# Lecture 3: Optimal Policy and Bellman Optimality Equation

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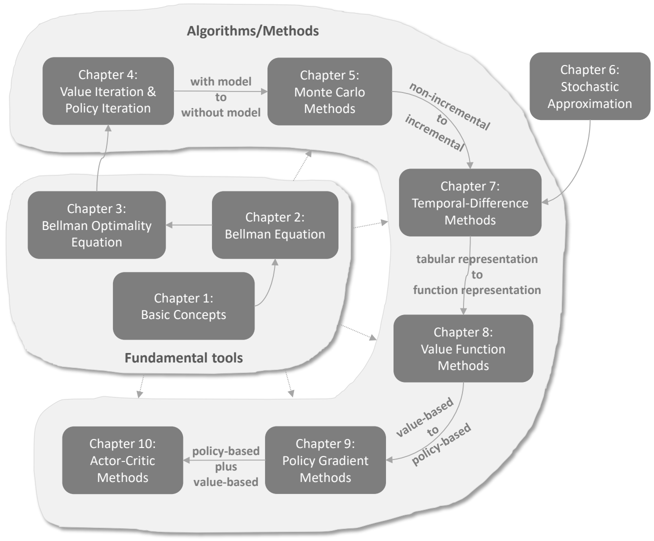
# Outline



Algorithms/Methods
Chapter 4: Value Iteration & Policy Iteration
with model to without model
Chapter 5: Monte Carlo Methods
non-incremental to incremental
Chapter 6: Stochastic Approximation
Chapter 3: Bellman Optimality Equation
Chapter 2: Bellman Equation
Chapter 1: Basic Concepts
Fundamental tools
Chapter 7: Temporal-Difference Methods
tabular representation to function representation
Chapter 8: Value Function Methods
value-based to policy-based
Chapter 10: Actor-Critic Methods
policy-based plus value-based
Chapter 9: Policy Gradient Methods

# Outline

In this lecture:

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

# Outline

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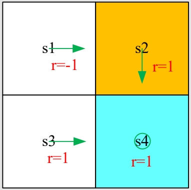
## Motivating examples



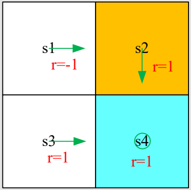

Exercise: write out the Bellman equation and solve the state values (set $\gamma = 0.9$)

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:

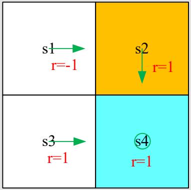
$$q_\pi(s_1, a_1) = -1 + \gamma v_\pi(s_1) = 6.2,$$

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

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

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

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




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

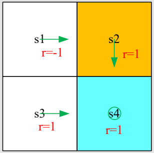
Answer: We can improve the policy based on action values.

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

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

通过原policy $\xrightarrow{\text{Bellman equation}}$ state values

$\downarrow$




发现更好的policy $\longleftarrow$ $s_1$的 action values

Observe the action values that we obtained just now:

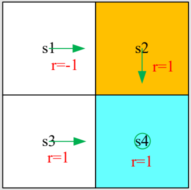
$$q_\pi(s_1, a_1) = 6.2, \quad q_\pi(s_1, a_2) = 8, \quad q_\pi(s_1, a_3) = 9,$$
$$q_\pi(s_1, a_4) = 6.2, \quad q_\pi(s_1, a_5) = 7.2.$$

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

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

# Motivating examples

在当前 Policy 中，$s_1$ 前下的动作 $a_3$ 的 action value 是最大的。但只是当前，如果 policy 更新了，$S_3$ $S_2$ $S_4$ 的动作不一样了，那 $a_3$ 不一定是最优的




通过多次迭代
最后终会是最优 Policy

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

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

如果$\pi_1$所有state value都大于$\pi_2$，则$\pi_1$更好

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*.

# Outline

Bellman equation 是先给定 Policy，之后再算 $v(s) = \dots v(s')$

**Bellman optimality equation (elementwise form):**

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

action value

Remarks:

- $p(r|s,a), p(s'|s,a)$, $r$, $\gamma$ are known. 这是 model 参数，已知
- $v(s), v(s')$ are unknown and to be calculated. 求 state value
- Is $\pi(s)$ known or unknown?

immidiate return

future return

**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 (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

# 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 $v = \max_\pi (r_\pi + \gamma P_\pi v)$ 有两个未知数π和v，但只有一个equation

**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 $\pi$:

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

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

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

**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 $c_1, c_2, c_3 \geq 0$.

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 $c_1, c_2, c_3$

$$q_3 = (c_1 + c_2 + c_3)q_3 = c_1 q_3 + c_2 q_3 + c_3 q_3 \geq c_1 q_1 + c_2 q_2 + c_3 q_3.$$

