Reinforcement Learning

Lecture 2: Planning & Learning

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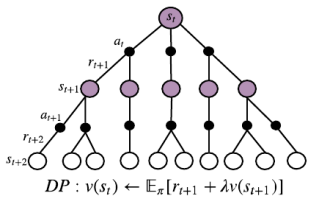
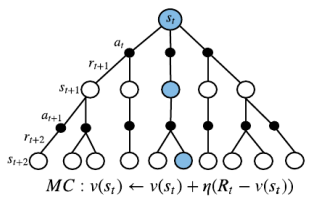
Lecture Outline

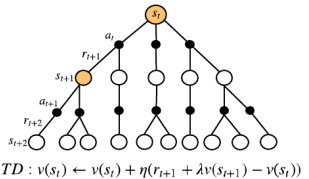
Lecture Outline (Cont'd)



Dynamic Programming (DP)



Monte Carlo (MC)



Temporal Difference (TD)

Lecture Outline

Learning v.s. Planning

Two fundamental problems in sequential decision making

- **Planning**
  - A model of the environment (e.g., state transition, reward function) is **known**
  - The agent performs computations with its model, **without** any external interaction
  - Example: **Dynamic Programming**
- **Learning**
  - The environment is initially **unknown**
  - The agent **interacts** with the model
  - The agent **learns** the optimal policy from experience
  - Example: **Monte Carlo methods**, **temporal difference learning** (**Q-learning**), **policy-based learning**, **model-based learning**

Example: Go Game

- **Planning**: Rules of Go are known
- Exhaustive search of the optimal move
- No need to play Go with others

- **Learning**: No need to know the rules
- Learn the optimal move from experience
- Practice makes perfect

Models: Finite MDPs

- Environment modelled by a finite MDP $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma \rangle$
- MDP model assumptions: **Markovianity** & **time-homogeneity**
- $\mathcal{S}$: state space (a **finite** set of states)
- $\mathcal{A}$: action space (a **finite** set of actions)
- $\mathcal{P}$: state transition probability matrix, $\mathcal{P}^{a}_{ss'} = \Pr(S_{t+1} = s' | A_t = a, S_t = s)$
- $\mathcal{R}$: reward function, $\mathcal{R}^{a}_{s} = \mathbb{E}(R_t | A_t = a, S_t = s)$
- γ: discounted factor $\in [\mathbf{0}, \mathbf{1}]$, allowed to be $\mathbf{1}$ if all sequences terminate (e.g., finite horizons)
- DP, MC and TD are **equally applicable** to settings with continuous state or action space

Bellman Equations

- Bellman equation for the (state) value function:

$$V^{\pi}(s) = \mathbb{E}^{\pi}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = s],$$

- or equivalently,

$$V^{\pi}(s) = \sum_{a \in \mathcal{A}} \pi(a|s) \Big[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V^{\pi}(s') \Big].$$

- Bellman optimality equation for the **optimal** value function:

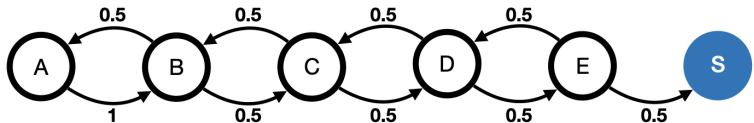
$$V^{\pi^{\text{opt}}}(s) = \max_a \mathbb{E}[R_t + \gamma V^{\pi^{\text{opt}}}(S_{t+1}) | A_t = a, S_t = s],$$

- or equivalently,

$$V^{\pi^{\text{opt}}}(s) = \max_{a \in \mathcal{A}} \Big[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V^{\pi^{\text{opt}}}(s') \Big].$$

Bellman Equation: The Random Walk Example

- Consider a simple **random walk** on a path:

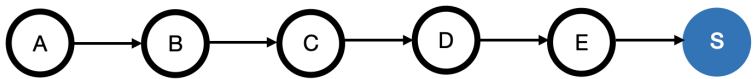


- Reward for transition to State S of value 1, zero reward for other transitions
- Bellman equations:

$$
\begin{aligned}
V^{\pi}(A) &= \mathbb{E}^{\pi}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = A] = \gamma V^{\pi}(B) \\
V^{\pi}(B) &= \mathbb{E}^{\pi}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = B] = \frac{\gamma}{2} V^{\pi}(C) + \frac{\gamma}{2} V^{\pi}(A) \\
&\vdots \\
V^{\pi}(E) &= \mathbb{E}^{\pi}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = E] = 1
\end{aligned}
$$

Bellman Optimality Equation: Random Walk

- The **random walk** example:



- Reward for transition to State $\boldsymbol{S}$ of value $\mathbf{1}$, zero reward for other transitions
- Bellman optimality equations:

$$
\begin{aligned}
\boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{A}) &= \max_{\boldsymbol{a}} \mathbb{E}[\boldsymbol{R_t} + \gamma \boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{S_{t+1}}) | \boldsymbol{A_t} = \boldsymbol{a}, \boldsymbol{S_t} = \boldsymbol{A}] = \gamma \boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{B}) \\
\boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{B}) &= \max_{\boldsymbol{a}} \mathbb{E}[\boldsymbol{R_t} + \gamma \boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{S_{t+1}}) | \boldsymbol{A_t} = \boldsymbol{a}, \boldsymbol{S_t} = \boldsymbol{B}] = \gamma \boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{C}) \\
&\vdots \\
\boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{E}) &= \max_{\boldsymbol{a}} \mathbb{E}[\boldsymbol{R_t} + \gamma \boldsymbol{V}^{\pi^{\text{opt}}}(\boldsymbol{S_{t+1}}) | \boldsymbol{A_t} = \boldsymbol{a}, \boldsymbol{S_t} = \boldsymbol{E}] = \mathbf{1}
\end{aligned}
$$

State-Action Value Function

Definition

The state-action value function (better known as the **Q-function**) is expected return starting from s and a under π,

$$Q^{\pi}(s,a) = \mathbb{E}^{\pi}(G_t|A_t = a, S_t = s) = \mathbb{E}^{\pi}\left(\sum_{i=0}^{+\infty} \gamma^i R_{i+t}|A_t = a, S_t = s\right).$$

- Q^{π} is **independent** of the time t in its definition, under **time-homogeneity**
- Q^{π} is the state value V^{π} under a Markov policy that implements a at the first time and follows π afterwards
- Reduces to action value function $\mathbb{E}^{\pi}(R_t|A_t = a)$ in Lecture 1 when $\gamma = 0$, $\mathcal{S} = \emptyset$

State-Action Value Function (Cont'd)

Relationships between V^π and Q^π

- $Q^\pi \rightarrow V^\pi$:

$$V^\pi(s) = \mathbb{E}^\pi(G_t|S_t = s) = \sum_{a \in \mathcal{A}} \pi(a|s)\mathbb{E}^\pi(G_t|A_t = a, S_t = s) = \sum_{a \in \mathcal{A}} \pi(a|s)Q^\pi(s, a)$$

