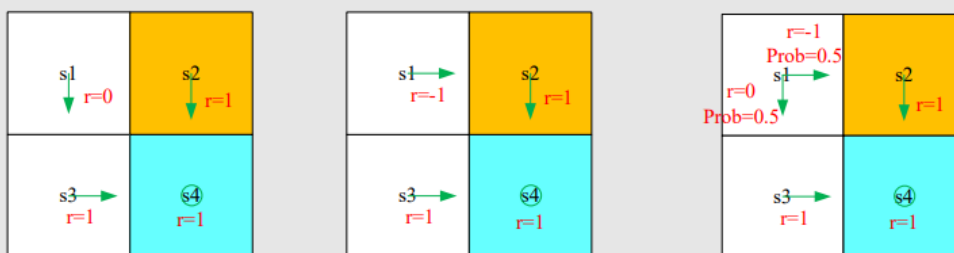
$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots$$

The **expectation** (or called **expected value or mean**) of  $G_t$  is defined as the state-value function or simply state value:

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

是关于s的函数，衡量当前状态价值高低，越大说明当前状态价值越高

Example:



Recall the returns obtained from  $s_1$  for the three examples:

$$v_{\pi_1}(s_1) = 0 + \gamma 1 + \gamma^2 1 + \dots = \gamma(1 + \gamma + \gamma^2 + \dots) = \frac{\gamma}{1 - \gamma}$$

$$v_{\pi_2}(s_1) = -1 + \gamma 1 + \gamma^2 1 + \dots = -1 + \gamma(1 + \gamma + \gamma^2 + \dots) = -1 + \frac{\gamma}{1 - \gamma}$$

$$v_{\pi_3}(s_1) = 0.5 \left( -1 + \frac{\gamma}{1 - \gamma} \right) + 0.5 \left( \frac{\gamma}{1 - \gamma} \right) = -0.5 + \frac{\gamma}{1 - \gamma}$$

期望计算

## 公式推导

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$$\begin{aligned} v_{\pi}(s) &= \mathbb{E}[R_{t+1} \mid S_t = s] + \gamma \mathbb{E}[G_{t+1} \mid S_t = s], \\ &= \underbrace{\sum_a \pi(a \mid s) \sum_r p(r \mid s, a) r}_{\text{mean of immediate rewards}} + \underbrace{\gamma \sum_a \pi(a \mid s) \sum_{s'} p(s' \mid s, a) v_{\pi}(s')}_{\text{mean of future rewards}}, \\ &= \sum_a \pi(a \mid s) [\sum_r p(r \mid s, a) r + \gamma \sum_{s'} p(s' \mid s, a) v_{\pi}(s')], \quad \forall s \in \mathcal{S} \end{aligned}$$

## Matrix vector

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## Solve the state values

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Given a policy, finding out the corresponding state values is called **policy evaluation!**

It is a fundamental problem in RL. It is the foundation to find better policies

- closed-form solution
- iterative solution

不同的策略可以得到相同的state value

通过state value可以评价策略好坏

## Action value

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选择action value大的值的action更新

state value呢?

计算action value:

- 先求state value, 再根据公式计算action value
- 直接计算action value

## 贝尔曼最优公式

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贝尔曼公式的特殊情况

- Core concepts: optimal state value and optimal policy
- A fundamental tool: the Bellman optimality equation (BOE)

## EXAMPLE

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更新: 选择action value最大的action

最优策略: 每次都选择action value最大的action

原因: 贝尔曼最优公式

What if we select the greatest action value? Then, **a new policy is obtained:**

$$\pi_{\text{new}}(a | s_1) = \begin{cases} 1 & a = a^* \\ 0 & a \neq a^* \end{cases}$$

where  $a^* = \arg \max_a q_\pi(s_1, a) = a_3$ .

## Definition

最优策略: A policy  $\pi^*$  is optimal if  $v_{\pi^*}(s) \geq v_\pi(s)$  for all  $s$  and for any other policy  $\pi$ .

The definition leads to many questions:

- Does the optimal policy exist? (所有状态state value都大于其他策略, 可能过于理想而不存在)
- Is the optimal policy unique? (是否存在多个最优策略)
- Is the optimal policy stochastic or deterministic? (该策略是确定性还是非确定性)
- How to obtain the optimal policy? (怎么得到)

To answer these questions, we study the Bellman optimality equation.

## BOE

$$\begin{aligned} v(s) &= \max_{\pi} \sum_a \pi(a | s) \left( \sum_r p(r | s, a) r + \gamma \sum_{s'} p(s' | s, a) v(s') \right), \quad \forall s \in \mathcal{S} \\ &= \max_{\pi} \sum_a \pi(a | s) q(s, a) \quad s \in \mathcal{S} \end{aligned}$$

若要max, 实际是对应最大的  $q(s, a)$

**Inspired by the above example**, considering that  $\sum_a \pi(a | s) = 1$ , we have

$$\max_{\pi} \sum_a \pi(a | s) q(s, a) = \max_{a \in \mathcal{A}(s)} q(s, a)$$

where the optimality is achieved when

$$\pi(a | s) = \begin{cases} 1 & a = a^* \\ 0 & a \neq a^* \end{cases}$$

where  $a^* = \arg \max_a q(s, a)$ .

与example处的结果一致

## Solve the optimality equation

固定 $v$ , 求解  $\pi$

实际问题:  $v = f(v)$

how to solve the equation?

## Contraction mapping theorem

Fixed point (不动点):  $x \in X$  is a fixed point of  $f: X \rightarrow X$  if

$$f(x) = x$$

Contraction **mapping** (or contractive **function**):  $f$  is a contraction mapping if

$$\|f(x_1) - f(x_2)\| \leq \gamma \|x_1 - x_2\|$$

where  $\gamma \in (0, 1)$ .

contraction function在求解 $x = f(x)$ 有三点性质

- Existence: there exists a fixed point  $x^*$  satisfying  $f(x^*) = x^*$ .
- Uniqueness: The fixed point  $x^*$  is unique.
- **Algorithm:** Consider a sequence  $\{x_k\}$  where  $x_{k+1} = f(x_k)$ , then  $x_k \rightarrow x^*$  as  $k \rightarrow \infty$ . Moreover, the convergence rate is exponentially fast. (利用迭代计算出 $x_k$ , when  $k \rightarrow \infty$ )

## solve

对于贝尔曼最优问题，其方程为 contractive function

(证明：满足  $\|f(x_1) - f(x_2)\| \leq \gamma \|x_1 - x_2\|$  即可，此处省略证明)

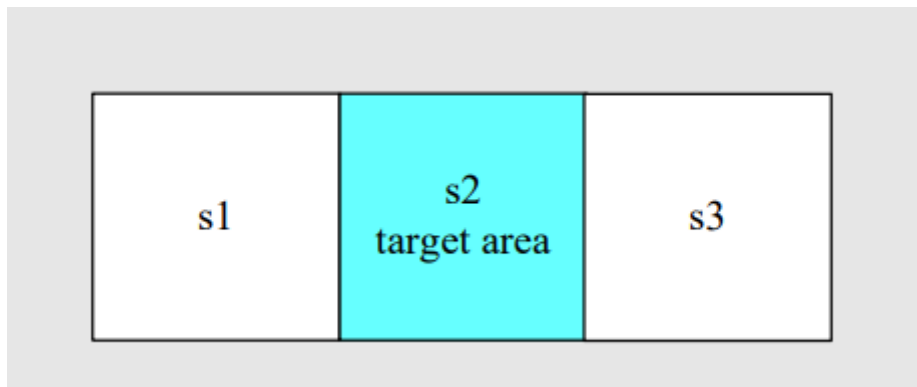
绕路：得到目标奖励越晚！和 $r$ 等于多少有关，但同时也受到  $\gamma$  的约束

因此求解：

$$\begin{aligned} v_{k+1}(s) &= \max_{\pi} \sum_a \pi(a | s) \left( \sum_r p(r | s, a) r + \gamma \sum_{s'} p(s' | s, a) v_k(s') \right) \\ &= \max_{\pi} \sum_a \pi(a | s) q_k(s, a) \\ &= \max_a q_k(s, a) \end{aligned}$$

设立初始的 $v_k$ ，不断迭代得到 $v_{k+1}$ 即可

## Example



The values of  $q(s, a)$

q-value table	$a_l$	$a_0$	$a_r$
$s_1$	$-1 + \gamma v(s_1)$	$0 + \gamma v(s_1)$	$1 + \gamma v(s_2)$
$s_2$	$0 + \gamma v(s_1)$	$1 + \gamma v(s_2)$	$0 + \gamma v(s_3)$
$s_3$	$1 + \gamma v(s_2)$	$0 + \gamma v(s_3)$	$-1 + \gamma v(s_3)$

Consider  $\gamma=0.9$  以及下面的初始条件

Our objective is to find  $v^*(s_i)$  and  $\pi^*k = 0$  :

v-value: select  $v_0(s_1) = v_0(s_2) = v_0(s_3) = 0$

q-value (using the previous table): \_\_\_\_\_

	$a_\ell$	$a_0$	$a_r$
$s_1$	-1	0	1
$s_2$	0	1	0
$s_3$	1	0	-1

关于policy: 采取greedy policy, select the greatest q-value

$$\pi(a_r | s_1) = 1, \quad \pi(a_0 | s_2) = 1, \quad \pi(a_\ell | s_3) = 1$$

v-value:  $v_1(s) = \max_a q_0(s, a)$

$$v_1(s_1) = v_1(s_2) = v_1(s_3) = 1$$

**This this policy good? Yes!**

但是注意, 此时虽然policy是最好的, 但是state value没有到最优!!! 因为此时k=1, 而对应的state value 要到无穷, 实际不用到无穷, 只需  $|v_{k+1} - v_k| < \sigma$ , 因此接下来的iteration, k=1

	$a_\ell$	$a_0$	$a_r$
$s_1$	-0.1	0.9	1.9
$s_2$	0.9	1.9	0.9
$s_3$	1.9	0.9	-0.1

然后Greedy policy (select the greatest q-value):

$$\pi(a_r | s_1) = 1, \quad \pi(a_0 | s_2) = 1, \quad \pi(a_\ell | s_3) = 1$$

k = 2, 3, ...

## Policy optimality

**回答上述的问题**

Suppose that  $v^*$  is the unique solution to  $v = \max_\pi (r_\pi + \gamma P_\pi v)$ , and  $v_\pi$  is the state value function satisfying  $v_\pi = r_\pi + \gamma P_\pi v_\pi$  for any given policy  $\pi$ , then

$$v^* \geq v_\pi, \quad \forall \pi$$

即最优的policy, **对应的state value大于每个地方的state value**

同时, 最优的policy怎么求? 贪心规则

For any  $s \in \mathcal{S}$ , the deterministic **greedy policy**

$$\pi^*(a | s) = \begin{cases} 1 & a = a^*(s) \\ 0 & a \neq a^*(s) \end{cases}$$

is an optimal policy solving the BOE. Here,

$$a^*(s) = \arg \max_a q^*(a, s),$$

where  $q^*(s, a) := \sum_r p(r | s, a)r + \gamma \sum_{s'} p(s' | s, a)v^*(s')$ .

## Analyzing optimal policies

即一些有趣的情况



比如  $\gamma$  较大时, 会比较远视, 当  $\gamma$  较小时, policy 会比较近视

且当 reward 线性变化时, 对应的最优 policy 不会变化

# Value Iteration & Policy Iteration

model-based

## Value iteration

### 原理

即贝尔曼最优公式的迭代求解法

start from  $v_0$

#### step1: Policy update (PU)

已知  $v_k$ , 求出 q-table, 然后找到最大的策略  $\pi_{k+1}$ , 然后更新

$$\pi_{k+1} = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_k)$$

#### step2: value update (VU)

将上面的  $\pi_{k+1}$  代入求解  $v_{k+1}$

$$v_{k+1} = r_{\pi_{k+1}} + \gamma P_{\pi_{k+1}} v_k$$

$v_k$  is not a state value, just a value

### 实践算法

#### Pseudocode: Value iteration algorithm

**Initialization:** The probability model  $p(r|s, a)$  and  $p(s'|s, a)$  for all  $(s, a)$  are known. Initial guess  $v_0$ .

