Reinforcement Learning

Lecture 1: Foundations of Reinforcement Learning

Chengchun Shi

Lecture Outline

Lecture Outline (Cont'd)

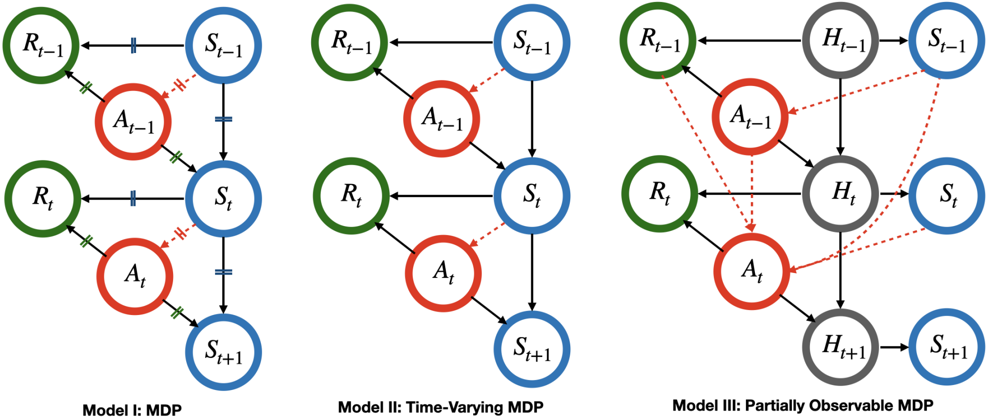
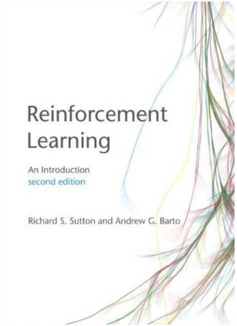


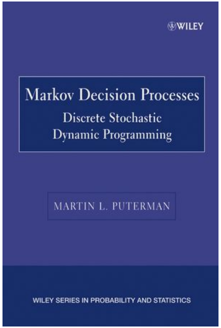
Figure: Causal diagrams for MDPs, TMDPs and POMDPs. Solid lines represent the causal relationships. Dashed lines indicate the information needed to implement the optimal policy. $\{H_t\}_t$ denotes latent variables. The parallel sign $\|$ indicates that the conditional probability function given parent nodes is equal.

Lecture Outline

Textbooks

- **Reinforcement Learning: An Introduction** (Second Edition) by Sutton and Barto (2018)
  - **Ebook** free online (link)
  - 50K citations so far
- **Markov decision processes: discrete stochastic dynamic programming** by Puterman (2014)





Useful Resources

- **Deepmind & UCL** reinforcement learning (RL) course by David Silver
  - **Course webpage** link
  - **Videos** available on Youtube
  - **Slides** available on webpage
- **UC Berkeley** PhD-level deep RL course by Sergey Levine
  - **Course webpage** link
  - Some more **resources** link
- Working draft on "**Reinforcement Learning: Theory and Algorithms**" by Alekh, Nan, Sham and Wen link

Applications

(a) Games

(b) Health Care

(c) Ridesharing

(d) Robotics

(e) Finance

(f) Automated Driving

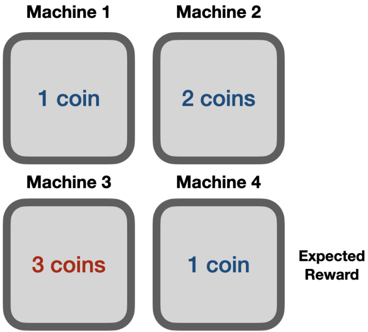
Lecture Outline

Multi-Armed Bandit (MAB) Problem

- The **simplest** RL problem
- A casino with **multiple** slot machines
- Playing each machine yields an independent **reward**.
- Limited knowledge (unknown reward distribution for each machine) and resources (**time**)
- **Objective**: determine which machine to pick at each time to maximize the expected **cumulative rewards**

Multi-Armed Bandit Problem (Cont'd)

- k-armed bandit problem (k machines)
- $A_t \in \{1, \cdots, k\}$: arm (machine) pulled (experimented) at time t
- $R_t \in \mathbb{R}$: reward at time t
- $Q(a) = \mathbb{E}(R_t | A_t = a)$ expected reward for each arm a (**unknown**)
- **Objective**: maximize $\sum_{t=1}^{T} \mathbb{E} R_t$.



Greedy Action Selection

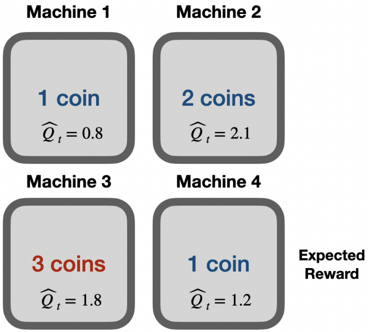
- **Action-value methods**: estimate the expected reward (i.e., value) of actions and use these estimates to select actions
- Estimated reward at time t:

$$\widehat{Q}_t(a) = \frac{\sum_{i=1}^{t} R_i \mathbb{I}(A_i = a)}{\sum_{i=1}^{t} \mathbb{I}(A_i = a)}$$

- **Greedy policy**:

$$A_t = \arg\max_a \widehat{Q}_{t-1}(a).$$

- Might be **suboptimal** in the long run.



Exploration-Exploitation Dilemma

- **Exploitation**: To maximize reward, the agent prefers the greedy policy that selects actions that maximizes the estimated expected reward.
- **Exploration**: To discover which actions yield a higher reward, the agent must try actions that it has less selected to improve the estimation accuracy.
- **Trade-off** between exploration and exploitation:
  - Neither exploration nor exploitation can be used exclusively.
  - The agent must try various actions and progressively favour high-reward actions.
- Practical algorithms: ε-**greedy**, **upper confidence bound** (UCB), **Thompson sampling**.

ε-Greedy

- **Input**: Choose a small value parameter $\varepsilon \in (0, 1)$.
- At each step **perform**:
  - With probability $\mathbf{1} - \varepsilon$: adopt the **greedy policy**;
  - With probability ε: choose a **randomly selected arm** from the set of all arms.
- Combines exploration and exploitation:
  - At each time, each arm is selected with probability at least $\boldsymbol{k}^{-1}\varepsilon$.
  - Greedy action is selected with probability $\mathbf{1} - \varepsilon + \boldsymbol{k}^{-1}\varepsilon$.

Incremental Implementation

- Average reward received from arm a by time t:

$$\widehat{Q}_t(a) = \mathbb{N}_t^{-1}(a) \sum_{i=1}^{t} \mathbb{I}(A_i = a) R_i,$$

  where $\mathbb{N}_t(a) = \sum_{i=1}^{t} \mathbb{I}(A_i = a)$.
- If arm a is selected at time $t+1$, then

$$\begin{aligned}
\widehat{Q}_{t+1}(a) &= \{\mathbb{N}_t(a) + 1\}^{-1} \left\{ \sum_{i=1}^{t} \mathbb{I}(A_i = a) R_i + R_{t+1} \right\} \\
&= \frac{\mathbb{N}_t(a)}{\mathbb{N}_t(a)+1} \left\{ \mathbb{N}_t^{-1}(a) \sum_{i=1}^{t} \mathbb{I}(A_i = a) R_i \right\} + \frac{R_{t+1}}{\mathbb{N}_t(a)+1} \\
&= \frac{\mathbb{N}_t(a)}{\mathbb{N}_t(a)+1} \widehat{Q}_t(a) + \frac{R_{t+1}}{\mathbb{N}_t(a)+1}.
\end{aligned}$$