- $V^\pi \rightarrow Q^\pi$:

$$\begin{aligned} Q^\pi(s, a) &= \mathbb{E}(R_t|A_t = a, S_t = s) + \gamma\mathbb{E}(G_{t+1}|A_t = a, S_t = s) \\ &= \mathbb{E}(R_t|A_t = a, S_t = s) + \gamma\mathbb{E}[\mathbb{E}^\pi(G_{t+1}|S_{t+1})|A_t = a, S_t = s] \\ &= \mathbb{E}[R_t + \gamma V^\pi(S_{t+1})|A_t = a, S_t = s] \end{aligned}$$

Dynamic Programming

Definition (Dynamic Programming)

A collection of algorithms used to compute optimal policies given **perfect** knowledge of the environment

- Dynamic programming (DP) is **rarely** used in practice (the environment is usually unknown)
- However, they provide a foundation for other solution methods
- "Dynamic programming" is used to solve many other statistical learning problems
  - Learning optimal **dynamic treatment regimes** (DTRs)
  - Multi-scale **change point detection**

Dynamic Programming Methods

- **Policy Iteration**: an iterative method that alternates between
  - **Policy Evaluation**
  - **Policy Improvement**

$$\pi_0 \longrightarrow V^{\pi_0} \longrightarrow \pi_1 \longrightarrow V^{\pi_1} \longrightarrow \cdots \longrightarrow \pi^{opt} \longrightarrow V^{\pi^{opt}}$$

- **Value Iteration**: simultaneously combine **policy evaluation** and **policy improvement**

$$V^{\pi_0} \longrightarrow V^{\pi_1} \longrightarrow V^{\pi_2} \longrightarrow \cdots \longrightarrow V^{\pi^{opt}} \longrightarrow \pi^{opt}$$

Lecture Outline

Policy Iteration: Policy Evaluation

- Computation of the (state) value function $\boldsymbol{V}^{\pi}$ for a given π
- According to the Bellman equation, for any $\boldsymbol{s}$,

$$\boldsymbol{V}^{\pi}(\boldsymbol{s}) = \sum_{\boldsymbol{a} \in \mathcal{A}} \pi(\boldsymbol{a}|\boldsymbol{s}) \Big[\mathcal{R}_{\boldsymbol{s}}^{\boldsymbol{a}} + \gamma \sum_{\boldsymbol{s}'} \mathcal{P}_{\boldsymbol{s}\boldsymbol{s}'}^{\boldsymbol{a}} \boldsymbol{V}^{\pi}(\boldsymbol{s}') \Big],$$

- written in matrix form, $\boldsymbol{V}^{\pi} = \mathcal{R} + \gamma \mathcal{P} \boldsymbol{V}^{\pi}$
- $\boldsymbol{V}^{\pi}$ is a column vector with one entry per state

$$\begin{bmatrix} \boldsymbol{V}^{\pi}(\boldsymbol{1}) \\ \vdots \\ \boldsymbol{V}^{\pi}(\boldsymbol{n}) \end{bmatrix} = \sum_{\boldsymbol{a} \in \mathcal{A}} \begin{bmatrix} \pi(\boldsymbol{a}|\boldsymbol{1}) \mathcal{R}_{\boldsymbol{1}}^{\boldsymbol{a}} \\ \vdots \\ \pi(\boldsymbol{a}|\boldsymbol{n}) \mathcal{R}_{\boldsymbol{n}}^{\boldsymbol{a}} \end{bmatrix} + \gamma \begin{bmatrix} \mathcal{P}_{\boldsymbol{11}} & \cdots & \mathcal{P}_{\boldsymbol{1n}} \\ \vdots & & \vdots \\ \mathcal{P}_{\boldsymbol{n1}} & \cdots & \mathcal{P}_{\boldsymbol{nn}} \end{bmatrix} \begin{bmatrix} \boldsymbol{V}^{\pi}(\boldsymbol{1}) \\ \vdots \\ \boldsymbol{V}^{\pi}(\boldsymbol{n}) \end{bmatrix},$$

where $\mathcal{P}_{\boldsymbol{ij}} = \sum_{\boldsymbol{a} \in \mathcal{A}} \pi(\boldsymbol{a}|\boldsymbol{i}) \mathcal{P}_{\boldsymbol{ij}}^{\boldsymbol{a}}$

Policy Evaluation (Cont'd)

- $\boldsymbol{V}^{\pi}$ is a solution of a system of $\boldsymbol{n}$ linear equations with $\boldsymbol{n}$ unknowns
- It can be computed directly

$$\begin{aligned} \boldsymbol{V}^{\pi} &= \mathcal{R} + \gamma \mathcal{P} \boldsymbol{V}^{\pi} \\ (\boldsymbol{I} - \gamma \mathcal{P}) \boldsymbol{V}^{\pi} &= \mathcal{R} \\ \boldsymbol{V}^{\pi} &= (\boldsymbol{I} - \gamma \mathcal{P})^{-1} \mathcal{R} \end{aligned}$$

- $\boldsymbol{I} - \gamma \mathcal{P}$ is **invertible** when γ is strictly smaller than $\mathbf{1}$, since

$$\boldsymbol{x}^{\top} (\boldsymbol{I} - \gamma \mathcal{P}) \boldsymbol{x} = (\mathbf{1} - \gamma) \|\boldsymbol{x}\|_2^2 + \gamma \sum_{i,j} \mathcal{P}_{ij} (\boldsymbol{x}_i - \boldsymbol{x}_j)^2 > \mathbf{0},$$

when $\boldsymbol{x} \neq \mathbf{0}$. The equality holds due to that each row of $\mathcal{P}$ sums up to $\mathbf{1}$.

Policy Evaluation: Algorithm

- **Iterative Policy Evaluation**: an iterative method that outputs a sequence of value functions $V_0, V_1, V_2, \cdots, V_k \rightarrow V^\pi$
- **Initial** value function V_0 is chosen arbitrarily subject to the **constraint** that at terminal state it has value $\mathbf{0}$
- **Iterative** update rule (according to the Bellman equation):

$$V_{k+1} = \mathcal{R} + \gamma \mathcal{P} V_k$$

- **Convergence** is guaranteed when γ is strictly smaller than $\mathbf{1}$ (more in appendix), or eventual termination is guaranteed from all states under π

Policy Evaluation: Pseudocode

- **Input**: a policy π, a threshold parameter $\epsilon > 0$
- **Initialization**: $V(s) = 0$ for any $s \in \mathcal{S}$
- **Repeat**:

