CSCI567 Machine Learning (Fall 2021)

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Administration

Reminder: HW5 is due on the coming Tuesday.

Quiz 2 logistics (**12/02, 5:00-7:40pm**):

- online via zoom, can take it wherever you want (SGM 123 is available)
- join the regular lecture zoom 10 minutes earlier (link available on course/DEN website; remember to sign in!), with your **camera on**
- A bit before 5pm, Crowdmark will send you the quiz.
- open-book/note, but *no collaboration or consultation*
- make a private Piazza post if you have clarification questions
- duration is 2.5 hours + 10 extra minutes for uploading; *$x\%$ penalty for x minutes late (past 7:40)*.

More on Quiz 2

Coverage: SVM + topics after Quiz 1; some other basic concepts (e.g. training error, regularization, kernel, etc.) might appear in conjunction.

Five problems in total

- one problem of 15 multiple-choice *multiple-answer* questions
  - *today's topics only appear here*
- four other homework-like problems, each has a couple sub-problems
- in total, **upload five scanned pdf/jpg/png's**, one for each problem
  - each can have multiple pages

Same tip: expect variants of questions from discussion/homework

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Outline

1. Review of last lecture
2. Multi-armed Bandits
3. Reinforcement learning

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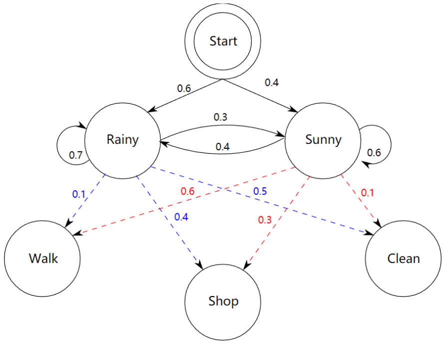
Hidden Markov Models

Model parameters:

- **initial distribution**
  $P(Z_1 = s) = \pi_s$
- **transition distribution**
  $P(Z_{t+1} = s' \mid Z_t = s) = a_{s,s'}$
- **emission distribution**
  $P(X_t = o \mid Z_t = s) = b_{s,o}$



Baum–Welch algorithm

Step 0 Initialize the parameters $(\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$

Step 1 (E-Step) Fixing the parameters, compute forward and backward messages for all sample sequences, then use these to compute $\gamma_s^{(n)}(t)$ and $\xi_{s,s'}^{(n)}(t)$ for each n, t, s, s'.

Step 2 (M-Step) Update parameters:

$$\pi_s \propto \sum_n \gamma_s^{(n)}(1), \quad a_{s,s'} \propto \sum_n \sum_{t=1}^{T-1} \xi_{s,s'}^{(n)}(t), \quad b_{s,o} \propto \sum_n \sum_{t: x_t = o} \gamma_s^{(n)}(t)$$

Step 3 Return to Step 1 if not converged

Viterbi Algorithm

Viterbi Algorithm

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

For each $t = 2, \ldots, T$,

- for each $s \in [S]$, compute

$$\delta_s(t) = b_{s,x_t} \max_{s'} a_{s',s} \delta_{s'}(t-1)$$

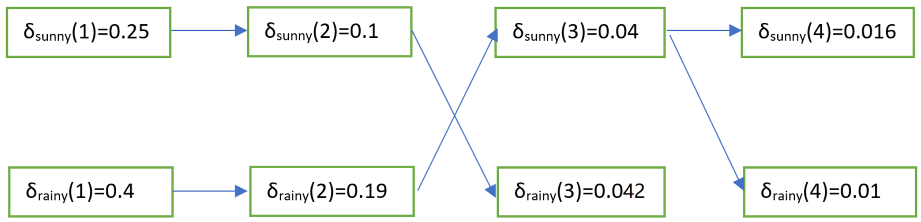
$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s} \delta_{s'}(t-1)$$

Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.
For each $t = T, \ldots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \ldots, z_T^*$.

Example

Arrows represent the "argmax", i.e. $\Delta_s(t)$.



The most likely path is **"rainy, rainy, sunny, sunny"**.

Viterbi Algorithm with missing data

Viterbi Algorithm with partial data $x_{1:T_0}$

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

For each $t = 2, \ldots, T$,

- for each $s \in [S]$, compute

$$\delta_s(t) = \begin{cases} b_{s,x_t} \max_{s'} a_{s',s}\delta_{s'}(t-1) & \text{if } t \le T_0 \\ \max_{s'} a_{s',s}\delta_{s'}(t-1) & \text{else} \end{cases}$$

$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s}\delta_{s'}(t-1).$$

Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.
For each $t = T, \ldots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \ldots, z_T^*$.

