Algorithmic and Theoretical Foundations of RL

MDP and Bellman Optimality

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Markov Chain

Definition 1 (Markov Chain)

Let $\mathcal{S} = \{s_1, \cdots, s_n\}$ be a finite state space. The discrete-time dynamic system $(s_t)_{t\in\mathbb{N}} \in \mathcal{S}$ is a Markov chain if it satisfies the Markov property:

$$P\left(s_{t+1} = s \mid s_t, s_{t-1}, \ldots, s_0\right) = P\left(s_{t+1} = s \mid s_t\right).$$

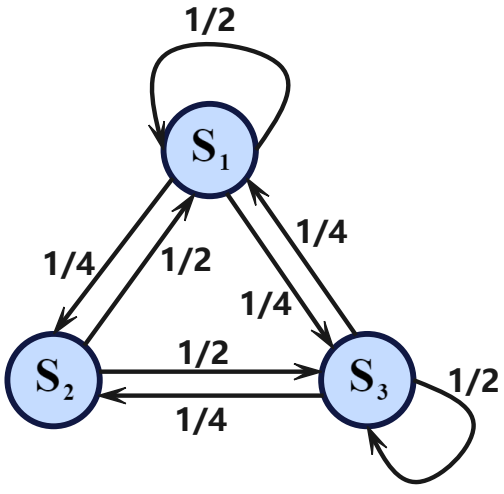
Transition Matrix:

$$P = \begin{bmatrix} p_{s_1s_1} & p_{s_1s_2} & \cdots & p_{s_1s_n} \\ p_{s_2s_1} & p_{s_2s_2} & \cdots & p_{s_2s_n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{s_ns_1} & p_{s_ns_2} & \cdots & p_{s_ns_n} \end{bmatrix}, \quad \text{where } p_{s_is_j} = P\left(s_{t+1} = s_i | s_t = s_j\right).$$

- Under some mild conditions, there exits a stationary distribution $x \in \Delta(\mathcal{S})$ such that $Px = x$.

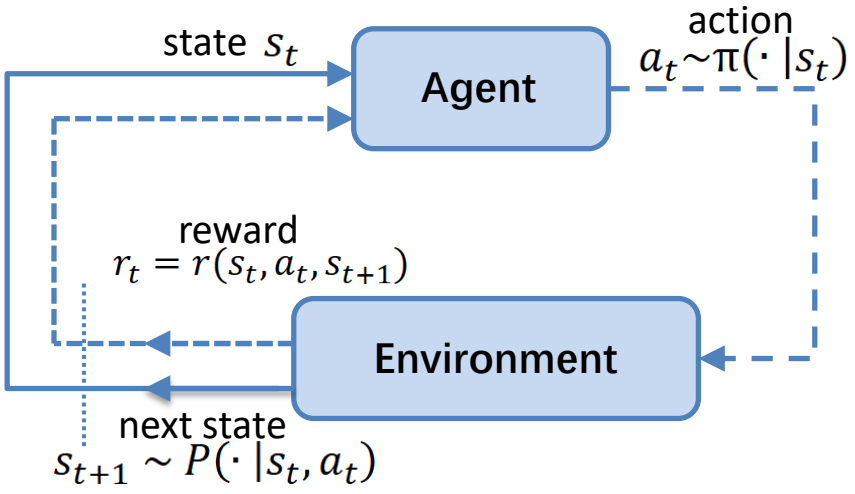
$\Delta(\mathcal{S})$ means the probability simplex on $\mathcal{S}$.

