Lecture 3: Optimal Policy and Bellman Optimality Equation

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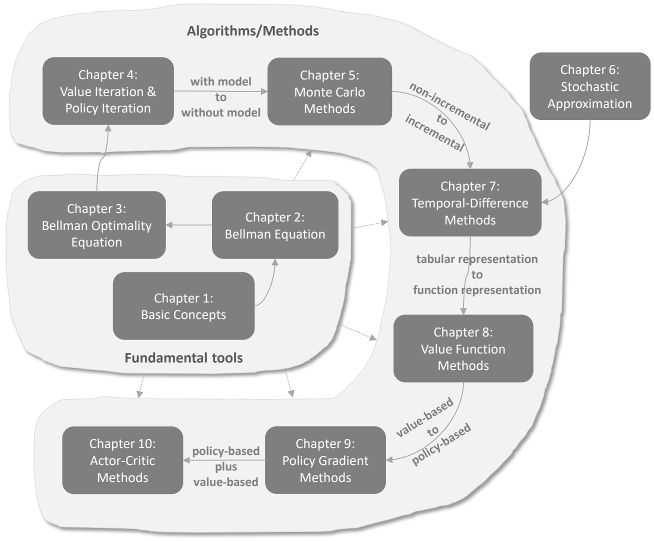
Outline



Algorithms/Methods
Chapter 4:
Value Iteration &
Policy Iteration
with model
to
without model
Chapter 5:
Monte Carlo
Methods
non-incremental
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Chapter 6:
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Methods
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Chapter 8:
Value Function
Methods
value-based
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Chapter 10:
Actor-Critic
Methods
Chapter 3:
Bellman Optimality
Equation
Chapter 2:
Bellman Equation
Chapter 1:
Basic Concepts
Fundamental tools

Outline

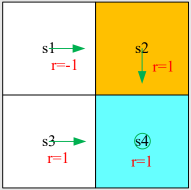
In this lecture:

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

Outline

Outline

Motivating examples



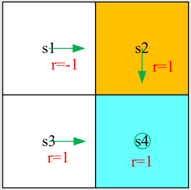
Exercise: write out the Bellman equation and solve the state values (set $\gamma = 0.9$)

Bellman equations:

$$
\begin{aligned}
v_\pi(s_1) &= -1 + \gamma v_\pi(s_2),\\
v_\pi(s_2) &= +1 + \gamma v_\pi(s_4),\\
v_\pi(s_3) &= +1 + \gamma v_\pi(s_4),\\
v_\pi(s_4) &= +1 + \gamma v_\pi(s_4).
\end{aligned}
$$

State values: $v_\pi(s_4) = v_\pi(s_3) = v_\pi(s_2) = 10, v_\pi(s_1) = 8$

Motivating examples



Exercise: calculate the action values of the five actions for s_1

Action values:

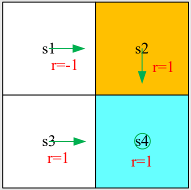
$$q_\pi(s_1,a_1) = -1 + \gamma v_\pi(s_1) = 6.2,$$

$$q_\pi(s_1,a_2) = -1 + \gamma v_\pi(s_2) = 8,$$

$$q_\pi(s_1,a_3) = 0 + \gamma v_\pi(s_3) = 9,$$

$$q_\pi(s_1,a_4) = -1 + \gamma v_\pi(s_1) = 6.2,$$

$$q_\pi(s_1,a_5) = 0 + \gamma v_\pi(s_1) = 7.2.$$



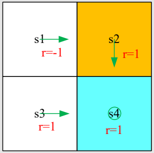
Question: While the policy is not good, how can we improve it?

Answer: We can improve the policy based on action values.