Algorithm

- **Input**: $0 < \varepsilon < 1$, termination time $\boldsymbol{T}$.
- **Initialization**: $\boldsymbol{t} = \mathbf{0}$, $\widehat{\boldsymbol{Q}}(\boldsymbol{a}) = \mathbf{0}$, $\mathbb{N}(\boldsymbol{a}) = \mathbf{0}$, for $\boldsymbol{a} = \mathbf{1}, \mathbf{2}, \cdots, \boldsymbol{k}$.
- **While** $\boldsymbol{t} < \boldsymbol{T}$:
  - **Update** $\boldsymbol{t}$: $\boldsymbol{t} \leftarrow \boldsymbol{t} + \mathbf{1}$.
  - ε**-greedy action selection**:

$$\boldsymbol{a}^* \leftarrow \begin{cases} \arg\max_{\boldsymbol{a}} \widehat{\boldsymbol{Q}}(\boldsymbol{a}), & \text{with probabiltiy } \mathbf{1} - \varepsilon, \\ \text{random arm}, & \text{with probabiltiy } \varepsilon. \end{cases}$$

  - **Receive reward** $\boldsymbol{R}$ from arm $\boldsymbol{a}^*$.
  - **Update** $\mathbb{N}(\boldsymbol{a}^*)$: $\mathbb{N}(\boldsymbol{a}^*) \leftarrow \mathbb{N}(\boldsymbol{a}^*) + \mathbf{1}$.
  - **Update** $\widehat{\boldsymbol{Q}}(\boldsymbol{a}^*)$:

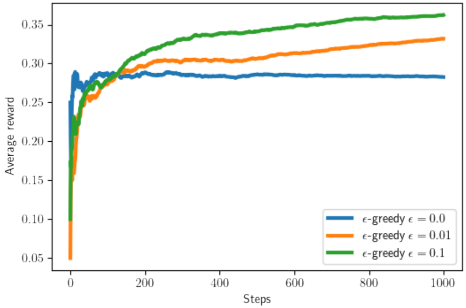
$$\widehat{\boldsymbol{Q}}(\boldsymbol{a}^*) \leftarrow \frac{\mathbb{N}(\boldsymbol{a}^*) - \mathbf{1}}{\mathbb{N}(\boldsymbol{a}^*)} \widehat{\boldsymbol{Q}}(\boldsymbol{a}^*) + \frac{\mathbf{1}}{\mathbb{N}(\boldsymbol{a}^*)} \boldsymbol{R}.$$

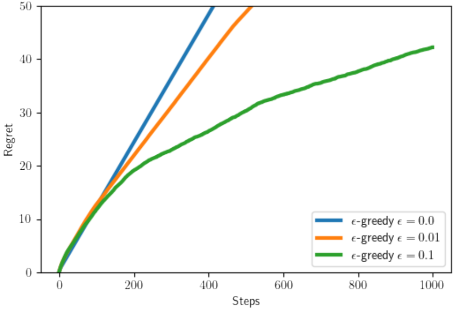
Example: Four Bernoulli Arms

Reward distributions	Bernoulli(0.1)	Bernoulli(0.4)	Bernoulli(0.1)	Bernoulli(0.1)

Best arm

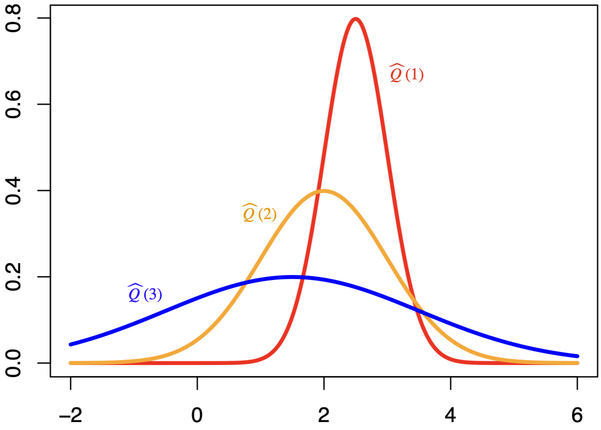
Example: Four Bernoulli Arms (Cont’d)





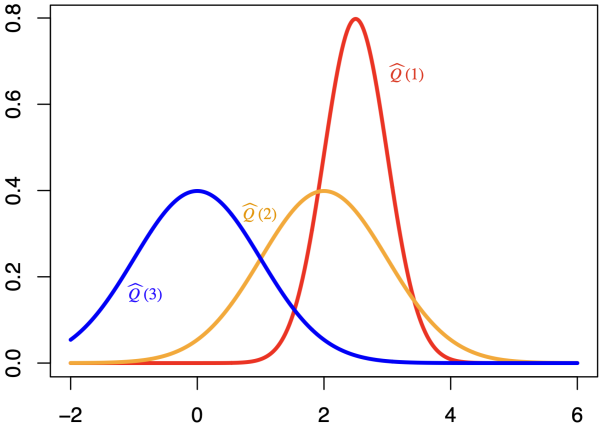
Optimism in the Face of Uncertainty

- The **optimistic principle**:
- The more **uncertain** we are about an action-value;
- The more **important** it is to explore that action;
- It could be the **best** action.
- Likely to pick blue action.
- **Different** from ε-greedy which selects arms uniformly random.



Optimism in the Face of Uncertainty (Cont'd)

- After picking blue action;
- Become less **uncertain** about the value;
- More likely to pick other actions;
- Until we home in on best action.



Upper Confidence Bound

- Estimate an **upper confidence** $U_t(a)$ for each action value such that

$$Q(a) \leq \widehat{Q}_t(a) + U_t(a),$$

  with high probability.
- $U_t(a)$ quantifies the **uncertainty** and depends on $\mathbb{N}_t(a)$ (number of times arm a has been selected up to time t)
  - Large $\mathbb{N}_t(a) \to$ small $U_t(a)$;
  - Small $\mathbb{N}_t(a) \to$ large $U_t(a)$.
- Select actions maximizing upper confidence bound

$$a^* = \arg\max_a [\widehat{Q}_t(a) + U_t(a)].$$

- Combines **exploration** ($U_t(a)$) and **exploitation** ($\widehat{Q}_t(a)$).

Upper Confidence Bound (Cont'd)

- Set $U_t(a) = \sqrt{c \log(t)/\mathbb{N}_t(a)}$ for some positive constant c.
- According to **Hoeffding's inequality** (link), when rewards are bounded between 0 and 1, the event

$$Q(a) \leq \widehat{Q}_t(a) + U_t(a),$$

holds with probability at least $1 - t^{-2c}$ (converges to 1 as $t \to \infty$).

Algorithm

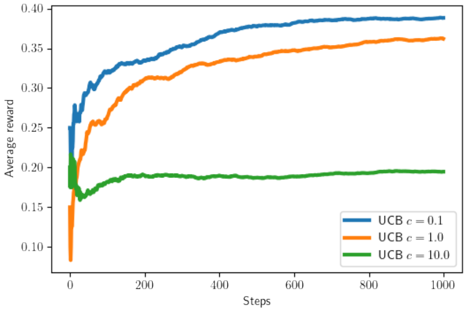
- **Input**: some positive constant c, termination time T.
- **Initialization**: $t = 0$, $\widehat{Q}(a) = 0$, $\mathbb{N}(a) = 0$, for $a = 1, 2, \cdots, k$.
- **While** $t < T$:
  - **Update** t: $t \leftarrow t + 1$.
  - **UCB action selection**:

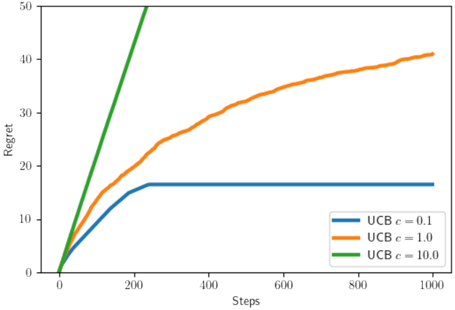
$$a^* \leftarrow \arg\max_a [\widehat{Q}(a) + \sqrt{c \log(t)/\mathbb{N}_t(a)}].$$

  - **Receive reward** R from arm a^*.
  - **Update** $\mathbb{N}(a^*)$: $\mathbb{N}(a^*) \leftarrow \mathbb{N}(a^*) + 1$.
  - **Update** $\widehat{Q}(a^*)$:

$$\widehat{Q}(a^*) \leftarrow \frac{\mathbb{N}(a^*) - 1}{\mathbb{N}(a^*)} \widehat{Q}(a^*) + \frac{1}{\mathbb{N}(a^*)} R.$$

Example: Four Bernoulli Arms (Revisited)





Thompson Sampling

- A **highly-competitive** algorithm to address exploration-exploitation trade-off.
- Impose **statistical models** for the reward distribution with parameter θ.
- Impose **prior distributions** for θ.
- At time t,
  - Use **Bayes rule** to update the **posterior distribution** of θ.
  - Sample a model parameter θ_t from the posterior distribution.
  - Compute action-value given θ_t, i.e., $\mathbb{E}(R|A=a,\theta_t)$.
  - Select action maximizing action-value

$$a^* = \arg\max_a \mathbb{E}(R|A=a,\theta_t).$$

- Posterior distribution quantifies the **uncertainty** of the estimated model parameter (**exploration**).
- $\mathbb{E}(R|A=a,\theta_t)$ estimates the oracle action value (**exploitation**).

