

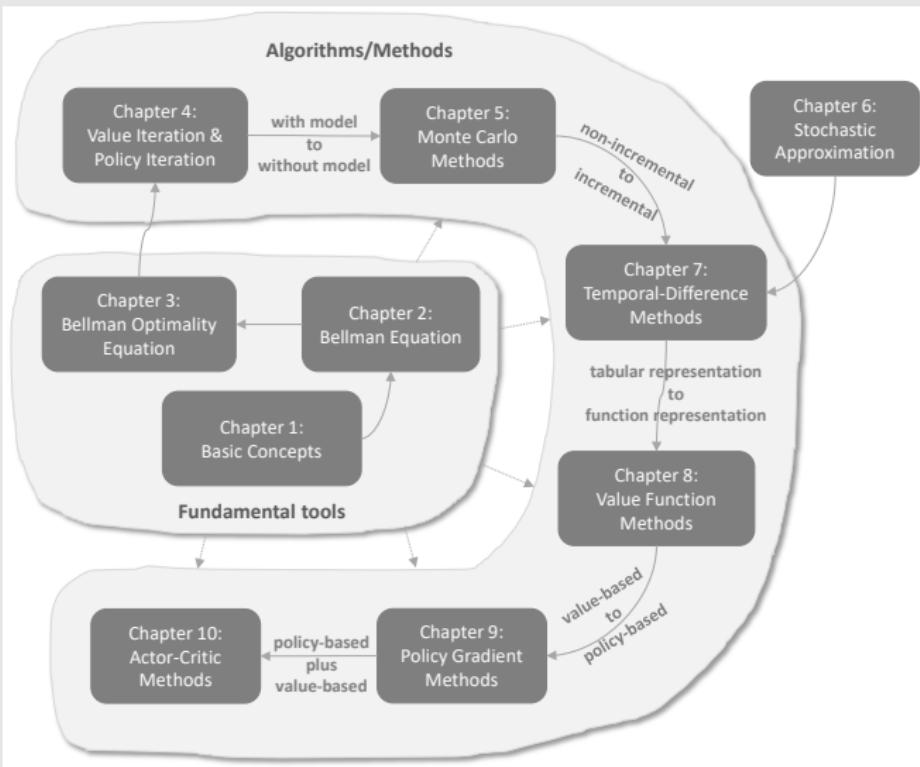
Lecture 3: Optimal Policy and Bellman Optimality Equation

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Outline



Outline

In this lecture:

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

Outline

1 Motivating examples

2 Definition of optimal policy

3 BOE: Introduction

4 BOE: Preliminaries

- BOE: Maximization on the right-hand side
- BOE: Rewrite as $v = f(v)$
- Contraction mapping theorem

5 BOE: Solution

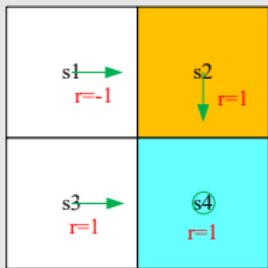
6 BOE: Optimality

7 Analyzing optimal policies

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Motivating examples



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

Answer: Bellman equations:

$$v_{\pi}(s_1) = -1 + \gamma v_{\pi}(s_2),$$

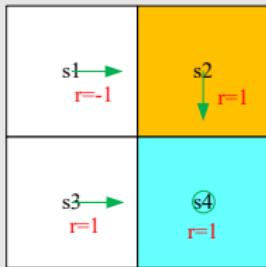
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State values: $v_{\pi}(s_4) = v_{\pi}(s_3) = v_{\pi}(s_2) = 10, v_{\pi}(s_1) = 8$

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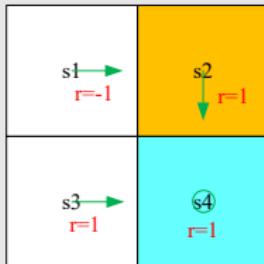
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Motivating examples



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

Answer: Action values:

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

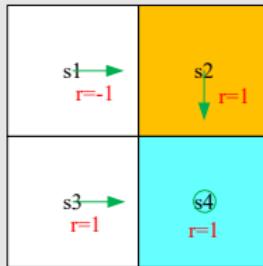
$$q_\pi(s_1, a_2) = -1 + \gamma v_\pi(s_2) = 8,$$

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

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

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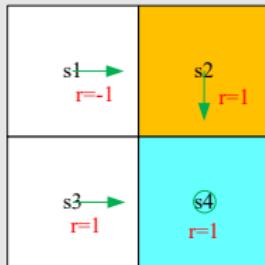
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Motivating examples



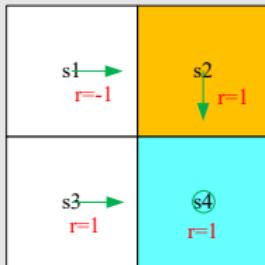
Question: While the policy is not good, how can we improve it?