Outline

1. Review of last lecture
2. Multi-armed Bandits
   - Online decision making
   - Motivation and setup
   - Exploration vs. Exploitation
3. Reinforcement learning

Decision making

Problems we have discussed so far:

- start with a training dataset
- learn a predictor or discover some patterns

But many real-life problems are about **learning continuously**:

- make a prediction/decision
- receive some feedback
- repeat

Broadly, these are called **online decision making problems**.

Examples

Amazon/Netflix/MSN **recommendation systems**:

- a user visits the website
- the system recommends some products/movies/news stories
- the system observes whether the user clicks on the recommendation

Playing games (Go/Atari/StarCraft/...) or **controlling robots**:

- make a move
- receive some reward (e.g. score a point) or loss (e.g. fall down)
- make another move...

Two formal setups

We discuss two such problems today:

- **multi-armed bandit**
- **reinforcement learning**

Mulit-armed bandits: motivation

Imagine going to a casino to play a slot machine

- it robs you, like a “bandit” with a single arm

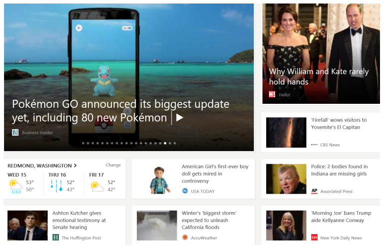
Of course there are many slot machines in the casino

- like a bandit with multiple arms (hence the name)
- **if I can play for 10 times, which machines should I play?**

Applications

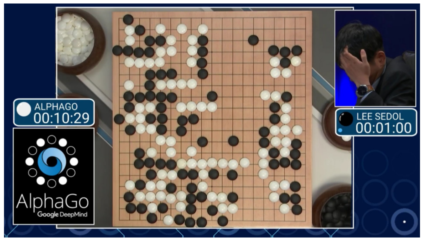
This simple model and its variants capture many real-life applications

- recommendation systems, each product/movie/news story is an arm (Microsoft MSN indeed employs a variant of bandit algorithm)
- game playing, each possible move is an arm (AlphaGo indeed has a bandit algorithm as one of the components)



Pokémon GO announced its biggest update yet, including 80 new Pokémon

Why William and Kate rarely hold hands



Formal setup

There are K **arms** (actions/choices/...)

The problem proceeds in rounds between the environment and a learner: for each time $t = 1, \ldots, T$

- the environment decides the reward for each arm $r_{t,1}, \ldots, r_{t,K}$
- the learner picks an arm $a_t \in [K]$
- the learner observes the reward for arm a_t, i.e., r_{t,a_t}

Importantly, *learner does not observe rewards for arms not selected!*

This kind of limited feedback is now usually referred to as bandit feedback

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Objective

What is the goal of this problem?

Maximizing total rewards $\sum_{t=1}^{T} r_{t,a_t}$ seems natural

But the absolute value of rewards is not meaningful, instead we should compare it to some *benchmark*. A classic benchmark is

$$\max_{a\in[K]} \sum_{t=1}^{T} r_{t,a}$$

i.e. the largest reward one can achieve by always playing a fixed arm

So we want to minimize

$$\max_{a\in[K]} \sum_{t=1}^{T} r_{t,a} - \sum_{t=1}^{T} r_{t,a_t}$$

This is called the **regret**: *how much I regret for not sticking with the best fixed arm in hindsight?*

Environments

How are the rewards generated by the environments?

- they could be generated via some fixed distribution
- they could be generated via some changing distribution
- they could be generated even completely arbitrarily/adversarially

We focus on a simple setting:

- rewards of arm a are i.i.d. samples of $\mathrm{Ber}(\mu_a)$, that is, $r_{t,a}$ is 1 with prob. μ_a, and 0 with prob. $1 - \mu_a$, independent of anything else.
- each arm has a different mean $(\mu_1, \ldots, \mu_K)$; the problem is essentially about finding the best arm $\operatorname{argmax}_a \mu_a$ as quickly as possible

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Empirical means

Let $\hat{\mu}_{t,a}$ be the **empirical mean** of arm a up to time t:

$$\hat{\mu}_{t,a} = \frac{1}{n_{t,a}} \sum_{\tau\le t: a_\tau = a} r_{\tau,a}$$

where

$$n_{t,a} = \sum_{\tau\le t} \mathbb{I}[a_\tau == a]$$

is the **number of times** we have picked arm a.

Concentration: $\hat{\mu}_{t,a}$ should be close to μ_a if $n_{t,a}$ is large

Exploitation only

Greedy

Pick each arm once for the first K rounds.