Illustrative Example



$$P = \begin{bmatrix} 1/2 & 1/2 & 1/4 \\ 1/4 & 0 & 1/4 \\ 1/4 & 1/2 & 1/2 \end{bmatrix}, \quad x = \begin{bmatrix} 2/5 \\ 1/5 \\ 2/5 \end{bmatrix}.$$

Markov Decision Process (MDP)

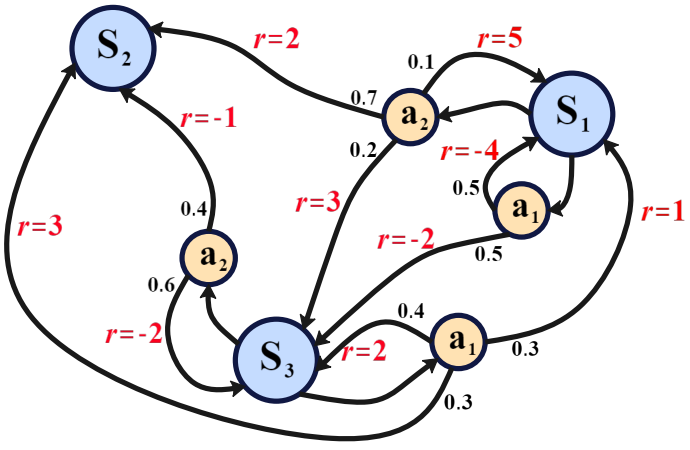


Markov chain augmented with decision and reward: $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, P, r, \gamma \rangle$

- $\mathcal{S}$: state space (状态空间)
- $P(\cdot|s, a)$: state transition model (状态转移模型)
- $\gamma \in [0, 1]$: discount factor (折扣因子)
- $\mathcal{A}$: action space (动作空间)
- $r(s, a, s')$: immediate reward (即时奖励),
  $r(s, a) = \sum_{s'} P(s'|s, a) r(s, a, s')$
- $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ (策略)

Without further specification, we assume $|\mathcal{S}| < \infty$, $|\mathcal{A}| < \infty$, and bounded immediate reward in this lecture for ease of discussion.

Illustrative Example



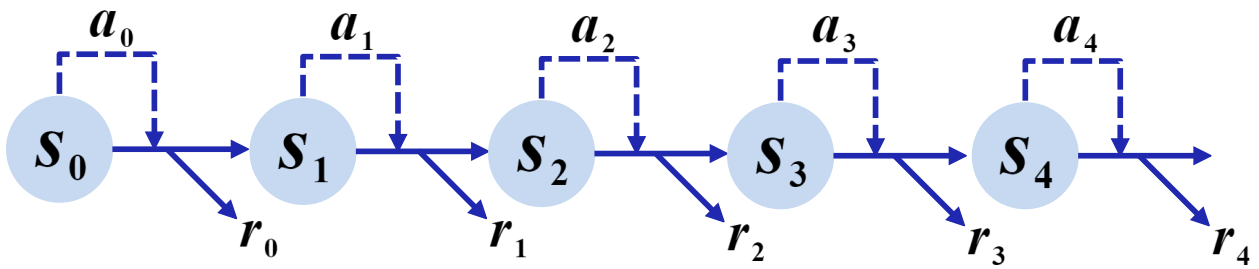
- three states: $\mathcal{S} = \{s_1, s_1, s_3\}$
- two actions: $\mathcal{A} = \{a_1, a_2\}$

Each edge is associated with a transition probability and a reward.

For instance, we can observe that:

- $P(s_3|s_3, a_2) = 0.6,\ P(s_2|s_3, a_2) = 0.4,$
- $r(s_3, a_2, s_3) = -2,\ r(s_3, a_2, s_2) = -1,$
- $r(s_3, a_2) = P(s_3|s_3, a_2)r(s_3, a_2, s_3) + P(s_2|s_3, a_2)r(s_3, a_2, s_2) = -1.6.$

State Value and Action Value



- Trajectory (轨迹):

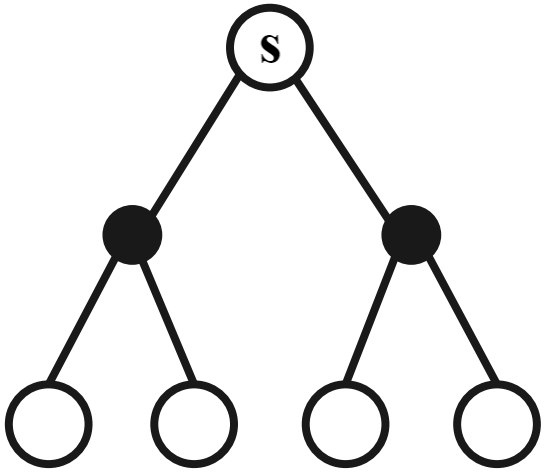
$$s_0, a_0, r_0, s_1, a_1, r_1, s_2, a_2, r_2, s_3, \cdots, \quad r_t = r(s_t, a_t, s_{t+1})$$