  $\Delta \leftarrow 0$

  For each $s \in \mathcal{S}$

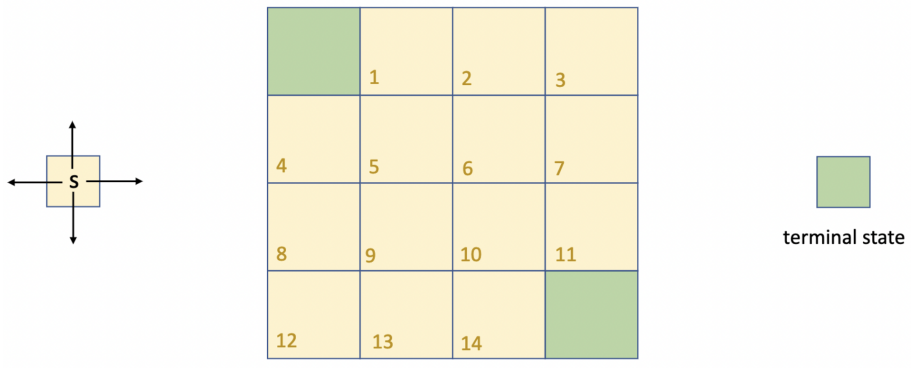
  $\nu \leftarrow V(s)$

  $V(s) \leftarrow \sum_{a \in \mathcal{A}} \pi(a|s) \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V(s') \right]$

  $\Delta \leftarrow \max(\Delta, |\nu - V(s)|)$

  until $\Delta < \epsilon$
- **Output** V

GridWorld Example



- Undiscounted, episodic, finite MDP task
- $\mathcal{A} = \{\textbf{up, down, right, left}\}$. Actions leading out of the grid leave state unchanged
- Rewards: for each transition, the reward of value $-\mathbf{1}$

GridWorld Example (Cont'd)

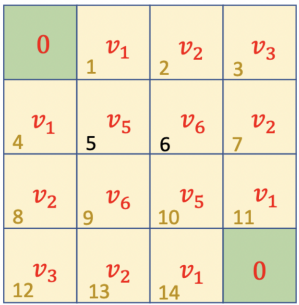
0	-14 1	-20 2	-22 3
-14 4	-18 5	-20 6	-20 7
-20 8	-20 9	-18 10	-14 11
-22 12	-20 13	-14 14	0

Figure: Values of uniform random policy

$$\pi(\boldsymbol{n}|\cdot) = \pi(\boldsymbol{s}|\cdot) = \pi(\boldsymbol{w}|\cdot) = \pi(\boldsymbol{e}|\cdot) = 0.25$$

GridWorld Example (Cont'd)

By **symmetry** and Bellman equation,



$$v_1 = \frac{1}{4}(-1 + v_2) + \frac{1}{4}(-1 + v_5) + \frac{1}{4}(-1 + 0) + \frac{1}{4}(-1 + v_1)$$

$$v_2 = \frac{1}{4}(-1 + v_3) + \frac{1}{4}(-1 + v_6) + \frac{1}{4}(-1 + v_1) + \frac{1}{4}(-1 + v_2)$$

$$v_3 = \frac{1}{4}(-1 + v_3) + \frac{1}{4}(-1 + v_2) + \frac{1}{4}(-1 + v_2) + \frac{1}{4}(-1 + v_3)$$

$$v_5 = \frac{1}{4}(-1 + v_6) + \frac{1}{4}(-1 + v_6) + \frac{1}{4}(-1 + v_1) + \frac{1}{4}(-1 + v_1)$$

$$v_6 = \frac{1}{4}(-1 + v_2) + \frac{1}{4}(-1 + v_5) + \frac{1}{4}(-1 + v_5) + \frac{1}{4}(-1 + v_2)$$

$$\Rightarrow (v_1, v_2, v_3, v_5, v_6) = (-14, -20, -22, -18, -20)$$

GridWorld Example (Cont'd)

$k = 0$

0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0

$k = 1$

0.0	-1.0	-1.0	-1.0
-1.0	-1.0	-1.0	-1.0
-1.0	-1.0	-1.0	-1.0
-1.0	-1.0	-1.0	0.0

$k = 2$

0.0	-1.7	-2.0	-2.0
-1.7	-2.0	-2.0	-2.0
-2.0	-2.0	-2.0	-1.7
-2.0	-2.0	-1.7	0.0

$k = 3$

0.0	-2.4	-2.9	-3.0
-2.4	-2.9	-3.0	-2.9
-2.9	-3.0	-2.9	-2.4
-3.0	-2.9	-2.4	0.0

$k = 10$

0.0	-6.1	-8.4	-9.0
-6.1	-7.7	-8.4	-8.4
-8.4	-8.4	-7.7	-6.1
-9.0	-8.4	-6.1	0.0

$k = \infty$

0.0	-14.	-20.	-22.
-14.	-18.	-20.	-20.
-20.	-20.	-18.	-14.
-22.	-20.	-14.	0.0

Figure: Value functions at each iteration

Policy Iteration: Policy Improvement

- Identify some π' that is no worse than π based on $\boldsymbol{V}^{\pi}$
- For any $\boldsymbol{s}$, consider a hybrid policy
  - implements $\boldsymbol{a}$ at the first time
  - follows π afterwards
- Its value is given by $\boldsymbol{Q}^{\pi}(\boldsymbol{s}, \boldsymbol{a})$ (can be computed based on $\boldsymbol{V}^{\pi}$)
- Select π' among the class of hybrid policies that **maximizes** the value

$$\pi'(\boldsymbol{s}) = \arg\max_{\boldsymbol{a}} \boldsymbol{Q}^{\pi}(\boldsymbol{s}, \boldsymbol{a})$$

- Its value is given by $\boldsymbol{Q}^{\pi}(\boldsymbol{s}, \pi'(\boldsymbol{s})) \geq \boldsymbol{V}^{\pi}(\boldsymbol{s})$, since the hybrid policy class contains π
- Surprisingly, according to **policy improvement theorem**, $\boldsymbol{V}^{\pi'}(\boldsymbol{s}) \geq \boldsymbol{V}^{\pi}(\boldsymbol{s})$ for any $\boldsymbol{s}$!

Policy Improvement (Cont'd)

Given a policy π, improve π by acting **greedily** with respect to V^{π},

$$\pi'(s) = \arg\max_{a} Q^{\pi}(s, a) = \arg\max_{a} \mathbb{E}[R_t + \gamma V^{\pi}(S_{t+1}) | A_t = a, S_t = s]$$
$$= \arg\max_{a} [\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V^{\pi}(s')]$$

Theorem

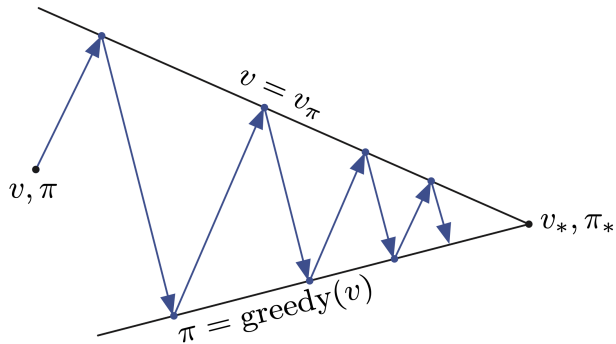
The greedy policy π' with respect to V^{π} is as good as or better than π,

$$V^{\pi'}(s) \geq V^{\pi}(s),$$

for any $s \in \mathcal{S}$.