For $t = K+1, \dots, T$, pick $a_t = \mathrm{argmax}_a \ \hat{\mu}_{t-1,a}$

What's wrong with this greedy algorithm?

Consider the following example:

- $K = 2, \mu_1 = 0.6, \mu_2 = 0.5$ (so arm 1 is the best)
- suppose the algorithm first picks arm 1 and sees reward 0, then picks arm 2 and sees reward 1 (this happens with decent probability)
- the algorithm will never pick arm 1 again!

The key challenge

All bandit problems face the same **dilemma**:

Exploitation vs. Exploration trade-off

- on one hand we want to exploit the arms that we think are good
- on the other hand we need to explore all arms often enough in order to figure out which one is better
- so each time we need to ask: *do I explore or exploit? and how?*

We next discuss **three ways** to trade off exploration and exploitation for our simple multi-armed bandit setting.

A natural first attempt

Explore–then–Exploit

Input: a parameter $T_0 \in [T]$

Exploration phase: for the first T_0 rounds, pick each arm for T_0/K times

Exploitation phase: for the remaining $T - T_0$ rounds, stick with the empirically best arm $\mathrm{argmax}_a \ \hat{\mu}_{T_0,a}$

Parameter T_0 clearly controls the exploration/exploitation trade-off

Issues of Explore–then–Exploit

It's pretty reasonable, but the disadvantages are also clear:

- not clear how to tune the hyperparameter T_0
- in the exploration phase, even if an arm is clearly worse than others based on a few pulls, it's still pulled for T_0/K times
- clearly it won't work if the environment is changing

A slightly better algorithm

ϵ-Greedy

Pick each arm once for the first K rounds.

For $t = K+1, \ldots, T$,

- with probability ϵ, explore: pick an arm uniformly at random
- with probability $1-\epsilon$, exploit: pick $a_t = \operatorname{argmax}_a \ \hat{\mu}_{t-1,a}$

Pros	**Cons**
always exploring and exploiting	need to tune ϵ
applicable to many other problems	same uniform exploration
first thing to try usually	

Is there a *more adaptive* way to explore?

More adaptive exploration

A simple modification of “Greedy” leads to the well-known:

Upper Confidence Bound (UCB) algorithm

For $t = 1, \ldots, T$, pick $a_t = \operatorname{argmax}_a \ \text{UCB}_{t,a}$ where

$$\text{UCB}_{t,a} \triangleq \hat{\mu}_{t-1,a} + 2\sqrt{\frac{\ln t}{n_{t-1,a}}}$$

- the first term in $\text{UCB}_{t,a}$ represents exploitation, while the second (bonus) term represents exploration
- the bonus term is large if the arm is not pulled often enough, which encourages exploration (adaptive due to the first term)
- a parameter-free algorithm, and *it enjoys optimal regret!*

Upper confidence bound

Why is it called upper confidence bound?

One can prove that with high probability,

$$\mu_a \leq \text{UCB}_{t,a}$$

so $\text{UCB}_{t,a}$ is indeed an upper bound on the true mean.

Another way to interpret UCB, “**optimism in face of uncertainty**”:

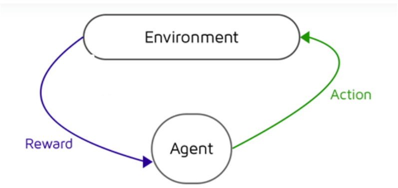
- true environment is unknown due to randomness (**uncertainty**)
- just pretend it's the most preferable one among all plausible environments (**optimism**)

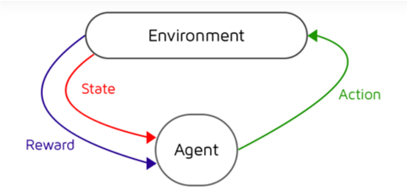
This principle is useful for many other bandit problems.

Outline

Motivation

Multi-armed bandit is among the simplest decision making problems with limited feedback.





It's often too simple to capture many real-life problems. One thing it fails to capture is the "state" of the learning agent, which has impacts on the reward of each action.

- e.g. for Atari games, after making one move, the agent moves to a different state, with possible different rewards for each action

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Reinforcement learning

Reinforcement learning (RL) is one way to deal with this issue.

Huge recent success when combined with deep learning techniques

- Atari games, poker, self-driving cars, etc.

