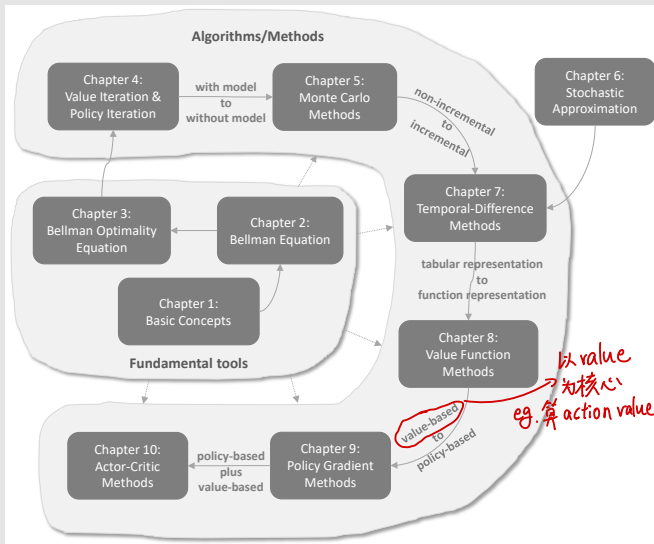


Lecture 9: Policy Gradient Methods

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Outline



In this lecture, we will move

- from value-based methods to policy-based methods
- from value function methods to policy function methods (or called policy gradient methods)

1 Basic idea of policy gradient

2 Metrics to define optimal policies

- Metric 1: Average value
- Metric 2: Average reward
- Summary of the two metrics

用梯度上升算法，
目标函数不同，要最大化

3 Gradients of the metrics

4 Gradient-ascent algorithm (REINFORCE)

5 Summary

- 1 Basic idea of policy gradient
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Basic idea of policy gradient

Previously, policies have been represented by tables:

- The action probabilities of all states are stored in a table $\pi(a|s)$. Each entry of the table is indexed by a state and an action.

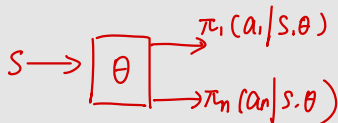
	a_1	a_2	a_3	a_4	a_5
s_1	$\pi(a_1 s_1)$	$\pi(a_2 s_1)$	$\pi(a_3 s_1)$	$\pi(a_4 s_1)$	$\pi(a_5 s_1)$
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
s_9	$\pi(a_1 s_9)$	$\pi(a_2 s_9)$	$\pi(a_3 s_9)$	$\pi(a_4 s_9)$	$\pi(a_5 s_9)$

Basic idea of policy gradient

Policies 的描述由表格 改为函数.

Now, policies can be represented by parameterized functions:

$$\pi(a|s, \theta)$$



where $\theta \in \mathbb{R}^m$ is a parameter vector.

- The function can be, for example, a neural network, whose input is s , output is the probability to take each action, and parameter is θ .
- **Advantage:** when the state space is large, the tabular representation will be of low efficiency in terms of storage and generalization.
- The function representation is also sometimes written as $\pi(a, s, \theta)$, $\pi_\theta(a|s)$, or $\pi_\theta(a, s)$.

Differences between tabular and function representations:

- First, how to define optimal policies?
 - In the tabular case, a policy π is optimal if it can maximize every state value.
 - In the function case, a policy π is optimal if it can maximize certain scalar metrics.

什么是最优策略？

表格: $V_{\pi^*}(S) \geq V_{\pi}(S)$ for $\forall \pi$

函数: 目标函数最优

Differences between tabular and function representations:

- Second, how to access the probability of an action?
 - In the tabular case, the probability of taking a at s can be directly accessed by looking up the tabular policy.
 - In the function case, we need to calculate the value of $\pi(a|s, \theta)$ given the function structure and the parameter.

Differences between tabular and function representations:

- Third, how to update policies?
 - In the tabular case, a policy π can be updated by directly changing the entries in the table.
 - In the function case, a policy π cannot be updated in this way anymore. Instead, it can only be updated by changing the parameter θ .

Basic idea of policy gradient

The basic idea of the policy gradient is simple:

目标函数

- First, metrics (or objective functions) to define optimal policies: $J(\theta)$, which can define optimal policies.
- Second, gradient-based optimization algorithms to search for optimal policies:

$$\theta_{t+1} = \theta_t + \alpha \nabla_{\theta} J(\theta_t) \leftarrow \text{梯度上升}$$

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

- What appropriate metrics should be used?
- How to calculate the gradients of the metrics?

