Lecture 9: Policy Gradient Methods

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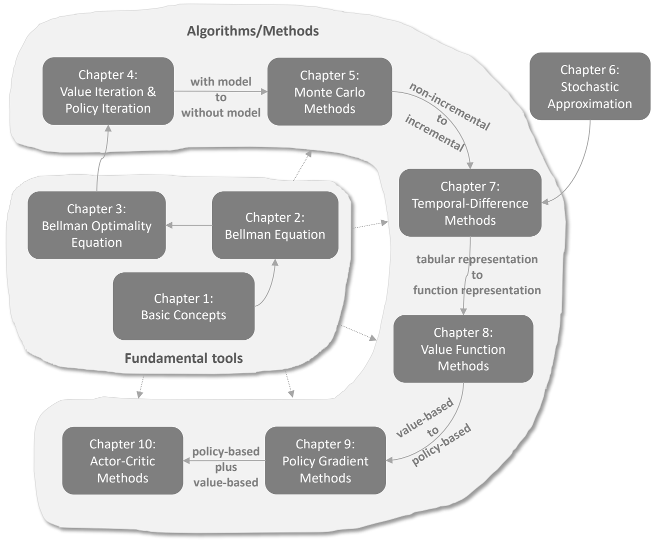
Outline



Algorithms/Methods
Chapter 4: Value Iteration & Policy Iteration
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Introduction

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)

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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

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*.

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:

- 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:

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

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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Metric 1: average value

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

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

- $\bar{v}_\pi$ 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

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

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: $\nabla_\theta \bar{v}_\pi = d^T \nabla_\theta v_\pi$
- In this case, we specifically denote d as d_0 and $\bar{v}_\pi$ as $\bar{v}_\pi^0$.

How to select d_0?

- One trivial way is to treat all the states equally important and hence select $d_0(s) = 1/|\mathcal{S}|$.
- 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,

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

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

Metric 1: average value

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

Case 2: d **depends** on the policy π.

- 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.
- The interpretation of selecting d_π is as follows.
  - d_π reflects the long-run behavior of the Markov decision process under a given policy π.
  - 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.

An important equivalent expression:

You will see the following metric often in the literature:

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

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

Answer: They are the same. That is because

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

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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 $S \sim d_\pi$,

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

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

Remarks:

- $\bar{r}_\pi$ 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:

- 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

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

where s_0 is the starting state of the trajectory.

Metrics to define optimal policies - Remarks

An important fact is that

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

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

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

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.

Remark 2 about the metrics:

- One complication is that the metrics can be defined in either the 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 $\bar{r}_\pi$ and $\bar{v}_\pi$?
- 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.

Outline

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.

Gradients of the metrics

I simply give the expression of the gradient without proof:

$$\nabla_\theta J(\theta) = \sum_{s\in\mathcal{S}} \eta(s) \sum_{a\in\mathcal{A}} \nabla_\theta \pi(a|s,\theta) q_\pi(s,a)$$

The above is a unified expression of many cases:

- $J(\theta)$ can be $\bar{v}_\pi$, $\bar{r}_\pi$, or $\bar{v}_\pi^0$.
- "$=$" 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:

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

First, why is this expression useful?

- Because we can use samples to approximate the gradient:

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

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

A compact and important expression of the gradient:

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

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

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

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:

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

Proof (continued): Then, we have

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

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.

Gradients of the metrics

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.

Outline

Now, we present the first policy gradient algorithm to find optimal policies!

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

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

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:

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

Gradient-ascent algorithm

- If $q_\pi(s_t, a_t)$ is estimated by Monte Carlo estimation, the algorithm has a specifics name, REINFORCE.
- REINFORCE is one of 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 $\{s_0, a_0, r_1, \ldots, s_{T-1}, a_{T-1}, r_T\}$ following $\pi(\theta)$.
  For $t = 0, 1, \ldots, T-1$:
    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?

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

- 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 $q_t(s_t, a_t)$.

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

  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 $q_t(s_t, a_t) > 0$).

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

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

Outline

Summary

Contents of this lecture:

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

Next lecture: Actor-critic