The foundation of RL is **Markov Decision Process (MDP)**,
a combination of Markov model (Lec 10) and multi-armed bandit

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Markov decision process

An MDP is parameterized by five elements

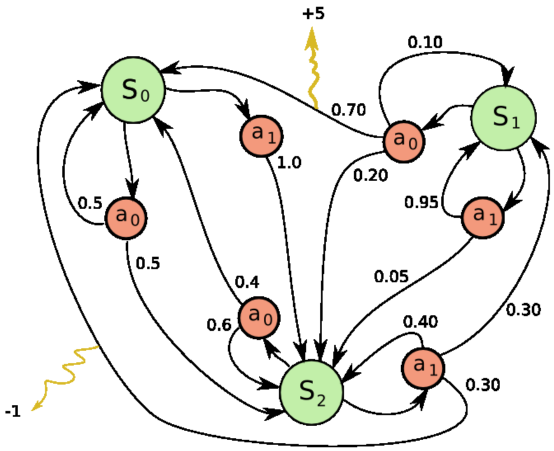
- $\mathcal{S}$: a set of possible states
- $\mathcal{A}$: a set of possible actions
- P: transition probability, $P_a(s, s')$ is the probability of transiting from state s to state s' after taking action a (Markov property)
- r: reward function, $r_a(s)$ is (expected) reward of action a at state s
- $\gamma \in (0, 1)$: discount factor, informally, reward of 1 from tomorrow is only counted as γ for today

Different from Markov models discussed in Lec 10, the state transition is influenced by the taken action.

Different from Multi-armed bandit, the reward depends on the state.

Example

3 states, 2 actions



Policy

A **policy** $\pi : \mathcal{S} \to \mathcal{A}$ indicates which action to take at each state.

If we start from state $s_0 \in \mathcal{S}$ and act according to a policy π, the discounted rewards for time $0, 1, 2, \dots$ are respectively

$$r_{\pi(s_0)}(s_0), \quad \gamma r_{\pi(s_1)}(s_1), \quad \gamma^2 r_{\pi(s_2)}(s_2), \quad \cdots$$

where $s_1 \sim P_{\pi(s_0)}(s_0, \cdot), \quad s_2 \sim P_{\pi(s_1)}(s_1, \cdot), \quad \cdots$

If we follow the policy forever, the total (discounted) reward is

$$\mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_{\pi(s_t)}(s_t)\right]$$

where the randomness is from $s_{t+1} \sim P_{\pi(s_t)}(s_t, \cdot)$.

Note: the discount factor allows us to consider an infinite learning process

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Optimal policy and Bellman equation

First goal: knowing all parameters, *how to find the optimal policy*

$$\operatorname*{argmax}_{\pi} \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_{\pi(s_t)}(s_t)\right] \quad ?$$

We first answer a related question: *what is the maximum reward one can achieve starting from an arbitrary state s?*

$$\begin{aligned} V(s) &= \max_{\pi} \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_{\pi(s_t)}(s_t) \;\middle|\; s_0 = s\right] \\ &= \max_{a \in \mathcal{A}} \left(r_s(a) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V(s') \right) \end{aligned}$$

V is called the **(optimal) value function**. It satisfies the above **Bellman equation**: $|\mathcal{S}|$ nonlinear equations with $|\mathcal{S}|$ unknowns, *how to solve it?*

Value Iteration

Value Iteration

Initialize $V_0(s)$ randomly for all $s \in \mathcal{S}$

For $k = 1, 2, \dots$ (until convergence)

$$V_k(s) = \max_{a \in \mathcal{A}} \left(r_s(a) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V_{k-1}(s') \right) \qquad \text{(Bellman upate)}$$

Knowing V, the optimal policy π^* is simply

$$\pi^*(s) = \operatorname*{argmax}_{a \in \mathcal{A}} \left(r_s(a) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V(s') \right)$$

Convergence of Value Iteration

Does Value Iteration always find the true value function V? **Yes!**

$$\begin{aligned} |V_k(s) - V(s)| &= \Bigg| \max_{a \in \mathcal{A}} \left(r_s(a) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V_{k-1}(s') \right) \\ &\qquad - \max_{a \in \mathcal{A}} \left(r_s(a) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V(s') \right) \Bigg| \\ &\le \gamma \max_{a \in \mathcal{A}} \left| \sum_{s' \in \mathcal{S}} P_a(s, s') \left(V_{k-1}(s') - V(s') \right) \right| \\ &\le \gamma \max_{a \in \mathcal{A}} \sum_{s' \in \mathcal{S}} P_a(s, s') \left| V_{k-1}(s') - V(s') \right| \\ &\le \gamma \max_{s''} \left| V_{k-1}(s'') - V(s'') \right| \le \cdots \le \gamma^k \max_{s''} \left| V_0(s'') - V(s'') \right| \end{aligned}$$

So the distance between V_k and V is shrinking *exponentially fast*.

