Artificial Intelligence

CS 165A

May 18, 2023

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Today

→ Bandits and exploration

Recap: Tabular MDP

- Discrete State, Discrete Action, Reward and Observation

$$S_t \in \mathcal{S} \quad A_t \in \mathcal{A} \quad R_t \in \mathbb{R} \quad \sout{O_t \in \mathcal{O}}$$

- Policy:
  - When the state is observable: $\pi : \mathcal{S} \to \mathcal{A}$
  - ~~Or when the state is not observable~~

$$\sout{\pi_t : (\mathcal{O} \times \mathcal{A} \times \mathbb{R})^{t-1} \to \mathcal{A}}$$

- Learn the best policy that maximizes the expected reward
  - Finite horizon (episodic) RL: $\pi^* = \arg\max_{\pi \in \Pi} \mathbb{E}[\sum_{t=1}^{T} R_t]$ T: horizon
  - Infinite horizon RL: $\pi^* = \arg\max_{\pi \in \Pi} \mathbb{E}[\sum_{t=1}^{\infty} \gamma^{t-1} R_t]$ γ: discount factor

Recap: Reward function and Value functions

- Immediate reward function r(s,a,s')
  - expected **immediate** reward

$$r(s,a,s') = \mathbb{E}[R_1 | S_1 = s, A_1 = a, S_2 = s']$$

$$r^{\pi}(s) = \mathbb{E}_{a \sim \pi(a|s)}[R_1 | S_1 = s]$$

- state value function: $V^{\pi}(s)$
  - expected **long-term** return when starting in *s* and following π

$$V^{\pi}(s) = \mathbb{E}_{\pi}[R_1 + \gamma R_2 + ... + \gamma^{t-1} R_t + ... | S_1 = s]$$

- state-action value function: $Q^{\pi}(s,a)$
  - expected **long-term** return when starting in *s*, performing *a,* and following π

$$Q^{\pi}(s,a) = \mathbb{E}_{\pi}[R_1 + \gamma R_2 + ... + \gamma^{t-1} R_t + ... | S_1 = s, A_1 = a]$$

Recap: Bellman equations – the fundamental equations of MDP and RL

- An alternative, recursive and more useful way of defining the V-function and Q function
  - V^{π} function Bellman equation

$$V^{\pi}(s) = \sum_{a} \pi(a|s) \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V^{\pi}(s')]$$

  - Q^{π} function Bellman equation

$$Q^{\pi}(s,a) = \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma \sum_{a'} \pi(a'|s') Q^{\pi}(s',a')]$$

  - V* function Bellman (optimality) equation

$$V^{*}(s) = \max_{a} \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V^{*}(s')]$$

  - Q* function Bellman (optimality) equation

$$Q^{*}(s,a) = \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma \max_{a'} Q^{*}(s',a')]$$

Recap: Policy Iterations and Value Iterations

- What are these algorithms for?
  - Algorithms of computing the V* and Q* functions from MDP parameters

- Policy Iterations

$$\pi_0 \rightarrow^E V^{\pi_0} \rightarrow^I \pi_1 \rightarrow^E V^{\pi_1} \rightarrow^I \ldots \rightarrow^I \pi^* \rightarrow^E V^*$$

- Value iterations

$$V_{k+1}(s) \leftarrow \max_a \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V_k(s')]$$

- How do we make sense of them?
  - Recursively applying the Bellman equations until convergence.

Matrix-form of Bellman Equations and Policy Evaluation

$$V^{\pi}(s) = \sum_{a} \pi(a|s) \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V^{\pi}(s')]$$

$$V^{\pi} = r^{\pi} + \gamma P_{\pi}^{T} V^{\pi}$$

$$V_{k+1}^{\pi}(s) \leftarrow \sum_{a} \pi(a|s) \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V_{k}^{\pi}(s')]$$

$$V_{k+1}^{\pi} \leftarrow r^{\pi} + \gamma P_{\pi}^{T} V_{k}^{\pi}$$

A reasonable question for the final: Matrix-form Bellman equation with Q^{π}

Matrix-form of Bellman Optimality Equation

$$V^*(s) = \max_a \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V^*(s')]$$

?

$$V_{k+1}(s) \leftarrow \max_a \sum_{s'} P(s'|s,a)[r(s,a,s') + \gamma V_k(s')]$$

?

Today's topic

- Exploration in the (multi-armed) Bandits problem

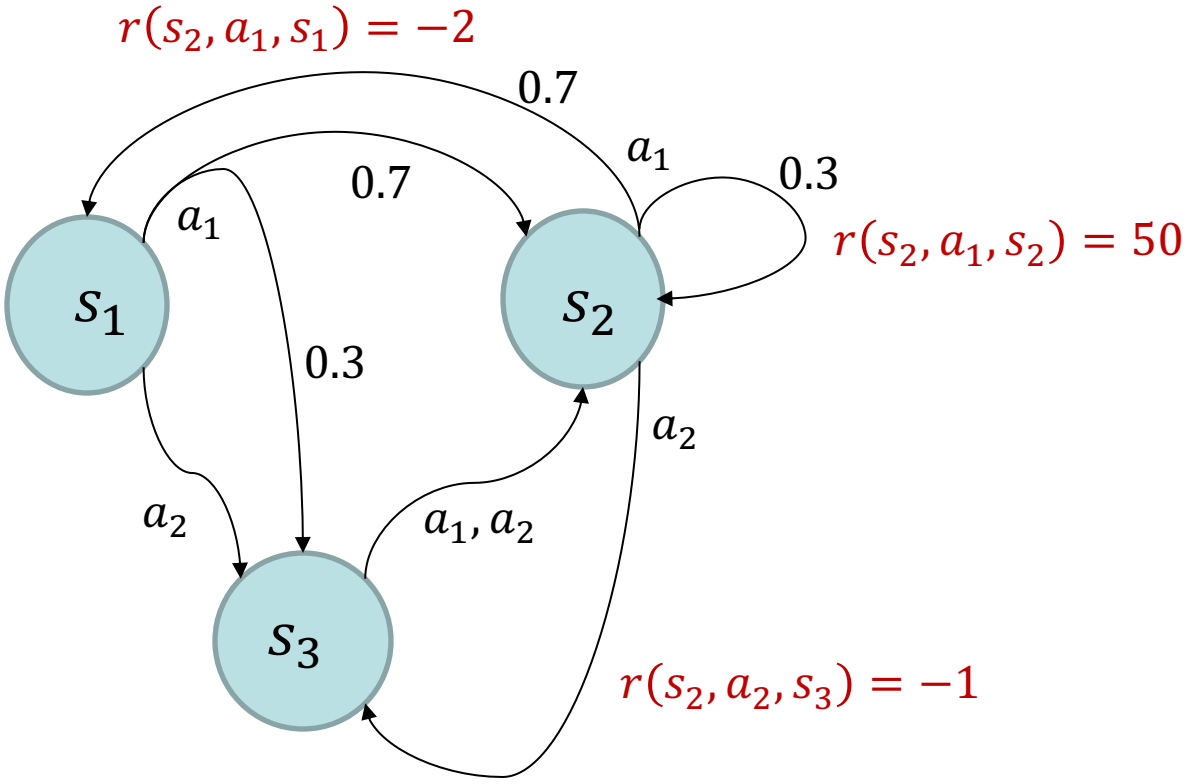
- Bandits algorithms
  - Explore-first
  - epsilon-greedy
  - Upper confidence bound