# Maximization on the right-hand side of BOE

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

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

通过上一页的例子，要让v(s)最大，就把权重全分配给action value最大的动作。

例：$q(s, a_3)$最大，则 $\pi(a_3|s) = 1$

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

matrix vector form

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:

定义域 =值域

- Fixed point: $x \in X$ is a fixed point of $f : X \to X$ if

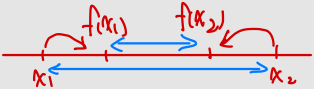
$$f(x) = x$$

- Contraction mapping (or contractive function): $f$ is a contraction mapping if

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

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

  - $\gamma$ 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.



Examples to demonstrate the concepts.

$f(x) = 0.5x$ 是一个 contraction mapping
$x=0$ 是该函数的不动点

### 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.*

收敛!!!

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 $\|A\| < 1$
  $x^* = 0$ is the unique fixed point. It can be solved iteratively by

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

# Outline

# 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*

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

*where $\gamma$ is the discount rate!*

For the proof of this lemma, see our book.

根据Banach不动点定理，一个压缩映射在完备空间上只有一个不动点
即：$v^*=f(v^*)$

Applying the contraction mapping theorem gives the following results.

用迭代法即可让 $v_{k+1} \longrightarrow v^*$

**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 $\gamma$.*

为什么不动点是最优的？ 因为 $v^*=f(v^*)=\max_\pi \cdots$ ，$v^*$就是max

**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 求$\pi^*$： 已知$v^*$，则用$v^*$去求所有的action value，并选择最大的action.

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

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?

# 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*

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

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 $\pi^*$ look like?

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

**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

圈起来的量是未知的
BOE即求这些未知

What factors determine the optimal state value and optimal policy?

It can be clearly seen from the BOE

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

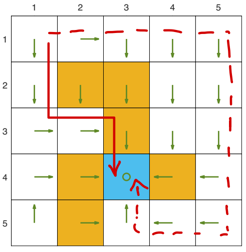
that there are three factors:

- System model: $p(s'|s,a)$, $p(r|s,a)$ ⟵ 由环境因素决定
- Reward design: $r$
- Discount rate: $\gamma$

由人设计，可更改

We next show how $r$ and $\gamma$ 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 |

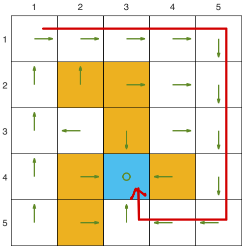
(a) $r_{\text{boundary}} = r_{\text{forbidden}} = -1$, $r_{\text{target}} = 1$, $\gamma = 0.9$

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

没有绕开 forbidden area，因为从长远来看，绕行的成本非常大（虚线）

γ变小，更加短视，选择绕行.（在BOE的式子可发现，
γ越小，immidiate return
的占比就更大）

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).

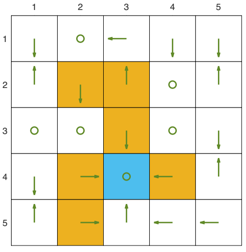
The optimal policy becomes shorted-sighted! Avoid all the forbidden areas!

# Analyzing optimal policies

BOE式子变为：$V(s) = \max_{\pi} \sum_{a} p(a|s) \left( p(r|a,s) r + 0 \right)$

If we change $\gamma$ to 0

$v^* = \max_{\pi} r_{\pi}$



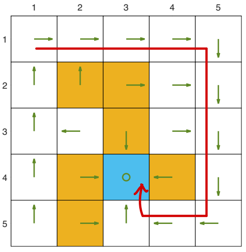

| | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 3 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 |
| 4 | 0.0 | 1.0 | 1.0 | 1.0 | 0.0 |
| 5 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 |

(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 $r_{\text{forbidden}} = -1$ 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

$r = r + 1$

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

The optimal policy remains the same!

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

**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 $v^*$:*

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

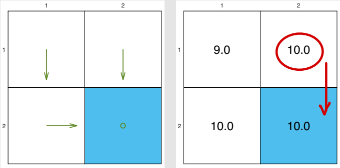
相当于：$v' = av^* + b'$

*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.*

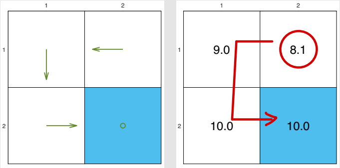
The proof is given in my book.

即使绕路在 reward 上没有 punishment。
discount rate 也会进行 punish.

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? optimal state value是唯一的 但optimal policy不是.
  - 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!