Learning MDPs

Now suppose we do not know the parameters of the MDP

- transition probability P
- reward function r

But we do still assume we can observe the states (in contrast to HMM), how do we find the optimal policy?

We discuss examples from two families of learning algorithms:

- **model-based** approaches
- **model-free** approaches

Model-based approaches

Key idea: learn the model P and r explicitly from samples

Suppose we have a sequence of interactions: $s_1, a_1, r_1, s_2, a_2, r_2, \ldots, s_T, a_T, r_T$, then the MLE for P and r are simply

$$P_a(s, s') \propto \#\text{transitions from } s \text{ to } s' \text{ after taking action } a$$
$$r_a(s) = \text{average observed reward at state } s \text{ after taking action } a$$

Having estimates of the parameters we can then apply value iteration to find the optimal policy.

Model-based approaches

How do we collect data $s_1, a_1, r_1, s_2, a_2, r_2, \ldots, s_T, a_T, r_T$?

Simplest idea: follow a random policy for T steps. This is similar to explore–then–exploit, and we know this is not the best way.

Let's adopt the ϵ-Greedy idea instead.

A sketch for model-based approaches

Initialize V, P, r randomly

For $t = 1, 2, \ldots$,

- **with probability ϵ, explore**: pick an action uniformly at random
- **with probability $1 - \epsilon$, exploit**: pick the optimal action based on V
- update the model parameters P, r
- update the value function V (via value iteration)

Model-free approaches

Key idea: do not learn the model explicitly. *What do we learn then?*

Define the $Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ function as

$$Q(s, a) = r_a(s) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') \max_{a' \in \mathcal{A}} Q(s', a')$$

In words, $Q(s, a)$ is the expected reward one can achieve starting from state s with action a, then acting optimally.

Clearly, $V(s) = \max_a Q(s, a)$.

Knowing $Q(s, a)$, the optimal policy at state s is simply $\operatorname{argmax}_a Q(s, a)$.

Model-free approaches learn the Q function directly from samples.

Temporal difference

How to learn the Q function?

$$Q(s,a) = r_a(s) + \gamma \sum_{s' \in \mathcal{S}} P_a(s,s') \max_{a' \in \mathcal{A}} Q(s',a')$$

On experience $\langle s_t, a_t, r_t, s_{t+1} \rangle$, with the current guess on Q, $r_t + \gamma \max_{a'} Q(s_{t+1}, a')$ is like a sample of the RHS of the equation.

So it's natural to do the following update:

$$\begin{aligned} Q(s_t,a_t) &\leftarrow (1-\alpha)Q(s_t,a_t) + \alpha \left(r_t + \gamma \max_{a'} Q(s_{t+1},a') \right) \\ &= Q(s_t,a_t) + \alpha \underbrace{\left(r_t + \gamma \max_{a'} Q(s_{t+1},a') - Q(s_t,a_t) \right)}_{\text{temporal difference}} \end{aligned}$$

α is like the learning rate

Q-learning

The simplest model-free algorithm:

Q-learning

Initialize Q randomly; denote the initial state by s_1.

For $t = 1, 2, \ldots,$

- **with probability** ϵ**, explore**: a_t is chosen uniformly at random
- **with probability** $1-\epsilon$**, exploit**: $a_t = \operatorname{argmax}_a Q(s_t, a)$
- execute action a_t, receive reward r_t, arrive at state s_{t+1}
- update the Q function

$$Q(s_t,a_t) \leftarrow (1-\alpha)Q(s_t,a_t) + \alpha \left(r_t + \gamma \max_{a} Q(s_{t+1},a) \right)$$

for some learning rate α.

Comparisons

	Model-based	Model-free
What it learns	model parameters $P, r, \ldots$	Q function
Space	$O(\lvert\mathcal{S}\rvert^2 \lvert\mathcal{A}\rvert)$	$O(\lvert\mathcal{S}\rvert \lvert\mathcal{A}\rvert)$
Performance	usually better	usually worse

There are many different algorithms and RL is an active research area.

Summary

A brief introduction to some online decision making problems:

- **Multi-armed bandits**
  - most basic problem to understand **exploration vs. exploitation**
  - algorithms: explore–then–exploit, ϵ-greedy, **UCB**
- **Markov decision process and reinforcement learning**
  - a combination of Markov models and multi-armed bandits
  - learning the optimal policy with a known MDP: **value iteration**
  - learning the optimal policy with an unknown MDP: model-based approach and model-free approach (e.g. **Q-learning**)