- Infinite horizon discounted return (折扣回报):

$$r_0 + \gamma r_1 + \gamma^2 r_2 + \cdots = \sum_{t=0}^{\infty} \gamma^t r_t$$

Here we consider infinite horizon discounted return which enable us to focus on the stationary policy. In finite horizon problems, it may be beneficial to select a different action depending on the remaining time steps which has the form $\pi(s) = (\pi_0(s), \pi_1(s), \cdots)$.

State Value and Action Value

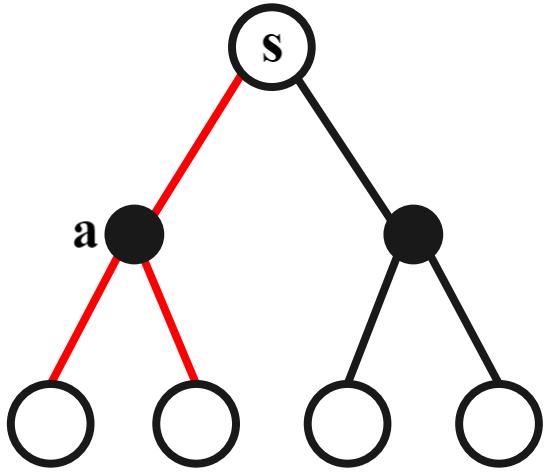


- State value (状态价值函数):

$$v_\pi(s) = \mathop{\mathbb{E}}_{\substack{a_t \sim \pi(\cdot|s_t), \\ s_{t+1} \sim P(\cdot|s_t, a_t)}} \left[\sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s \right], \forall s \in \mathcal{S}$$

The expectation is indeed taken with respect to all possible random trajectories whose distribution is determined by π and P. Later, we often simplify the expression for the expectation to $\mathbb{E}_\pi$.

State Value and Action Value



- Action (or state-action) value (q-value, 动作价值函数):

$$q_\pi(s,a) = \mathop{\mathbb{E}}_{\substack{s_{t+1}\sim P(\cdot|s_t,a_t),\\ a_{t+1}\sim\pi(\cdot|s_{t+1})}} \left[\sum_{t=0}^{\infty}\gamma^t r_t | s_0 = s, a_0 = a\right], \forall (s,a) \in \mathcal{S}\times\mathcal{A}$$

State Value and Action Value

- The relation between the state value and the action value is given by

$$v_\pi(s) = \sum_a \pi(a|s) q(s,a).$$

- Computing the expectation seems not easy. However, the MDP structure enables us to compute the values by finding the solutions to linear systems (i.e., Bellman equations).

Bellman Equations

Theorem 1 (Bellman Equations)

Given an MDP, for any policy π, the values satisfy the following expectation equations:

$$v_\pi(s) = \sum_a \pi(a|s) \underbrace{\sum_{s'} P(s' \mid s, a) \left(r(s, a, s') + \gamma v_\pi(s')\right)}_{q_\pi(s,a)},$$

$$q_\pi(s, a) = \sum_{s'} P(s' \mid s, a) \Big(r(s, a, s') + \gamma \underbrace{\sum_{a' \in \mathcal{A}} \pi(a' \mid s') q_\pi(s', a')}_{v_\pi(s')} \Big).$$

- For any $v \in \mathbb{R}^{|\mathcal{S}|}$, define **Bellman Operator**

$$[\mathcal{T}_\pi v](s) = \sum_a \pi(a|s) \sum_{s'} P(s' \mid s, a) \left(r(s, a, s') + \gamma v(s')\right).$$