**Aim:** Search the optimal state value and an optimal policy solving the Bellman optimality equation.

While  $v_k$  has not converged in the sense that  $\|v_k - v_{k-1}\|$  is greater than a predefined small threshold, for the  $k$ th iteration, do

For every state  $s \in \mathcal{S}$ , do

For every action  $a \in \mathcal{A}(s)$ , do

$$\text{q-value: } q_k(s, a) = \sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a)v_k(s')$$

$$\text{Maximum action value: } a_k^*(s) = \arg \max_a q_k(a, s)$$

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

$$\text{Value update: } v_{k+1}(s) = \max_a q_k(a, s)$$

# Policy iteration

## 原理

start from  $\pi_0$

### step1: policy evaluation (PE)

计算state value, 因为state value实际上表征的就是策略的好坏

已知  $\pi_k$ , 求  $v_{\pi_k}$

NOTE: 此处有两种计算方法, 一种是直接计算, 一种是迭代计算

$$v_{\pi_k} = r_{\pi_k} + \gamma P_{\pi_k} v_{\pi_k}$$

### step2: policy improvement (PI)

update policy, 用greedy算法得到  $\pi_{k+1}$

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

policy iteration 和value iteration的关系

- 证明policy iteration算法收敛时, 用到value iteration收敛的结果
- 是 iteration的极端

▷ Q2: In the policy improvement step, why is the new policy  $\pi_{k+1}$  better than  $\pi_k$ ?

- Lemma (Policy Improvement)

If  $\pi_{k+1} = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_{\pi_k})$ , then  $v_{\pi_{k+1}} \geq v_{\pi_k}$  for any  $k$ .

## 实践编程算法

## Pseudocode: Policy iteration algorithm

**Initialization:** The probability model  $p(r|s, a)$  and  $p(s'|s, a)$  for all  $(s, a)$  are known. Initial guess  $\pi_0$ .

**Aim:** Search for the optimal state value and an optimal policy.

While the policy has not converged, for the  $k$ th iteration, do

*Policy evaluation:*

Initialization: an arbitrary initial guess  $v_{\pi_k}^{(0)}$

While  $v_{\pi_k}^{(j)}$  has not converged, for the  $j$ th iteration, do

For every state  $s \in \mathcal{S}$ , do

$$v_{\pi_k}^{(j+1)}(s) = \sum_a \pi_k(a|s) \left[ \sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a)v_{\pi_k}^{(j)}(s') \right]$$

*Policy improvement:*

For every state  $s \in \mathcal{S}$ , do

For every action  $a \in \mathcal{A}(s)$ , do

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

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

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

**靠近目标的策略会先变好，远离目标的策略会后变好**

原因：greedy action，当靠近目标时，target是最greedy的，而greedy则依靠周围的情况，如果周围乱七八糟，得到的策略也不一定是最好的

## Truncated policy iteration

上述两个算法的一般化！

	Policy iteration algorithm	Value iteration algorithm	Comments
1) Policy:	$\pi_0$	N/A	
2) Value:	$v_{\pi_0} = r_{\pi_0} + \gamma P_{\pi_0} v_{\pi_0}$	$v_0 := v_{\pi_0}$	
3) Policy:	$\pi_1 = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_{\pi_0})$	$\pi_1 = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_0)$	The two policies are the same
4) Value:	$v_{\pi_1} = r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}$	$v_1 = r_{\pi_1} + \gamma P_{\pi_1} v_0$	$v_{\pi_1} \geq v_1$ since $v_{\pi_1} \geq v_{\pi_0}$
5) Policy:	$\pi_2 = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_{\pi_1})$	$\pi'_2 = \arg \max_{\pi} (r_{\pi} + \gamma P_{\pi} v_1)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Consider the step of solving  $v_{\pi_1} = r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}$  :

$$\begin{aligned}
v_{\pi_1}^{(0)} &= v_0 \\
\text{value iteration} \leftarrow v_1 &\leftarrow v_{\pi_1}^{(1)} = r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}^{(0)} \\
v_{\pi_1}^{(2)} &= r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}^{(1)} \\
&\vdots \\
\text{truncated policy iteration} \leftarrow \bar{v}_1 &\leftarrow v_{\pi_1}^{(j)} = r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}^{(j-1)} \\
&\vdots \\
\text{policy iteration} \leftarrow v_{\pi_1} &\leftarrow v_{\pi_1}^{(\infty)} = r_{\pi_1} + \gamma P_{\pi_1} v_{\pi_1}^{(\infty)}
\end{aligned}$$

- The **value** iteration algorithm computes **once**.
- The **policy** iteration algorithm computes an **infinite number of iterations**.
- The **truncated** policy iteration algorithm computes a **finite number of iterations** (say  $j$ ). The rest iterations from  $j$  to  $\infty$  are **truncated**.

#### Pseudocode: Truncated policy iteration algorithm

**Initialization:** The probability model  $p(r|s, a)$  and  $p(s'|s, a)$  for all  $(s, a)$  are known. Initial guess  $\pi_0$ .

**Aim:** Search for the optimal state value and an optimal policy.

While the policy has not converged, for the  $k$ th iteration, do

*Policy evaluation:*

Initialization: select the initial guess as  $v_k^{(0)} = v_{k-1}$ . The maximum iteration is set to be  $j_{\text{truncate}}$ .

While  $j < j_{\text{truncate}}$ , do

For every state  $s \in \mathcal{S}$ , do

$$v_k^{(j+1)}(s) = \sum_a \pi_k(a|s) \left[ \sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a) v_k^{(j)}(s') \right]$$

Set  $v_k = v_k^{(j_{\text{truncate}})}$

*Policy improvement:*

For every state  $s \in \mathcal{S}$ , do

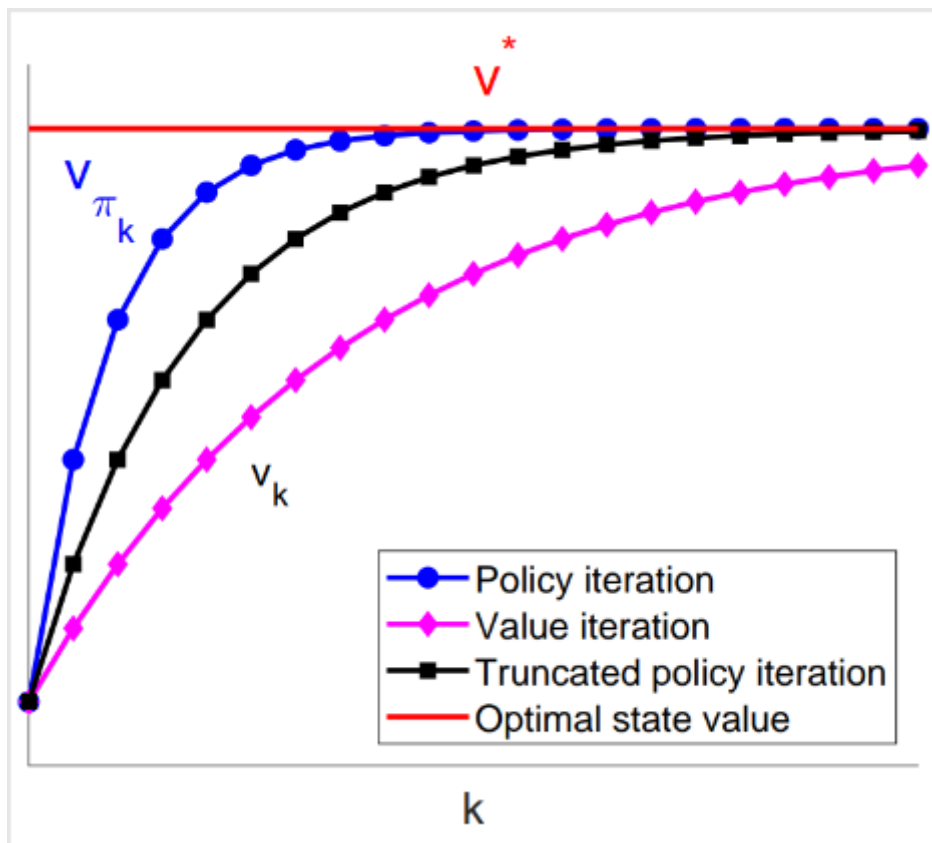
For every action  $a \in \mathcal{A}(s)$ , do

$$q_k(s, a) = \sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a) v_k(s')$$

$$a_k^*(s) = \arg \max_a q_k(s, a)$$

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

limited times



# Monte Carlo Learning

**Model Free** -> monte carlo estimation

**Core: policy iteration -> model-free**

## Example

许多次采样！通过平均值来代替期望！数据理论支持：大数定理！

大量实验来近似！为什么蒙特卡罗？因为没有模型，只能实验

**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!**

## MC Basic

**model-free**最大区别的点在于PI中的计算action value

**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:

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

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

## 计算action value

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

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

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

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

## 具体Policy iteration

### step1: policy evaluation

在求解state value时，用期望代替原本用模型求解的答案

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  $q_{\pi_k}(s, a)$ .

### step2: policy improvement

NOTE:

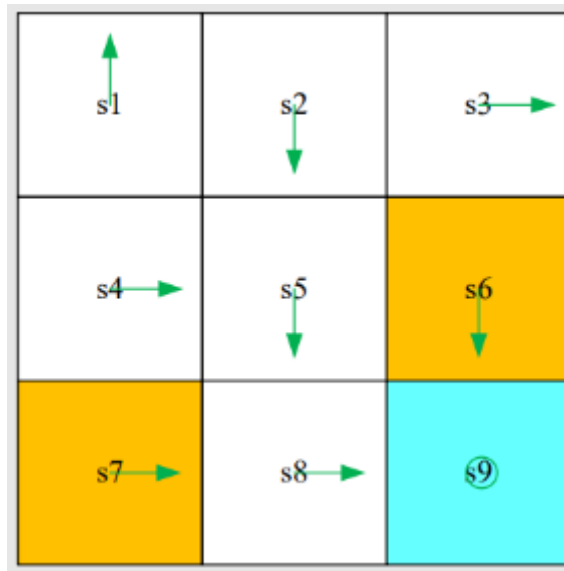
- **useful to reveal the core idea, not practical due to low efficiency**
- **直接估计action value! 而不是估计state value**

still is convergent

注意：此处的action value是估计的！

## Example1

episode lenth!



Task:

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

与model-based区别在哪? 不能直接用公式

Step1: 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!** (统计计算期望!)
- 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

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

Step2: 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!

## Example2

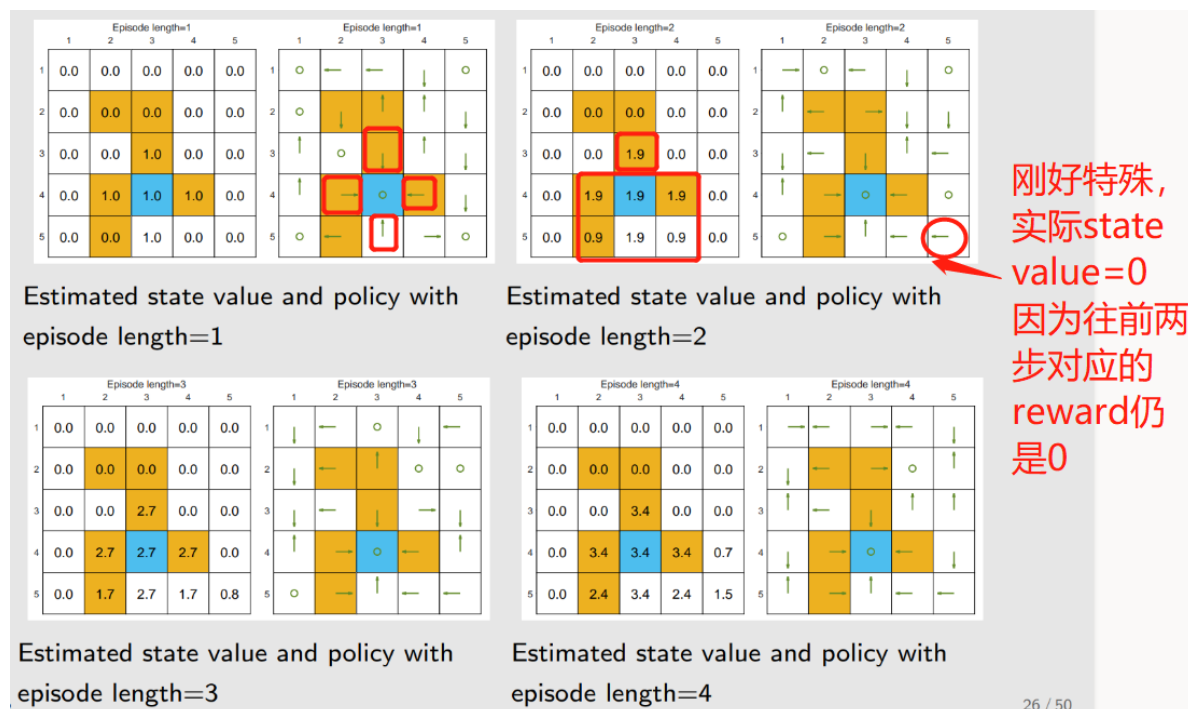
### the impact of episode length

所谓episode length, 可以理解为探索长度

length=1  $\rightarrow q_{\pi_0}(s_1, a_1) = -1$

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

且是从target处开始逆向优化!!