Proof can be found in the Appendix.

Policy Iteration: Revisit



- **Policy Evaluation**: Compute $\boldsymbol{V}^{\boldsymbol{\pi}}$ via iterative policy evaluation
- **Policy Improvement**: Generate $\boldsymbol{\pi}'$ via greedy policy improvement

Policy Iteration: Pseudocode

- **Initialization**: $V(s) = 0$, $\pi(s) \in \mathcal{A}$ arbitrarily for any $s \in \mathcal{S}$
- **Repeat**:

  $\Delta \leftarrow 0$

  For each $s \in \mathcal{S}$

  $\nu \leftarrow V(s)$

  $V(s) \leftarrow \sum_{a \in \mathcal{A}} \pi(a|s) \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V(s') \right]$

  $\Delta \leftarrow \max(\Delta, |\nu - V(s)|)$

  until $\Delta < \epsilon$
- **policystable** $\leftarrow$ **True**
- **For each** $s \in \mathcal{S}$:

  $b \leftarrow \pi(s)$

  $\pi(s) \leftarrow \arg\max_a [\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V(s')]$

  If $b \neq \pi(s)$ **then policystable** $\leftarrow$ **False**
- **If policystable**, **then Return** π, **else** go to bullet point #2

Lecture Outline

Value Iteration

- Policy iteration is **computationally inefficient**, as each iteration requires executing policy evaluation which requires multiple iterations
- According to the Bellman optimality equation,

$$V^{\pi^{\text{opt}}}(s) = \max_{a \in \mathcal{A}} \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V^{\pi^{\text{opt}}}(s') \right].$$

- **Value iteration** idea: iteratively apply the above updates

$$V_{k+1}(s) = \max_{a \in \mathcal{A}} \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V_k(s') \right].$$

- Drive the optimal deterministic policy

$$\pi^{opt}(s) = \arg\max_{a \in \mathcal{A}} \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V^{\pi^{\text{opt}}}(s') \right].$$

- **Convergence** is guaranteed when γ is strictly smaller than $\mathbf{1}$ (more in Appendix), or eventual termination is guaranteed from all states.

Value Iteration: Pseudocode

- **Initialization**: $\boldsymbol{V}(\boldsymbol{s}) = \mathbf{0}$, $\pi(\boldsymbol{s}) \in \mathcal{A}$ arbitrarily for any $\boldsymbol{s} \in \mathcal{S}$
- **Repeat**:

  $\Delta \leftarrow \mathbf{0}$

  For each $\boldsymbol{s} \in \mathcal{S}$

  $\nu \leftarrow \boldsymbol{V}(\boldsymbol{s})$

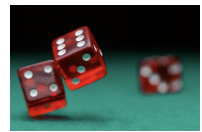
  $\boldsymbol{V}(\boldsymbol{s}) \leftarrow \max_{\boldsymbol{a} \in \mathcal{A}} \left[\mathcal{R}_{\boldsymbol{s}}^{\boldsymbol{a}} + \gamma \sum_{\boldsymbol{s}'} \mathcal{P}_{\boldsymbol{s}\boldsymbol{s}'}^{\boldsymbol{a}} \boldsymbol{V}(\boldsymbol{s}') \right]$

  $\Delta \leftarrow \mathbf{max}(\Delta, |\nu - \boldsymbol{V}(\boldsymbol{s})|)$

  until $\Delta < \epsilon$
- **Output**: optimal deterministic policy given by

$$\pi^{opt}(\boldsymbol{s}) = \arg\max_{\boldsymbol{a} \in \mathcal{A}} \left[\mathcal{R}_{\boldsymbol{s}}^{\boldsymbol{a}} + \gamma \sum_{\boldsymbol{s}'} \mathcal{P}_{\boldsymbol{s}\boldsymbol{s}'}^{\boldsymbol{a}} \boldsymbol{V}^{\pi^{\mathbf{opt}}}(\boldsymbol{s}') \right].$$

Example: Gambler's Problem

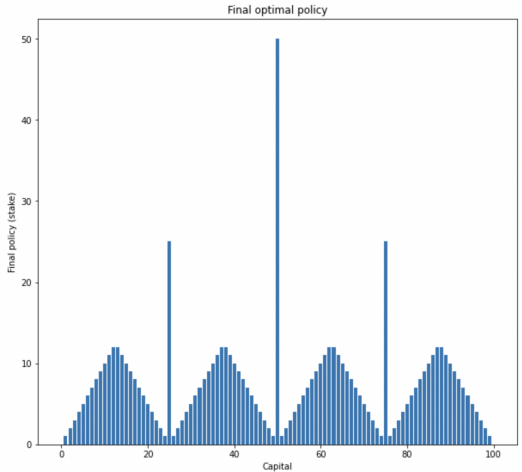


- A gambler makes bets on the outcomes of a sequence of coin flips
- The gambler must decide for each coin flip what proportion of capital to stake
- If **the outcome of the coin flip = heads**, then:
  The gambler **wins** as much money as they have staked on this flip
- Else:
  The gambler **loses** their stake
- The game ends when the gambler reaches the goal of **£100** or **runs out of money**

Example: Gambler's Problem (Cont'd)

- Undiscounted, episodic, finite MDP task
- $\mathcal{S}$: $\{0, 1, \cdots, 99, 100\}$, termination states 0 and 100
- $\mathcal{A}(s)$: $\{1, 2, \cdots, \min(s, 100 - s)\}$, depends on the state
- Pr(outcome of coin flip is heads) $= p$ (known parameter)

Example: Gambler's Problem, the Optimal Policy



Some Technical Questions

- How do we know that value iteration converges to $\boldsymbol{V}^{\pi^{\text{opt}}}$?
- Or that iterative policy evaluation converges to $\boldsymbol{V}^{\pi}$?
- And therefore that policy iteration converges to $\boldsymbol{V}^{\pi^{\text{opt}}}$?
- Is the solution unique?
- These questions are resolved by **Banach fixed-point theorem** (more in the appendix)

Lecture Outline

MC Policy Evaluation

- Defined for **episodic** tasks
  - Value functions are updated upon completion of an episode
  - Different from **step-by-step** methods (e.g., temporal difference learning)
- **Objective**: estimate the value function V^{π} for a given policy π, from a set of episodes obtained by following π

$$S_0, A_0, R_0, \cdots, S_T \sim \pi$$

- V^{π} is the expected return $\mathbb{E}^{\pi}(\sum_{0 \leq t \leq T} \gamma^t R_t | S_0 = s)$
- Monte Carlo idea: use **empirical mean** return to approximate **expected return**
- Types of MC methods:
  - **First-visit MC method**: $V^{\pi}(s)$ estimated by the average of returns following **each first visit** to s in a set of episodes
  - **Every-visit MC method**: $V^{\pi}(s)$ estimated by the average of returns following **each visit** to s in a set of episodes