In particular, the current policy $\pi(a|s_1)$ is

$$\pi(a|s_1) = \begin{cases} 1 & a = a_2 \\ 0 & a \neq a_2 \end{cases}$$

Motivating examples

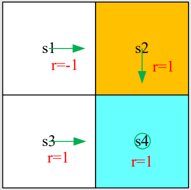


Observe the action values that we obtained just now:

$$q_\pi(s_1, a_1) = 6.2, \quad q_\pi(s_1, a_2) = 8, \quad q_\pi(s_1, a_3) = 9,$$
$$q_\pi(s_1, a_4) = 6.2, \quad q_\pi(s_1, a_5) = 7.2.$$

What if we select the greatest action value? Then, the new policy is

$$\pi_{\text{new}}(a|s_1) = \begin{cases} 1 & a = a_3 \\ 0 & a \neq a_3 \end{cases}$$



Question: why doing this can improve the policy?

- Intuition: easy! Actions with greater values are better.
- Math: nontrivial! Will be introduced in this and next lectures!

Outline

Optimal policy

The state value could be used to evaluate if a policy is good or not: if

$$v_{\pi_1}(s) \geq v_{\pi_2}(s) \quad \text{for all } s \in \mathcal{S}$$

then π_1 is "better" than π_2.

Definition

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

The definition leads to many questions:

- Does the optimal policy exist?
- Is the optimal policy unique?
- Is the optimal policy stochastic or deterministic?
- How to obtain the optimal policy?

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

Outline

Bellman optimality equation (BOE)

Bellman optimality equation (elementwise form):

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

Remarks:

- $p(r|s,a), p(s'|s,a)$, r, γ are known.
- $v(s), v(s')$ are unknown and to be calculated.
- Is $\pi(s)$ known or unknown?

Bellman optimality equation (matrix-vector form):

$$v = \max_{\pi}(r_\pi + \gamma P_\pi v)$$

where the elements corresponding to s or s' are

$$[r_\pi]_s \triangleq \sum_a \pi(a|s) \sum_r p(r|s,a) r,$$

$$[P_\pi]_{s,s'} = p(s'|s) \triangleq \sum_a \pi(a|s) \sum_{s'} p(s'|s,a)$$

Here $\max_\pi$ is performed elementwise:

$$\max_{\pi} \begin{bmatrix} * \\ \vdots \\ * \end{bmatrix} = \begin{bmatrix} \max_{\pi(s_1)} * \\ \vdots \\ \max_{\pi(s_n)} * \end{bmatrix}$$

Bellman optimality equation (BOE)

Bellman optimality equation (matrix-vector form):

$$v = \max_{\pi}(r_\pi + \gamma P_\pi v)$$

- BOE is tricky yet elegant!
  - Why elegant? It describes the optimal policy and optimal state value in an elegant way.
  - Why tricky? There is a maximization on the right-hand side, which may not be straightforward to see how to compute.
- This lecture will answer all the following questions:
  - Algorithm: how to solve this equation?
  - Existence: does this equation have solutions?
  - Uniqueness: is the solution to this equation unique?
  - Optimality: how is it related to optimal policy?

Outline

Outline

BOE: elementwise form

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

BOE: matrix-vector form $v = \max_\pi (r_\pi + \gamma P_\pi v)$

Example (How to solve two unknowns from one equation)

Solve two unknown variables $x, a \in \mathbb{R}$ from the following equation:

$$x = \max_a (2x - 1 - a^2).$$

To solve them, first consider the right hand side. Regardless the value of x, $\max_a (2x - 1 - a^2) = 2x - 1$ where the maximization is achieved when $a = 0$. Second, when $a = 0$, the equation becomes $x = 2x - 1$, which leads to $x = 1$. Therefore, $a = 0$ and $x = 1$ are the solution of the equation.