注意上面非0的state value, 对应为最优的策略

### Conclusion:

- The episode length should be sufficiently long.
- The episode length does not have to be infinitely long.

## MC Exploring Start

### MC Basic的推广

如何更新? 引入Visit!

### MC Basic: Initial visit

Exploring: 在计算一次episode时, 其同时访问了其他的state-action pairs, 因此可以计算其他的action value, 提高效率



▷ The episode also visits other state-action pairs.

$$\begin{aligned} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_4} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots & \text{ [original episode]} \\ s_2 \xrightarrow{a_4} s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots & \text{ [episode starting from } (s_2, a_4)] \\ s_1 \xrightarrow{a_2} s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots & \text{ [episode starting from } (s_1, a_2)] \\ s_2 \xrightarrow{a_3} s_5 \xrightarrow{a_1} \dots & \text{ [episode starting from } (s_2, a_3)] \\ s_5 \xrightarrow{a_1} \dots & \text{ [episode starting from } (s_5, a_1)] \end{aligned}$$

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**: 只用第一次出现的进行估计!
- **every-visit method**: 后面出现的都可以利用来估计!

**When to update the policy**

- first method: 把**所有episode**的return收集后再开始估计, 然后改进
- second method: 得到**一个episode**的return就开始估计, 直接改进, 得到一个改进一个 (最后仍会收敛)

## GPI

**GPI: generalized policy iteration**

- 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.
- 不需要十分精确估计! 但最后仍能收敛

**Exploring的缺点: 每一个state action pair都要有一个episode, 以防漏掉**

如何解决? 看下面!

## MC $\xi$ -Greedy

为什么要探索? 不是按照贪心就可以得到最优策略吗?

为什么用这个策略? **不需要exploring starts**

Soft policy: A policy is called soft if **the probability to take any action is positive**.

此处的soft policy:  $\xi$ -Greedy

原因: episode够长, 只要用1个或几个就可以覆盖其他所有state action pair

## Definition

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

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

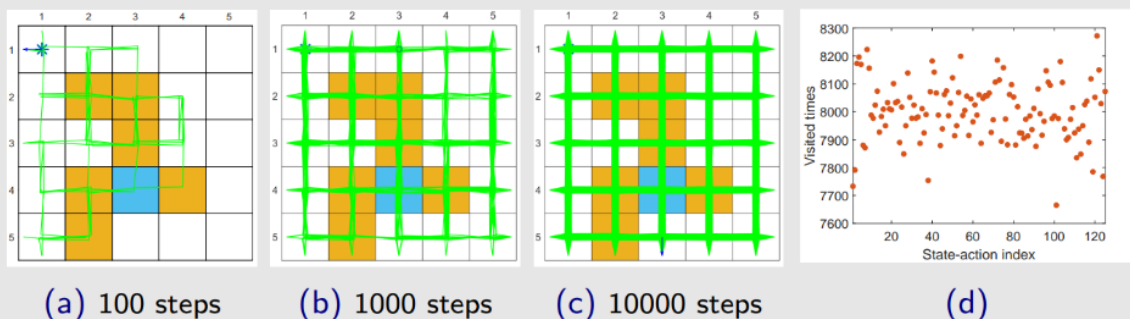
$$1 - \frac{\varepsilon}{|\mathcal{A}(s)|} (|\mathcal{A}(s)| - 1) = 1 - \varepsilon + \frac{\varepsilon}{|\mathcal{A}(s)|} \geq \frac{\varepsilon}{|\mathcal{A}(s)|}$$

- Why use  $\varepsilon$  - greedy? **Balance** between **exploitation and exploration!!!** (充分利用和探索性)
- When  $\varepsilon=0$ , it becomes **greedy!** Less exploration but more exploitation!
- When  $\varepsilon=1$ , it becomes a **uniform distribution (均匀分布)**. More exploration but less exploitation.

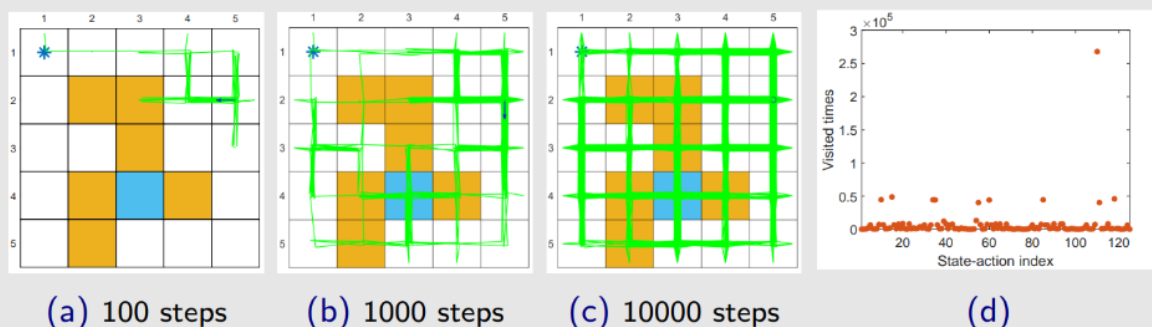
在选择数据时, 我们利用every visit, 因为action pair可能会被访问很多次, 如果用first visit, 则会导致数据浪费

## Example

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



When  $\varepsilon$  is small, the exploration ability of the policy is also small.



## Conclusion

- The advantage of  $\varepsilon$ -greedy policies is that they have stronger exploration ability so that the exploring starts condition is not required.

- The disadvantage is that  $\varepsilon - greedy$  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  $\varepsilon - Greedy$  algorithm is only optimal in the set  $\Pi_\varepsilon$  of all  $\varepsilon - greedy$  policies.
- $\varepsilon$  **cannot be too large**.
- 当  $\varepsilon$  为0.1或很小时，得到的policy与greedy policy一致，当变大时，得到的最终的policy与greedy有出入

# Stochastic Approximation

## Mean estimation Example

how to calculate the mean

- **The first way**, which is trivial, is to **collect all the samples** then calculate the average.
- **The second way** can avoid this drawback because it calculates the average in an **incremental** and **iterative** manner.

We can use

$$w_{k+1} = w_k - \frac{1}{k}(w_k - x_k).$$

to calculate the mean  $\bar{x}$  incrementally:(上述公式可推导)

$$\begin{aligned} w_1 &= x_1 \\ w_2 &= w_1 - \frac{1}{1}(w_1 - x_1) = x_1 \\ w_3 &= w_2 - \frac{1}{2}(w_2 - x_2) = x_1 - \frac{1}{2}(x_1 - x_2) = \frac{1}{2}(x_1 + x_2) \\ w_4 &= w_3 - \frac{1}{3}(w_3 - x_3) = \frac{1}{3}(x_1 + x_2 + x_3) \\ &\vdots \\ w_{k+1} &= \frac{1}{k} \sum_{i=1}^k x_i \end{aligned}$$

将  $\frac{1}{k}$  替换成  $\alpha_k$ ，即为对应的a special **SA algorithm** and also a **special stochastic gradient descent algorithm**

## Robbins-Monro algorithm

### Description

**Stochastic approximation (SA):**

- SA is powerful in the sense that it **does not require to know the expression of the objective function nor its derivative**.

**Robbins-Monro (RM) algorithm:**

- There is a pioneering work in the field of **stochastic approximation**.
- The famous **stochastic gradient descent** algorithm is a special form of the RM algorithm. (SGD)
- It can be used to analyze the **mean estimation algorithms** introduced in the beginning.

用于求解  $g(w) = 0$  的解

The Robbins-Monro (RM) algorithm can solve this problem:

$$w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k), \quad k = 1, 2, 3, \dots$$

where

- $w_k$  is the  $k$  th estimate of the **root**
- $\tilde{g}(w_k, \eta_k) = g(w_k) + \eta_k$  is the  $k$ th **noisy observation**
- $a_k$  is a **positive** coefficient. ( $a_k > 0$ )  
The function  $g(w)$  is a **black box!** This algorithm **relies on data**:
- Input sequence:  $\{w_k\}$
- Noisy output sequence:  $\{\tilde{g}(w_k, \eta_k)\}$   
Philosophy: without model, we need data!
- Here, the model refers to the expression of the function.

## Example

Excise: manually solve  $g(w) = w - 10$  using the RM algorithm.

Set:  $w_1 = 20, a_k \equiv 0.5, \eta_k = 0$  (i.e., no observation error)

$$\begin{aligned} w_1 &= 20 \implies g(w_1) = 10 \\ w_2 &= w_1 - a_1 g(w_1) = 20 - 0.5 * 10 = 15 \implies g(w_2) = 5 \\ w_3 &= w_2 - a_2 g(w_2) = 15 - 0.5 * 5 = 12.5 \implies g(w_3) = 2.5 \\ &\vdots \\ w_k &\rightarrow 10 \end{aligned}$$

## Convergence analysis

A rigorous convergence result is given below

Theorem (Robbins-Monro Theorem)

In the Robbins-Monro algorithm, if

1.  $0 < c_1 \leq \nabla_w g(w) \leq c_2$  for all  $w$ ;
2.  $\sum_{k=1}^{\infty} a_k = \infty$  and  $\sum_{k=1}^{\infty} a_k^2 < \infty$ ;
3.  $\mathbb{E}[\eta_k | \mathcal{H}_k] = 0$  and  $\mathbb{E}[\eta_k^2 | \mathcal{H}_k] < \infty$ ;  
where  $\mathcal{H}_k = \{w_k, w_{k-1}, \dots\}$ , then  $w_k$  **converges with probability 1 (w.p.1)**(概率收敛) to the root  $w^*$  satisfying  $g(w^*) = 0$

- $a_k$  要收敛到0, 但不要收敛太快,

## Application to mean estimation

estimation algorithm

$$w_{k+1} = w_k + \alpha_k (x_k - w_k).$$

We know that

- If  $\alpha_k = 1/k$ , then  $w_{k+1} = 1/k \sum_{i=1}^k x_i$ .
- If  $\alpha_k$  is not  $1/k$ , the convergence was not analyzed.

we show that this algorithm is a **special case of the RM algorithm**. Then, its **convergence naturally** follows

下面将证明上述方程为RM算法

1. Consider a function:

$$g(w) \doteq w - \mathbb{E}[X]$$

Our aim is to solve  $g(w) = 0$ . If we can do that, then we can obtain  $\mathbb{E}[X]$ .

2. The observation we can get is

$$\tilde{g}(w, x) \doteq w - x$$

because we can only **obtain samples of  $X$** . Note that

$$\begin{aligned}\tilde{g}(w, \eta) &= w - x = w - x + \mathbb{E}[X] - \mathbb{E}[X] \\ &= (w - \mathbb{E}[X]) + (\mathbb{E}[X] - x) \doteq g(w) + \eta,\end{aligned}$$

3. The RM algorithm for solving  $g(x) = 0$  is

$$w_{k+1} = w_k - \alpha_k \tilde{g}(w_k, \eta_k) = w_k - \alpha_k (w_k - x_k),$$

which is exactly the **mean estimation algorithm**.