Thompson Sampling (Bernoulli Bandit Example)

- **Statistical models**:
  - Reward of the ath arm follows a Bernoulli distribution with mean $\theta(a)$.
  - $\theta(a)$ follows a Beta(α, β) distribution (**prior**).
  - **Conjugate** distribution of binomial, i.e. posterior distribution is Beta as well
  - α and β measures the beliefs for **success** and **failure**
- **Bayesian inference**:
  - $\theta(a)$ follows a Beta$(S_a + \alpha, F_a + \beta)$ distribution (**posterior**) where (S_a, F_a) corresponds to the success and failure counters under arm a.
- **Compute action value**:

$$\mathbb{E}(R|A = a, \theta_t) = \theta_t(a).$$

Algorithm (Bernoulli Bandit Example[1])

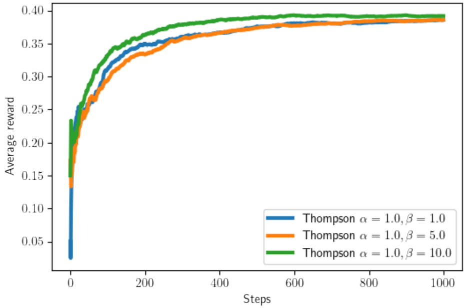
- **Input**: hyper-parameters α, $\beta > 0$, termination time T.
- **Initialization**: $t = 0$, $S_a = F_a = 0$, for $a = 1, 2, \cdots, k$.
- **While** $t < T$:
  - **Update** t: $t \leftarrow t + 1$.
  - **Posterior sampling**: For $a = 1, 2, \cdots, k$, sample

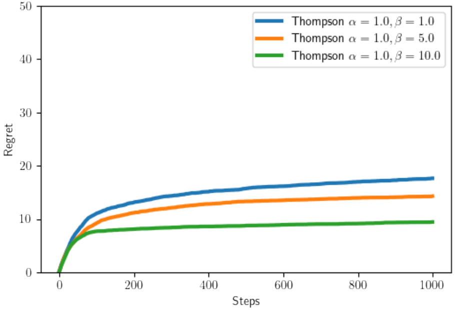
$$\theta_a \sim \mathrm{Beta}(S_a + \alpha, F_a + \beta)$$

  - **Action selection**: $a^* \leftarrow \arg\max_a \theta_a$.
  - **Receive reward** R from arm a^*.
  - **Update** S_a and F_a:
    - If $R = 1$, $S_a \leftarrow S_a + 1$;
    - If $R = 0$, $F_a \leftarrow F_a + 1$.

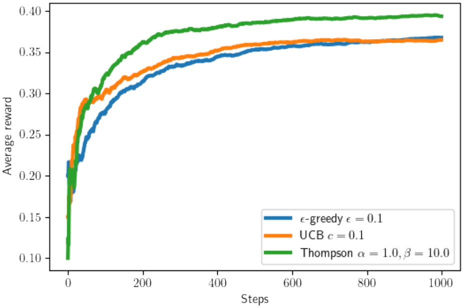
[1] The general algorithm can be found in Chapelle and Li [2011]

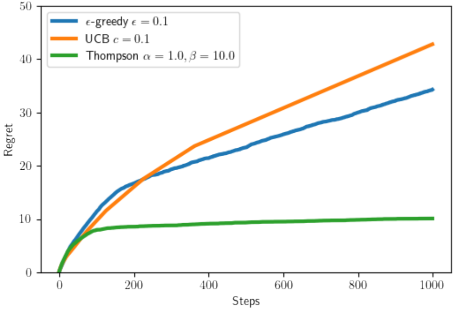
Example: Four Bernoulli Arms (Revisited)





Example: Four Bernoulli Arms (Cont'd)





Theory

Define the **regret** T, $\mathcal{R}(T)$ as the difference between the cumulative reward under the **best action** and that under the **selected actions**, up to time T.

Theorem (UCB, Auer et al. [2002])

The **expected regret** *of the UCB algorithm* $\mathbb{E}\mathcal{R}(T)$ *is upper bounded by* $C_1 \log(T)$ *for some constant* $C_1 > 0$.

Theorem (TS, Agrawal and Goyal [2012])

The **expected regret** *of the Thompson sampling algorithm* $\mathbb{E}\mathcal{R}(T)$ *is upper bounded by* $C_2 \log(T)$ *for some constant* $C_2 > 0$.

- Both algorithms achieve logarithmic expected regret.
- Their performances are nearly the same as the oracle method that works as if the best action were known.

Lecture Outline

1. Introduction to Reinforcement Learning (RL)

1.1 Multi-Armed Bandits

1.2 Contextual Bandits

2. Markov Decision Processes (MDPs)

2.1 Time-Varying MDPs (TMDPs)

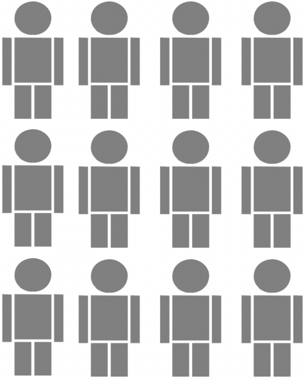
2.2 Partially Observable MDPs (POMDPs)

3. The Existence of the Optimal Stationary Policy

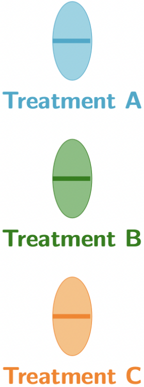
Contextual Bandits

- Extension of MAB with **contextual** information.
- A **widely-used** model in medicine and technological industries.
- At time $\boldsymbol{t}$, the agent
  - Observe a context $\boldsymbol{S_t}$;
  - Select an action $\boldsymbol{A_t}$;
  - Receives a reward $\boldsymbol{R_t}$ (depends on both $\boldsymbol{S_t}$ and $\boldsymbol{A_t}$).
- **Objective**: maximize cumulative reward.
- ε-**greedy**, **UCB** and **Thompson sampling** can be similarly adopted [see e.g., Chu et al., 2011, Agrawal and Goyal, 2013, Zhou et al., 2020, Zhang et al., 2020].