- Readings:
  - AIMA 17.3
  - Sutton and Barto: Chapter 2

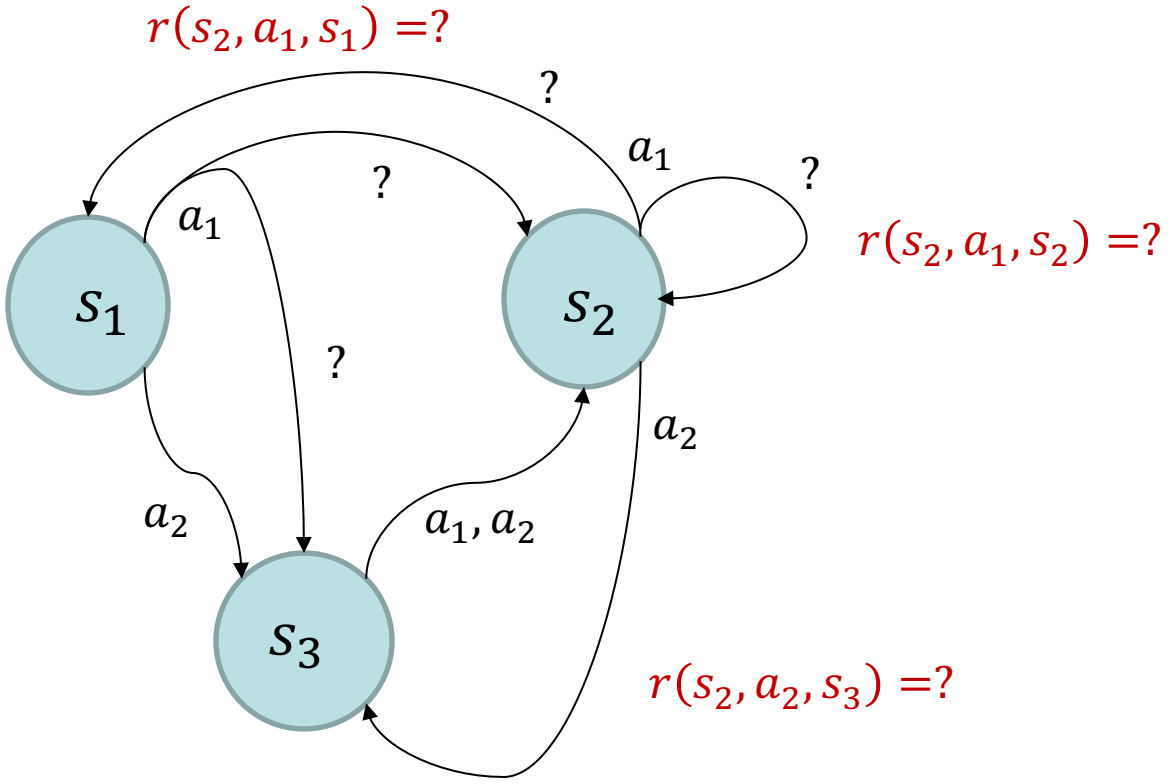
Solving MDP with VI or PI is offline planning

- The agent is given how the environment works
- The agent works out the optimal policy in its mind.
- The agent never really starts to play at all.
- No learning is happening.

State-space diagram representation of an MDP: An example with 3 states and 2 actions.



What happens if you do not know the rewards / transition probabilities?



Then you have to learn by interacting with the unknown environment.

You cannot use only offline planning!

Exploration: Try unknown actions to see what happens.

Exploitation: Maximize utility using what we know.

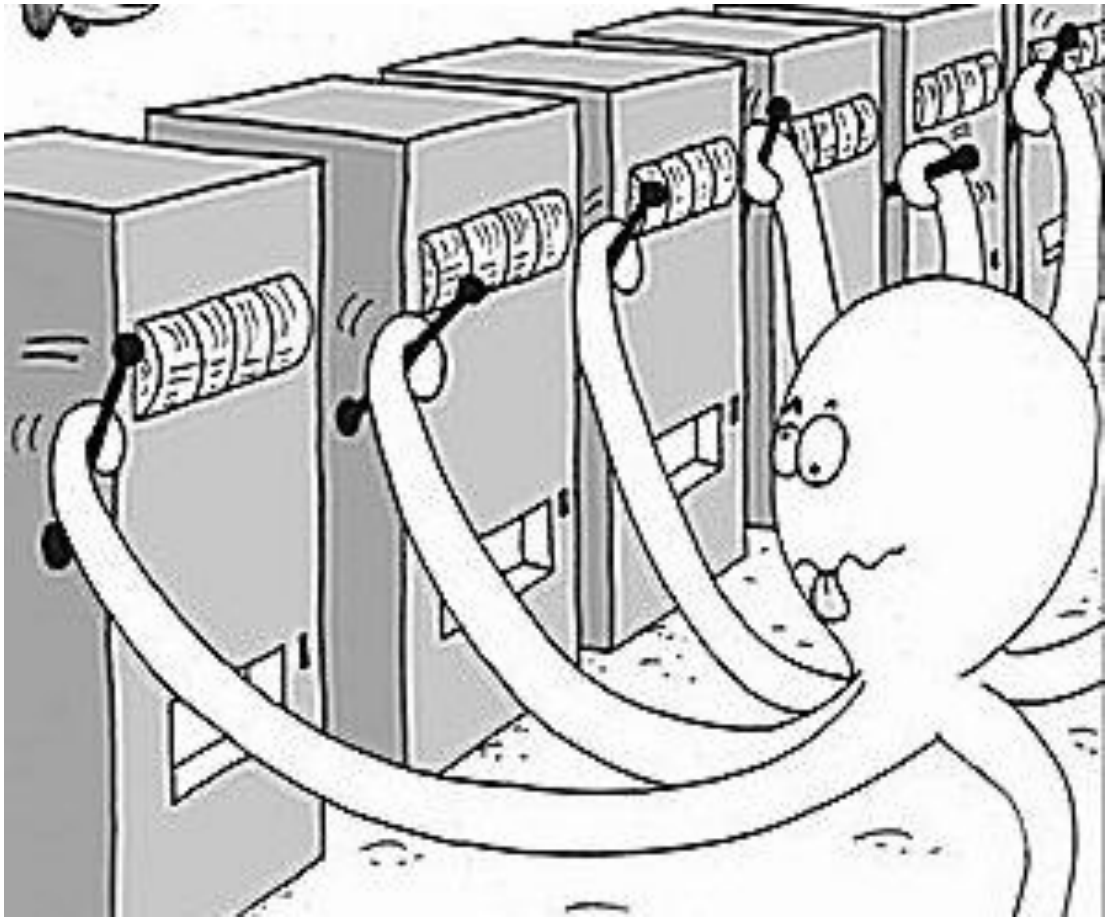
Let us tackle different aspects of the RL problem one at a time