The convergence naturally follows.

## SGD

### introduction

SGD is a **special RM** algorithm.

The **mean estimation** algorithm is a **special SGD algorithm**

SGD: 常用于**解决优化问题**(实际还是求根问题?)

最小化: 梯度下降

最大化: 梯度上升

- GD (gradient descent)

$$w_{k+1} = w_k - \alpha_k \nabla_w \mathbb{E}[f(w_k, X)] = w_k - \alpha_k \mathbb{E}[\nabla_w f(w_k, X)]$$

drawback: the **expected value** is difficult to **obtain**.

- BGD: **No model, use data to estimate the mean**

$$\begin{aligned}\mathbb{E}[\nabla_w f(w_k, X)] &\approx \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i) \\ w_{k+1} &= w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n \nabla_w f(w_k, x_i).\end{aligned}$$

Drawback: it requires **many samples** in each iteration for each  $w_k$ .

- SGD

- $$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k)$$

compared to the BGD, let  $n = 1$

## example

We next consider an example:

$$\min_w J(w) = \mathbb{E}[f(w, X)] = \mathbb{E} \left[ \frac{1}{2} \|w - X\|^2 \right],$$

where

$$f(w, X) = \|w - X\|^2/2 \quad \nabla_w f(w, X) = w - X$$

**answer**

- The SGD algorithm for solving the above problem is

$$w_{k+1} = w_k - \alpha_k \nabla_w f(w_k, x_k) = w_k - \alpha_k (w_k - x_k)$$

- Note:
  - It is **the same as the mean estimation** algorithm we presented before.
  - That mean estimation algorithm is a **special SGD** algorithm.

## convergence

**Core: 证明SGD是RM算法, 就可以证明其是收敛的**

We next show that SGD is a special RM algorithm. Then, the convergence naturally follows. The aim of SGD is to minimize

$$J(w) = \mathbb{E}[f(w, X)]$$

This problem can be converted to a root-finding problem:

$$\nabla_w J(w) = \mathbb{E}[\nabla_w f(w, X)] = 0$$

Let

$$g(w) = \nabla_w J(w) = \mathbb{E}[\nabla_w f(w, X)]$$

Then, the aim of SGD is to find the root of  $g(w) = 0$ .

**用RM算法解决上述问题**

What we can measure is

$$\begin{aligned} \tilde{g}(w, \eta) &= \nabla_w f(w, x) \\ &= \underbrace{\mathbb{E}[\nabla_w f(w, X)]}_{g(w)} + \underbrace{\nabla_w f(w, x) - \mathbb{E}[\nabla_w f(w, X)]}_{\eta}. \end{aligned}$$

Then, the RM algorithm for solving  $g(w) = 0$  is

$$w_{k+1} = w_k - a_k \tilde{g}(w_k, \eta_k) = w_k - a_k \nabla_w f(w_k, x_k).$$

- It is exactly the SGD algorithm.
- Therefore, SGD is a **special RM algorithm**.

## pattern

由于梯度具有随机性, 收敛是否存在随机性呢? 即  $w_k$  是否会绕一大圈再回到  $w^*$

**不存在**

通过**相对误差**来证明

$$\delta_k \doteq \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w f(w_k, X)]|}$$

Since  $\mathbb{E}[\nabla_w f(w^*, X)] = 0$ , we further have

$$\delta_k = \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w f(w_k, X)] - \mathbb{E}[\nabla_w f(w^*, X)]|} = \frac{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}{|\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)(w_k - w^*)]|}.$$

**上式用了中值定理**

where the last equality is due to the mean value theorem and  $\tilde{w}_k \in [w_k, w^*]$

Suppose  $f$  is strictly convex such that

$$\nabla_w^2 f \geq c > 0$$

for all  $w, X$ , where  $c$  is a **positive bound**.

Then, the denominator of  $\delta_k$  becomes

$$\begin{aligned} |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)(w_k - w^*)]| &= |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)](w_k - w^*)| \\ &= |\mathbb{E}[\nabla_w^2 f(\tilde{w}_k, X)]| |w_k - w^*| \geq c |w_k - w^*| \end{aligned}$$

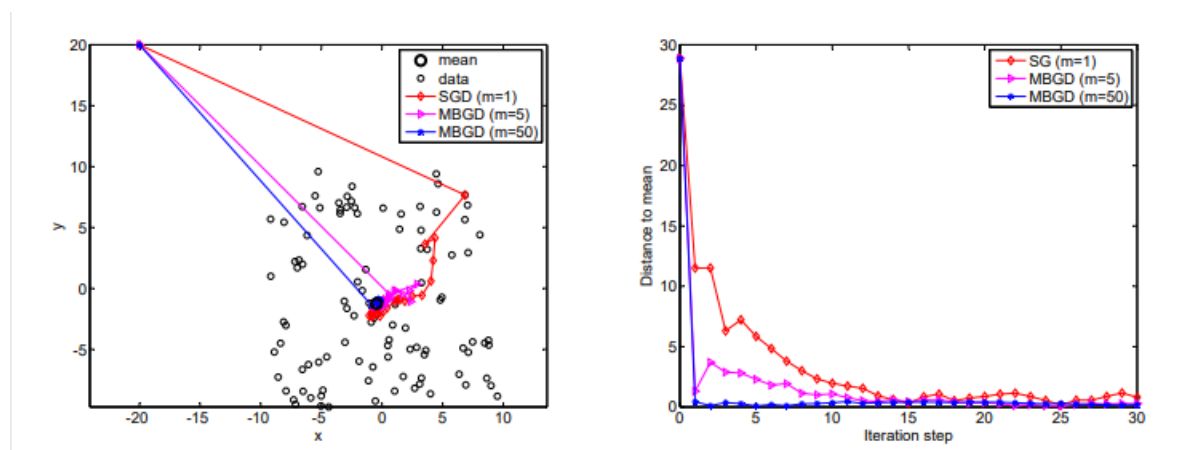
Substituting the above inequality to  $\delta_k$  gives

$$\delta_k \leq \frac{\overbrace{|\nabla_w f(w_k, x_k) - \mathbb{E}[\nabla_w f(w_k, X)]|}^{\text{stochastic gradient}}}{\underbrace{c |w_k - w^*|}_{\text{distance to the optimal solution}}}.$$

因此,

- 当  $w_k$  与  $w^*$  相距较远时, 分母很大, 此时从另外一个角度而言, 相对误差很小, 分子很小, 因此随机梯度和真实梯度基本一致, 意味着算法的趋势朝着真实值, 也就是  $w^*$  前进
- 当  $w_k$  与  $w^*$  相距较近时, 分母很小, 此时从另外一个角度而言, 相对误差较大, 分子较大, 此时则存在随机性, 即其不一定能够准确收敛到  $w^*$

因此证明了, 不会有收敛的随机性!



- Although the initial guess of the mean is **far away from the true value**, the SGD estimate can **approach** the neighborhood of the true value **fast**.
- When the estimate is **close to the true value**, it exhibits certain **randomness** but still approaches the true value gradually

# Temporal-Difference Learning

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Model-free

迭代式算法

## Motivating example

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三个例子

**First**, consider the simple mean estimation problem: calculate

$$w = \mathbb{E}[X]$$

based on some iid samples  $\{x\}$  of  $X$ .

- By writing  $g(w) = w - \mathbb{E}[X]$ , we can reformulate the problem to a root-finding problem

$$g(w) = 0.$$

- Since we can only obtain samples  $\{x\}$  of  $X$ , the noisy observation is

$$\tilde{g}(w, \eta) = w - x = (w - \mathbb{E}[X]) + (\mathbb{E}[X] - x) \doteq g(w) + \eta.$$

- Then, according to the last lecture, we know the RM algorithm for solving  $g(w) = 0$  is

$$w_{k+1} = w_k - \alpha_k \tilde{g}(w_k, \eta_k) = w_k - \alpha_k (w_k - x_k)$$

**Second**

$$w = \mathbb{E}[v(X)]$$

$$g(w) = w - \mathbb{E}[v(X)]$$

$$\tilde{g}(w, \eta) = w - v(x) = (w - \mathbb{E}[v(X)]) + (\mathbb{E}[v(X)] - v(x)) \doteq g(w) + \eta$$

$$w_{k+1} = w_k - \alpha_k \tilde{g}(w_k, \eta_k) = w_k - \alpha_k [w_k - v(x_k)]$$

**Finally**

$$w = \mathbb{E}[R + \gamma v(X)]$$

$$w_{k+1} = w_k - \alpha_k \tilde{g}(w_k, \eta_k) = w_k - \alpha_k [w_k - (r_k + \gamma v(x_k))]$$

## TD learning of state values

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没有模型的情况下，求解贝尔曼公式



求解贝尔曼公式其实就是求解RM算法

## Description

The data/experience required by the algorithm:

- $(s_0, r_1, s_1, \dots, s_t, r_{t+1}, s_{t+1}, \dots)$  or  $\{(s_t, r_{t+1}, s_{t+1})\}_t$  generated following the given policy  $\pi$ .

The TD algorithm can be annotated as

$$\underbrace{v_{t+1}(s_t)}_{\text{new estimate}} = \underbrace{v_t(s_t)}_{\text{current estimate}} - \alpha_t(s_t) \overbrace{[v_t(s_t) - [r_{t+1} + \gamma v_t(s_{t+1})]]}^{\text{TD error } \delta_t},$$

$\underbrace{[r_{t+1} + \gamma v_t(s_{t+1})]}_{\text{TD target } \bar{v}_t}$

Here,

$$\bar{v}_t \doteq r_{t+1} + \gamma v(s_{t+1})$$

is called the TD target.

$$\delta_t \doteq v(s_t) - [r_{t+1} + \gamma v(s_{t+1})] = v(s_t) - \bar{v}_t$$

is called the TD error.

It is clear that the **new estimate**  $v_{t+1}(s_t)$  is a **combination** of the **current estimate**  $v_t(s_t)$  and the **TD error**.

**TD target** 实际就是  $v_\pi$ , 即策略的state value, 因为没有模型, 最开始并不知道完整的state value, 需要不断采样, 不断更新, 到最后的state value (而不是最优策略)

That is because the algorithm drives  $v(s_t)$  towards  $\bar{v}_t$ .

### TD error

- It is a **difference** between two consequent time steps.
- It reflects the deficiency between  $v_t$  and  $v_\pi$ . To see that, denote

$$\delta_{\pi,t} \doteq v_\pi(s_t) - [r_{t+1} + \gamma v_\pi(s_{t+1})]$$

## The idea of the algorithm

**Q: What does this TD algorithm do mathematically?**

**A: It solves the Bellman equation of a given policy  $\pi$  without model.**

引入新的贝尔曼公式

First, a new expression of the Bellman equation.

The definition of state value of  $\pi$  is

$$v_\pi(s) = \mathbb{E}[R + \gamma G \mid S = s], \quad s \in \mathcal{S}$$

where  $G$  is discounted return. Since

$$\mathbb{E}[G \mid S = s] = \sum_a \pi(a \mid s) \sum_{s'} p(s' \mid s, a) v_\pi(s') = \mathbb{E}[v_\pi(S') \mid S = s],$$

where  $S'$  is the next state, we can rewrite (4) as

$$v_{\pi}(s) = \mathbb{E} [R + \gamma v_{\pi}(S') \mid S = s], \quad s \in \mathcal{S}$$

Equation (5) is another expression of the Bellman equation. It is sometimes called the **Bellman expectation equation**, an important tool to design and analyze TD algorithms.