Maximization on the right-hand side of BOE

Fix $v'(s)$ first and solve π:

$$
\begin{aligned}
v(s) &= \max_\pi \sum_a \pi(a|s) \left(\sum_r p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v(s') \right), \quad \forall s \in \mathcal{S} \\
&= \max_\pi \sum_a \pi(a|s)q(s,a) = \max_\pi \left[\pi(a_1|s)q(s,a_1) + \cdots + \pi(a_5|s)q(s,a_5) \right] \\
&\doteq \max_{c_1,\ldots,c_5} \left[c_1 q(s,a_1) + \cdots + c_5 q(s,a_5) \right], \qquad c_1 + \cdots + c_5 = 1
\end{aligned}
$$

Example (How to solve $\max_\pi \sum_a \pi(a|s)q(s,a)$)

Suppose $q_1, q_2, q_3 \in \mathbb{R}$ are given. Find c_1^*, c_2^*, c_3^* solving

$$\max_{c_1,c_2,c_3} c_1q_1 + c_2q_2 + c_3q_3.$$

where $c_1 + c_2 + c_3 = 1$ and $c_1, c_2, c_3 \geq 0$.

Answer: Suppose $q_3 \geq q_1, q_2$. Then, the optimal solution is $c_3^* = 1$ and $c_1^* = c_2^* = 0$. That is because for any c_1, c_2, c_3

$$q_3 = (c_1 + c_2 + c_3)q_3 = c_1q_3 + c_2q_3 + c_3q_3 \geq c_1q_1 + c_2q_2 + c_3q_3.$$

Maximization on the right-hand side of BOE

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

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

where the optimality is achieved when

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

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

Outline

Solve the Bellman optimality equation

The BOE is $v = \max_\pi(r_\pi + \gamma P_\pi v)$. Let

$$f(v) := \max_\pi(r_\pi + \gamma P_\pi v)$$

Then, the Bellman optimality equation becomes

$$v = f(v)$$

where

$$[f(v)]_s = \max_\pi \sum_a \pi(a|s)q(s,a), \quad s \in \mathcal{S}$$

This equation looks very simple. How to solve it?

Outline

Some concepts:

- Fixed point: $x \in X$ is a fixed point of $f : X \to X$ 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 $\gamma \in (0, 1)$.

  - γ must be strictly less than 1 so that many limits such as $\gamma^k \to 0$ as $k \to 0$ hold.
  - Here $\|\cdot\|$ can be any vector norm.

Examples to demonstrate the concepts.

Example

- $x = f(x) = 0.5x$, $x \in \mathbb{R}$.

  It is easy to verify that $x = 0$ is a fixed point since $0 = 0.5 \times 0$. Moreover, $f(x) = 0.5x$ is a contraction mapping because $\|0.5x_1 - 0.5x_2\| = 0.5\|x_1 - x_2\| \leq \gamma\|x_1 - x_2\|$ for any $\gamma \in [0.5, 1)$.

- $x = f(x) = Ax$, where $x \in \mathbb{R}^n, A \in \mathbb{R}^{n \times n}$ and $\|A\| \leq \gamma < 1$.

  It is easy to verify that $x = 0$ is a fixed point since $0 = A0$. To see the contraction property, $\|Ax_1 - Ax_2\| = \|A(x_1 - x_2)\| \leq \|A\|\|x_1 - x_2\| \leq \gamma\|x_1 - x_2\|$. Therefore, $f(x) = Ax$ is a contraction mapping.

Theorem (Contraction Mapping Theorem)

For any equation that has the form of $x = f(x)$, if f is a contraction mapping, then

- **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 $x_k \to x^*$ as $k \to \infty$. Moreover, the convergence rate is exponentially fast.*

For the proof of this theorem, see the book.

Examples:

- $x = 0.5x$, where $f(x) = 0.5x$ and $x \in \mathbb{R}$
  $x^* = 0$ is the unique fixed point. It can be solved iteratively by
  $$x_{k+1} = 0.5x_k$$
- $x = Ax$, where $f(x) = Ax$ and $x \in \mathbb{R}^n, A \in \mathbb{R}^{n\times n}$ and $\|A\| < 1$
  $x^* = 0$ is the unique fixed point. It can be solved iteratively by
  $$x_{k+1} = Ax_k$$

Outline

Let's come back to the Bellman optimality equation:

$$v = f(v) = \max_{\pi}(r_\pi + \gamma P_\pi v)$$

Theorem (Contraction Property)

$f(v)$ is a contraction mapping satisfying

$$\|f(v_1) - f(v_2)\| \leq \gamma \|v_1 - v_2\|$$

where γ is the discount rate!