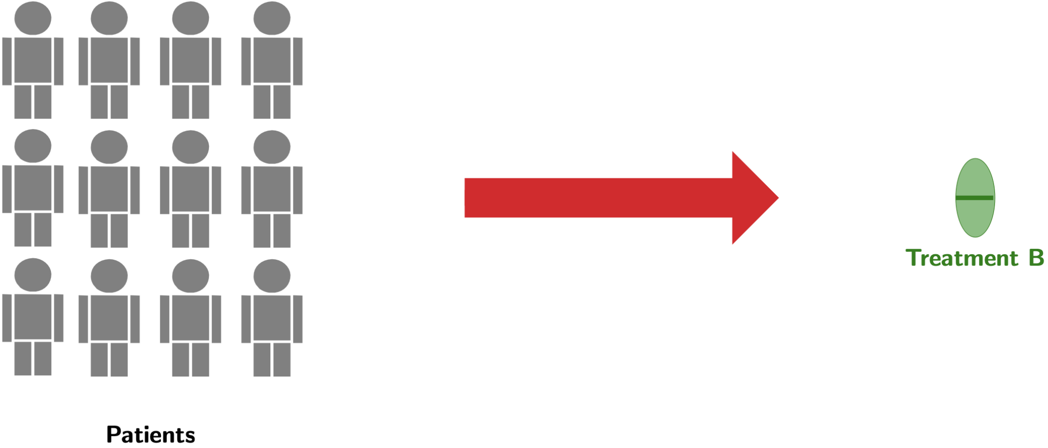
Application I: Precision Medicine



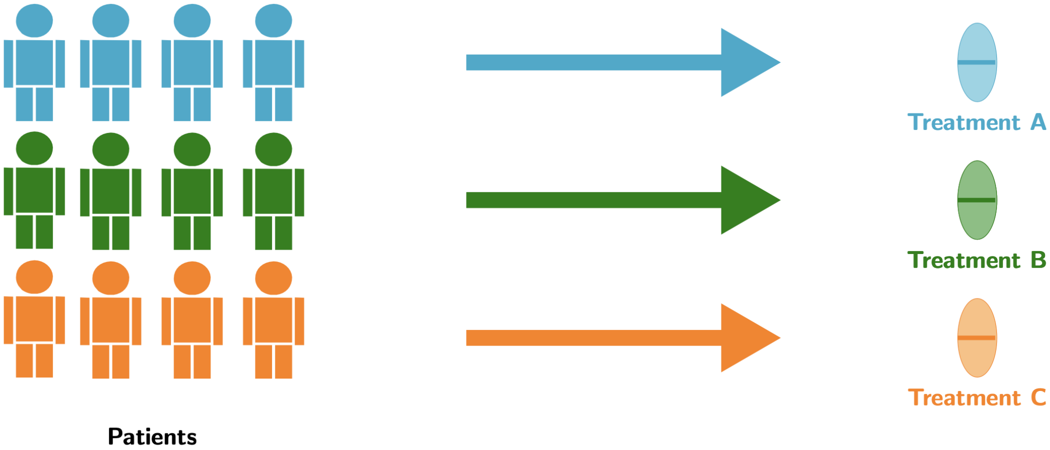
Patients



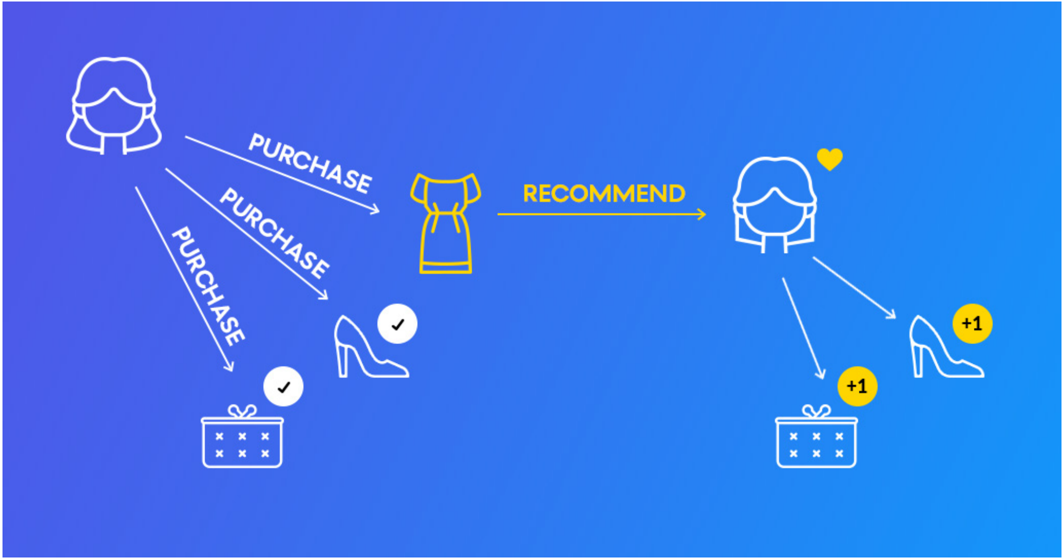
One-Size-Fits-All



Individualized Treatment Regime

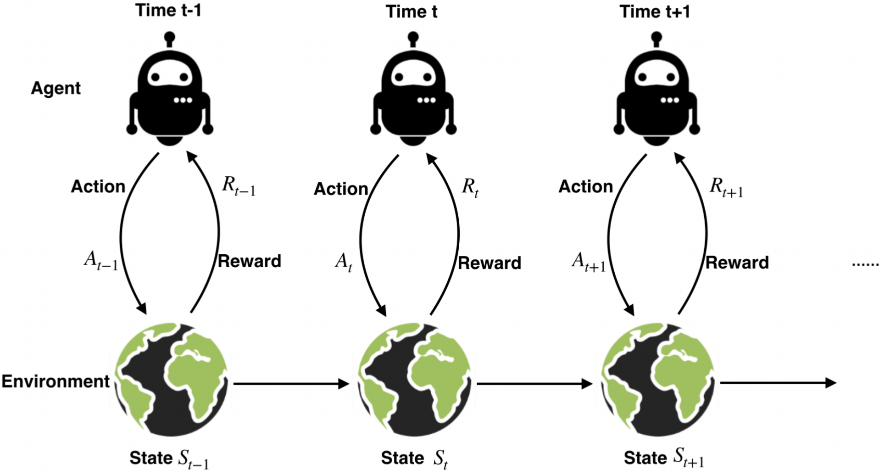


Application II: Personalized Recommendation



Lecture Outline

Sequential Decision Making



Objective: find an optimal policy that maximizes the cumulative reward

Markov Decision Processes

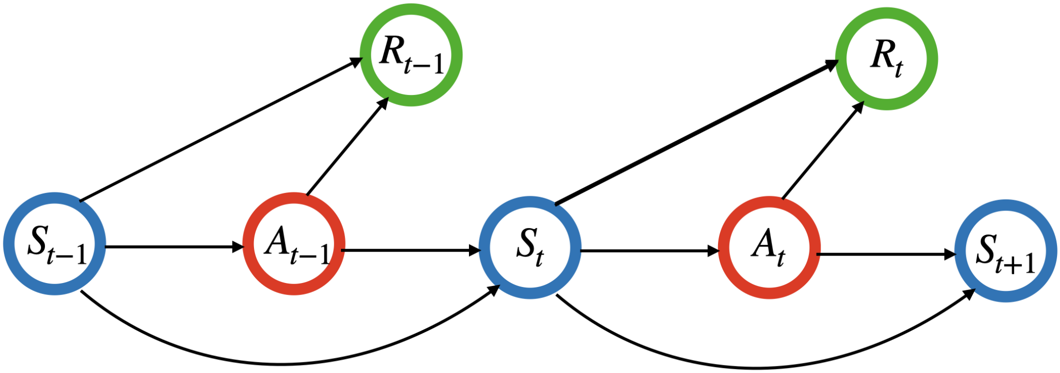
Definition

$\{S_t, A_t, R_t\}_t$ forms a Markov decision process if and only if

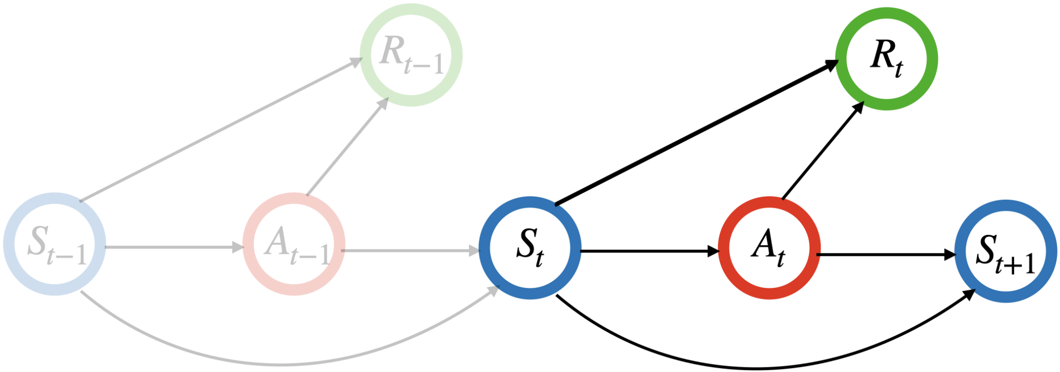
- $\Pr(S_{t+1}, R_t | A_t, S_t) = \Pr(S_{t+1}, R_t | A_t, S_t, R_{t-1}, A_{t-1}, S_{t-1}, \cdots)$ (Markovianity)
- $\Pr(S_{t+1}, R_t | A_t = a, S_t = s) = \Pr(S_t, R_{t-1} | A_{t-1} = a, S_{t-1} = s)$ (time-homogeneity)

- The current **state-action** pair captures all relevant information from the history
- When A_t depends the history only through S_t, $\{S_t, A_t, R_t\}_t$ forms a Markov chain.