**TD算法是计算贝尔曼公式的一个RM算法**

**Second, solve the Bellman equation in (5) using the RM algorithm.**

In particular, by defining

$$g(v(s)) = v(s) - \mathbb{E} [R + \gamma v_{\pi}(S') \mid s],$$

we can rewrite (5) as

$$g(v(s)) = 0$$

Since we can only obtain the samples  $r$  and  $s'$  of  $R$  and  $S'$ , the noisy observation we have is

$$\begin{aligned} \tilde{g}(v(s)) &= v(s) - [r + \gamma v_{\pi}(s')] \\ &= \underbrace{(v(s) - \mathbb{E} [R + \gamma v_{\pi}(S') \mid s])}_{g(v(s))} + \underbrace{(\mathbb{E} [R + \gamma v_{\pi}(S') \mid s] - [r + \gamma v_{\pi}(s')])}_{\eta}. \end{aligned}$$

therefore

$$\begin{aligned} v_{k+1}(s) &= v_k(s) - \alpha_k \tilde{g}(v_k(s)) \\ &= v_k(s) - \alpha_k (v_k(s) - [r_k + \gamma v_{\pi}(s'_k)]), \quad k = 1, 2, 3, \dots \end{aligned}$$

To **remove the two assumptions** in the RM algorithm, we can modify it

- One modification is that  $\{(s, r, s')\}$  is **changed to**  $\{(s_t, r_{t+1}, s_{t+1})\}$  so that the algorithm can **utilize the sequential samples** in an episode.
- Another modification is that  $v_{\pi}(s')$  is **replaced by an estimate of it** because we don't know it in advance.

## convergence

### Theorem (Convergence of TD Learning)

By the TD algorithm (1),  $v_t(s)$  converges with probability 1 to  $v_{\pi}(s)$  for all  $s \in \mathcal{S}$  as  $t \rightarrow \infty$  if  $\sum_t \alpha_t(s) = \infty$  and  $\sum_t \alpha_t^2(s) < \infty$  for all  $s \in \mathcal{S}$ .

## Comparison

TD/Sarsa learning	MC learning
Online: TD learning is online. It can update the state/action values immediately after receiving a reward.	Offline: MC learning is offline. It has to wait until an episode has been completely collected.
Continuing tasks: Since TD learning is online, it can handle both episodic and continuing tasks.	Episodic tasks is offline, it can only handle episodic tasks that has terminate states.

TD/Sarsa learning	MC learning
Bootstrapping: TD bootstraps because the update of a value relies on the previous estimate of this value. Hence, it requires initial guesses.	Non-bootstrapping: MC is not bootstrapping, because it can directly estimate state/action values without any initial guess.
Low estimation variance: TD has lower than MC because there are fewer random variables. For instance, Sarsa requires $R_{t+1}, S_{t+1}, A_{t+1}$ .	High estimation variance: To estimate $q_{\pi}(s_t, a_t)$ , we need samples of $R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots$ . Suppose the length of each episode is $L$ . There are $ \mathcal{A} ^L$ possible episodes.

## Sarsa

### Description

**Core Idea:** that is to use **an algorithm to solve the Bellman equation of a given policy**.

The **complication emerges** when we try to **find optimal policies and work efficiently**

Next, we introduce, Sarsa, an algorithm that can directly estimate **action values**.

估计action value, 从而更新, 改进策略, Policy evaluation+Policy improvement

如何估计呢? not model, need data

也是求解了一个**action value**相关的贝尔曼公式!

收敛性:  $q_t(s, a) - > q_{\pi}(s, a)$

在policy evaluation (update q-value) 后立马policy improvement (update policy)

First, our aim is to **estimate the action values of a given policy  $\pi$** .

Suppose we have some **experience**  $\{(s_t, a_t, r_{t+1}, s_{t+1}, a_{t+1})\}_t$ . (Sarsa)

We can use the following **Sarsa algorithm** to estimate the action values:

$$q_{t+1}(s_t, a_t) = q_t(s_t, a_t) - \alpha_t(s_t, a_t) [q_t(s_t, a_t) - [r_{t+1} + \gamma q_t(s_{t+1}, a_{t+1})]],$$

$$q_{t+1}(s, a) = q_t(s, a), \quad \forall (s, a) \neq (s_t, a_t),$$

where  $t = 0, 1, 2, \dots$

NOTE: 第二个条件是当某个state action pair没被访问时, **将保持原状**

- $q_t(s_t, a_t)$  is an **estimate** of  $q_{\pi}(s_t, a_t)$ ;
- $\alpha_t(s_t, a_t)$  is the **learning rate depending on**  $s_t, a_t$ .

如何policy improvement?

For each episode, do

- If the current  $s_t$  is not the target state, do

- **Update q-value (policy evaluation) :**

$$q_{t+1}(s_t, a_t) = q_t(s_t, a_t) - \alpha_t(s_t, a_t) [q_t(s_t, a_t) - [r_{t+1} + \gamma q_t(s_{t+1}, a_{t+1})]]$$

- ○ **Update policy (policy) :**

$$\pi_{t+1}(a \mid s_t) = 1 - \frac{\epsilon}{|\mathcal{A}|}(|\mathcal{A}| - 1) \text{ if } a = \arg \max_a q_{t+1}(s_t, a)$$

$$\pi_{t+1}(a \mid s_t) = \frac{\epsilon}{|\mathcal{A}|} \text{ otherwise}$$

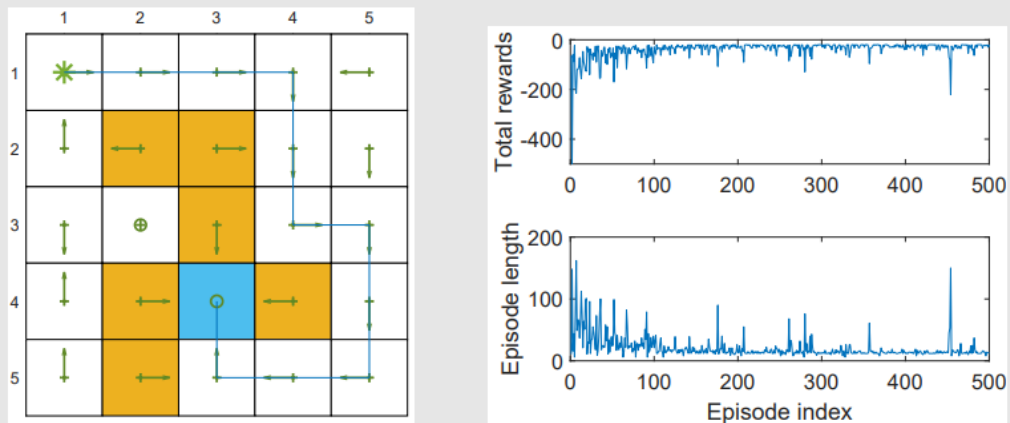
## Example

The task is to find a good path **from a specific starting state** to the **target state**

So:

### Results:

- The left figures above show the final policy obtained by Sarsa.
  - Not all states have the optimal policy.
- The right figures show the total reward and length of every episode.
  - The metric of total reward per episode will be frequently used.



## Expected Sarsa

## Description

A variant of Sarsa is the Expected Sarsa algorithm:

$$\begin{aligned} q_{t+1}(s_t, a_t) &= q_t(s_t, a_t) - \alpha_t(s_t, a_t) [q_t(s_t, a_t) - (r_{t+1} + \gamma \mathbb{E}[q_t(s_{t+1}, A)])], \\ q_{t+1}(s, a) &= q_t(s, a), \quad \forall (s, a) \neq (s_t, a_t), \end{aligned}$$

where

$$\mathbb{E}[q_t(s_{t+1}, A)] = \sum_a \pi_t(a \mid s_{t+1}) q_t(s_{t+1}, a) \doteq v_t(s_{t+1})$$

is the **expected value** of  $q_t(s_{t+1}, a)$  under policy  $\pi_t$ .

Compared to Sarsa:

- The **TD target** is changed from  $r_{t+1} + \gamma q_t(s_{t+1}, a_{t+1})$  as in Sarsa to  $r_{t+1} + \gamma \mathbb{E}[q_t(s_{t+1}, A)]$  as in Expected Sarsa.
- Need more **computation**. But it is beneficial in the sense that it **reduces the estimation variances** because it **reduces random variables** in Sarsa from  $\{s_t, a_t, r_{t+1}, s_{t+1}, a_{t+1}\}$  to  $\{s_t, a_t, r_{t+1}, s_{t+1}\}$ . (因为遍历了所有的action)

## n-step Sarsa

n-step Sarsa: can unify Sarsa and Monte Carlo learning The definition of action value is

$$\begin{aligned} \text{Sarsa} &\leftarrow G_t^{(1)} = R_{t+1} + \gamma q_\pi(s_{t+1}, A_{t+1}), \\ G_t^{(2)} &= R_{t+1} + \gamma R_{t+2} + \gamma^2 q_\pi(s_{t+2}, A_{t+2}), \\ &\vdots \\ \text{n-step Sarsa} &\leftarrow G_t^{(n)} = R_{t+1} + \gamma R_{t+2} + \dots + \gamma^n q_\pi(s_{t+n}, A_{t+n}), \\ &\vdots \\ \text{MC} &\leftarrow G_t^{(\infty)} = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots \end{aligned}$$

- Sarsa aims to solve

$$q_\pi(s, a) = \mathbb{E}[G_t^{(1)} | s, a] = \mathbb{E}[R_{t+1} + \gamma q_\pi(s_{t+1}, A_{t+1}) | s, a].$$

- MC learning aims to solve

$$q_\pi(s, a) = \mathbb{E}[G_t^{(\infty)} | s, a] = \mathbb{E}[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots | s, a].$$

- An intermediate algorithm called n-step Sarsa aims to solve

$$q_\pi(s, a) = \mathbb{E}[G_t^{(n)} | s, a] = \mathbb{E}[R_{t+1} + \gamma R_{t+2} + \dots + \gamma^n q_\pi(s_{t+n}, A_{t+n}) | s, a] -$$

The algorithm of n-step Sarsa is

$$q_{t+1}(s_t, a_t) = q_t(s_t, a_t) - \alpha_t(s_t, a_t) [q_t(s_t, a_t) - [r_{t+1} + \gamma r_{t+2} + \dots + \gamma^n q_t(s_{t+n}, a_{t+n})]].$$

n-step Sarsa is **more general** because it becomes the (one-step) Sarsa algorithm when  $n = 1$  and the MC learning algorithm when  $n = \infty$ .

## Q-learning

### Description

Core Idea: 求解贝尔曼最优公式

$$\begin{aligned} q_{t+1}(s_t, a_t) &= q_t(s_t, a_t) - \alpha_t(s_t, a_t) \left[ q_t(s_t, a_t) - \left[ r_{t+1} + \gamma \max_{a \in \mathcal{A}} q_t(s_{t+1}, a) \right] \right], \\ q_{t+1}(s, a) &= q_t(s, a), \quad \forall (s, a) \neq (s_t, a_t) \end{aligned}$$

引入了 behavior policy, target policy

## off-Policy Vs on-policy

off-policy: 比如我behavior policy可以用探索性比较强的, 比如action的选择可以均匀分布, 以此来得到更多experience

而对应的target policy为了得到最优的策略, 直接选择greedy policy, 而不是  $\epsilon$ -greedy, 因为此时我已经不缺探索性了

on-policy: 而behavior policy=target policy, 比如 Sarsa, uses  $\epsilon$ -greedy policies to **maintain certain exploration ability**, 但由于一般设置较小, 其对应的探索能力有限, 因为如果设置较大, 最后优化效果并不好

## Value Function

### Example

**Core Idea:** 用曲线拟合替代tables 表示state value

最简单: 直线拟合

$$\hat{v}(s, w) = as + b = \underbrace{\begin{bmatrix} s, 1 \end{bmatrix}}_{\phi^T(s)} \underbrace{\begin{bmatrix} a \\ b \end{bmatrix}}_w = \phi^T(s)w$$

where

- $w$  is the parameter vector
- $\phi(s)$  the feature vector of  $s$
- $\hat{v}(s, w)$  is linear in  $w$

当然, 也可以用二阶, 三阶, 高阶拟合

$$\hat{v}(s, w) = as^2 + bs + c = \underbrace{\begin{bmatrix} s^2, s, 1 \end{bmatrix}}_{\phi^T(s)} \underbrace{\begin{bmatrix} a \\ b \\ c \end{bmatrix}}_w = \phi^T(s)w.$$

优点: 存储方面, 存储的维数大幅减少,

同时, 泛化能力很好

When a state  $s$  is visited, the parameter  $w$  is updated so that the values of some other unvisited states can also be updated.

## Algorithm for state value estimation

### Objective function

The objective function is

$$J(w) = \mathbb{E} \left[ \left( v_\pi(S) - \hat{v}(S, w) \right)^2 \right]$$

- Our goal is to find the best  $w$  that can **minimize**  $J(w)$ .