These questions will be answered in detail in this lecture.

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- 2 Metrics to define optimal policies**
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1 Basic idea of policy gradient

目标函数

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Metric 1: average value

state value 的加权平均

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

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

所有 $d(s)$ 之和 = 1

- \bar{v}_π 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

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

Metric 1: average value

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

Case 1: d is **independent** of the policy π .

- This case is relatively simple because the gradient of the metric is easier to calculate: $\nabla_{\theta} \bar{v}_{\pi} = d^T \nabla_{\theta} v_{\pi}$ ← d 和 π 没关系, 则求梯度时只求 $\nabla_{\theta} v_{\pi}$ 即可
- In this case, we specifically denote d as d_0 and \bar{v}_{π} as \bar{v}_{π}^0 .

How to select d_0 ?

- One trivial way is to treat all the states **equally important** and hence select $d_0(s) = 1/|S|$. 一种情况: uniformly distribution.
- Another important case is that we are only interested in **a specific state** s_0 . For example, the episodes in some tasks always start from the same state s_0 . Then, we only care about the long-term return starting from s_0 . In this case,

另一种: 某-状态 s_0 特别重要,

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

In this case, $\bar{v}_{\pi} = v_{\pi}(s_0)$

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

Case 2: d depends on the policy π . d 和 π 有关系

- A common way is to select d as $d_\pi(s)$, which is the stationary distribution under π . Details of stationary distribution can be found in the last lecture and the book. 一般 d_π 是 stationary distribution, 即在长时间执行 π 和,
- The interpretation of selecting d_π is as follows. agent 出现在 S 的概率.
 - d_π reflects the long-run behavior of the Markov decision process under a given policy π .
$$d_\pi^T P_\pi = d_\pi^T$$
 - 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.

Metric 1: average value

An important equivalent expression:

You will see the following metric often in the literature:

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

Question: What is its relationship to the metric we introduced just now?

Answer: **They are the same.** That is because

$$\begin{aligned} J(\theta) &= \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t R_{t+1} \right] = \sum_{s \in \mathcal{S}} d(s) \mathbb{E} \left[\underbrace{\sum_{t=0}^{\infty} \gamma^t R_{t+1} | S_0 = s}_{\text{discounted return } G_t} \right] \\ &= \sum_{s \in \mathcal{S}} d(s) \underbrace{v_{\pi}(s)}_{\text{discounted return } G_t} \\ &= \bar{v}_{\pi} \end{aligned}$$

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Metric 2: average reward

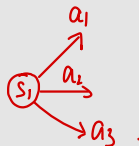
The second metric is **average one-step reward** or simply **average reward**:

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

where $S \sim d_\pi$,

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

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



$$\begin{aligned} r_\pi(s_1) &= \pi(a_1|s_1) r(s_1, a_1) \\ &\quad + \pi(a_2|s_1) r(s_1, a_2) \\ &\quad + \pi(a_3|s_1) r(s_1, a_3) \end{aligned}$$

Remarks:

- \bar{r}_π is simply a weighted average of immediate rewards.
- $r_\pi(s)$ is the average immediate reward that can be obtained from s .
- d_π is the stationary distribution.

An important equivalent expression:

从 s_0 开始的一条链 .

- Suppose an agent follows a given policy and generate a trajectory with the rewards as (R_1, R_2, \dots) .
- The average single-step reward along this trajectory is

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} [R_1 + R_2 + \dots + R_n | S_0 = s_0] \\ &= \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[\sum_{t=0}^{n-1} R_{t+1} | S_0 = s_0 \right] \end{aligned}$$

where s_0 is the starting state of the trajectory.

Metrics to define optimal policies - Remarks

除以 n 后, 自动算出 $d_\pi(s)$ 了.
有点像大数定律.

An important fact is that

$$\begin{aligned}\lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[\sum_{t=0}^{n-1} R_{t+1} | S_0 = s_0 \right] &= \lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[\sum_{t=0}^{n-1} R_{t+1} \right] \\ &= \sum_s d_\pi(s) r_\pi(s) \\ &= \bar{r}_\pi\end{aligned}$$

在无穷多步之后, S_0 是从哪开始
已经不重要了, trajectory 会涉及

✓ 所有的 states

Remarks:

- Highlight: the starting state s_0 does not matter.
- The derivation of the equation is nontrivial and can be found in my book.