- Markov Decision Processes:
  - Dynamics are given no need to learn

- **Bandits: Explore-Exploit in simple settings**
  - RL without dynamics

- Full Reinforcement Learning
  - Learning MDPs

Slot machines and Multi-arm bandits



Multi-arm bandits: Problem setup

- No state. k-actions $a \in \mathcal{A} = \{1, 2, ..., k\}$
- You decide which arm to pull in every iteration

$$A_1, A_2, ..., A_T$$

- You collect a cumulative payoff of $\sum_{t=1}^{T} R_t$
- The goal of the agent is to maximize the expected payoff.
  - For future payoffs?
  - For the expected cumulative payoff?

Key differences from MDPs

- Simplified:
  - No state-transitions

- But:
  - We are not given the expected reward r(s, a, s')
  - We need to learn the optimal policy by trials-and-errors.

A 10-armed bandits example

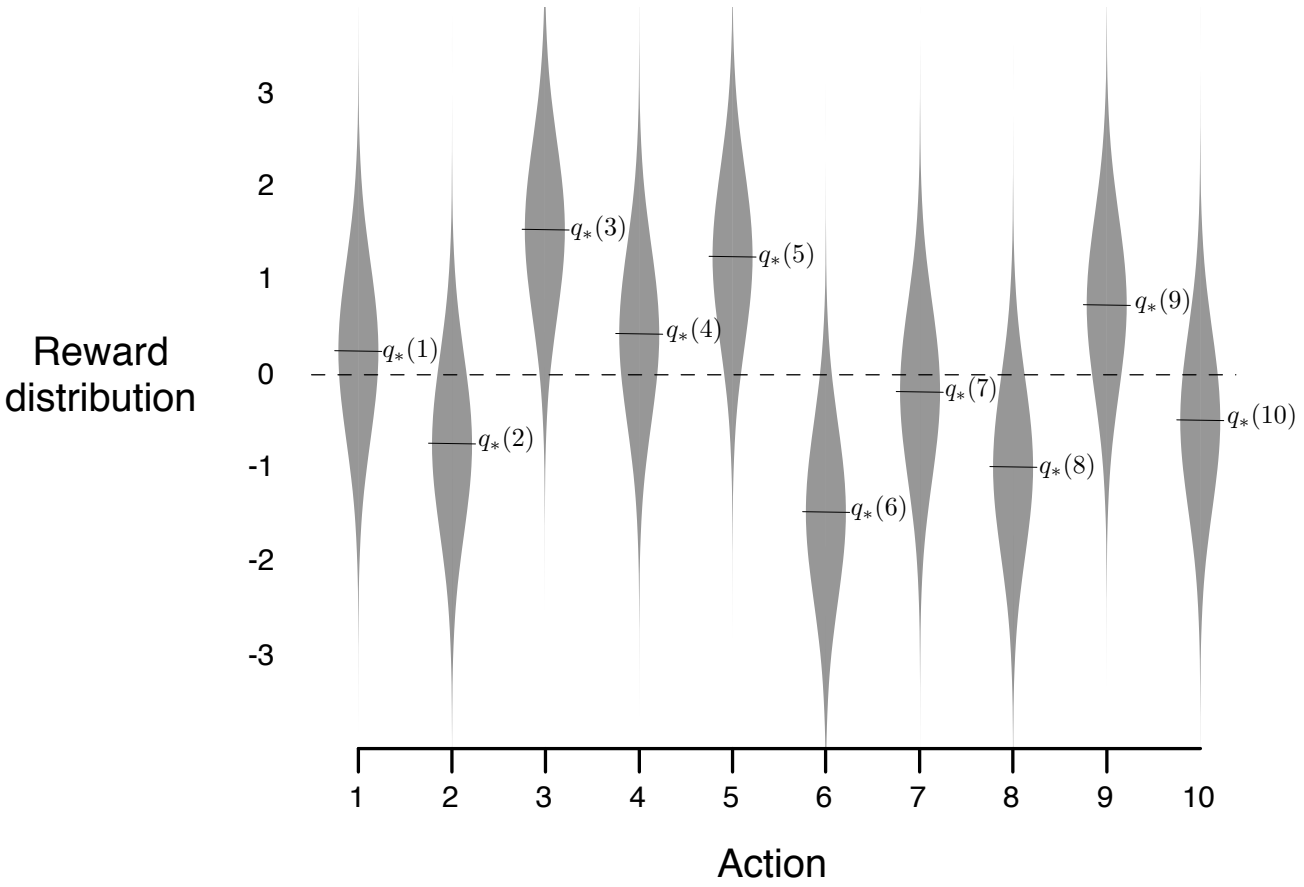


Figure 2.1: An example bandit problem from the 10-armed testbed. The true value $q_*(a)$ of each of the ten actions was selected according to a normal distribution with mean zero and unit variance, and then the actual rewards were selected according to a mean $q_*(a)$ unit variance normal distribution, as suggested by these gray distributions.

How do we measure the performance of an **online learning agent**?

- The notion of "Regret":
  - I wish I have done things differently.
  - Comparing to the best actions in the hindsight, how much worse did I do.