- The **expectation** is with respect to the random variable  $S \in \mathcal{S}$ . What is the **probability distribution** of  $S$ ?
- This is often confusing because we have not discussed the **probability distribution of states** so far in this book.
- There are **several ways to define** the probability distribution of  $S$ .

first way: uniform distribution

$$J(w) = \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w))^2 \right] = \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} (v_\pi(s) - \hat{v}(s, w))^2$$

缺点：有些状态离target area较远，并不重要，被访问次数较少，对应的权重应小

**second way: stationary distribution.**

Let  $\{d_\pi(s)\}_{s \in \mathcal{S}}$  denote the stationary distribution of the Markov process under policy  $\pi$ . By definition,  $d_\pi(s) \geq 0$  and  $\sum_{s \in \mathcal{S}} d_\pi(s) = 1$ .

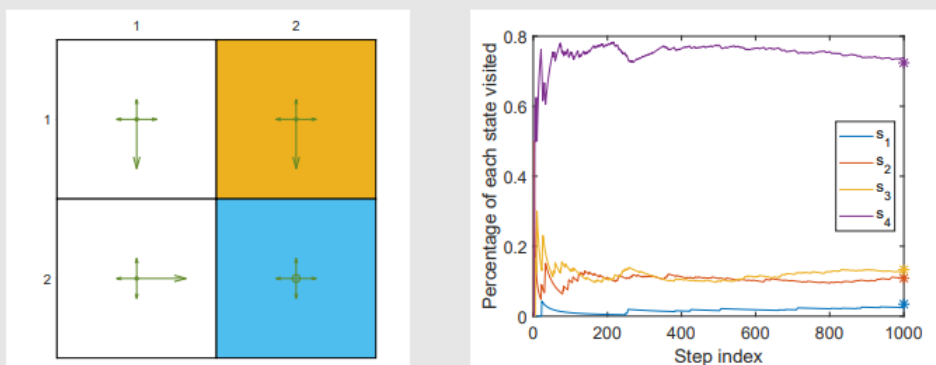
$$J(w) = \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w))^2 \right] = \sum_{s \in \mathcal{S}} d_\pi(s) (v_\pi(s) - \hat{v}(s, w))^2$$

为什么叫稳态？因为要足够多次的step，等系统稳定后，基本不再改变时

Illustrative example:

- Given a policy shown in the figure.
- Let  $n_\pi(s)$  denote the number of times that  $s$  has been visited in a very long episode generated by  $\pi$ .
- Then,  $d_\pi(s)$  can be approximated by

$$d_\pi(s) \approx \frac{n_\pi(s)}{\sum_{s' \in \mathcal{S}} n_\pi(s')}$$



**Figure:** Long-run behavior of an  $\epsilon$ -greedy policy with  $\epsilon = 0.5$ .

可以证明，最后的  $d_\pi(s)$  为转移矩阵的特征向量

[Book All-in-one.pdf](#)

# Optimization algorithms

那究竟如何优化呢？

最小化：梯度下降

$$w_{k+1} = w_k - \alpha_k \nabla_w J(w_k)$$

The true gradient is

$$\begin{aligned}\nabla_w J(w) &= \nabla_w \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w))^2 \right] \\ &= \mathbb{E} \left[ \nabla_w (v_\pi(S) - \hat{v}(S, w))^2 \right] \\ &= 2 \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w)) (-\nabla_w \hat{v}(S, w)) \right] \\ &= -2 \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w)) \nabla_w \hat{v}(S, w) \right]\end{aligned}$$

use the **stochastic gradient**

$$w_{t+1} = w_t + \alpha_t (v_\pi(s_t) - \hat{v}(s_t, w_t)) \nabla_w \hat{v}(s_t, w_t)$$

系数2已经合并到常数里了

注意到  $v_\pi$  未知，因此要进行替代

两种替代方式：Monte Carlo learning和TD Learning（但是此种替代并不严谨，优化的并不是上述true error，而是projected Bellman error）

- First, Monte Carlo learning with function approximation  
Let  $g_t$  be the **discounted return starting from  $s_t$  in the episode**. Then,  $g_t$  can be used to approximate  $v_\pi(s_t)$ . The algorithm becomes

$$w_{t+1} = w_t + \alpha_t (g_t - \hat{v}(s_t, w_t)) \nabla_w \hat{v}(s_t, w_t)$$

- Second, TD learning with function approximation  
By the spirit of TD learning,  $r_{t+1} + \gamma \hat{v}(s_{t+1}, w_t)$  can be viewed as an approximation of  $v_\pi(s_t)$ . Then, the algorithm becomes

$$w_{t+1} = w_t + \alpha_t [r_{t+1} + \gamma \hat{v}(s_{t+1}, w_t) - \hat{v}(s_t, w_t)] \nabla_w \hat{v}(s_t, w_t)$$

## Selection of function approximators

究竟如何选择相关函数，1阶？2阶？

一阶的好处：简洁，参数少

- The theoretical properties of the TD algorithm in the linear case can be much better understood than in the nonlinear case.
- Linear function approximation is still powerful in the sense that the **tabular representation is merely a special case of linear function approximation**.

坏处：难以拟合非线性情况

Recall that the TD-Linear algorithm is

$$w_{t+1} = w_t + \alpha_t [r_{t+1} + \gamma \phi^T(s_{t+1}) w_t - \phi^T(s_t) w_t] \phi(s_t),$$

- When  $\phi(s_t) = e_{s_t}$ , the above algorithm becomes

$$w_{t+1} = w_t + \alpha_t (r_{t+1} + \gamma w_t(s_{t+1}) - w_t(s_t)) e_{s_t}.$$



This is a vector equation that merely updates the  $s_t$  th entry of  $w_t$ .

- Multiplying  $e_{s_t}^T$  on both sides of the equation gives

$$w_{t+1}(s_t) = w_t(s_t) + \alpha_t (r_{t+1} + \gamma w_t(s_{t+1}) - w_t(s_t)),$$

which is exactly the tabular TD algorithm.

## Examples

## Summary of the story

## theoretical analysis

- The algorithm

$$w_{t+1} = w_t + \alpha_t [r_{t+1} + \gamma \hat{v}(s_{t+1}, w_t) - \hat{v}(s_t, w_t)] \nabla_w \hat{v}(s_t, w_t)$$

does not minimize the following objective function:

$$J(w) = \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w))^2 \right]$$

Different objective functions:

- Objective function 1: **True value error**

$$J_E(w) = \mathbb{E} \left[ (v_\pi(S) - \hat{v}(S, w))^2 \right] = \|\hat{v}(w) - v_\pi\|_D^2$$

- Objective function 2: **Bellman error**

$$J_{BE}(w) = \|\hat{v}(w) - (r_\pi + \gamma P_\pi \hat{v}(w))\|_D^2 \doteq \|\hat{v}(w) - T_\pi(\hat{v}(w))\|_D^2$$

where  $T_\pi(x) \doteq r_\pi + \gamma P_\pi x$

- Objective function 3: **Projected Bellman error**

$$J_{PBE}(w) = \|\hat{v}(w) - MT_\pi(\hat{v}(w))\|_D^2$$

where  $M$  is a **projection matrix**. (投影变换矩阵, 即无论  $w$  怎么选, 两者都有距离时, 该投影变换矩阵能将二者error变为0)

**The TD-Linear algorithm minimizes the projected Bellman error.**

Details can be found in the book.

## Sarsa with function approximation

**Core Idea:** 利用Sarsa估计action value

So far, we merely considered the problem of **state value estimation**. That is we hope

$$\hat{v} \approx v_\pi$$

To search for optimal policies, we need to **estimate action values**.

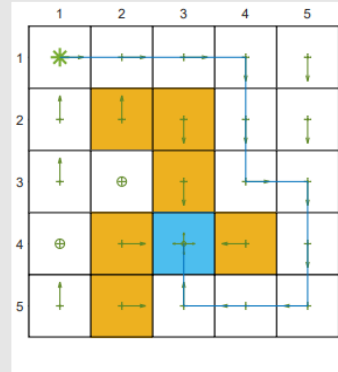
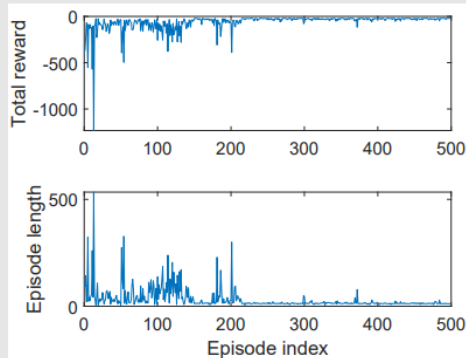
The Sarsa algorithm with value function approximation is

$$w_{t+1} = w_t + \alpha_t [r_{t+1} + \gamma \hat{q}(s_{t+1}, a_{t+1}, w_t) - \hat{q}(s_t, a_t, w_t)] \nabla_w \hat{q}(s_t, a_t, w_t).$$

This is **the same as** the algorithm we introduced previously in this lecture **except that**  $\hat{v}$  is replaced by  $\hat{q}$ .

Illustrative example:

- Sarsa with *linear function* approximation.
- $\gamma = 0.9$ ,  $\epsilon = 0.1$ ,  $r_{\text{boundary}} = r_{\text{forbidden}} = -10$ ,  $r_{\text{target}} = 1$ ,  $\alpha = 0.001$ .



## Q-learning with function approximation

**Core Idea:** 利用q-learning的方式更新action value

The q-value update rule is

$$w_{t+1} = w_t + \alpha_t \left[ r_{t+1} + \gamma \max_{a \in \mathcal{A}(s_{t+1})} \hat{q}(s_{t+1}, a, w_t) - \hat{q}(s_t, a_t, w_t) \right] \nabla_w \hat{q}(s_t, a_t, w_t)$$

which is the same as Sarsa except that  $\hat{q}(s_{t+1}, a_{t+1}, w_t)$  is replaced by  $\max_{a \in \mathcal{A}(s_{t+1})} \hat{q}(s_{t+1}, a, w_t)$

## Deep Q-learning

DQN: 原本算法计算变量梯度, 涉及到神经网络底层, 因此要进行改进

Deep Q-learning aims to minimize the objective function/loss function:

$$J(w) = \mathbb{E} \left[ \left( R + \gamma \max_{a \in \mathcal{A}(S')} \hat{q}(S', a, w) - \hat{q}(S, A, w) \right)^2 \right],$$

where  $(S, A, R, S')$  are random variables.

- This is actually the Bellman optimality error. That is because

$$q(s, a) = \mathbb{E} \left[ R_{t+1} + \gamma \max_{a \in \mathcal{A}(S_{t+1})} q(S_{t+1}, a) \mid S_t = s, A_t = a \right], \quad \forall s, a$$

The value of  $R + \gamma \max_{a \in \mathcal{A}(S')} \hat{q}(S', a, w) - \hat{q}(S, A, w)$  **should be zero** in the expectation sense

均匀采样的数学原因：

# Policy Function

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**Core Idea: 函数表达策略!**

**value-based to policy based**

优化目标函数来求最优策略

$\theta$ 是参数，可以是神经网络，用以计算  $\pi(a|s)$

## Basic idea of Policy gradient

---

The basic idea of the policy gradient is simple:

- First, metrics (or objective functions) to define **optimal policies**:  $J(\theta)$ , which can define optimal policies. (定义目标函数)
- Second, **gradient-based optimization algorithms** to search for optimal policies: (优化目标函数)

$$\theta_{t+1} = \theta_t + \alpha \nabla_{\theta} J(\theta_t)$$

Although the idea is simple, the complication emerges when we try to answer the following questions.

- What **appropriate metrics** should be used? (选择什么函数合适)
- How to calculate the gradients of the metrics? (如何优化?)