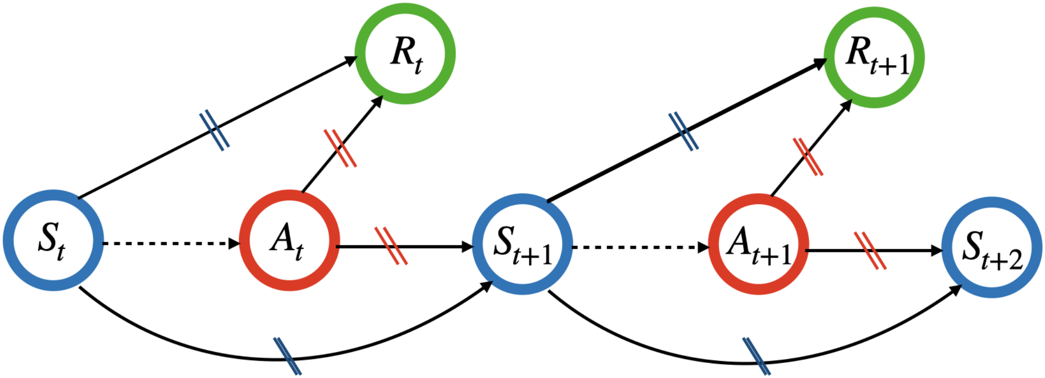
Markov Assumption



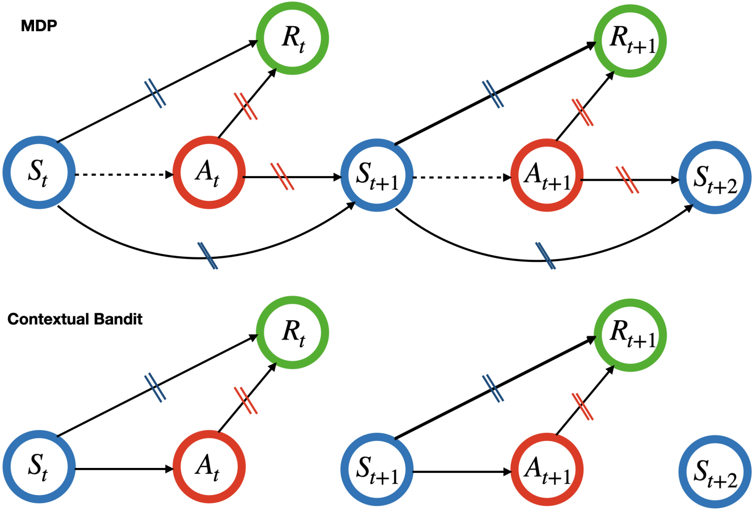
Markov Assumption



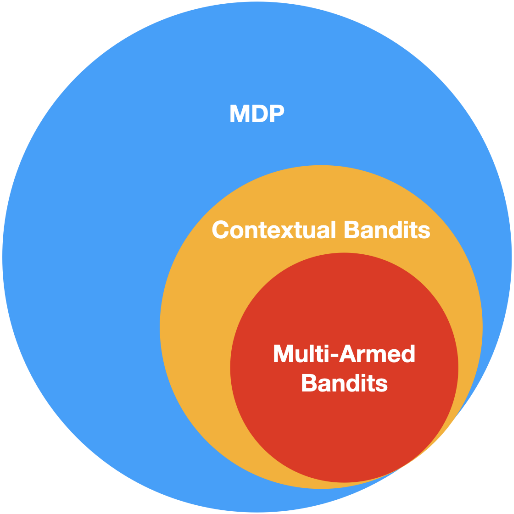
Stationarity Assumption



MDP vs Contextual Bandits



MDP v.s. Contextual Bandits (Cont'd)



Lecture Outline

Time-Varying MDPs

- The **time-homogeneity** assumption is likely to be violated in real applications (e.g., mobile health, ridesharing)
- **Nonstationarity** *is the case most commonly encountered in reinforcement learning* [Sutton and Barto, 2018]

Definition

$\{S_t, A_t, R_t\}_t$ forms a time-varying Markov decision process iff

$$\Pr(S_{t+1}, R_t | A_t, S_t) = \Pr(S_{t+1}, R_t | A_t, S_t, R_{t-1}, A_{t-1}, S_{t-1}, \cdots) \qquad \text{(Markovianity)}$$

Causal Diagram: TMDP

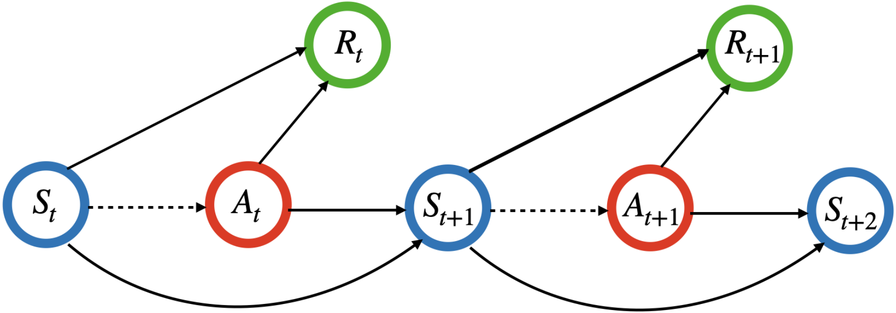
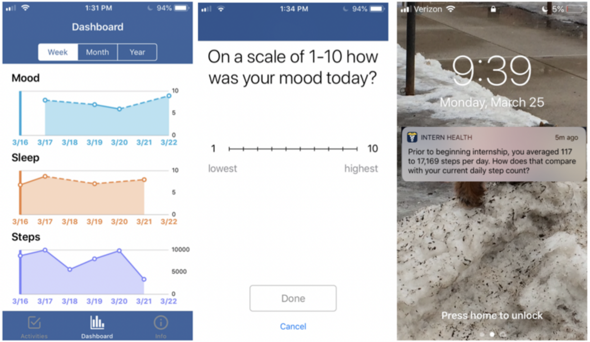


Figure: Causal diagrams for MDPs. Solid lines represent causal relationships. The parent nodes for the action is **not** specified in the model. $\boldsymbol{A_t}$ could either depend on $\boldsymbol{S_t}$ or the history.