- For MAB, the regret is defined as follow

$$T \max_{a \in [k]} \mathbb{E}[R_t|a] - \sum_{t=1}^{T} \mathbb{E}_{a \sim \pi} \left[\mathbb{E}[R_t|a] \right]$$

Greedy strategy

- Expected reward

$$q_*(a) \doteq \mathbb{E}[R_t \mid A_t = a] .$$

- Estimate the expected reward

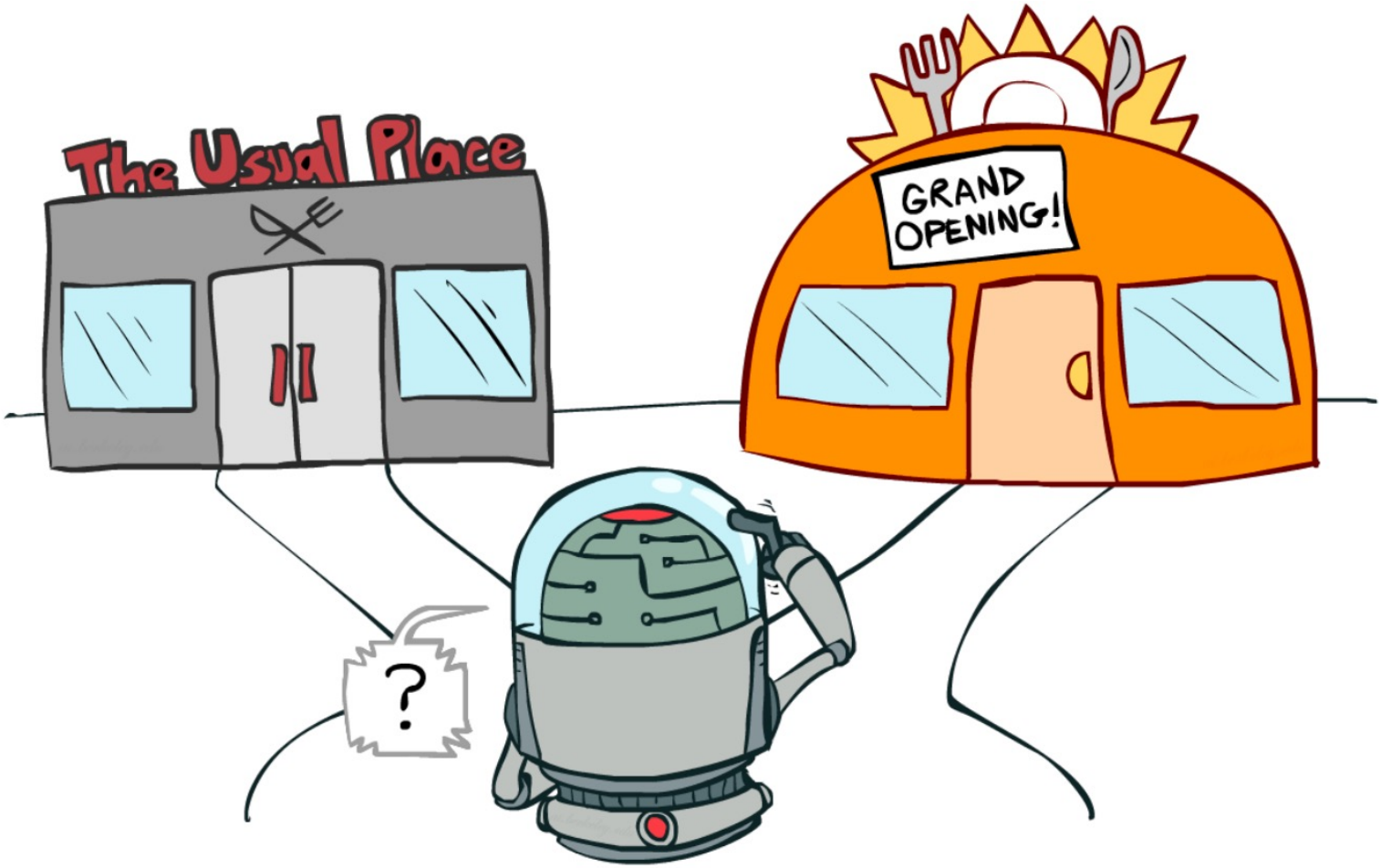
$$Q_t(a) \doteq \frac{\text{sum of rewards when } a \text{ taken prior to } t}{\text{number of times } a \text{ taken prior to } t}$$

$$= \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbb{1}_{A_i=a}}{\sum_{i=1}^{t-1} \mathbb{1}_{A_i=a}}$$

- Choose $A_t \doteq \arg\max_a Q_t(a),$

What is the issue with this strategy?

Exploration vs. Exploitation



(Illustration from Dan Klein and Pieter Abbeel's course in UC Berkeley)

Exploration first strategy

- Let's spend the first N step exploring.
  - Play each action for N / k times.

$$Q_t(a) = \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbb{1}_{A_i=a}}{\sum_{i=1}^{t-1} \mathbb{1}_{A_i=a}}$$

- For t = N +1, N+2, …, T:

$$A_t \doteq \arg\max_a Q_t(a),$$

All (you need to know) about Statistics in one slide, two theorems.

- Statistics is about using **samples** from a distribution to infer the properties of the distribution itself (**population**)
  - $X_1, X_2, X_3, \ldots, X_n \sim P$

- Law of large number
  - Average ---> Mean $\bar{X} := \frac{1}{n}\sum_{i=1}^{n} X_i \to \mathbb{E}[X_1]$

- Central limit theorem
  - The rate is sqrt(1/n) $\sqrt{n} \cdot \left(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathbb{E}[X_1] \right) \to N(0, \mathrm{Var}(X_1))$

Random variables are difficult to work with, but with statistics, a lot of the properties are more-or-less deterministic, thanks to LLN.

- Statistics is about using **samples** from a distribution to infer the properties of the distribution itself (**population**)
  - $X_1, X_2, X_3, \ldots, X_n \sim P$

- **(Simplified version of the) Hoeffding's Inequality**:
  - with high probability,

$$\left| \frac{1}{n} \sum_{i=1}^{n} X_i - \mathbb{E}[X_1] \right| = O(1/\sqrt{n})$$

*If you try each arm multiple times, then you have a good idea what the expected reward is.

How does Exploration-First work?