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



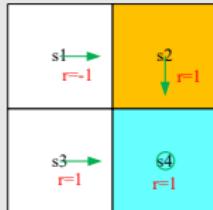
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Motivating examples



Observe the action values that we obtained just now:

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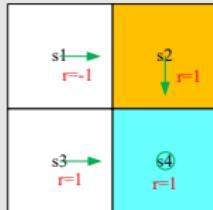
$$q_{\pi}(s_1, a_4) = 6.2, \quad q_{\pi}(s_1, a_5) = 7.2.$$

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

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

The new policy can avoid the forbidden area and seems better.

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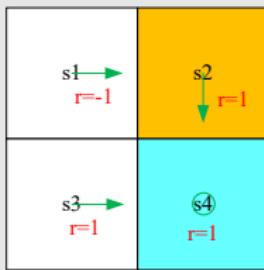
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Motivating examples



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!

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Optimal policy

State value can be used to evaluate whether 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 .

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 need the Bellman optimality equation.

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

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Bellman optimality equation (BOE)

Bellman optimality equation (elementwise form):

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

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Remarks:

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

Bellman optimality equation (BOE)

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_{π} 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)

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

- 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?

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Maximization on the right-hand side of BOE

BOE: elementwise form

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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 :

$$\begin{aligned} v(s) &= \max_{\pi} \sum_a \pi(a|s) \left(\sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a)v(s') \right), \quad \forall s \in \mathcal{S} \\ &= \max_{\pi} \sum_a \pi(a|s)q(s, a) = \max_{\pi} [\pi(a_1|s)q(s, a_1) + \dots + \pi(a_5|s)q(s, a_5)] \\ &\doteq \max_{c_1, \dots, c_5} [c_1q(s, a_1) + \dots + c_5q(s, a_5)], \quad c_1 + \dots + c_5 = 1 \end{aligned}$$

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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 $c_1, c_2, c_3 \geq 0$.

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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

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

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

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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?

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Preliminaries: Contraction mapping theorem

Some concepts:

- **Fixed point:** $x \in X$ 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 $\gamma \in (0, 1)$.

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

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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

$$\|0.5x_1 - 0.5x_2\| = 0.5\|x_1 - x_2\| \leq \gamma\|x_1 - x_2\| \text{ for any } \gamma \in [0.5, 1).$$

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- $x = f(x) = Ax$, 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,

$$\|Ax_1 - Ax_2\| = \|A(x_1 - x_2)\| \leq \|A\|\|x_1 - x_2\| \leq \gamma\|x_1 - x_2\|. \text{ Therefore, } f(x) = Ax \text{ is a contraction mapping.}$$

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 $\{x_k\}$ generated by*

$$x_{k+1} = f(x_k)$$

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

For the proof of this theorem, see the book.

Preliminaries: Contraction mapping theorem

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 $\|A\| < 1$
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- 1 Motivating examples
- 2 Definition of optimal policy
- 3 BOE: Introduction
- 4 BOE: Preliminaries
 - BOE: Maximization on the right-hand side
 - BOE: Rewrite as $v = f(v)$
 - Contraction mapping theorem
- 5 BOE: Solution
- 6 BOE: Optimality
- 7 Analyzing optimal policies

Contraction property of BOE

Let's come back to the Bellman optimality equation:

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

The proof is omitted here and can be found in my book.

Contraction property of BOE

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 that satisfies

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

where γ is the discount rate!

The proof is omitted here and can be found in my book.

Solve the Bellman optimality equation

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

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

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

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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?

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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 my book.

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

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Optimal policy

What does an optimal policy π^* look like?

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

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

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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.

Analyzing optimal policies

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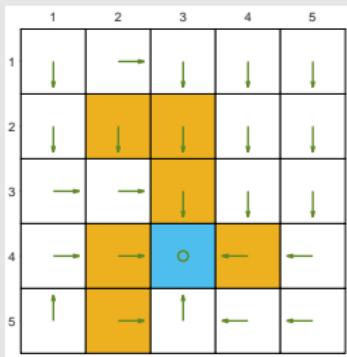
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Analyzing optimal policies

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



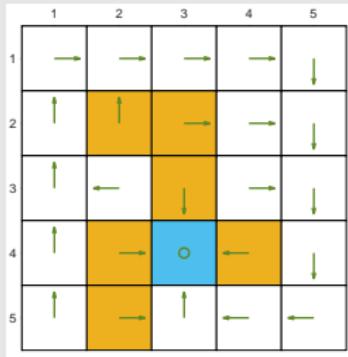
	1	2	3	4	5
1	5.8	5.6	6.2	6.5	5.8
2	6.5	7.2	8.0	7.2	6.5
3	7.2	8.0	10.0	8.0	7.2
4	8.0	10.0	10.0	10.0	8.0
5	7.2	9.0	10.0	9.0	8.1

(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!!