For the proof of this lemma, see our book.

Applying the contraction mapping theorem gives the following results.

Theorem (Existence, Uniqueness, and Algorithm)

For the BOE $v = f(v) = \max_\pi(r_\pi + \gamma P_\pi v)$, there always exists a solution v^* and the solution is unique. The solution could be solved iteratively by

$$v_{k+1} = f(v_k) = \max_\pi(r_\pi + \gamma P_\pi v_k) \tag{1}$$

This sequence $\{v_k\}$ converges to v^* exponentially fast given any initial guess v_0. The convergence rate is determined by γ.

Important: The algorithm in (1) is called the value iteration algorithm. We will analyze it in the next lecture! This lecture focuses more on the fundamental properties.

Outline

Policy optimality

Suppose v^* is the solution to the Bellman optimality equation. It satisfies

$$v^* = \max_\pi (r_\pi + \gamma P_\pi v^*)$$

Suppose

$$\pi^* = \arg\max_\pi (r_\pi + \gamma P_\pi v^*)$$

Then

$$v^* = r_{\pi^*} + \gamma P_{\pi^*} v^*$$

Therefore, π^* is a policy and $v^* = v_{\pi^*}$ is the corresponding state value.

Is π^* the optimal policy? Is v^* the greatest state value can be achieved?

Policy optimality

Theorem (Policy Optimality)

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

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

For the proof, please see our book.

Now we understand why we study the BOE. That is because it describes the optimal state value and optimal policy.

Optimal policy

What does an optimal policy π^* look like?

$$\pi^*(s) = \arg\max_{\pi} \sum_a \pi(a|s) \underbrace{\left(\sum_r p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v^*(s') \right)}_{q^*(s,a)}$$

Theorem (Greedy Optimal Policy)

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

Outline

Analyzing optimal policies

What factors determine the optimal state value and optimal policy?

It can be clearly seen from the BOE

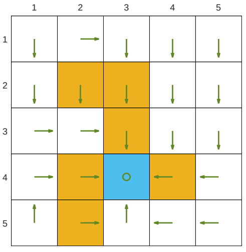
$$v(s) = \max_{\pi} \sum_a \pi(a|s) \left(\sum_r p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v(s') \right)$$

that there are three factors:

- System model: $p(s'|s,a)$, $p(r|s,a)$
- Reward design: r
- Discount rate: γ

We next show how r and γ can affect the optimal policy.

The optimal policy and the corresponding optimal state value are obtained by solving the BOE.

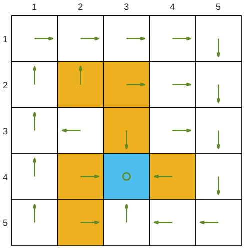


	1	2	3	4	5
1	5.8	5.6	6.2	6.5	5.8
2	6.5	7.2	8.0	7.2	6.5
3	7.2	8.0	10.0	8.0	7.2
4	8.0	10.0	10.0	10.0	8.0
5	7.2	9.0	10.0	9.0	8.1

(a) $r_{\text{boundary}} = r_{\text{forbidden}} = -1$, $r_{\text{target}} = 1$, $\gamma = 0.9$

The optimal policy dares to take risks: entering forbidden areas!!

If we change $\gamma = 0.9$ to $\gamma = 0.5$



	1	2	3	4	5
1	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.1
3	0.0	0.0	2.0	0.1	0.1
4	0.0	2.0	2.0	2.0	0.2
5	0.0	1.0	2.0	1.0	0.5

(b) The discount rate is $\gamma = 0.5$. Others are the same as (a).

The optimal policy becomes shorted-sighted! Avoid all the forbidden areas!

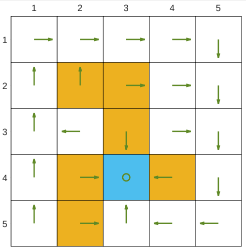
Analyzing optimal policies

If we change γ to 0

(c) The discount rate is $\gamma = 0$. Others are the same as (a).