The Bellman equation can be rewritten as

$$v_\pi = \mathcal{T}_\pi v_\pi.$$

Matrix Form of Bellman Equation

The linear matrix-vector equation for the bellman equation for state value is given by:

$$v_\pi = \underbrace{r_\pi + \gamma P^\pi v_\pi}_{\mathcal{T}_\pi v_\pi},$$

where

$$\begin{bmatrix} v_\pi(s_1) \\ \vdots \\ v_\pi(s_n) \end{bmatrix} = \begin{bmatrix} r_\pi(s_1) \\ \vdots \\ r_\pi(s_n) \end{bmatrix} + \gamma \begin{bmatrix} p^\pi_{s_1 s_1} & \dots & p^\pi_{s_1 s_n} \\ \vdots & \ddots & \vdots \\ p^\pi_{s_n s_1} & \dots & p^\pi_{s_n s_n} \end{bmatrix} \begin{bmatrix} v_\pi(s_1) \\ \vdots \\ v_\pi(s_n) \end{bmatrix},$$

and the entries of r_π and P^π are

$$r_\pi(s) = \sum_a \pi(a|s) \sum_{s'} P(s'|s,a) r(s,a,s') \quad \text{and} \quad p^\pi_{ss'} = \sum_a \pi(a|s) P(s'|s,a).$$

Only consider the matrix form of the bellman equation for state value.

Matrix Form of Bellman Equation

Properties:

- $P^\pi \mathbf{1} = \mathbf{1}$, $|\lambda(P^\pi)| \leq 1$ for any eigenvalue of P^π
- $(I - \gamma P^\pi)$ is invertible
- $(I - \gamma P^\pi)^{-1} \geq I$
- if a vector $r \geq 0$, then $(I - \gamma P^\pi)^{-1} r \geq r \geq 0$

Solutions:

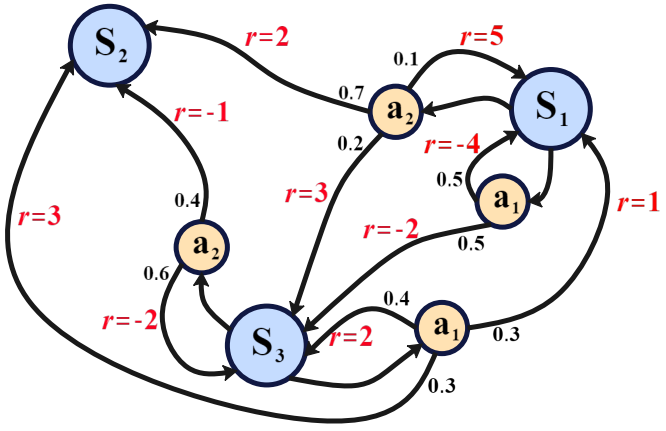
- Direct solution:

$$v_\pi = (\mathrm{I} - \gamma P^\pi)^{-1} r_\pi$$

- Iterative solution:

$$v_{k+1} = r_\pi + \gamma P_\pi v_k = \mathcal{T}_\pi v_k,$$
$$v_k \to v_\pi = (\mathrm{I} - \gamma P^\pi)^{-1} r_\pi \text{ as } k \to \infty$$

Illustrative Example



Consider the policy $\pi(a|s) = 0.5$ for each state s and each action a and $\gamma = 0.9$:

$$P^\pi = \begin{bmatrix} 0.3 & 0.35 & 0.35 \\ 0 & 1 & 0 \\ 0.15 & 0.35 & 0.5 \end{bmatrix},$$

$$r_\pi = [-0.25, 0, 0.2]^T,$$

$$v_\pi = [-0.21, 0, 0.31]^T.$$

We can also verify the correctness of v_π. Taking the state s_0 as an example, it is not hard to show that

$$\begin{aligned} v_\pi(s_3) =& \sum_a \pi(a|s_3) \sum_{s'} p(s'|s_3, a) \left(r(s_3, a, s') + \gamma v_\pi(s')\right) \\ =& 0.5\left(-1.6 + 0.9 \times 0.6 \times 0.31\right) + 0.5\left(2 + 0.9(0.4 \times 0.31 - 0.3 \times 0.21)\right) \\ =& 0.31. \end{aligned}$$

Assume s_2 will always transfers to s_2 with reward 0 no matter what action is taken.