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Summary of the two metrics

Metric	Expression 1	Expression 2	Expression 3
\bar{v}_π	$\sum_{s \in \mathcal{S}} d(s) v_\pi(s)$	$\mathbb{E}_{S \sim d}[v_\pi(S)]$	$\lim_{n \rightarrow \infty} \mathbb{E} \left[\sum_{t=0}^n \gamma^t R_{t+1} \right]$
\bar{r}_π	$\sum_{s \in \mathcal{S}} d_\pi(s) r_\pi(s)$	$\mathbb{E}_{S \sim d_\pi}[r_\pi(S)]$	$\lim_{n \rightarrow \infty} \frac{1}{n} \mathbb{E} \left[\sum_{t=0}^{n-1} R_{t+1} \right]$

Table: Summary of the different but equivalent expressions of \bar{v}_π and \bar{r}_π .

Summary of the two metrics

\bar{V}_π 和 \bar{r}_π 的取值由 θ 决定

Remark 1 about the metrics:

- All these metrics are functions of π .
- Since π is parameterized by θ , these metrics are functions of θ .
- In other words, different values of θ can generate different metric values.

Therefore, we can search for the optimal values of θ to maximize these metrics.
This is the basic idea of policy gradient methods.

Summary of the two metrics

$$\begin{aligned} V_t &= r_{t+1} + \gamma V_{t+1} \\ &= r_{t+1} + \gamma (r_{t+2} + \gamma V_{t+2}) \\ &= \dots \end{aligned}$$

Remark 2 about the metrics:

- One complication is that the metrics can be defined in either the ~~discounted~~ discounted case where $\gamma \in (0, 1)$ or the undiscounted case where $\gamma = 1$.
- The undiscounted case is nontrivial.
- We only consider the discounted case so far in this book. For details about the undiscounted case, see the book.

Remark 3 about the metrics:

- What is the relationship between \bar{r}_π and \bar{v}_π ?
- The two metrics are **equivalent** (not equal) to each other. Specifically, in the discounted case where $\gamma < 1$, it holds that

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

Therefore, they can be **maximized simultaneously**. See the proof in the book.

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Gradients of the metrics

Given a metric, we next

- derive its gradient
- and then, apply gradient-based methods to optimize the metric.

The gradient calculation is one of the most complicated parts of policy gradient methods! That is because

- first, we need to distinguish different metrics $\bar{v}_\pi, \bar{r}_\pi, \bar{v}_\pi^0$
- second, we need to distinguish discounted and undiscounted cases.

\bar{v}_π^0 指的是 $d_\pi(s)$ 和 π 是没有关系的

$d_\pi(s)$ 和 π 有关系: stationary distribution.

Gradients of the metrics

probability distribution (就是 $d_\pi(s)$)

I simply give the expression of the gradient without proof:

$$\nabla_\theta J(\theta) = \sum_{s \in \mathcal{S}} \underbrace{\eta(s)}_{\text{策略梯度}} \sum_{a \in \mathcal{A}} \underbrace{\nabla_\theta \pi(a|s, \theta) q_\pi(s, a)}_{\text{action value}}.$$

The above is a **unified expression of many cases**:

- $J(\theta)$ can be \bar{v}_π , \bar{r}_π , or \bar{v}_π^0 .
- “=” may denote strict equality, approximation, or proportional to.
- η is a distribution or weight of the states.

The derivation of this expression is **very complex**.

Details are not given here. Interested readers can read my book.

For most readers, it is sufficient to know this expression.

A compact and important expression of the gradient:

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

↓ S 满足 η 分布, A 满足 π 分布

First, why is this expression useful?

- Because we can use samples to approximate the gradient:

用采样近似

$$\nabla_{\theta} J \approx \nabla_{\theta} \ln \pi(a|s, \theta) q_{\pi}(s, a)$$

where s, a are samples. This is the idea of stochastic gradient descent.

A compact and important expression of the gradient:

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

Second, how to prove the above equation?