- Assume: 0 < reward < 1
- After N rounds, *with high probability*

$$Q_t(a) \approx q_*(a) \pm C\sqrt{\frac{k}{N}}$$

Hoeffding's inequality!

- Do this for all k arms.

- (w.h.p.) The regret is smaller than

$$N + C(T - N)\sqrt{k/N}$$

How does Exploration-First work?

- (High probability) Regret bound:

$$N + C(T - N)\sqrt{k/N}$$

- Choose N to minimize the regret

$$N = O(T^{2/3}k^{1/3})$$

- Final regret bound:

$$O(T^{2/3}k^{1/3})$$

ε-Greedy strategy: one way to balance exploration and exploitation

- You choose with probability 1- ε

$$A_t \doteq \arg\max_a Q_t(a),$$

- With probability ε, choose an action uniformly at random!
  - Including the argmax.

- Carefully choose ε parameter.

Let's analyze ε-Greedy!

- By Hoeffding's inequality, at every t
  - w.h.p. each arm is chosen at least 0.5 ε t / k times.
  - w.h.p.,

$$Q_t(a) \approx q_*(a) \pm C\sqrt{k/\epsilon t}$$

- Regret bound is

$$\epsilon T + \sum_{t=1}^{T} C\sqrt{\frac{k}{\epsilon t}}$$

Convergent and divergent series

$$1 + 1/2^2 + 1/3^2 + ... + 1/T^2 = ?$$

$$1 + 1/2 + 1/3 + ... + 1/T = ?$$

$$1 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + ... + \frac{1}{\sqrt{T}} = ?$$

On the side, check out Riemann's Zeta Function…

Let's analyze ε-Greedy!

- Regret bound

$$\epsilon T \ + \sum_{t=1}^{T} C\sqrt{\frac{k}{\epsilon t}} \ \leq \epsilon T + O\left(\sqrt{\frac{Tk}{\epsilon}}\right)$$

- Choose the optimal ε to minimize the bound?

- Work it out yourself that you get T^{2/3} just like in Explore-First.

Upper Confidence Bound algorithm (UCB)

- At time t, choose the action

$$A_t \leftarrow \underset{a}{\operatorname{argmax}} \left[Q_t(a) + c\sqrt{\frac{\log(1+t)}{N_t(a)}} \right]$$

- Idea: Be optimistic
  - Choose an option that maximizes the upper confidence bound.

$$\mathbb{E}[\text{Regret}] = O(\sqrt{Tk})$$

- The proof is out of the scope of this course. For those who are interested, please look up. It's not difficult.

Example: Two-Armed Bandits

- k=2. Expected reward $r(a = 1) = 0.8,\ r(a = 2) = 0.5$

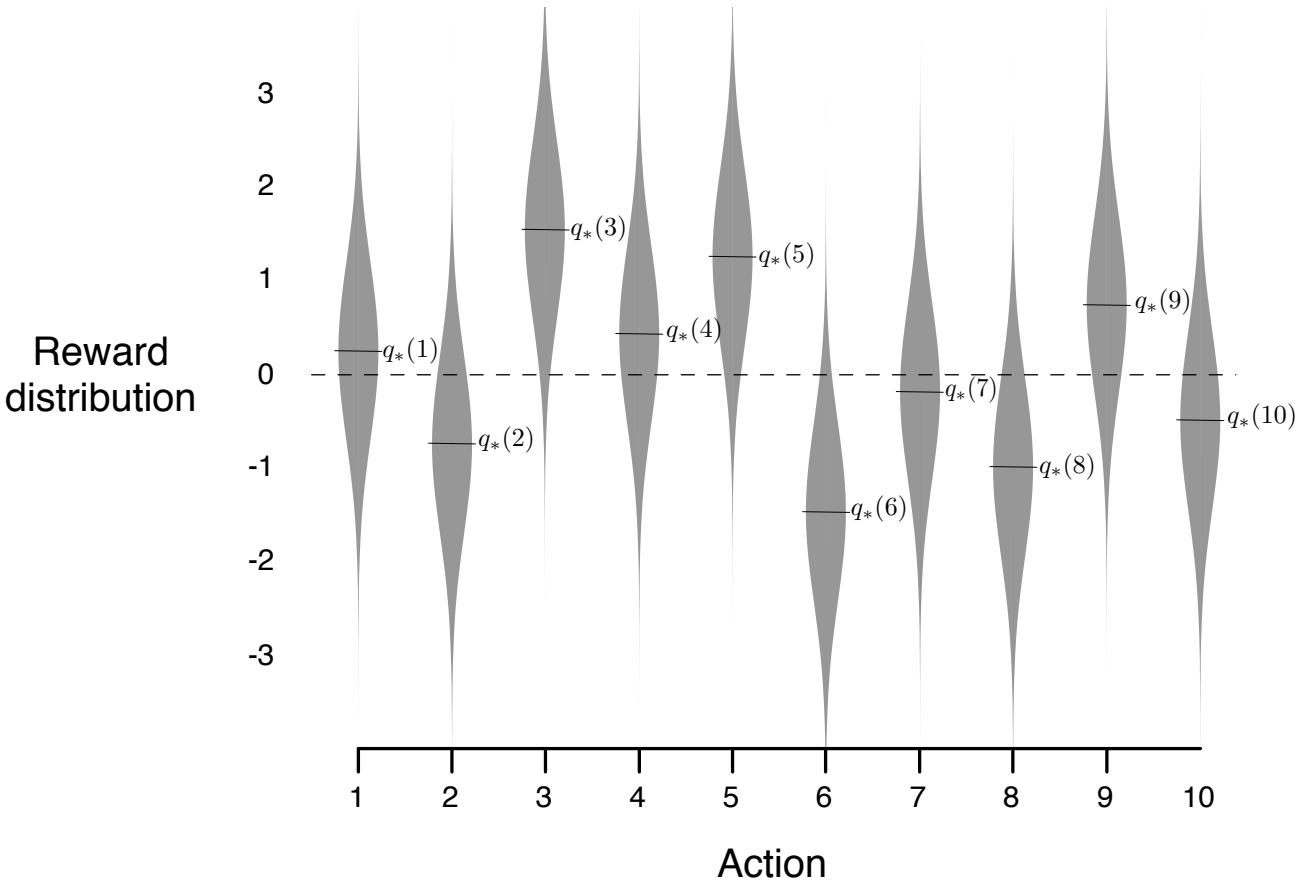
- Question: what is the Q-function for this problem?
  - If episodical with horizon T= 1.
  - If discounted with $0 \leq \gamma < 1$

- What is the optimal policy?