Mobile Health Example: Intern Health Study

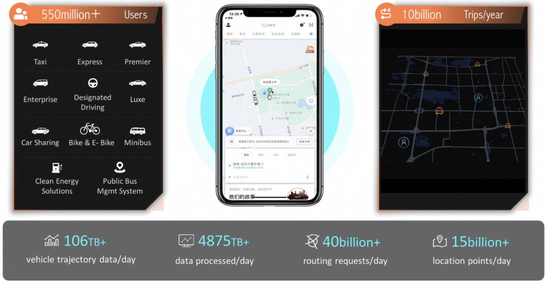
- **Mental health** management
- **Subject**: First-year medical interns
- S_t: Interns' **mood scores**, **sleep hours** and **step counts**
- A_t: Send **text notifications** or not
- R_t: **Mood scores** or **step counts**

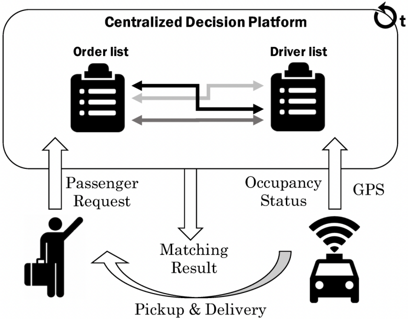


(i) App Dashboard (ii) Mood EMA (iii) Notifications

- The study lasts for half an year
- Treatment effects are usually **time-inhomogeneous** (decays over time)
- Leading to TMDPs

Ridesharing Example: Order-Dispatching





- S_t: **Supply** (number of available drivers) and **demand** (number of call orders)
- A_t: **Order-dispatching**: match a driver with an order
- R_t: **Passengers' answer rate/Drivers' income**
- Weekday-weekend differences, peak and off-peak differences lead to **time-inhomogeneity**

Lecture Outline

Partially Observable MDPs

- Difference between MDPs and POMDPs: states **fully-observable** or **partially-observable**
- The fully-observability assumption might be violated in practice
- In healthcare, patients' characteristics might not be fully recorded

Causal Diagram: POMDP

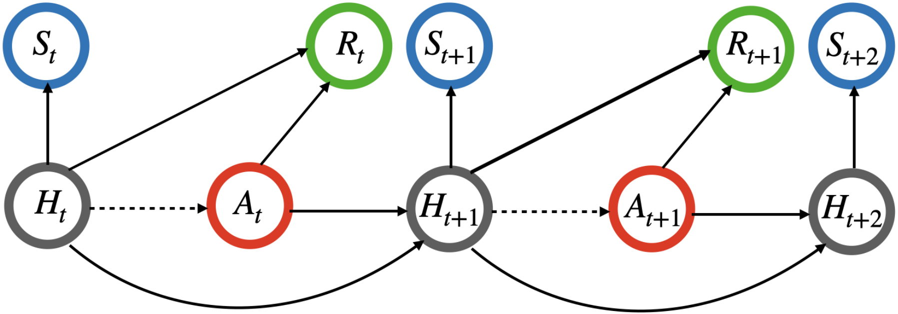
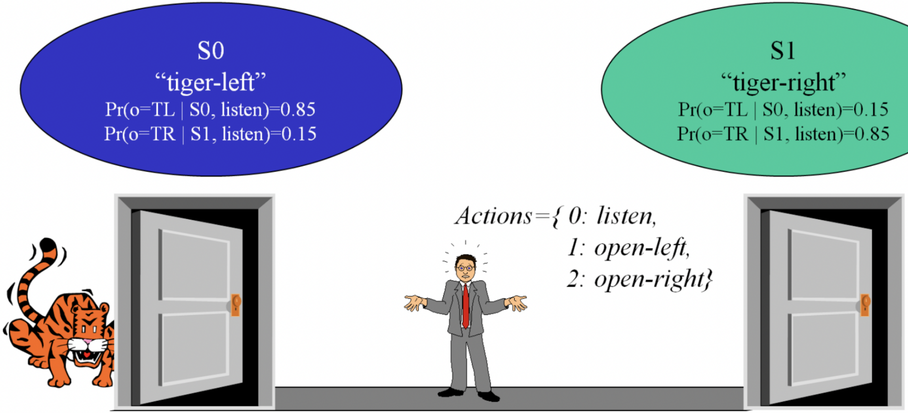


Figure: Causal diagrams for MDPs. Solid lines represent causal relationships. $\{H_t\}_t$ denotes latent states. The parent nodes for the action is **not** specified in the model. A_t could either depend on S_t or the history.

Example: the Tiger Problem



Reward Function

- *Penalty for wrong opening: -100*
- *Reward for correct opening: +10*
- *Cost for listening action: -1*

Observations

- *to hear the tiger on the left (TL)*
- *to hear the tiger on the right(TR)*

Example: the Tiger Problem (Cont'd)

Suppose we choose to listen at each time

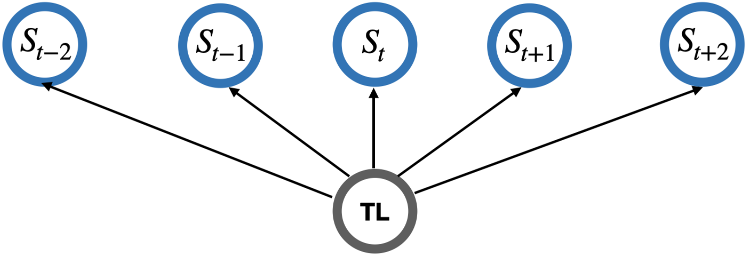


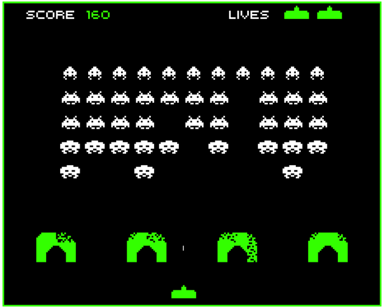
Figure: Causal diagram for the tiger problem. TL denotes the tiger location. S_t denotes the inferred location of the tiger at time t.

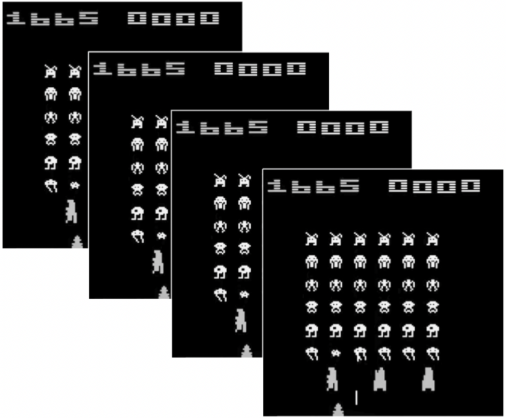
Converting non-MDPs into MDPs

- MDP assumptions: Markovianity & time-homogeneity
- To ensure **time-homogeneity**: include time variables in the state
- In ridesharing, include dummy variables weekdays/weekends & peak/off-peak hours
- In mobile health, use more recent observations
- To ensure **Markovianity**: concatenate measurements over multiple time steps

Stacking Frames in Atari Games

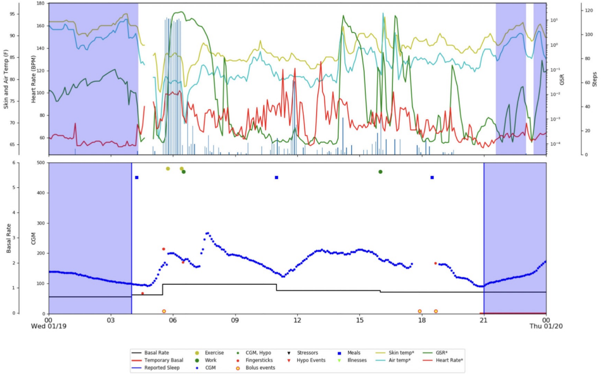
Input is a stack of 4 most recent frames [Mnih et al., 2015]





Concatenating Observations in Diabetes Study

- Management of **Type-I diabetes**
- **Subject**: Patients with diabetes.
- S_t: Patient's **glucose levels**, **food intake**, **exercise intensity**
- A_t: **Insulin doses** injected
- R_t: **Index of Glycemic Control** (function of patient's glucose level)



- Markovianity holds when concatenating 4 most recent observations [Shi et al., 2020]
- Concatenating observations also yield better policies