Proof: Consider the function $\ln \pi$ where \ln is the natural logarithm. It is easy to see that

$$\nabla_{\theta} \ln \pi(a|s, \theta) = \frac{\nabla_{\theta} \pi(a|s, \theta)}{\pi(a|s, \theta)}$$

$$\begin{aligned}\nabla \ln x &= \frac{1}{x} \\ \nabla \ln f(x) &= \frac{1}{f(x)} \cdot \nabla f(x)\end{aligned}$$

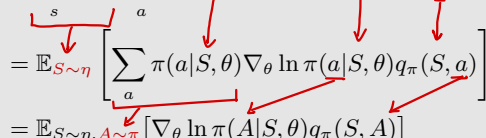
and hence

$$\nabla_{\theta} \pi(a|s, \theta) = \pi(a|s, \theta) \nabla_{\theta} \ln \pi(a|s, \theta).$$

A compact and important expression of the gradient:

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

Proof (continued): Then, we have

$$\begin{aligned}\nabla_{\theta} J &= \sum_s \eta(s) \sum_a \nabla_{\theta} \pi(a|s, \theta) q_{\pi}(s, a) \\ &= \sum_s \eta(s) \sum_a \pi(a|s, \theta) \nabla_{\theta} \ln \pi(a|s, \theta) q_{\pi}(s, a) \\ &= \mathbb{E}_{S \sim \eta} \left[\sum_a \pi(a|S, \theta) \nabla_{\theta} \ln \pi(a|S, \theta) q_{\pi}(S, a) \right] \\ &= \mathbb{E}_{S \sim \eta, A \sim \pi} [\nabla_{\theta} \ln \pi(A|S, \theta) q_{\pi}(S, A)]\end{aligned}$$


The diagram illustrates the derivation of the gradient expression. Red arrows indicate the mapping of variables between the equations:

- From the first equation to the second, s is mapped to S and a is mapped to A .
- From the second equation to the third, s is mapped to S and a is mapped to A .
- From the third equation to the fourth, S is mapped to S and A is mapped to A .

Remarks: It is required by $\ln \pi(a|s, \theta)$ that for any s, a, θ

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

- This can be achieved by using softmax functions that can normalize the entries in a vector from $(-\infty, +\infty)$ to $(0, 1)$.
 - For example, for any vector $x = [x_1, \dots, x_n]^T$,

$$z_i = \frac{e^{x_i}}{\sum_{j=1}^n e^{x_j}}$$

where $z_i \in (0, 1)$ and $\sum_{i=1}^n z_i = 1$.

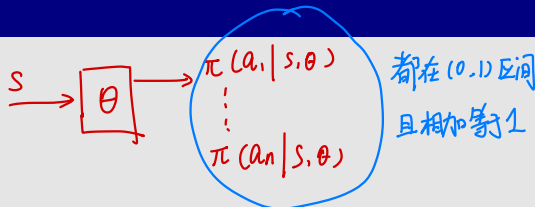
- Specifically, the policy function has the form of

$$\pi(a|s, \theta) = \frac{e^{h(s, a, \theta)}}{\sum_{a' \in \mathcal{A}} e^{h(s, a', \theta)}}$$

where $h(s, a, \theta)$ is another function to be learned.

归一化

在 (0, 1) 区间



Remarks:

- Such a form based on the softmax function can be realized by a neural network whose input is s and parameter is θ . The network has $|\mathcal{A}|$ outputs, each of which corresponds to $\pi(a|s, \theta)$ for an action a . The activation function of the output layer should be softmax.
- Since $\pi(a|s, \theta) > 0$ for all a , the parameterized policy is stochastic and hence exploratory.
 - There also exist deterministic policy gradient (DPG) methods. We will study in the next lecture.

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Now, we present [the first policy gradient algorithm](#) to find optimal policies!

1) The gradient-ascent algorithm maximizing $J(\theta)$ is

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

2) Since the true gradient is unknown, we can replace it by a stochastic one:

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

3) Furthermore, since q_{π} is unknown, it can be replaced by an estimate:

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

Gradient-ascent algorithm

- If $q_\pi(s_t, a_t)$ is estimated by Monte Carlo estimation, the algorithm has a specific name, **REINFORCE**.
- REINFORCE is one of the earliest and simplest policy gradient algorithms.
- Many other policy gradient algorithms such as the actor-critic methods can be obtained by extending REINFORCE (next lecture).