Example: UCB on a Two Armed Bandit

- A run of UCB algorithm with c = 2.
  1. Initialize $\mathrm{Q}_1(a) = \infty, \forall\, a \in \{1,2\}$. UCB: $\bar{Q}_1(a) = \infty$.
  2. Pick action $\mathrm{A}_1 = 1$. (break ties arbitrarily), receive a reward of 0.
     a. Update $N_2(a) \leftarrow N_1(a) + 1(\mathrm{A}_1 = \mathrm{a})$
     b. Update $\mathrm{Q}_2(1) = 0/1 = 0,\ Q_2(2) = \infty$
     c. Update $\bar{Q}_2(1) \leftarrow Q_2(1) + 2\sqrt{\frac{\log 2}{1}} \approx 0 + 1.67, \bar{Q}_2(2) = \infty$
  3. Pick action $a = 2$ (because of what?), receive a reward of 1.
     a. Update $N_3(2) \leftarrow N_2(2) + 1, \mathrm{Q}_3(2) \leftarrow 1$
     b. Update $\bar{Q}_3(2) \leftarrow Q_3(2) + 2\sqrt{\frac{\log 2}{1}} \approx 1 + 1.67$
     c. Keep $N_3(1), Q_3(1), \bar{Q}_3(1)$ unchanged.
  4. Which action to pick at next?
  5. …

A 10-armed bandits benchmark



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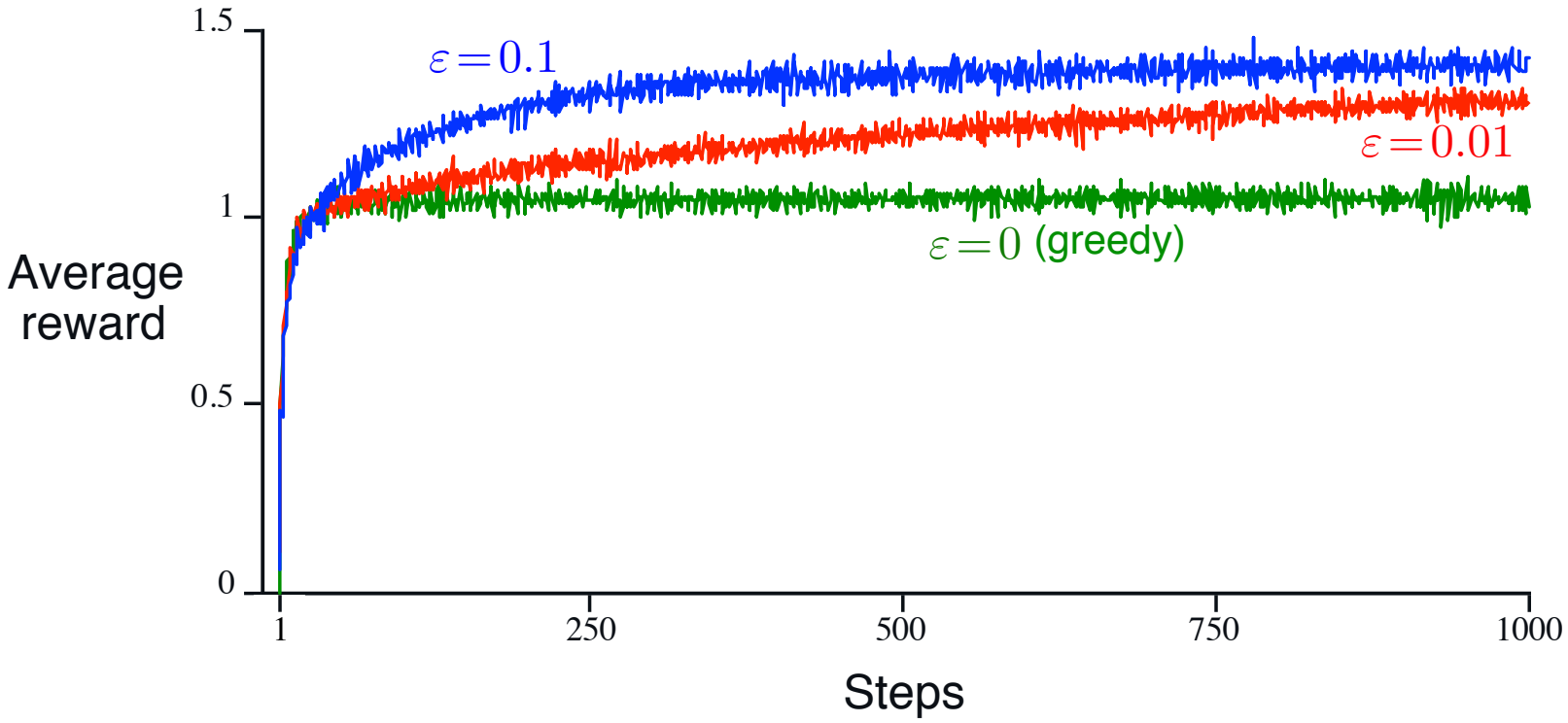
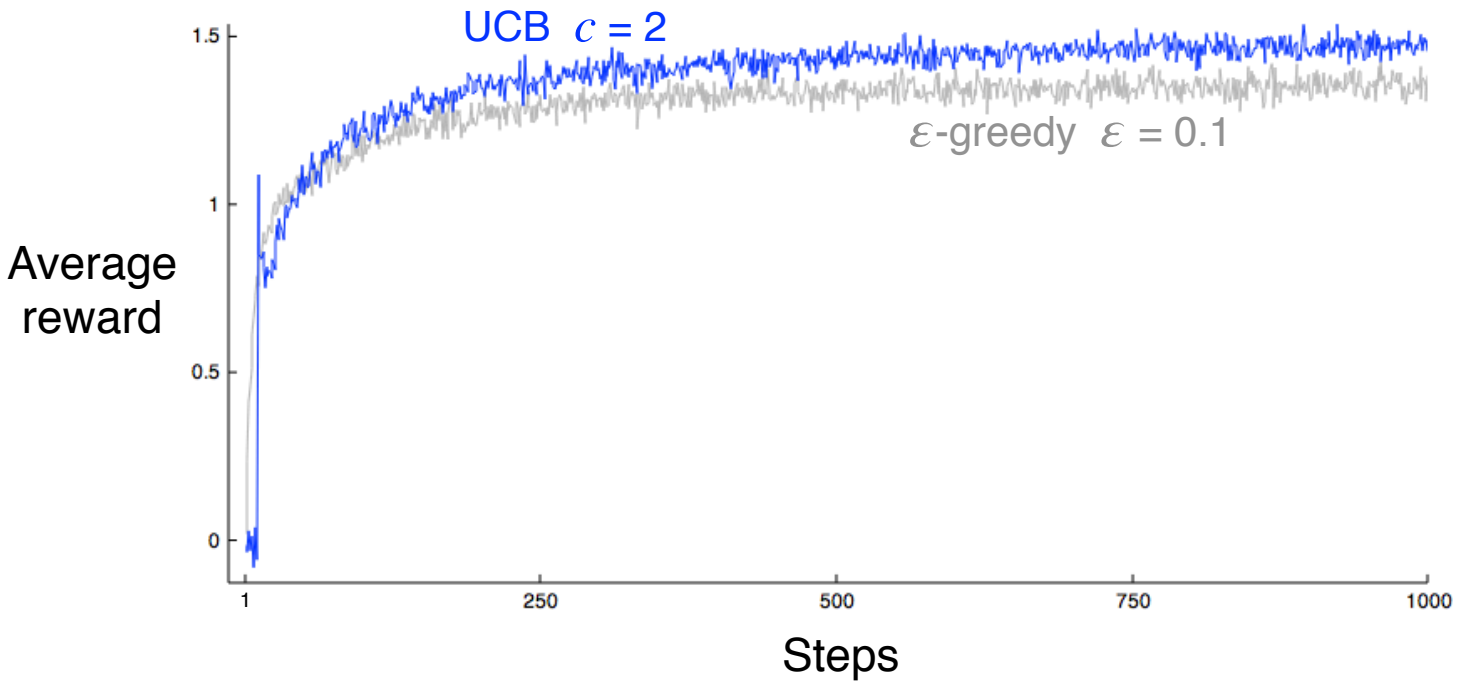
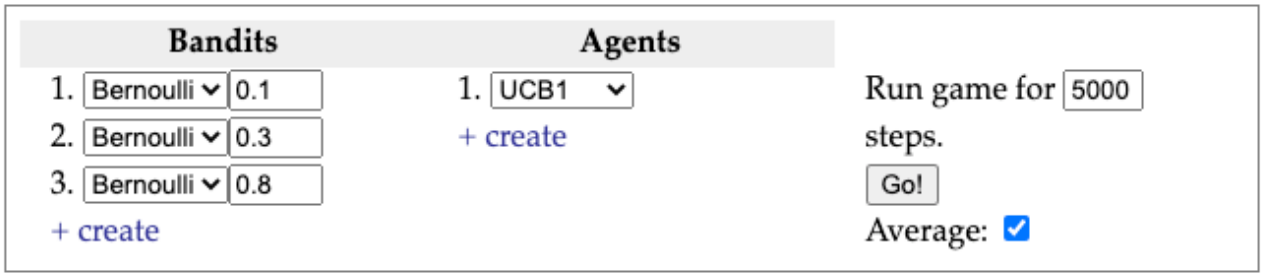
Comparing the different algorithms