First-Visit MC Policy Evaluation: Pseudocode

- **Initialization**:
  $\boldsymbol{N}$ (counter), $\boldsymbol{N}(\boldsymbol{s}) \leftarrow \mathbf{0}$ for all $\boldsymbol{s} \in \mathcal{S}$
  Returns$(\boldsymbol{s}) \leftarrow$ an empty list, for all $\boldsymbol{s} \in \mathcal{S}$
- **Repeat**:
  Generate an episode following policy π
  For each distinct $\boldsymbol{s}$ appearing in the episode
    $\boldsymbol{G} \leftarrow$ return following the first occurrence of $\boldsymbol{s}$
    $\boldsymbol{N}(\boldsymbol{s}) \leftarrow \boldsymbol{N}(\boldsymbol{s}) + \mathbf{1}$
    Returns$(\boldsymbol{s}) \leftarrow$ **Returns**$(\boldsymbol{s}) + \boldsymbol{G}$
- **Output**:
  For each distinct $\boldsymbol{s}$
    $\boldsymbol{N}^{-1}(\boldsymbol{s})$**Returns**$(\boldsymbol{s})$

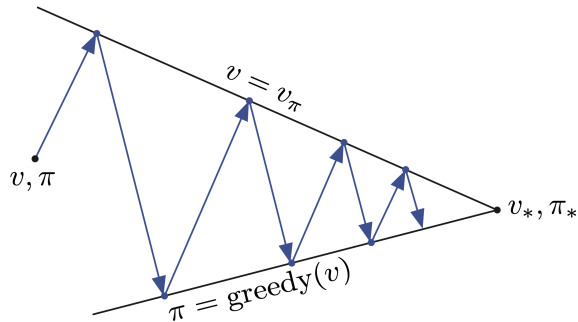
Every-Visit MC Policy Evaluation: Pseudocode

- **Initialization**:
  $N \leftarrow$ counter, $N(s) \leftarrow 0$ for all $s \in \mathcal{S}$
  $\text{Returns}(s) \leftarrow$ an empty list, for all $s \in \mathcal{S}$
- **Repeat**:
  Generate an episode following policy π
  For each s appearing in the episode
    $G \leftarrow$ return following the occurrence of s
    $N(s) \leftarrow N(s) + 1$
    $\text{Returns}(s) \leftarrow \text{Returns}(s) + G$
- **Output**:
  For each distinct s
    $N^{-1}(s)\text{Returns}(s)$

Lecture Outline

MC Control with Generalized Policy Iteration

- **Objective**: use MC estimation to learn the optimal policy.
- Integrate policy iteration with MC methods



- **Policy Evaluation**: Compute $\boldsymbol{V}^{\boldsymbol{\pi}}$ via MC policy evaluation
- **Policy Improvement**: Generate π' via greedy policy improvement?

Policy Iteration Using State-Action Value Function

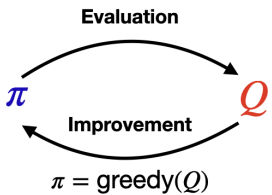
- Greedy policy improvement over $\boldsymbol{V}^{\pi}$ requires model of MDP

$$\pi'(\boldsymbol{s}) = \arg\max_{\boldsymbol{a}}[\mathcal{R}_{\boldsymbol{s}}^{\boldsymbol{a}} + \gamma \sum_{\boldsymbol{s}'} \mathcal{P}_{\boldsymbol{ss}'}^{\boldsymbol{a}} \boldsymbol{V}^{\pi}(\boldsymbol{s}')]$$

- Greedy policy improvement over $\boldsymbol{Q}^{\pi}(\boldsymbol{s}, \boldsymbol{a})$ is model free

$$\pi'(\boldsymbol{s}) = \arg\max_{\boldsymbol{a}} \boldsymbol{Q}^{\pi}(\boldsymbol{s}, \boldsymbol{a})$$

MC Version of Policy Iteration



$$\pi_0 \longrightarrow Q^{\pi_0} \longrightarrow \pi_1 \longrightarrow Q^{\pi_1} \longrightarrow \cdots \longrightarrow \pi^{opt} \longrightarrow Q^{\pi^{opt}}$$

- **Policy Evaluation**: MC estimation of state-action value function
- **Policy Improvement**: Improve the policy wrt the current state-action value function

MC Estimation of State-Action Values

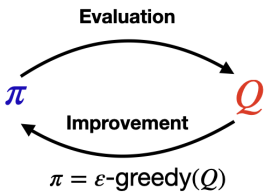
- Many state-action pairs may never be visited under a policy
  - Ex. if π is deterministic, only **one** state-action pair is observed for each distinct state
  - Need to ensure **exploration**!
- Two approaches for ensuring exploration:
  - **Exploring starts**: the first step of each episode starts at a state-action pair and every such pair has non-zero probability of being selected at the start
  - **Stochastic policies**: use policies that ensures a non-zero probability of selecting each action from the set of available actions in each given state

MC Control with ε-Greedy Exploration

- Simplest idea for ensuring continual exploration
- All $\boldsymbol{m}$ actions are tried with non-zero probabilities
- With probability $\mathbf{1} - \varepsilon$ choose the **greedy** action
- With probability ε choose an action at **random**

$$\pi(\boldsymbol{a}|\boldsymbol{s}) = \begin{cases} \varepsilon/\boldsymbol{m} + \mathbf{1} - \varepsilon, & \text{if } \boldsymbol{a} = \arg\max_{\boldsymbol{a}'} \boldsymbol{Q}(\boldsymbol{s}, \boldsymbol{a}') \\ \varepsilon/\boldsymbol{m}, & \text{otherwise} \end{cases}$$

MC Control with ε-Greedy Exploration (Cont'd)



$$\pi_0 \longrightarrow Q^{\pi_0} \longrightarrow \pi_1 \longrightarrow Q^{\pi_1} \longrightarrow \cdots \longrightarrow \pi^{\varepsilon,opt} \longrightarrow Q^{\pi^{\varepsilon,opt}}$$

Pseudocode

- **Initialization**:

  $\boldsymbol{N}$ (counter), $\boldsymbol{N}(\boldsymbol{s}, \boldsymbol{a}) \leftarrow \mathbf{0}$ for all $\boldsymbol{s} \in \mathcal{S}$, $\boldsymbol{a} \in \mathcal{A}$

  $\textbf{Returns}(\boldsymbol{s}, \boldsymbol{a}) \leftarrow$ empty lists, for all $\boldsymbol{s} \in \mathcal{S}$, $\boldsymbol{a} \in \mathcal{A}$

  $\pi \leftarrow$ arbitrary ε-greedy policy

  $\boldsymbol{Q} \leftarrow$ arbitrary

- **Repeat**:

  Generate an episode using exploring starts and policy π

  For each distinct $(\boldsymbol{s}, \boldsymbol{a})$ appearing in the episode

  $\boldsymbol{G} \leftarrow$ return following the first occurrence of $(\boldsymbol{s}, \boldsymbol{a})$

  $\boldsymbol{N}(\boldsymbol{s}, \boldsymbol{a}) \leftarrow \boldsymbol{N}(\boldsymbol{s}, \boldsymbol{a}) + \mathbf{1}$

  $\textbf{Returns}(\boldsymbol{s}, \boldsymbol{a}) \leftarrow \textbf{Returns}(\boldsymbol{s}, \boldsymbol{a}) + \boldsymbol{G}$

  $\boldsymbol{Q}(\boldsymbol{s}, \boldsymbol{a}) \leftarrow \textbf{Returns}(\boldsymbol{s}, \boldsymbol{a}) / \boldsymbol{N}(\boldsymbol{s}, \boldsymbol{a})$

  For each distinct $\boldsymbol{s}$:

$$\pi(\boldsymbol{a}|\boldsymbol{s}) \leftarrow \begin{cases} \varepsilon/\boldsymbol{m} + \mathbf{1} - \varepsilon, & \text{if } \boldsymbol{a} = \arg\max \boldsymbol{Q}(\boldsymbol{s}, \boldsymbol{a}) \\ \varepsilon/\boldsymbol{m}, & \text{otherwise} \end{cases}$$

Lecture Outline

TD Learning v.s. MC Methods v.s. DP Algorithms

(TD) Learning: a learning method that combines ideas from Monte Carlo (MC) methods and dynamic programming (DP)

Algorithms	DP	MC	TD
Planning	✔	✗	✗
Learning	✗	✔	✔
Model-free	✗	✔	✔
Step-by-step	✔	✗	✔
Episode-by-episode	✗	✔	✗
Episodic task	✔	✔	✔
Continuous task	✔	✗	✔

Lecture Outline

MC Prediction

- **Objective**: learns V^{π} from experience under π
- MC Policy Evaluation: $V(s) \leftarrow$ **average**[**Returns**(s)]
- Incremental update for every-visit MC prediction:

$$V(S_t) \leftarrow V(S_t) + \alpha_t[G_t - V(S_t)]$$

  where α_t is $\frac{1}{\#[\textbf{Returns}(S_t)]}$ at time t
- We may regard G_t as a **target**
- The update can be performed after return G_t is observed
- i.e. after the episode is completed

TD Prediction

- Unlike MC methods, TD methods wait only until **next time step**
- The simplest TD method (so called TD(**0**)) considers the update

$$V(S_t) \leftarrow V(S_t) + \alpha_t[R_t + \gamma V(S_{t+1}) - V(S_t)]$$

- This update rule has $R_t + \gamma V(S_{t+1})$ as the **target**
- Considered as a **bootstrap** method: update in part based on an existing estimate
- Different from "bootstrap" in statistics: a resampling method (e.g., sample with replacement) for **uncertainty quantification** of a given estimate

MC vs TD update

- Notice that under the MDP assumption

$$
\begin{aligned}
V^{\pi}(s) &= \mathbb{E}^{\pi}(G_t | S_t = s) && (1)\\
&= \mathbb{E}^{\pi}(\sum_{k=0}^{\infty} \gamma^k R_{t+k} | S_t = s)\\
&= \mathbb{E}^{\pi}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = s] && (2)
\end{aligned}
$$

- MC methods use as the target the random variable in (1)
- TD methods use as the target the random variable in (2)
  - **Immediate reward** and estimate of the **future value**

TD: Pseudocode

- **Input**: π policy to be evaluated, step size α
- **Initialization**: V arbitrary
- **Repeat** for each episode:
  - **Initialize** state s
  - **Repeat** for each step of the episode:
    - $a \leftarrow$ action given by π for s
    - Take action a, observe reward r and next state s'
    - $V(s) \leftarrow V(s) + \alpha[r + \gamma V(s') - V(s)]$
    - $s \leftarrow s'$
  - **until** s is a terminal state

Pros & Cons of MC vs TD

- MC must wait until the **end** of episode
- MC learns from **complete** sequences
- MC only works for **episodic** (terminating) environments

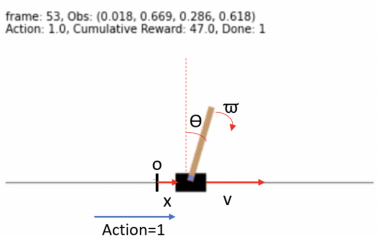
- TD can learn online after **each step**
- TD can learn from **incomplete** sequences
- TD works in **continuing** environments

Pros & Cons of MC vs TD (Cont'd)

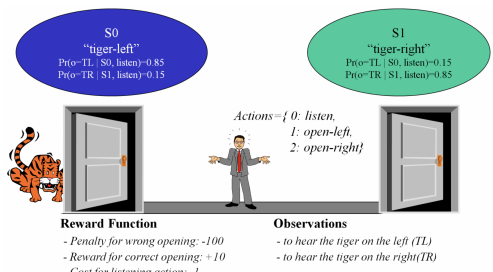
- Bias/Variance Trade-Off
- Return G_t is **unbiased** estimate of $V^\pi(S_t)$
- Oracle target $R_t + \gamma V^\pi(S_{t+1})$ is **unbiased** estimate of $V^\pi(S_t)$
- TD target $R_t + \gamma V(S_{t+1})$ is **biased** estimate of $V^\pi(S_t)$
- TD target has much lower **variance** than the return
  - Return depends on **many** random actions, transitions, rewards
  - TD target depends on **one** random action, transition, reward
- MC has **high variance, zero bias, insensitive to initialization**
- TD has **low variance, some bias, sensitive to initialization**

Pros & Cons of MC vs TD (Cont'd)

- TD exploits **Markov** & **stationary** properties
- Relies on the **Bellman equation**
- More **efficient** in MDP environments



- MC **does** not exploit these properties
- More **flexible** in non-MDP environments (e.g., POMDP)



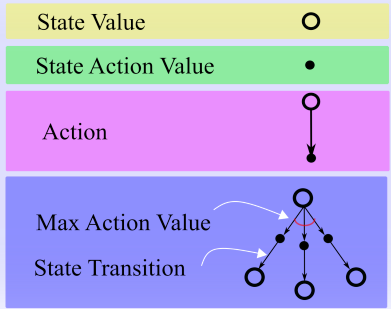
Rate of Convergence

- For i.i.d. random variables $\boldsymbol{X_1}, \cdots, \boldsymbol{X_n}$ with mean $\boldsymbol{\mu}$ and variance $\boldsymbol{\sigma^2}$,

$$\sqrt{\boldsymbol{n}}(\bar{\boldsymbol{X}} - \boldsymbol{\mu}) \to N(\boldsymbol{0}, \boldsymbol{\sigma^2}),$$

  according to CLT.
- $\bar{\boldsymbol{X}}$ converges to $\boldsymbol{\mu}$ at a rate of $\boldsymbol{n^{-1/2}}$.
- For $\boldsymbol{n}$ episodes with $\boldsymbol{T}$ time points per episode, first-visit MC converges at a rate of $\boldsymbol{n^{-1/2}}$.
- For $\boldsymbol{n}$ episodes with $\boldsymbol{T}$ time points per episode, TD converges at a rate of $(\boldsymbol{nT})^{-1/2}$, with proper choice of step sizes.
- First-visit MC requires $\boldsymbol{n} \to \infty$ to be consistent
- TD requires either $\boldsymbol{n}$ or $\boldsymbol{T} \to \infty$ to be consistent