Pseudocode: Policy Gradient by Monte Carlo (REINFORCE)

Initialization: Initial parameter θ ; $\gamma \in (0, 1)$; $\alpha > 0$.

Goal: Learn an optimal policy to maximize $J(\theta)$.

For each episode, do

 Generate an episode $\{s_0, a_0, r_1, \dots, s_{T-1}, a_{T-1}, r_T\}$ following $\pi(\theta)$.

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

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

Policy update: $\theta \leftarrow \theta + \alpha \nabla_\theta \ln \pi(a_t | s_t, \theta) q_t(s_t, a_t)$

Remark 1: How to do sampling?

$$\mathbb{E}_{S \sim \eta, A \sim \pi} \left[\nabla_{\theta} \ln \pi(A|S, \theta_t) q_{\pi}(S, A) \right] \longrightarrow \nabla_{\theta} \ln \pi(a|s, \theta_t) q_{\pi}(s, a)$$

- How to sample S ?
 - $S \sim \eta$, where the distribution η is a long-run behavior under π .
 - In practice, people usually do not care about it.
- How to sample A ?
 - $A \sim \pi(A|S, \theta)$. Hence, a_t should be sampled following $\pi(\theta_t)$ at s_t .
 - Therefore, **policy gradient methods are on-policy**.

Remark 2: How to interpret this algorithm?

Since

$$\nabla_{\theta} \ln \pi(a_t | s_t, \theta_t) = \frac{\nabla_{\theta} \pi(a_t | s_t, \theta_t)}{\pi(a_t | s_t, \theta_t)}$$

the algorithm can be rewritten as

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

Therefore, we have the important expression of the algorithm:

$$\theta_{t+1} = \theta_t + \alpha \beta_t \nabla_{\theta} \pi(a_t | s_t, \theta_t)$$

The interpretation of

$$\theta_{t+1} = \theta_t + \alpha \beta_t \nabla_{\theta} \pi(a_t | s_t, \theta_t)$$

is as follows. Suppose that α is sufficiently small.

Interpretation:

- If $\beta_t > 0$, the probability of choosing (s_t, a_t) is increased:

$$\pi(a_t | s_t, \theta_{t+1}) > \pi(a_t | s_t, \theta_t)$$

- If $\beta_t < 0$, the probability of choosing (s_t, a_t) is lower:

$$\pi(a_t | s_t, \theta_{t+1}) < \pi(a_t | s_t, \theta_t)$$

Math: When $\theta_{t+1} - \theta_t$ is sufficiently small, the definition of differential implies

$$\begin{aligned}\pi(a_t | s_t, \theta_{t+1}) &\approx \pi(a_t | s_t, \theta_t) + (\nabla_{\theta} \pi(a_t | s_t, \theta_t))^T (\theta_{t+1} - \theta_t) \\ &= \pi(a_t | s_t, \theta_t) + \alpha \beta_t (\nabla_{\theta} \pi(a_t | s_t, \theta_t))^T (\nabla_{\theta} \pi(a_t | s_t, \theta_t)) \\ &= \pi(a_t | s_t, \theta_t) + \alpha \beta_t \|\nabla_{\theta} \pi(a_t | s_t, \theta_t)\|^2\end{aligned}$$

Gradient-ascent algorithm

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

Interpretation (continued): β_t can balance exploration and exploitation.

The reason is as follows.

- First, β_t is proportional to $q_t(s_t, a_t)$.

$$\text{greater } q_t(s_t, a_t) \implies \text{greater } \beta_t \implies \text{greater } \pi(a_t|s_t, \theta_{t+1})$$

Therefore, the algorithm intends to exploit actions with greater values.

- Second, β_t is inversely proportional to $\pi(a_t|s_t, \theta_t)$ (when $q_t(s_t, a_t) > 0$).

$$\text{smaller } \pi(a_t|s_t, \theta_t) \implies \text{greater } \beta_t \implies \text{greater } \pi(a_t|s_t, \theta_{t+1})$$

Therefore, the algorithm intends to explore actions that have low probabilities.

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Contents of this lecture:

- Metrics for optimality
- Gradients of the metrics
- Gradient-ascent algorithm
- A special case: REINFORCE

Next lecture: Actor-critic