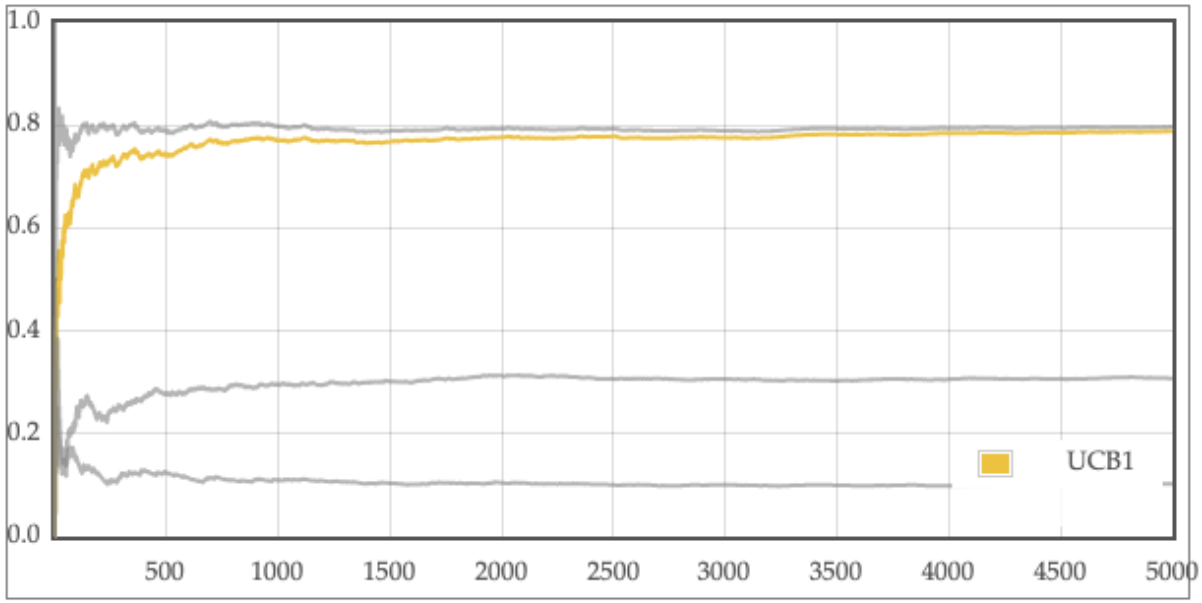


UCB vs. ε-Greedy



Live Demo of an Agent Solving Multi-Armed Bandits





Credit Mark Reid: http://mark.reid.name/code/bandits/

Variants of Bandits problems

- Online Learning from Expert Advice
  - Adversarial chooses the outcome
  - You observe outcome of other arms as well
  - Compare against the best arm in the hindsight

Remark: In all these problems, there are algorithms with provably low-regret.

- Adversarial k-Armed Bandits
  - Same as above. But you observe only your arm.

- Nonstationary Bandits
  - Stochastic but the reward distribution changes over time.
  - Compare against the best arm for each time.

- Contextual bandits: you have a state in each time point.