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Optimal Values and Optimal Policy

Definition:

- Optimal state value: $v^*(s) = \max_\pi v_\pi(s), \forall s \in \mathcal{S}$
- Optimal action value: $q^*(s,a) = \max_\pi q_\pi(s,a), \forall s \in \mathcal{S}, a \in \mathcal{A}$

Theorem 2 (Existence of optimal policy)

For an MDP, there exists a deterministic optimal policy π^* such that

$$v_{\pi*}(s) = v^*(s), \quad q_{\pi^*}(s,a) = q^*(s,a).$$

For conciseness, we only consider stationary policies.

Proof of Theorem 2

Given the optimal values $v^*(s)$, $s \in \mathcal{S}$, define the following deterministic policy

$$\pi^*(a|s) = \begin{cases} 1 & \text{if } a = \arg\max_a \mathbb{E}_{s'}\left[r(s,a,s') + \gamma v^*(s')\right] \\ 0 & \text{otherwise.} \end{cases}$$

We are going to show that $v^*(s) = v^{\pi^*}(s)$.

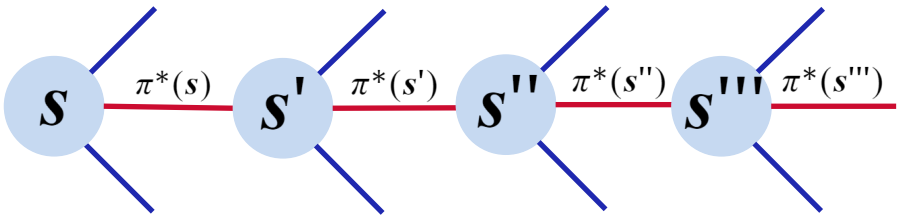
By the Bellman equation we have

$$\begin{aligned} v^*(s) = \max_\pi v_\pi(s) &= \max_\pi \left\{\mathbb{E}_\pi\left[r(s,a,s') + \gamma v_\pi(s')\right]\right\} \\ &\leq \max_\pi \left\{\mathbb{E}_\pi\left[r(s,a,s') + \gamma v^*(s')\right]\right\} \\ &= \max_a \left\{r(s,a,s') + \gamma v^*(s')\right\} \\ &= \mathbb{E}_{s'}\left[r(s,\pi^*(s),s') + \gamma v^*(s')\right], \end{aligned}$$

where with a slight abuse of notation, we use $a^*(s)$ to denote the action that π^* selects at s.

We use $\pi^*(s)$ to denote the action π^* chooses.

Proof of Theorem 2 (Cont'd)



Iterating this procedure yields

$$
\begin{aligned}
v^*(s) &\leq \mathbb{E}_{s'}\left[r(s,\pi^*(s),s') + \gamma v^*(s')\right] \\
&\leq \mathbb{E}_{s'}\left[r(s,\pi^*(s),s') + \gamma \mathbb{E}_{s''}\left[r(s',\pi^*(s'),s'') + \gamma v^*(s'')\right]\right] \\
&\leq \cdots\cdots \\
&\leq \mathbb{E}\left[r(s,\pi^*(s),s') + \gamma r(s',\pi^*(s'),s'') + \gamma^2 r(s'',\pi^*(s''),s''') + \cdots\right\} \\
&= v_{\pi^*}(s).
\end{aligned}
$$

By the definition of v^*, we conclude that $v^*(s) = v_{\pi^*}(s)$. Moreover, a similar argument can show that $q_{\pi^*}(s,a) = q^*(s,a)$ for the same policy π^*.

Proof of Theorem 2 (More Compact Form)

Define (in an elementwise way)

$$\pi^* = \arg\max_{\pi} \left(r_\pi + P^\pi v^* \right).$$

Then, $\forall \pi$, one has

$$v_\pi \leq r_{\pi^*} + P^{\pi^*} v^* \quad \Rightarrow \quad v_* \leq r_{\pi^*} + P^{\pi^*} v^*.$$

Let $v_0 = v^*$ and define

$$v_{k+1} = r_{\pi^*} + P^{\pi^*} v_k, \ k = 0, 1, \cdots$$

Then $v_{k+1} \to v_{\pi^*}$. Moreover, if $v_k \geq v_*$, it can be easily verified $v_{k+1} \geq v_*$. By taking a limit, we have $v_{\pi^*} \geq v^*$. By the definition of v^*, there must hold $v^*(s) = v_{\pi^*}(s)$.

