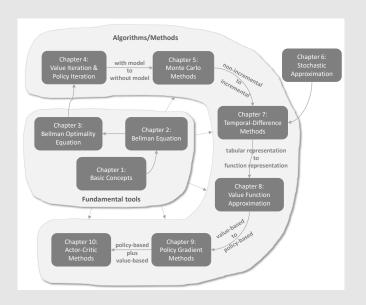
# Lecture 3: Optimal Policy and Bellman Optimality Equation

Shiyu Zhao



Shiyu Zhao

#### In this lecture:

• Core concepts: optimal state value and optimal policy

• A fundamental tool: Bellman optimality equation (BOE)

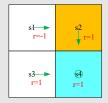
Shiyu Zhao 2 / 45

- 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

Shiyu Zhao 3/45

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

Bellman equations:

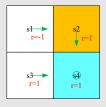
$$v_{\pi}(s_1) = -1 + \gamma v_{\pi}(s_2),$$
  

$$v_{\pi}(s_2) = +1 + \gamma v_{\pi}(s_4),$$
  

$$v_{\pi}(s_3) = +1 + \gamma v_{\pi}(s_4),$$
  

$$v_{\pi}(s_4) = +1 + \gamma v_{\pi}(s_4).$$

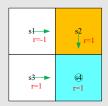
State values:  $v_{\pi}(s_4) = v_{\pi}(s_3) = v_{\pi}(s_2) = 10, v_{\pi}(s_1) = 8$ 



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

$$\begin{aligned} q_{\pi}(s_1, a_1) &= -1 + \gamma v_{\pi}(s_1) = 6.2, \\ q_{\pi}(s_1, a_2) &= -1 + \gamma v_{\pi}(s_2) = 8, \\ q_{\pi}(s_1, a_3) &= 0 + \gamma v_{\pi}(s_3) = 9, \\ q_{\pi}(s_1, a_4) &= -1 + \gamma v_{\pi}(s_1) = 6.2, \\ q_{\pi}(s_1, a_5) &= 0 + \gamma v_{\pi}(s_1) = 7.2. \end{aligned}$$

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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

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

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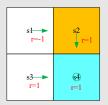
Observe the action values that we obtained just now:

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

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

$$\pi_{\mathsf{new}}(a|s_1) = \left\{ \begin{array}{ll} 1 & a = a_3 \\ 0 & a \neq a_3 \end{array} \right.$$

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## 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!

Shiyu Zhao 9 / 45

- 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

Shiyu Zhao 10 / 45

# Optimal policy

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

$$v_{\pi_1}(s) \ge v_{\pi_2}(s)$$
 for all  $s \in \mathcal{S}$ 

then  $\pi_1$  is "better" than  $\pi_2$ .

#### Definition

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?
- 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.

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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

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# Bellman optimality equation (BOE)

## Bellman optimality equation (elementwise form):

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

#### Remarks:

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

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# 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  $s^\prime$  are

$$\begin{split} [r_{\pi}]_s &\triangleq \sum_a \pi(a|s) \sum_r p(r|s,a)r, \\ [P_{\pi}]_{s,s'} &= p(s'|s) \triangleq \sum_a \pi(a|s) \sum_{s'} p(s'|s,a) \end{split}$$

Here  $\max_{\pi}$  is performed elementwise.

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# 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?

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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

Shiyu Zhao 16/45

- 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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# Maximization on the right-hand side of BOE

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.

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# Maximization on the right-hand side of BOE

Fix v'(s) first and solve  $\pi$ :

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

$$= \max_{\pi} \sum_{a} \pi(a|s)q(s, a) = \max_{\pi} \left[ \pi(a_1|s)q(s, a_1) + \dots + \pi(a_5|s)q(s, a_5) \right]$$

$$\doteq \max_{c_1, \dots, c_5} \left[ c_1 q(s, a_1) + \dots + c_5 q(s, a_5) \right], \quad c_1 + \dots + c_5 = 1$$

## 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

$$\max_{c_1, c_2, c_3} c_1 q_1 + c_2 q_2 + c_3 q_3.$$

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

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  $c_1,c_2,c_3$ 

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

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

Shiyu Zhao 20 / 4

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

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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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- 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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#### 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

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

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

- $\gamma$  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.

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

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## 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.

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#### 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

$$x_{k+1} = Ax_k$$

Shiyu Zhao 27/45

- 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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# 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 satisfying

$$||f(v_1) - f(v_2)|| \le \frac{\gamma}{\|v_1 - v_2\|}$$

where  $\gamma$  is the discount rate!

For the proof of this lemma, see our book.

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# 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

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

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

**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.

Shiyu Zhao 30 / 45

- 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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# Policy optimality

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

Is  $\pi^*$  the optimal policy? Is  $v^*$  the greatest state value can be achieved?

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# Policy optimality

## Theorem (Policy Optimality)

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

$$v^* \ge v_{\pi}, \quad \forall \pi$$

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.

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# Optimal policy

What does an optimal policy  $\pi^*$  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  $q^*(s, a) \doteq \sum_r p(r|s, a)r + \gamma \sum_{s'} p(s'|s, a)v^*(s')$ .

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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

Shiyu Zhao 35 / 45

What factors determine the optimal state value and optimal policy? It can be clearly seen from the BOE

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

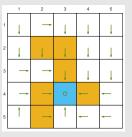
that there are three factors:

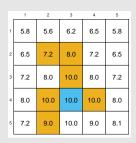
- System model: p(s'|s, a), p(r|s, a)
- ullet Reward design: r
- Discount rate:  $\gamma$

We next show how r and  $\gamma$  can affect the optimal policy.

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



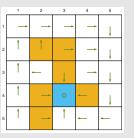


(a) 
$$r_{\rm boundary} = r_{\rm forbidden} = -1$$
,  $r_{\rm target} = 1$ ,  $\gamma = 0.9$ 

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

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



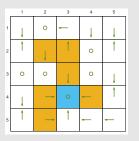


(b) The discount rate is  $\gamma=0.5$ . Others are the same as (a).

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

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If we change  $\gamma$  to 0





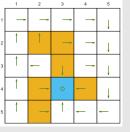
(c) The discount rate is  $\gamma = 0$ . Others are the same as (a).

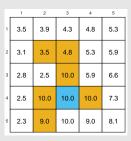
The optimal policy becomes extremely short-sighted! Also, choose the action that has the greatest *immediate reward*! Cannot reach the target!

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If we increase the punishment when entering forbidden areas: change

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





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

The optimal policy would also avoid the forbidden areas.

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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!

Shiyu Zhao 41 / 45

# 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  $v^*$ :

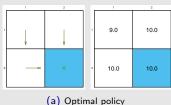
$$v' = av^* + \frac{b}{1 - \gamma} \mathbf{1},$$

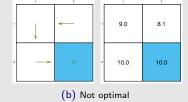
where  $\gamma \in (0,1)$  is the discount rate and  $\mathbf{1} = [1,\ldots,1]^T$ . Consequently, the optimal policies are invariant to the affine transformation of the reward signals.

The proof is given in my book.

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## Meaningless detour?





(a) Optimal policy

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

Answer: Wrong! 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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# 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:

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

Shiyu Zhao 44 / 45

## 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!

Shiyu Zhao 45 / 45