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

Outline

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

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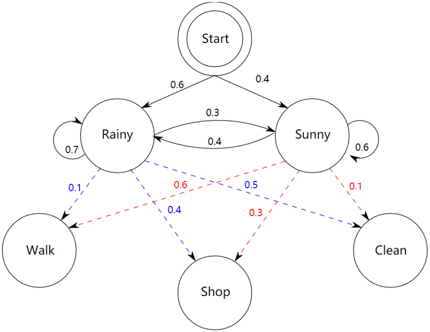
Hidden Markov Models

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

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

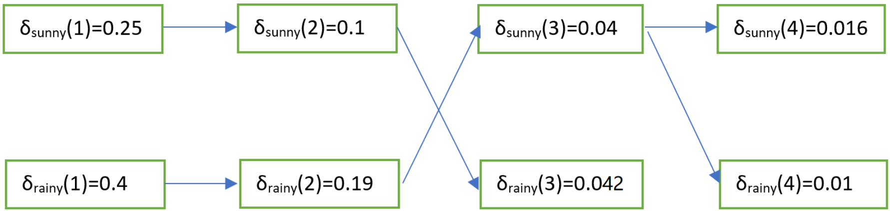
$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s} \delta_{s'}(t-1)$$

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

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

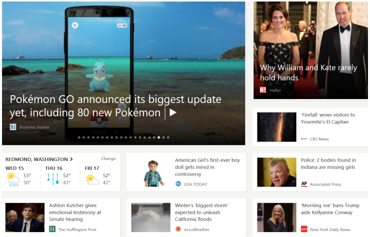
Of course there are many slot machines in the casino

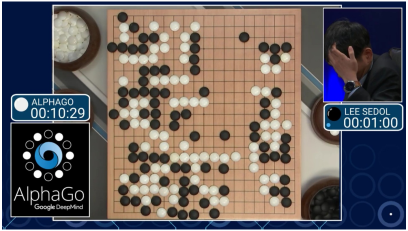
- like a bandit with multiple arms (hence the name)
- **if I can play for 10 times, which machines should I play?**

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)





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

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 $\mathrm{argmax}_a\, \mu_a$ as quickly as possible

Empirical means

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

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

where

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

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 $t = K + 1, \ldots, T$, 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 $\text{argmax}_a \ \hat{\mu}_{T_0,a}$

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 $a_t = \mathrm{argmax}_a \ \hat{\mu}_{t-1,a}$

Pros

- always exploring and exploiting
- applicable to many other problems
- first thing to try usually

Cons

- need to tune ϵ
- same uniform exploration

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 $a_t = \operatorname{argmax}_a \ \mathrm{UCB}_{t,a}$ where

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

- the first term in $\mathrm{UCB}_{t,a}$ 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,

$$\mu_a \le \mathsf{UCB}_{t,a}$$

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

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

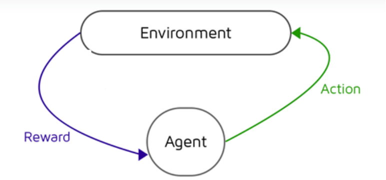
- true environment is unknown due to randomness (**uncertainty**)
- just pretend it's the most preferable one among all plausible environments (**optimism**)

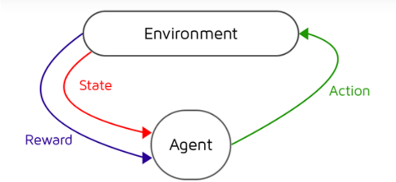
This principle is useful for many other bandit problems.

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

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

Markov decision process

An MDP is parameterized by five elements

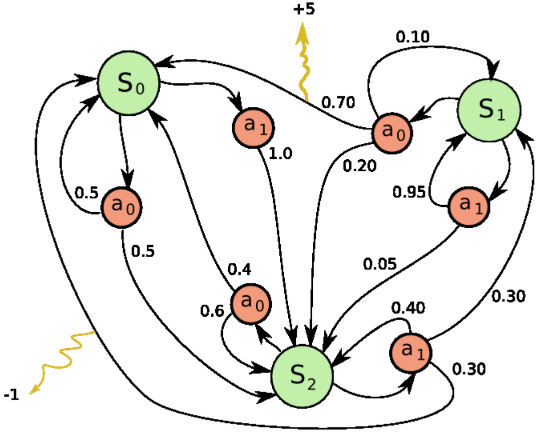
- $\mathcal{S}$: a set of possible states
- $\mathcal{A}$: a set of possible actions
- P: transition probability, $P_a(s, s')$ is the probability of transiting from state s to state s' after taking action a (Markov property)
- r: reward function, $r_a(s)$ is (expected) reward of action a at state s
- $\gamma \in (0, 1)$: 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 $0, 1, 2, \ldots$ are respectively

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

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

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

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 $k = 1, 2, \ldots$ (until convergence)

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

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 $Q : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ 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**)