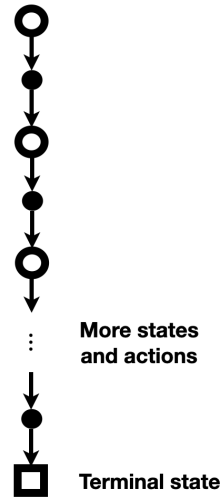
Backup Diagram



Taken from `https://towardsdatascience.com/all-about-backup-diagram-fefb25aaf804`

Backup Diagram (Cont'd)

TD



MC

SARSA: an On-Policy TD Control

- **SARSA**: a TD method for **policy optimisation**
  - Follows the pattern of policy iteration
  - Uses TD prediction method for **policy evaluation**
  - Uses ε-greedy exploration for **policy improvement**
- Similar to MC control, estimate state-action value $\boldsymbol{Q}^{\pi}(\boldsymbol{s}, \boldsymbol{a})$ (instead of the state value $\boldsymbol{V}^{\pi}(\boldsymbol{s})$) for the control problem
- Different from MC control, update the state-value **every time step**

Bellman Equations

- Bellman equation for the (state) value function:

$$V^{\pi}(s) = \mathbb{E}[R_t + \gamma V^{\pi}(S_{t+1}) | S_t = s].$$

- Bellman equation for the state-action value function:

$$Q^{\pi}(s, a) = \mathbb{E}\left[R_t + \gamma \sum_{a'} \pi(a' | S_{t+1}) Q^{\pi}(S_{t+1}, a') | A_t = a, S_t = s\right],$$

or equivalently,

$$Q^{\pi}(s, a) = \mathbb{E}^{\pi}[R_t + \gamma Q^{\pi}(S_{t+1}, A_{t+1}) | A_t = a, S_t = s].$$

SARSA

- Incremental estimation of the state-action value function:

$$Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \alpha[R_t + \gamma Q(S_{t+1}, A_{t+1}) - Q(S_t, A_t)],$$

  for non-terminal state S_{t+1}
- If S_{t+1} is a terminal state, $Q(S_{t+1}, A_{t+1}) = 0$
- This update uses every element of the quintuple of variables:

$$\underset{S\ \ A\ \ R\ \ S\ \ A}{(S_t, A_t, R_t, S_{t+1}, A_{t+1})}$$

SARSA: Pseudocode

- **Initialization**: Q arbitrary
- **Repeat** for each episode:
  - **Initialize** state s
  - **Choose** action a from s using policy derived from Q (ε-greedy)
  - **Repeat** for each step of the episode:
    - Take action a, observe reward r and next state s'
    - $a' \leftarrow$ action from s' using policy derived from Q (ε-greedy)
    - $Q(s,a) \leftarrow Q(s,a) + \alpha[r + \gamma Q(s',a') - Q(s,a)]$
    - $s \leftarrow s'$, $a \leftarrow a'$
  - **until** s is a terminal state

Convergence of SARSA

Theorem

SARSA converges to the optimal Q-function, $Q(s,a) \rightarrow Q^{\pi^{\text{opt}}}(s,a)$ *for any* s *and* a*, if*

- *All state-action pairs are explored infinitely many times,*

$$\sum_{t=0}^{\infty} \mathbb{I}(S_t = s, A_t = a) = \infty.$$

- *The policy converges to a greedy policy,*

$$\lim_{t \rightarrow \infty} \pi_t(a|s) = \mathbb{I}(a = \arg\max_{a'} Q_t(s,a'))$$

- *Robbins-Monro sequence of step-sizes (Robbins and Monro, 1951),*

$$\sum_{t=0}^{\infty} \alpha_t = \infty \text{ and } \sum_{t=0}^{\infty} \alpha_t^2 < \infty$$

Convergence of SARSA (Cont'd)

- Condition 1: All state-action pairs are **explored** infinitely many times

  $\Rightarrow \varepsilon$ to be strictly positive

- Condition 2: The policy converges to a **greedy** policy

  $\Rightarrow \varepsilon_t$ decays to zero as t grows to infinity

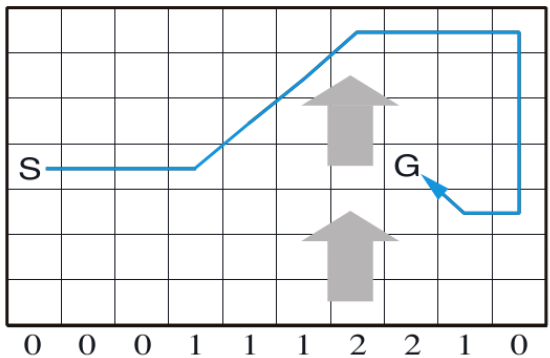
- Condition 3: Robbins-Monro sequence of step-sizes

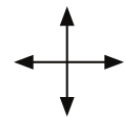
$$\sum_{t=0}^{\infty} \alpha_t = \infty \text{ and } \sum_{t=0}^{\infty} \alpha_t^2 < \infty$$

$\Rightarrow \alpha_t$ proportional to t^{-c} for $1/2 < c \leq 1$.

$\sum_t t^{-c} = \infty$ when $c \leq 1$ and $\sum_t t^{-c} < \infty$ when $c > 1$

Windy Gridworld Example





Actions

- An **episodic** task
- Rewards of -1 until **goal** is reached
- Strength of wind indicated by numbers

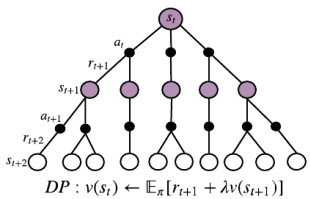
Windy Gridworld Example (Cont'd)

```
Optimal policy is:
['R' 'D' 'R' 'R' 'R' 'R' 'R' 'R' 'R' 'D']
['R' 'R' 'U' 'L' 'R' 'R' 'R' 'U' 'R' 'D']
['L' 'U' 'R' 'R' 'R' 'R' 'R' 'R' 'R' 'D']
['R' 'R' 'R' 'R' 'R' 'R' 'U' 'G' 'R' 'D']
['R' 'D' 'D' 'R' 'R' 'R' 'U' 'D' 'L' 'L']
['D' 'D' 'D' 'R' 'R' 'U' 'U' 'D' 'R' 'U']
['R' 'R' 'U' 'R' 'U' 'U' 'U' 'U' 'R' 'L']
['0' '0' '0' '1' '1' '1' '2' '2' '1' '0']
```