Analyzing optimal policies

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



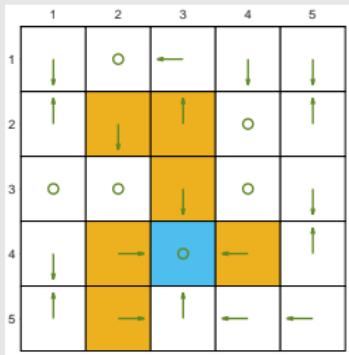
	1	2	3	4	5
1	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.1
3	0.0	0.0	2.0	0.1	0.1
4	0.0	2.0	2.0	2.0	0.2
5	0.0	1.0	2.0	1.0	0.5

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

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

Analyzing optimal policies

If we change γ to 0



	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	0.0
3	0.0	0.0	1.0	0.0	0.0
4	0.0	1.0	1.0	1.0	0.0
5	0.0	0.0	1.0	0.0	0.0

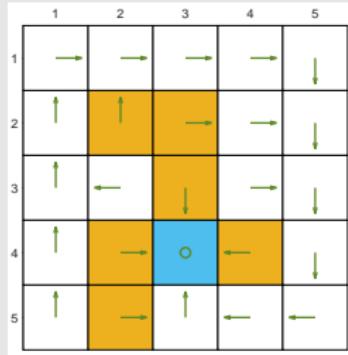
(c) The discount rate is $\gamma = 0$. Others are the same as (a).

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

Analyzing optimal policies

If we increase the punishment when entering forbidden areas: change

$$r_{\text{forbidden}} = -1 \text{ to } r_{\text{forbidden}} = -10$$



	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.

Analyzing optimal policies

What if we change $r \rightarrow ar + b$ ($a > 0$)?

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^* :

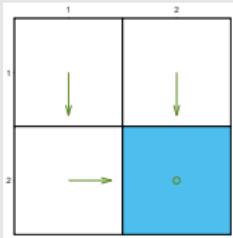
$$v' = av^* + \frac{b}{1 - \gamma} \mathbf{1},$$

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

The proof is given in my book.

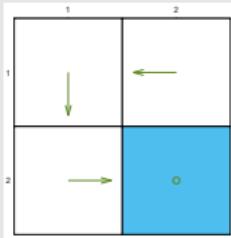
Analyzing optimal policies

Meaningless detour?



(a) Optimal policy

1	2	
1	9.0	10.0
2	10.0	10.0



(b) Not optimal

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

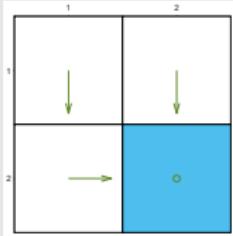
Answer: We do punish by using the discount rate!

Policy (a): return = $1 + \gamma 1 + \gamma^2 1 + \dots = 1/(1 - \gamma) = 10$

Policy (b): return = $0 + \gamma 0 + \gamma^2 1 + \gamma^3 1 + \dots = \gamma^2/(1 - \gamma) = 8.1$

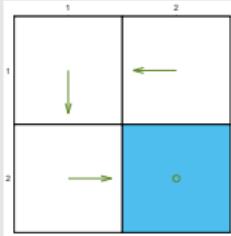
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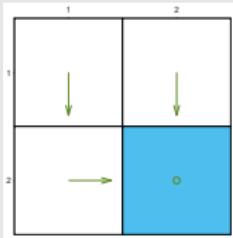
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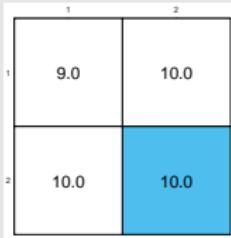
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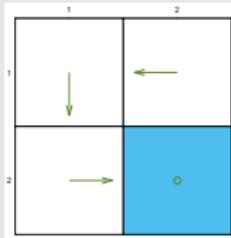
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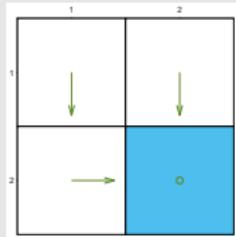
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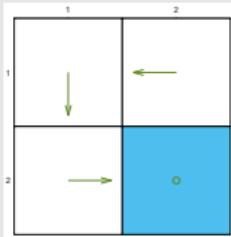
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Summary

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?
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 - Iterative algorithm suggested by the contraction mapping theorem
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