The optimal policy becomes extremely short-sighted! Also, choose the action that has the greatest *immediate reward*! Cannot reach the target!

If we increase the punishment when entering forbidden areas: change $r_{\text{forbidden}} = -1$ to $r_{\text{forbidden}} = -10$



	1	2	3	4	5
1	3.5	3.9	4.3	4.8	5.3
2	3.1	3.5	4.8	5.3	5.9
3	2.8	2.5	10.0	5.9	6.6
4	2.5	10.0	10.0	10.0	7.3
5	2.3	9.0	10.0	9.0	8.1

(d) $r_{\text{forbidden}} = -10$. Others are the same as (a).

The optimal policy would also avoid the forbidden areas.

What if we change $r \to ar + b$?

For example,

$$r_{\text{boundary}} = r_{\text{forbidden}} = -1, \quad r_{\text{target}} = 1, \quad r_{\text{otherstep}} = 0$$

becomes

$$r_{\text{boundary}} = r_{\text{forbidden}} = 0, \quad r_{\text{target}} = 2, \quad r_{\text{otherstep}} = 1$$

The optimal policy remains the same!

What matters is not the absolute reward values! It is their relative values!

Analyzing optimal policies (optional)

Theorem (Optimal Policy Invariance)

Consider a Markov decision process with $v^* \in \mathbb{R}^{|\mathcal{S}|}$ as the optimal state value satisfying $v^* = \max_\pi(r_\pi + \gamma P_\pi v^*)$. If every reward r is changed by an affine transformation to $ar + b$, where $a, b \in \mathbb{R}$ and $a > 0$, then the corresponding optimal state value v' is also an affine transformation of v^*:

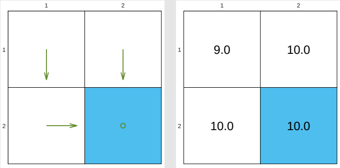
$$v' = av^* + \frac{b}{1-\gamma}\mathbf{1},$$

where $\gamma \in (0, 1)$ is the discount rate and $\mathbf{1} = [1, \ldots, 1]^T$. Consequently, the optimal policies are invariant to the affine transformation of the reward signals.

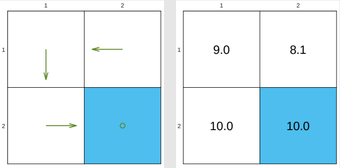
The proof is given in my book.

Analyzing optimal policies

Meaningless detour?



(a) Optimal policy



(b) Not optimal

Question: Why does the optimal policy not take meaningless detours? We don't punish for taking detours because $r_{\text{otherstep}} = 0$.

Answer: Wrong! We do punish by using the discount rate!

Policy (a): $\text{return} = 1 + \gamma 1 + \gamma^2 1 + \cdots = 1/(1-\gamma) = 10.$

Policy (b): $\text{return} = 0 + \gamma 0 + \gamma^2 1 + \gamma^3 1 + \cdots = \gamma^2/(1-\gamma) = 8.1$

Summary

Bellman optimality equation:

- Elementwise form:

$$v(s) = \max_{\pi} \sum_{a} \pi(a|s) \underbrace{\left(\sum_{r} p(r|s,a)r + \gamma \sum_{s'} p(s'|s,a)v(s') \right)}_{q(s,a)}, \quad \forall s \in \mathcal{S}$$

- Matrix-vector form:

$$v = \max_{\pi} (r_\pi + \gamma P_\pi v)$$

Summary

Questions about the Bellman optimality equation:

- Existence: does this equation have solutions?
  - Yes, by the contraction mapping theorem
- Uniqueness: is the solution to this equation unique?
  - Yes, by the contraction mapping theorem
- Algorithm: how to solve this equation?
  - Iterative algorithm suggested by the contraction mapping theorem
- Optimality: why we study this equation
  - Because its solution corresponds to the optimal state value and optimal policy.

Finally, we understand why it is important to study the BOE!