CSCI567 Machine Learning (Spring 2021)

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Outline

1. Review of last lecture
2. Multi-armed Bandits

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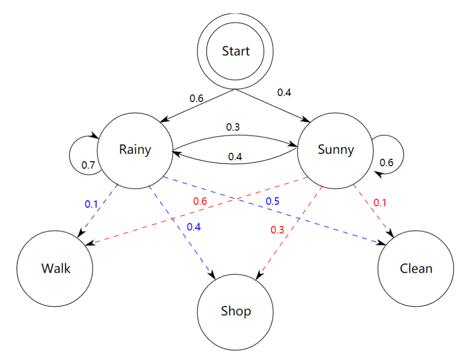
Hidden Markov Models

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

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

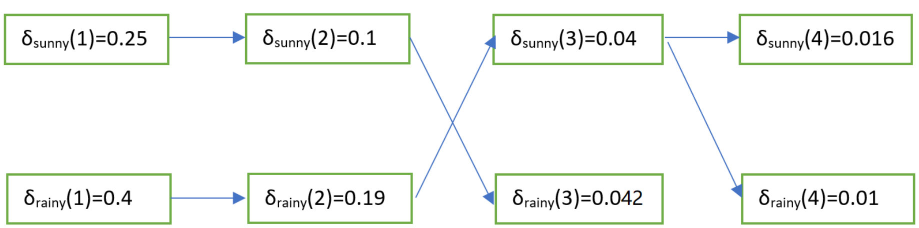
$$\Delta_s(t) = \operatorname*{argmax}_{s'} a_{s',s} \delta_{s'}(t-1)$$

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:

- **multi-armed bandit** (this lecture)
- **reinforcement learning** (next lecture)

Mulit-armed bandits: motivation

Imagine going to a casino to play a slot machine

- invariably it takes your money like a "bandit".

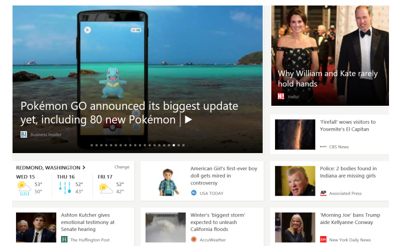
Of course there are many slot machines in the casino

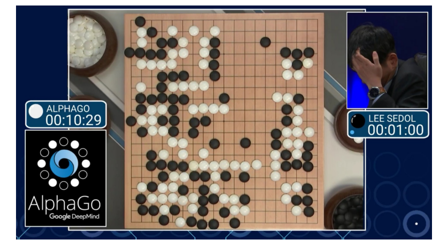
- like a bandit with multiple arms (hence the name)
- **if I can play for 10 times, which machines should I play?**

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 $\text{Ber}(\mu_a)$, 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

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

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 alg. first pick arm 1 and see reward 0, then pick arm 2 and see 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 $a_t = \text{argmax}_a \ \hat{\mu}_{t-1,a}$

Pros	**Cons**
• always exploring and exploiting • applicable to many other problems • first thing to try usually	• 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 $a_t = \text{argmax}_a \ \text{UCB}_{t,a}$ 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,

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

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.