Lecture Outline

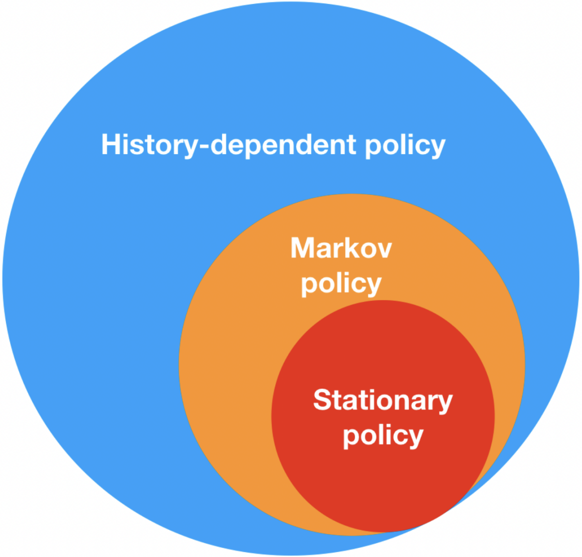
The Agent's Policy

- The agent implements a **mapping** π_t from the observed data to a probability distribution over actions at each time step
- The collection of these mappings $\pi = \{\pi_t\}_t$ is called **the agent's policy**:

$$\pi_t(a|\bar{s}) = \Pr(A_t = a|\bar{S}_t = \bar{s}),$$

  where $\bar{S}_t = (S_t, R_{t-1}, A_{t-1}, S_{t-1}, \cdots, R_0, A_0, S_0)$ is the set of **observed data history** up to time t.
- **History-Dependent** Policy: π_t depends on $\bar{S}_t$.
- **Markov** Policy: π_t depends on $\bar{S}_t$ only through S_t.
- **Stationary** Policy: π is Markov & π_t is **homogeneous** in t, i.e., $\pi_0 = \pi_1 = \cdots$.

The Agent's Policy (Cont'd)



The Agent's Policy (Cont'd)

- The collection of these mappings $\pi = \{\pi_t\}_t$ is called **the agent's policy**:

$$\pi_t(a|\bar{s}) = \Pr(A_t = a|\bar{S}_t = \bar{s}),$$

  where $\bar{S}_t = (S_t, R_{t-1}, A_{t-1}, S_{t-1}, \cdots, R_0, A_0, S_0)$.

- **Random** Policy: $\pi_t(\bullet|\bar{s})$ is a probability distribution over the action space
- **Deterministic** Policy: each probability distribution is degenerate
  - i.e., for any t and $\bar{s}$, $\pi_t(a|\bar{s}) = 1$ for some a and 0 for other actions
  - use $\pi_t(\bar{s})$ to denote the action that the agent selects

Goals, Objectives and the Return

The agent's goal: find a policy that maximizes the **expected return** received in long run

Definition (Return, Average Reward Setting)

The **return** G_t is the average reward from time-step t.

$$G_t = \lim_{T \to \infty} \frac{1}{T} \sum_{i=t}^{t+T-1} R_i.$$

Definition (Return, Discounted Reward Setting)

The **return** G_t is the cumulative discounted reward from time-step t.

$$G_t = \sum_{i=0}^{+\infty} \gamma^i R_{i+t}.$$

Discounted Reward Setting (Our Focus)

Definition (Return)

The **return** G_t is the cumulative discounted reward from time-step t.

$$G_t = \sum_{i=0}^{+\infty} \gamma^i R_{i+t}.$$

- The **discount factor** $0 \leq \gamma < 1$ represents the **trade-off** between **immediate** and **future** rewards.
- The value of receiving reward R after k time steps is $\gamma^k R$.
- $\gamma = 0$ leads to "**myopic**" evaluation
- γ close to 1 leads to "**far-sighted**" evaluation (close to the average reward)

Why Discount?

- **Mathematically convenient**: avoids infinite returns.
- **Computationally convenient**: easier to develop practical algorithms.
- In finance, immediate rewards earn more **interests** than delayed rewards
- Animal/human behaviour shows **preference** for immediate reward
  - Go to bed late and you'll be tired tomorrow
  - Eat heartily in winter and you'll need to trim fat in summer
- Possible to set $\gamma = \mathbf{1}$ in **finite horizon** settings (number of decision steps is finite; e.g., precision medicine applications where patients receive only a finite number of treatments)

(State) Value Function

Definition

The (state) value function $V^\pi(s)$ is expected return starting from s under π,

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

- V^π is **independent** of the time t in its definition, under **time-homogeneity**
- $\mathbb{E}^\pi$ denotes the expectation assuming the system follows π

Bellman Equation

Definition

The Bellman equation for the state value function is given by

$$\boldsymbol{V}^{\boldsymbol{\pi}}(\boldsymbol{s}) = \mathbb{E}^{\boldsymbol{\pi}}\{\boldsymbol{R}_{\boldsymbol{t}} + \gamma \boldsymbol{V}^{\boldsymbol{\pi}}(\boldsymbol{S}_{\boldsymbol{t}+1}) | \boldsymbol{S}_{\boldsymbol{t}} = \boldsymbol{s}\}.$$

- The value function can be **decomposed** into two parts:
  - Immediate reward $\boldsymbol{R}$
  - discounted value of success state $\gamma \boldsymbol{V}^{\boldsymbol{\pi}}(\boldsymbol{S}_{\boldsymbol{t}+1})$
- Forms the basis for **value evaluation** (more in later lectures)

Bellman Equation (Proof)

$$
\begin{aligned}
V^{\pi}(s) &= \mathbb{E}^{\pi}(G_t | S_t = s) \\
&= \mathbb{E}^{\pi}(R_t + \gamma(R_{t+1} + \gamma R_{t+2} + \cdots) | S_t = s) \\
&= \mathbb{E}^{\pi}(R_t | S_t = s) + \gamma \mathbb{E}^{\pi}(G_{t+1} | S_t = s) \\
&= \mathbb{E}^{\pi}(R_t | S_t = s) + \gamma \mathbb{E}^{\pi}\{\mathbb{E}^{\pi}(G_{t+1} | S_{t+1}, S_t) | S_t = s\} \\
&= \mathbb{E}^{\pi}(R_t | S_t = s) + \gamma \mathbb{E}^{\pi}\{\mathbb{E}^{\pi}(G_{t+1} | S_{t+1}) | S_t = s\} \\
&= \mathbb{E}^{\pi}(R_t | S_t = s) + \gamma \mathbb{E}^{\pi}\{V^{\pi}(S_{t+1}) | S_t = s\},
\end{aligned}
$$

The second last equation holds due to the **Markov assumption**.

Bellman Optimality Equation

Definition

The Bellman optimality equation for the state-value function is given by

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

- According to the Bellman equation,

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

- The optimal policy selects the action that maximizes the value: $\mathbb{E}^{\pi^{\text{opt}}} = \max_a \mathbb{E}$

Existence of Optimal Stationary Policy in MDPs

Theorem (See also Puterman [2014], Theorem 6.2.10)

Assume the state-action space is **discrete** *and the rewards are* **bounded***. Then there exists an* **optimal stationary policy** $\pi^{opt} = \{\pi_t^{opt}\}_t$ *such that*

- $\pi_1^{opt} = \pi_2^{opt} = \cdots = \pi_t^{opt} = \cdots$
- $\mathbb{E}^{\pi^{opt}} G_0 \geq \mathbb{E}^{\pi} G_0$ *for any* **history-dependent** *policy* π

- When the system dynamics satisfies the **Markov** and **time-homogeneity** assumption, so does the **optimal policy**.
- Lay the **foundation** for most existing RL algorithms
- Simplify the calculation since it suffices to focus on stationary policies

Sketch of the Proof [Shi et al., 2020]

Goal HR, MR, SR denote classes of history-dependent, Markov and stationary policies. To show $\sup_{\pi \in \mathrm{SR}} V^{\pi}(s) = \sup_{\pi \in \mathrm{HR}} V^{\pi}(s)$ for any s.

Step 1 Show $\sup_{\pi \in \mathrm{MR}} V^{\pi}(s) = \sup_{\pi \in \mathrm{HR}} V^{\pi}(s)$ for any s under Markovianity.

Step 2 Show for any function ν that satisfies the **Bellman optimality equation**,

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

$\nu(s) = \sup_{\pi \in \mathrm{MR}} V^{\pi}(s)$ for any s.