Remark

It is not hard to see that π^* can be rewritten as

$$\pi^*(a|s) = \begin{cases} 1 & \text{if } a = \arg\max_a q^*(s,a) \\ 0 & \text{otherwise.} \end{cases}$$

Thus, if we know $q^*(s,a)$, we immediately have the optimal policy. This observation forms the foundation of Q-learning.

- Finding the optimal policy looks challenging since there are at least as many as $|\mathcal{A}|^{|\mathcal{S}|}$ deterministic policies to test. However, we can leverage the MDP structure to transfer this problem into a dynamic programming problem. The key is hidden in Bellman optimality equations.

Bellman Optimality Equations

Theorem 3

The optimal values satisfy the following Bellman optimality equations:

$$v^*(s) = \max_a \sum_{s'} P\left(s'|s,a\right)\left(r(s,a,s') + \gamma v^*\left(s'\right)\right),$$

$$q^*(s,a) = \sum_{s'} P\left(s'|s,a\right)\left(r(s,a,s') + \gamma \max_{a' \in \mathcal{A}} q^*(s',a')\right).$$

Proof: Since $v^*(s) = v_{\pi^*}(s)$, by Bellman equation for $v_{\pi^*}(s)$, we have

$$\begin{aligned} v^*(s) = v_{\pi^*}(s) &= \mathbb{E}_{\pi^*}\left[r(s,a,s') + \gamma v_{\pi^*}(s')\right] \\ &= \mathbb{E}_{\pi^*}\left[r(s,a,s') + \gamma v^*(s')\right] \\ &= \max_a \mathbb{E}_{s'}\left[r(s,a,s') + \gamma v^*(s')\right]. \end{aligned}$$

In the remaining part, we restrict our discussion on Bellman optimality equation for optimal state value. The one for action value can be similarly discussed.

Existence and Uniqueness of Solution of Bellman Optimality Equation

Fixed Point Theorem

Definition 2 (Contraction mapping)

Let (X, d) be a complete metric space. Then a map $T : X \to X$ is called a contraction mapping on X if there exists $\rho \in [0, 1)$ such that $d(T(x), T(y)) \leq \rho \cdot d(x, y)$ for all $x, y \in X$.

Theorem 4 (Fixed point theorem)

Let (X, d) be a non-empty complete metric space with a contraction mapping $T : X \to X$. Then T admits a unique fixed point x^* in X (i.e. $T(x^*) = x^*$). Furthermore, x^* can be obtained as follows: start with an arbitrary element $x_0 \in X$ and define a sequence $(x_k)_{k \in \mathbb{N}}$ by $x_k = T(x_{k-1})$ for $k \geq 1$. Then $\lim_{k \to \infty} x_k = x^*$.

Existence and Uniqueness of Solution of Bellman Optimality Equation

Contraction Property of Bellman Optimality Operator

Bellman optimality operator of state value:

$$[\mathcal{T}v](s) = \max_a \sum_{s'} P\left(s'|s,a\right)\left(r(s,a,s') + \gamma v\left(s'\right)\right),$$

It is straightforward to see that $\mathcal{T}$ is monotone, that is $Tv_1 \leq Tv_2$ if $v_1 \leq v_2$.

Theorem 5

The Bellman optimality operator of state value is a contraction with respect to infinity norm,

$$\|\mathcal{T}v_1 - \mathcal{T}v_2\|_\infty \leq \gamma \|v_1 - v_2\|_\infty.$$

It follows that there exists a unique solution for Bellman optimality equation of state value.

Proof: The proof is based directly on the following observation:

$$|\max_a f(a) - \max_a g(a)| \leq \max_a |f(a) - g(a)|.$$

Questions?