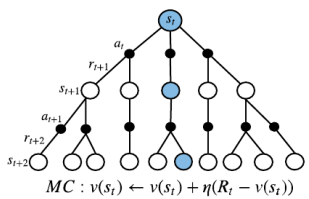
Summary

- Planning v.s. Learning
- Dynamic programming v.s. Monte Carlo v.s. Temporal Difference
- Policy Iteration v.s. Value Iteration
- Policy Evaluation v.s. Policy Improvement
- MC Prediction v.s. MC Control
- TD Prediction v.s. SARSA
- γ-Contraction, Banach Fixed Point Theorem

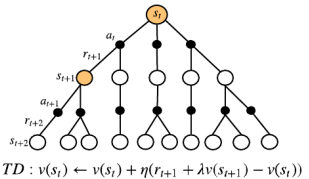
Summary (Cont'd)



Dynamic Programming (DP)



Monte Carlo (MC)



Temporal Difference (TD)

Appendix: Proof of Policy Improvement Theorem

Consider a sequence of policies:

- π_0: a given stationary policy π
- π_k: a Markov policy that implements π' at the first k times and follows π afterwards
- π_∞: the greedy policy π'

We show in the appendix

- **Step 1**: π_1 is no worse than π_0, i.e., $Q^\pi(s, \pi'(s)) \geq V^\pi(s)$
- **Step 2**: π_{k+1} is no worse than π_k for any $k \geq 1$

This proves the policy improvement theorem

Appendix: Policy Improvement Theorem, Step 1

- π_0: a given stationary policy π
- π_1: a Markov policy that implements π' at the initial time and follows π afterwards
- By definition,

$$\pi'(s) = \arg\max_a Q^\pi(s, a)$$

- This yields

$$Q^\pi(s, \pi'(s)) = \max_a Q^\pi(s, a) \geq \sum_a \pi(a|s) Q^\pi(s, a) = V^\pi(s)$$

- i.e., π_1 is no worse than π_0

Appendix: Policy Improvement Theorem, Step 2

- π_k: a Markov policy that implements π' at the first k times and follows π afterwards
- The difference between two value functions is given by

$$V^{\pi_{k+1}}(s) - V^{\pi_k}(s) = \gamma^k \mathbb{E}^{\pi'}[Q^{\pi}(S_k, \pi'(S_k))|S_0 = s] - \gamma^k \mathbb{E}^{\pi'}[V^{\pi}(S_k)|S_0 = s]$$

- Results in Step 1 yield $Q^{\pi}(S_k, \pi'(S_k)) \geq V^{\pi}(S_k)$, and hence $V^{\pi_{k+1}}(s) \geq V^{\pi_k}(s)$
- i.e., π_{k+1} is no worse than π_k

Appendix: Bellman Expectation Operator

Definition

Define the Bellman Expectation Operator T^π as a function that maps a given value function V into another value function $T^\pi V$ such that

$$T^\pi V(s) = \sum_{a \in \mathcal{A}} \pi(a|s) \Big[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a V(s') \Big], \qquad \forall s \in \mathcal{S}.$$

- The Bellman equation can be rewritten as $V^\pi = T^\pi V^\pi$
- This operator is a γ-**contraction**, i.e. it makes value function closer by at least γ

$$\max_s |T^\pi V_1(s) - T^\pi V_2(s)| = \gamma \max_s \Big| \sum_{a,s'} \pi(a|s) \mathcal{P}_{ss'}^a [V_1(s') - V_2(s')] \Big|$$

$$\leq \gamma \max_s |V_1(s) - V_2(s)| \max_s \Big| \sum_{a,s'} \pi(a|s) \mathcal{P}_{ss'}^a \Big| = \gamma \max_s |V_1(s) - V_2(s)|$$

- Iterative Policy Evaluation: $V_0 \to T^\pi V_0 \to T^\pi T^\pi V_0 \to \cdots$

Appendix: Banach Fix Point Theorem

Theorem

Suppose $\boldsymbol{T}$ *is a* γ*-contraction. Then under certain conditions,*

- $\boldsymbol{T}$ *admits a* **unique** *fix point* $\boldsymbol{V}^*$*, i.e.* $\boldsymbol{T}\boldsymbol{V}^* = \boldsymbol{V}^*$*;*
- $\boldsymbol{V}^*$ *can be found as follows: define a sequence* $\{\boldsymbol{V_k}\}_{\boldsymbol{k}}$ *such that* $\boldsymbol{V_{k+1}} = \boldsymbol{T}\boldsymbol{V_k}$*. Then* $\boldsymbol{V}^* = \boldsymbol{\lim_k V_k}$

- Proof can be found here
- $\boldsymbol{T}^{\boldsymbol{\pi}}$ is has a unique fix point
- $\boldsymbol{V}^{\boldsymbol{\pi}}$ is the fix point, according to the Bellman equation
- Iterative policy evaluation converges to $\boldsymbol{V}^{\boldsymbol{\pi}}$

Appendix: Bellman Optimality Operator

Definition

Define the Bellman Expectation Operator $\boldsymbol{T}$ as a function that maps a given value function $\boldsymbol{V}$ into another value function $\boldsymbol{TV}$ such that

$$\boldsymbol{TV}(s) = \max_{a \in \mathcal{A}} \left[\mathcal{R}_s^a + \gamma \sum_{s'} \mathcal{P}_{ss'}^a \boldsymbol{V}(s') \right], \qquad \forall s \in \mathcal{S}.$$

- The Bellman optimality equation can be rewritten as $\boldsymbol{V}^{\pi^{\text{opt}}} = \boldsymbol{T}\boldsymbol{V}^{\pi^{\text{opt}}}$
- This operator is a γ-**contraction** as well

$$\begin{aligned} \max_s |\boldsymbol{TV_1}(s) - \boldsymbol{TV_2}(s)| &= \gamma \max_{s,a} \left| \sum_{s'} \mathcal{P}_{ss'}^a [\boldsymbol{V_1}(s') - \boldsymbol{V_2}(s')] \right| \\ &\leq \gamma \max_{s'} |\boldsymbol{V_1}(s') - \boldsymbol{V_2}(s')| \end{aligned}$$

Appendix: Convergence of Dynamic Programming

- $\boldsymbol{T}$ has a unique fix point
- $\boldsymbol{V}^{\pi^{\text{opt}}}$ is the fix point, according to the Bellman optimality equation
- According to the Banach fix point theorem, **value iteration** converges to $\boldsymbol{V}^{\pi^{\text{opt}}}$
- **Policy iteration** (that integrates iterative policy evaluation & policy improvement) converges to $\boldsymbol{\pi}^{opt}$

Questions