## Metrics to define optimal policies

---

**Two metrics** (两种优化函数)

都是关于  $\pi$  的函数，且  $\pi$  是  $\theta$  的函数

The first metric is the **average state value** or simply called **average value**

### Average value

求出每个state的state value然后求mean

$$\bar{v}_{\pi} = \sum_{s \in \mathcal{S}} d(s) v_{\pi}(s)$$

- $\bar{v}_{\pi}$  is a **weighted average** of the state values.
- $d(s) \geq 0$  is the **weight** for state  $s$ .
- Since  $\sum_{s \in \mathcal{S}} d(s) = 1$ , we can interpret  $d(s)$  as a probability distribution. Then, the metric can be written as

$$\bar{v}_{\pi} = \mathbb{E}[v_{\pi}(S)]$$

where  $S \sim d$ .

How to select the **distribution d**? There are **two cases**.

- The first case is that  $d$  is **independent** of the policy  $\pi$ . (另外一种就是依赖于决策)

不依赖又分两种：均匀 (equally important) 和非均匀 (only interested in a specific state  $s_0$ )

we only care about the long-term return **starting from**  $s_0$

$$d_0(s_0) = 1, \quad d_0(s \neq s_0) = 0$$

- The second case is that  $d$  depends on the policy  $\pi$ .
- A common way to select  $d$  as  $d_\pi(s)$ , which is the stationary distribution under  $\pi$ .
- One basic property of  $d_\pi$  is that it satisfies

$$d_\pi^T P_\pi = d_\pi^T$$

where  $P_\pi$  is the **state transition probability matrix**.

- The interpretation of selecting  $d_\pi$  is as follows.
- If one state is frequently visited in the long run, it is **more important and deserves more weight**.
- If a state is **hardly visited**, then we give it less weight.

等价描述:

$$J(\theta) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t R_{t+1} \right]$$

## Average reward

求出每个state的immediate reward然后求mean

$$\bar{r}_\pi \doteq \sum_{s \in \mathcal{S}} d_\pi(s) r_\pi(s) = \mathbb{E}[r_\pi(S)]$$

where  $S \sim d_\pi$ . Here,

$$r_\pi(s) \doteq \sum_{a \in \mathcal{A}} \pi(a | s) r(s, a)$$

is the average of the one-step immediate reward that can be obtained starting from state  $s$ , and

$$r(s, a) = \mathbb{E}[R | s, a] = \sum_r r p(r | s, a)$$

- The weight  $d_\pi$  is the **stationary distribution**.
- As its name suggests,  $\bar{r}_\pi$  is simply a weighted average of the one-step immediate rewards.

有一个等价描述

- Suppose an agent follows a given policy and generate a trajectory with the rewards as  $(R_{t+1}, R_{t+2}, \dots)$ .
- The average single-step reward along this trajectory is

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E}[R_{t+1} + R_{t+2} + \dots + R_{t+n} | S_t = s_0] \\ &= \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[ \sum_{k=1}^n R_{t+k} | S_t = s_0 \right] \end{aligned}$$

where  $s_0$  is the starting state of the trajectory.

Proof:

$$\begin{aligned}\lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[ \sum_{k=1}^n R_{t+k} \mid S_t = s_0 \right] &= \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[ \sum_{k=1}^n R_{t+k} \right] \\ &= \sum_s d_\pi(s) r_\pi(s) \\ &= \bar{r}_\pi\end{aligned}$$

- Intuitively,  $\bar{r}_\pi$  is more **short-sighted** because it merely considers the immediate rewards, whereas  $\bar{v}_\pi$  considers the **total reward overall steps**.
- However, the two metrics are **equivalent** to each other. (两个metric等价, 因为当一个达到极值时, 另一个必然也到达极值) In the discounted case where  $\gamma < 1$ , it holds that

$$\bar{r}_\pi = (1 - \gamma) \bar{v}_\pi$$

## Gradients of the metrics

---

Core Idea: 如何求梯度?

Summary of the results about the gradients:

$$\begin{aligned}\nabla_\theta J(\theta) &= \sum_{s \in \mathcal{S}} \eta(s) \sum_{a \in \mathcal{A}} \nabla_\theta \pi(a \mid s, \theta) q_\pi(s, a) \\ &= \mathbb{E} [\nabla_\theta \ln \pi(A \mid S, \theta) q_\pi(S, A)]\end{aligned}$$

where

- $J(\theta)$  can be  $\bar{v}_\pi, \bar{r}_\pi$ , or  $\bar{v}_\pi^0$ .
- "=" may denote **strict equality**, **approximation**, or **proportional to**.
- $\eta$  is a **distribution** or **weight** of the states.

Some remarks: Because we need to calculate  $\ln \pi(a \mid s, \theta)$ , we must **ensure** that for all  $s, a, \theta$

$$\pi(a \mid s, \theta) > 0$$

- This can be archived by using **softmax functions** that can normalize the entries in a vector from  $(-\infty, +\infty)$  to  $(0, 1)$ .

## Gradient-ascent algorithm

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Core Idea: 具体怎么优化函数?

对于期望, 利用采样近似; 对于未知数, 比如  $q_\pi(s_t, a_t)$ , 也要近似替代, 两种方法替代

1: Monte-Carlo 对应 Reinforce

2: TD methods 对应 **Actor-Critic**

$$\theta_{t+1} = \theta_t + \alpha \underbrace{\left( \frac{q_t(s_t, a_t)}{\pi(a_t | s_t, \theta_t)} \right)}_{\beta_t} \nabla_{\theta} \pi(a_t | s_t, \theta_t)$$

The coefficient  $\beta_t$  can well balance **exploration** and **exploitation**.

- First,  $\beta_t$  is **proportional** to  $q_t(s_t, a_t)$ .
- If  $q_t(s_t, a_t)$  is great, then  $\beta_t$  is great. (即return大的action, 后续选到该action的概率就大! 体现剥削性)
- Therefore, the algorithm intends to **enhance actions with greater values**.
- Second,  $\beta_t$  is **inversely proportional** to  $\pi(a_t | s_t, \theta_t)$ .
- If  $\pi(a_t | s_t, \theta_t)$  is small, then  $\beta_t$  is large. (即其他action 本身概率小的话, 则后续选到他的概率会增大, 体现探索性)
- Therefore, the algorithm intends to **explore actions that have low probabilities**.

伪代码!

### Pseudocode: Policy Gradient by Monte Carlo (REINFORCE)

**Initialization:** A parameterized function  $\pi(a|s, \theta)$ ,  $\gamma \in (0, 1)$ , and  $\alpha > 0$ .

**Aim:** Search for an optimal policy maximizing  $J(\theta)$ .

For the  $k$ th iteration, do

Select  $s_0$  and generate an episode following  $\pi(\theta_k)$ . Suppose the episode is  $\{s_0, a_0, r_1, \dots, s_{T-1}, a_{T-1}, r_T\}$ .

For  $t = 0, 1, \dots, T - 1$ , do

**Value update:**  $q_t(s_t, a_t) = \sum_{k=t+1}^T \gamma^{k-t-1} r_k$

**Policy update:**  $\theta_{t+1} = \theta_t + \alpha \nabla_{\theta} \ln \pi(a_t | s_t, \theta_t) q_t(s_t, a_t)$

$\theta_k = \theta_T$

## Actor-Critic Methods

### The Simplest AC (QAC)

实际是Policy gradient, 只不过结合了value function

Core Idea: **利用TD估计, 称为actor-critic**

何为actor: policy update

何为critic: policy evaluation

对应运用TD算法估计action-value的

## The simplest actor-critic algorithm (QAC)

**Aim:** Search for an optimal policy by maximizing  $J(\theta)$ .

At time step  $t$  in each episode, do

Generate  $a_t$  following  $\pi(a|s_t, \theta_t)$ , observe  $r_{t+1}, s_{t+1}$ , and then generate  $a_{t+1}$  following  $\pi(a|s_{t+1}, \theta_t)$ .

Critic (value update):

$$w_{t+1} = w_t + \alpha_w [r_{t+1} + \gamma q(s_{t+1}, a_{t+1}, w_t) - q(s_t, a_t, w_t)] \nabla_w q(s_t, a_t, w_t)$$

Actor (policy update):

$$\theta_{t+1} = \theta_t + \alpha_\theta \nabla_\theta \ln \pi(a_t | s_t, \theta_t) q(s_t, a_t, w_{t+1})$$

## A2C

### Baseline invariance

**Core Idea:** introduce a baseline to reduce variance

$$\begin{aligned} \nabla_\theta J(\theta) &= \mathbb{E}_{S \sim \eta, A \sim \pi} [\nabla_\theta \ln \pi(A | S, \theta_t) q_\pi(S, A)] \\ &= \mathbb{E}_{S \sim \eta, A \sim \pi} [\nabla_\theta \ln \pi(A | S, \theta_t) (q_\pi(S, A) - b(S))] \end{aligned}$$

NOTE: 该函数为**s**的函数，且添加后对期望没有影响，但会影响方差

**relative proof**

$$\begin{aligned} \mathbb{E}_{S \sim \eta, A \sim \pi} [\nabla_\theta \ln \pi(A | S, \theta_t) b(S)] &= \sum_{s \in \mathcal{S}} \eta(s) \sum_{a \in \mathcal{A}} \pi(a | s, \theta_t) \nabla_\theta \ln \pi(a | s, \theta_t) b(s) \\ &= \sum_{s \in \mathcal{S}} \eta(s) \sum_{a \in \mathcal{A}} \nabla_\theta \pi(a | s, \theta_t) b(s) \\ &= \sum_{s \in \mathcal{S}} \eta(s) b(s) \sum_{a \in \mathcal{A}} \nabla_\theta \pi(a | s, \theta_t) \\ &= \sum_{s \in \mathcal{S}} \eta(s) b(s) \nabla_\theta \sum_{a \in \mathcal{A}} \pi(a | s, \theta_t) \\ &= \sum_{s \in \mathcal{S}} \eta(s) b(s) \nabla_\theta 1 = 0 \end{aligned}$$

- Why? Because  $\text{tr}[\text{var}(X)] = \mathbb{E}[X^T X] - \bar{x}^T \bar{x}$  and

$$\begin{aligned} \mathbb{E}[X^T X] &= \mathbb{E}[(\nabla_\theta \ln \pi)^T (\nabla_\theta \ln \pi) (q_\pi(S, A) - b(S))^2] \\ &= \mathbb{E}[\|\nabla_\theta \ln \pi\|^2 (q_\pi(S, A) - b(S))^2] \end{aligned}$$

Imagine  $b$  is huge (e.g., 1 million)

**b**存在最优解，但由于过于复杂，我们一般用  $v_\pi(s)$  替代

## algorithm

$$\begin{aligned}\theta_{t+1} &= \theta_t + \alpha \mathbb{E} [\nabla_{\theta} \ln \pi(A | S, \theta_t) [q_{\pi}(S, A) - v_{\pi}(S)]] \\ &\doteq \theta_t + \alpha \mathbb{E} [\nabla_{\theta} \ln \pi(A | S, \theta_t) \delta_{\pi}(S, A)]\end{aligned}$$

where

$$\delta_{\pi}(S, A) \doteq q_{\pi}(S, A) - v_{\pi}(S)$$

is called the advantage function (why called advantage?).

当  $q_{\pi}(S)$  大于  $v_{\pi}(S)$ , 说明该state action-pair优秀!

进行进一步变换

$$\begin{aligned}\theta_{t+1} &= \theta_t + \alpha \nabla_{\theta} \ln \pi(a_t | s_t, \theta_t) \delta_t(s_t, a_t) \\ &= \theta_t + \alpha \frac{\nabla_{\theta} \pi(a_t | s_t, \theta_t)}{\pi(a_t | s_t, \theta_t)} \delta_t(s_t, a_t) \\ &= \theta_t + \underbrace{\alpha \left( \frac{\delta_t(s_t, a_t)}{\pi(a_t | s_t, \theta_t)} \right)}_{\text{step size}} \nabla_{\theta} \ln \pi(a_t | s_t, \theta_t)\end{aligned}$$

同样能平衡 exploration 和 exploitation, 而且更好, 因为分子是相对值 (作差), 而QAC是绝对值

进一步, 对应的  $\delta_{\pi}(S, A)$  可以由TD算法估计得到

伪代码:

### Advantage actor-critic (A2C) or TD actor-critic

**Aim:** Search for an optimal policy by maximizing  $J(\theta)$ .

At time step  $t$  in each episode, do

Generate  $a_t$  following  $\pi(a|s_t, \theta_t)$  and then observe  $r_{t+1}, s_{t+1}$ .