Step 3 Show the existence of $\pi^* \in \mathrm{SR}$ such that V^{π^*} satisfies the Bellman optimality equation. This together with Step 2 yields

$$\sup_{\pi \in \mathrm{SR}} V^{\pi}(s) = \sup_{\pi \in \mathrm{MR}} V^{\pi}(s).$$

Sketch of the Proof (Step 1)

The key to Step 1 is to show for any $\pi \in \mathbf{HR}$ and any s, there exists a Markov policy $\dot{\pi} = \{\dot{\pi}_t\}_{t \geq 0}$ where $\dot{\pi}_t$ depends on S_t only such that

$$\Pr^{\pi}(A_t = a, S_t = s' | S_0 = s) = \Pr^{\dot{\pi}}(A_t = a, S_t = s' | S_0 = s), \tag{1}$$

for any $t \geq 0, a, s'$ where the probabilities $\Pr^{\pi}$ and $\Pr^{\dot{\pi}}$ are taken by assuming the system dynamics follow π and $\dot{\pi}$, respectively.
Under the **Markov assumption**, we have

$$\mathbb{E}^{\pi}(R_t | S_0 = s) = \mathbb{E}^{\pi}[r(S_t, A_t) | S_0], \qquad \forall t \geq 0.$$

This together with (1) yields that

$$\mathbb{E}^{\pi}(R_t | S_0 = s) = \mathbb{E}^{\dot{\pi}}(R_t | S_0 = s), \qquad \forall t \geq 0,$$

and hence $V^{\pi}(s) = V^{\dot{\pi}}(s)$.

Sketch of the Proof (Step 2)

First, by iteratively apply the inequality

$$\nu(s) \geq \max_a \mathbb{E}[R_t + \gamma\nu(S_{t+1})|A_t = a, S_t = s]$$

we can show that $\nu(s) \geq \sup_{\pi \in \mathrm{MR}} V^{\pi}(s)$ for any s
Second, define the operator

$$\mathcal{L}\nu(s) = \max_a \mathbb{E}[\nu(S_{t+1})|A_t = a, S_t = s]$$

The operator $\mathcal{I} - \gamma\mathcal{L}$ is bounded and linear, and is thus invertible and its inverse equals $\sum_{k\geq 0} \gamma^k \mathcal{L}^k$. This together with

$$\nu(s) \leq \max_a \mathbb{E}[R_t + \gamma\nu(S_{t+1})|A_t = a, S_t = s]$$

yields that $\nu(s) \leq \sup_{\pi \in \mathrm{MR}} V^{\pi}(s)$ for any s

Sketch of the Proof (Step 3)

For any function ν, define the norm $\|\nu\|_\infty = \sup_s |\nu(s)|$. We have for any ν_1 and ν_2 that

$$
\begin{aligned}
\sup_s \Big| \max_a \mathbb{E}[R_t + \gamma \nu_1(S_{t+1}) | A_t = a, S_t = s] \\
- \max_a \mathbb{E}[R_t + \gamma \nu_2(S_{t+1}) | A_t = a, S_t = s] \Big| \\
\leq \gamma \max_a \sup_s |\mathbb{E}[\nu_1(S_{t+1}) - \nu_2(S_{t+1}) | A_t = a, S_t = s]| \\
\leq \gamma \|\nu_1 - \nu_2\|_\infty
\end{aligned}
$$

By **Banach's fix point theorem**, there exists a unique value function ν_0 that satisfies the optimal Bellman equation. This together with the first two steps completes the proof.

Existence of Optimal Markov Policy in TMDPs

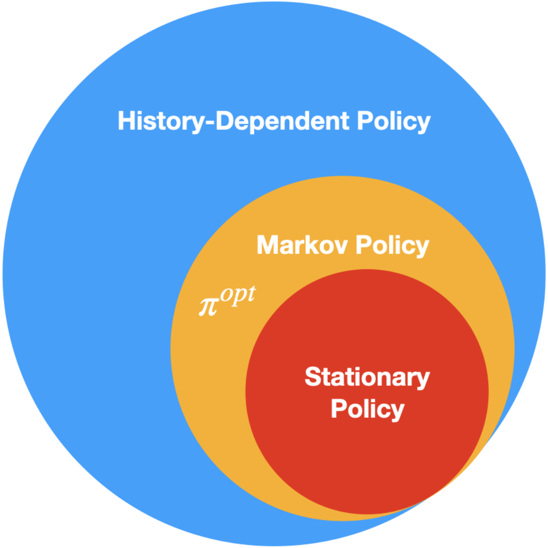
Theorem (See also Puterman [2014], Theorem 5.5.1)

Assume the state-action space is **discrete**. *Then there exists an* **optimal Markov policy** $\pi^{opt} = \{\pi_t^{opt}\}_t$ *such that*

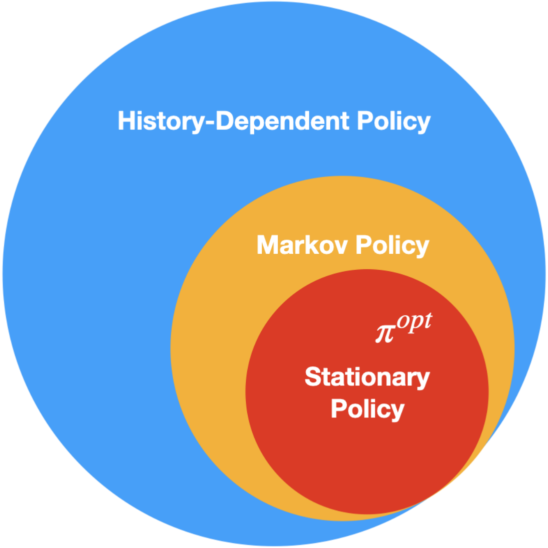
- *each* π_t^{opt} *depends on the data history only through* S_t
- $\mathbb{E}^{\pi^{opt}} G_0 \geq \mathbb{E}^{\pi} G_0$ *for any* **history-dependent** *policy* π

When the system dynamics satisfies the **Markov** assumption, so does the **optimal policy**.

In TMDPs


History-Dependent Policy
Markov Policy
π^{opt}
Stationary
Policy

In MDPs


History-Dependent Policy
Markov Policy
π^{opt}
Stationary Policy

Summary

- Exploration-exploitation tradeoff
- ϵ-greedy
- Upper confidence bound
- Thompson sampling

- Multi-armed bandits
- Contextual bandits
- Markov decision processes

Summary (Cont'd)

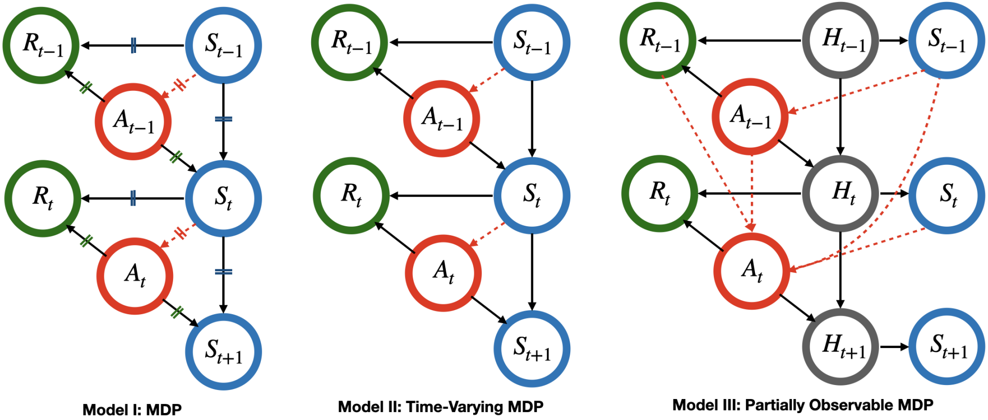


Figure: Causal diagrams for MDPs, TMDPs and POMDPs. Solid lines represent the causal relationships. Dashed lines indicate the information needed to implement the optimal policy. $\{H_t\}_t$ denotes latent variables. The parallel sign $\parallel$ indicates that the conditional probability function given parent nodes is equal.

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Questions