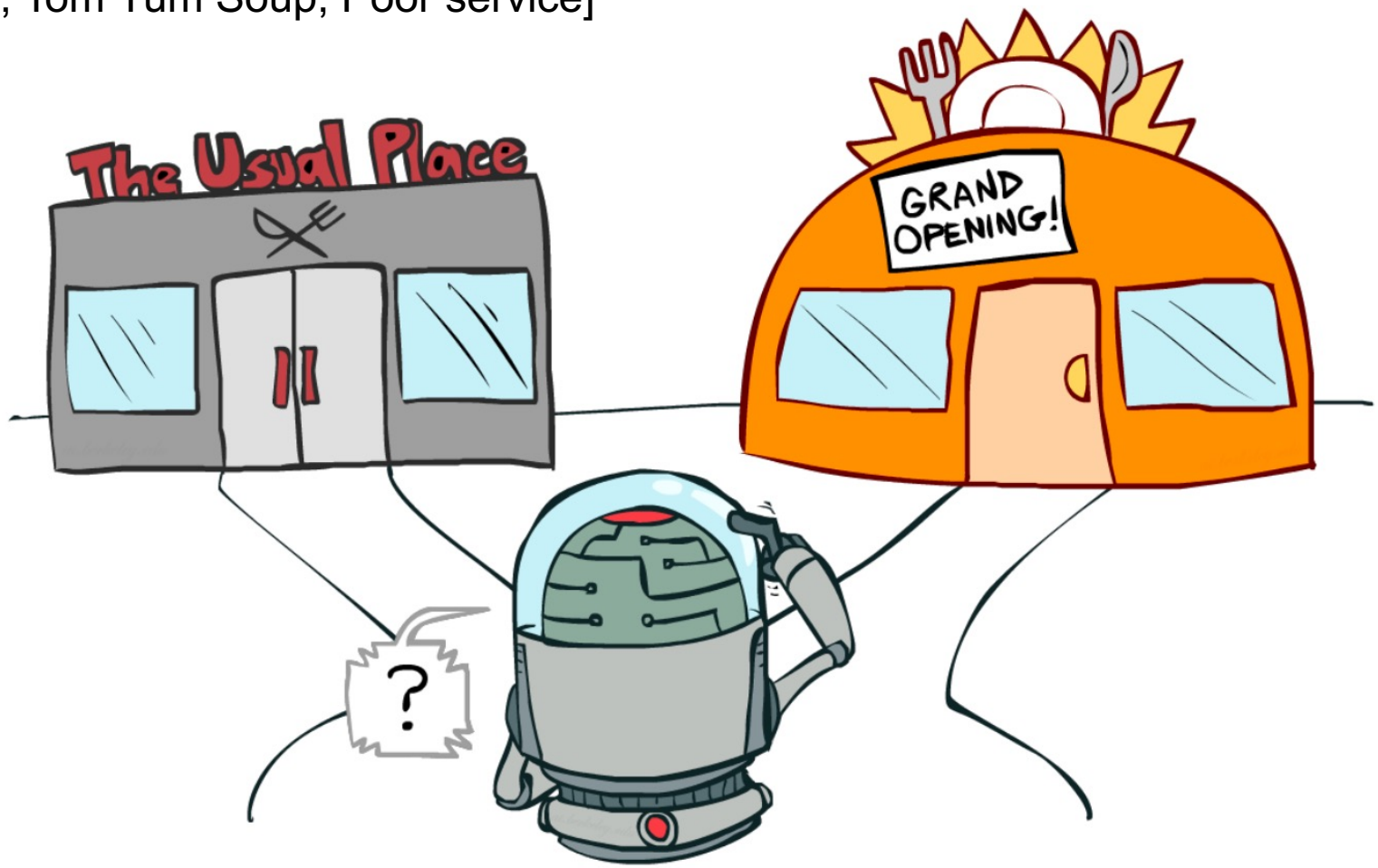
Do I have to try, if I have features?

Features:

[Noodles, Tom Yum Soup, Poor service]

Features:

[Burger, Fries, Onion Ring, Fried Chicken]



(Illustration from Dan Klein and Pieter Abbeel's course in UC Berkeley)

We know how to use with features, don't we?

- Classifier agent
  - Take features of a restaurant as input
  - Output a prediction of "will I like the food?"
- Train with supervised learning
  - Using the my previous visits to the restaurants
  - Using Yelp reviews

Why can't we just use that?

How to explore?

Contextual Bandits: Problem Setup

- For each round t = 1, 2, 3, …, T:
  - A context $x_t \sim$ unknown distribution i.i.d.
  - Agent picks an action $a_t = 1,2,3,..,K$
  - Reward $r_t \sim D(. \mid x_t, a_t)$

- Agent's goals:
  - Learn the best policy out of many policies Π
  - Minimize the cumulative regret

A finite family of policies

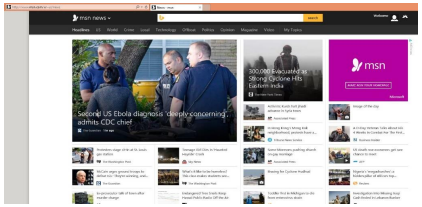
$$T \cdot \max_{\pi \in \Pi} \mathbb{E}_{\pi}[r_t(x_t, a_t)] - \mathbb{E}_{\text{Agent's policy}} \left[\sum_{t=1}^{T} r_t(x_t, a_t) \right]$$

Reward from the best policy

Reward collected by the Agent

Applications of Contextual Bandits

Personalized news?

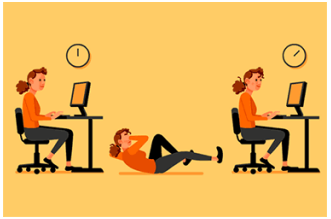


Repeatedly:

1. Observe features of user+articles
2. Choose a news article.
3. Observe click-or-not

Goal: Maximize fraction of clicks

Health advice?



Repeatedly:

1. Observe features of user+advice
2. Choose an advice.
3. Observe steps walked

Goal: Healthy behaviors (e.g. step count)

amazon

Recommendations

buy or not buy

Exploration vs. Exploitation in Contextual Bandits.

- Challenging because:
  - Infinite state space, never see the same context again.
  - Exponentially large policy space
- Ideas:
  - ExploreFirst, ε-Greedy $O(T^{2/3})$
  - UCB? But how do we construct Confidence Interval for an exponentially large set of policies?
- Optimal regret:

$$O(\sqrt{KT \log |\Pi|})$$

Next lecture

- Reinforcement learning for MDPs
  - Model-based vs model-free algorithms
  - Online policy iterations
  - Temporal difference learning

- Readings:
  - AIMA Ch 22.1- 22.4
  - Sutton and Barto: Ch 5, Ch 6, Ch 9.1