TD error (advantage function):

$$\delta_t = r_{t+1} + \gamma v(s_{t+1}, w_t) - v(s_t, w_t)$$

Critic (value update):

$$w_{t+1} = w_t + \alpha_w \delta_t \nabla_w v(s_t, w_t)$$

Actor (policy update):

$$\theta_{t+1} = \theta_t + \alpha_{\theta} \delta_t \nabla_{\theta} \ln \pi(a_t | s_t, \theta_t)$$

由于已经是stochastic, 所以不需要  $\epsilon$ -greedy

## Off-policy AC

有两个概率分布, 用其中一个概率分布计算另外一个概率分布的期望!



## Example

$$p_0(X = +1) = 0.5, \quad p_0(X = -1) = 0.5$$

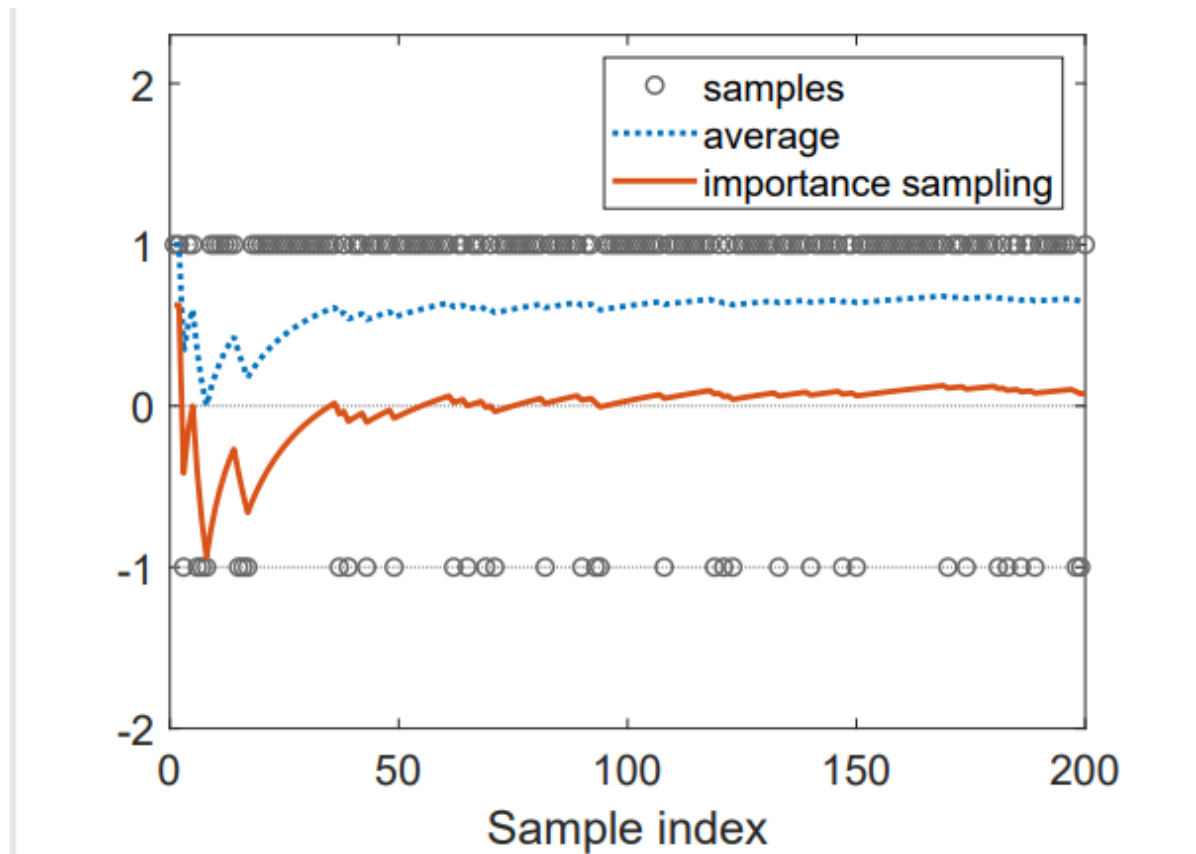
$$p_1(X = +1) = 0.8, \quad p_1(X = -1) = 0.2$$

The expectation is

$$\mathbb{E}_{X \sim p_1}[X] = (+1) \cdot 0.8 + (-1) \cdot 0.2 = 0.6$$

If we use the average of the samples, then without suprising

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \rightarrow \mathbb{E}_{X \sim p_1}[X] = 0.6 \neq \mathbb{E}_{X \sim p_0}[X]$$



## Importance sampling

Note that

$$\mathbb{E}_{X \sim p_0}[X] = \sum_x p_0(x)x = \sum_x p_1(x) \underbrace{\frac{p_0(x)}{p_1(x)}}_{f(x)} x = \mathbb{E}_{X \sim p_1}[f(X)]$$

- Thus, **we can estimate**  $\mathbb{E}_{X \sim p_1}[f(X)]$  **in order to estimate**  $\mathbb{E}_{X \sim p_0}[X]$ .
- How to estimate  $\mathbb{E}_{X \sim p_1}[f(X)]$  ? Easy. Let (即对  $f(x_i)$  采样)

$$\bar{f} \doteq \frac{1}{n} \sum_{i=1}^n f(x_i), \quad \text{where } x_i \sim p_1$$

Then,

$$\mathbb{E}_{X \sim p_1}[\bar{f}] = \mathbb{E}_{X \sim p_1}[f(X)]$$

$$\text{var}_{X \sim p_1}[\bar{f}] = \frac{1}{n} \text{var}_{X \sim p_1}[f(X)]$$

Therefore,  $\bar{f}$  is a good approximation for  $\mathbb{E}_{X \sim p_1}[f(X)] = \mathbb{E}_{X \sim p_0}[X]$

- $\frac{p_0(x_i)}{p_1(x_i)}$  is called the importance weight.
- If  $p_1(x_i) = p_0(x_i)$ , the importance weight is **one** and  $\bar{f}$  becomes  $\bar{x}$ .
- If  $p_0(x_i) \geq p_1(x_i)$ ,  $x_i$  can be more often sampled by  $p_0$  than  $p_1$ . The importance weight ( $>1$ ) can emphasize the importance of this sample.
- 举个栗子：当  $p_0 > p_1$  时，说明原本这个样本概率较大， $p_0$  较大，但是在  $p_1$  内较少出现，因此很珍贵，要加大其比重！

## off-policy gradient

- Suppose  $\beta$  is the **behavior policy** that generates **experience samples**.
- Our aim is to use these samples to **update** a target policy  $\pi$  that can minimize the metric

$$J(\theta) = \sum_{s \in \mathcal{S}} d_\beta(s) v_\pi(s) = \mathbb{E}_{S \sim d_\beta} [v_\pi(S)]$$

where  $d_\beta$  is the **stationary distribution** under policy  $\beta$ .

So, in the discounted case where  $\gamma \in (0, 1)$ , the **gradient** of  $J(\theta)$  is

$$\nabla_\theta J(\theta) = \mathbb{E}_{S \sim \rho, A \sim \beta} \left[ \frac{\pi(A | S, \theta)}{\beta(A | S)} \nabla_\theta \ln \pi(A | S, \theta) q_\pi(S, A) \right]$$

where  $\beta$  is the behavior policy and  $\rho$  is a **state distribution**.

## The algorithm

### Off-policy actor-critic based on importance sampling

**Initialization:** A given behavior policy  $\beta(a|s)$ . A target policy  $\pi(a|s, \theta_0)$  where  $\theta_0$  is the initial parameter vector. A value function  $v(s, w_0)$  where  $w_0$  is the initial parameter vector.

**Aim:** Search for an optimal policy by maximizing  $J(\theta)$ .

At time step  $t$  in each episode, do

Generate  $a_t$  following  $\beta(s_t)$  and then observe  $r_{t+1}, s_{t+1}$ .

**TD error (advantage function):**

$$\delta_t = r_{t+1} + \gamma v(s_{t+1}, w_t) - v(s_t, w_t)$$

**Critic (value update):**

$$w_{t+1} = w_t + \alpha_w \frac{\pi(a_t | s_t, \theta_t)}{\beta(a_t | s_t)} \delta_t \nabla_w v(s_t, w_t)$$

**Actor (policy update):**

$$\theta_{t+1} = \theta_t + \alpha_\theta \frac{\pi(a_t | s_t, \theta_t)}{\beta(a_t | s_t)} \delta_t \nabla_\theta \ln \pi(a_t | s_t, \theta_t)$$

## DPG

## introduction

Up to now, the policies used in the policy gradient methods are all **stochastic** since  $\pi(a|s, \theta) > 0$  for every  $(s, a)$ .

Can we use deterministic policies in the policy gradient methods?

- Benefit: it can handle **continuous action**. (即action有无数个, 此时不能用随机的action, 必须确定性的action)
- Now, the deterministic policy is specifically denoted as

$$a = \mu(s, \theta) \doteq \mu(s)$$

- $\mu$  is a **mapping** from  $\mathcal{S}$  to  $\mathcal{A}$ . (从state映射到action space, 每个状态有确定性的动作)
- $\mu$  can be **represented by, for example, a neural network** with the input as  $s$ , the output as  $a$ , and the parameter as  $\theta$ .
- We may write  $\mu(s, \theta)$  in short as  $\mu(s)$ .

## deterministic policy gradient

$$J(\theta) = \mathbb{E}[v_\mu(s)] = \sum_{s \in \mathcal{S}} d_0(s) v_\mu(s)$$

where  $d_0(s)$  is a probability distribution satisfying  $\sum_{s \in \mathcal{S}} d_0(s) = 1$ .

- $d_0$  is selected to be independent of  $\mu$ . The gradient in this case is easier to calculate.
- There are two special yet important cases of selecting  $d_0$ .
  - The first special case is that  $d_0(s_0) = 1$  and  $d_0(s \neq s_0) = 0$ , where  $s_0$  is a specific starting state of interest.
  - The second special case is that  $d_0$  is the stationary distribution of a behavior policy that is different from the  $\mu$ .

In the discounted case where  $\gamma \in (0, 1)$ , the gradient of  $J(\theta)$  is

$$\begin{aligned} \nabla_\theta J(\theta) &= \sum_{s \in \mathcal{S}} \rho_\mu(s) \nabla_\theta \mu(s) (\nabla_a q_\mu(s, a)) \Big|_{a=\mu(s)} \\ &= \mathbb{E}_{S \sim \rho_\mu} \left[ \nabla_\theta \mu(S) (\nabla_a q_\mu(S, a)) \Big|_{a=\mu(S)} \right] \end{aligned}$$

Here,  $\rho_\mu$  is a state distribution.

## algorithm

**Initialization:** A given behavior policy  $\beta(a|s)$ . A deterministic target policy  $\mu(s, \theta_0)$  where  $\theta_0$  is the initial parameter vector. A value function  $v(s, w_0)$  where  $w_0$  is the initial parameter vector.

**Aim:** Search for an optimal policy by maximizing  $J(\theta)$ .

At time step  $t$  in each episode, do

Generate  $a_t$  following  $\beta$  and then observe  $r_{t+1}, s_{t+1}$ .

TD error:

$$\delta_t = r_{t+1} + \gamma q(s_{t+1}, \mu(s_{t+1}, \theta_t), w_t) - q(s_t, a_t, w_t)$$

Critic (value update):

$$w_{t+1} = w_t + \alpha_w \delta_t \nabla_w q(s_t, a_t, w_t)$$

Actor (policy update):

$$\theta_{t+1} = \theta_t + \alpha_\theta \nabla_\theta \mu(s_t, \theta_t) (\nabla_a q(s_t, a, w_{t+1}))|_{a=\mu(s_t)}$$

Remarks:

- This is an off-policy implementation where the behavior policy  $\beta$  may be different from  $\mu$ .
- $\beta$  can also be replaced by  $\mu + \text{noise}$ .
- How to select the function to represent  $q(s, a, w)$ ?
  - **Linear function:**  $q(s, a, w) = \phi^T(s, a)w$  where  $\phi(s, a)$  is the feature vector. Details can be found in the DPG paper.
  - **Neural networks:** deep deterministic policy gradient (DDPG) method.

Over!