# **CSCI 567: Machine Learning**

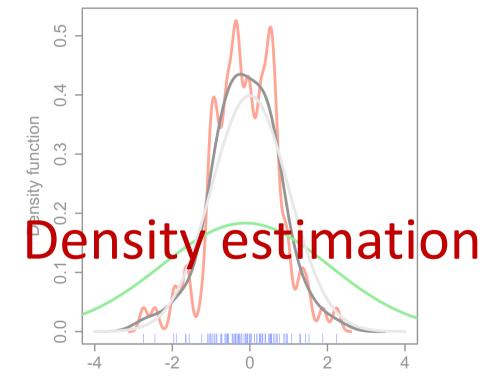
Vatsal Sharan Spring 2024

Lecture 12, Apr 12



# Administrivia

- Exam 2 is on April 26 in class (1pm-3:20pm)
  - Similar format to Exam 1
  - Syllabus is lecture 6 (multiclass classification & neural networks) onwards
- Project mid-term check-ins next week
  - Short report due on Monday April 15 on Gradescope
- Today's plan:
  - Density estimation & Naïve Bayes
  - Multi-armed bandits
  - Reinforcement Learning



Х

# **Density estimation**

- Introduction
- Parametric methods
- Non-parametric methods

# Introduction

With clustering using GMMs, our high-level goal was the following:

Given a training set  $x_1, \ldots, x_n$ , estimate a density function p that could have generated this dataset (via  $x_i \overset{i.i.d.}{\sim} p$ ).

This is a special case of the general problem of *density estimation*, an important unsupervised learning problem.

Density estimation is useful for many downstream applications

- we have seen clustering already, will see more today
- these applications also *provide a way to measure quality of the density estimator*

# **Density estimation**

- Introduction
- Parametric methods
- Non-parametric methods

#### **Parametric methods: generative models**

Parametric estimation assumes a generative model parametrized by  $\theta$ :

$$p(\boldsymbol{x}) = p(\boldsymbol{x} ; \boldsymbol{\theta})$$

Examples:

• GMM: 
$$p(\boldsymbol{x}; \boldsymbol{\theta}) = \sum_{j=1}^{k} \pi_j N(\boldsymbol{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$
 where  $\boldsymbol{\theta} = \{\pi_j, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\}$ 

• Multinomial: a discrete variable with values in  $\{1, 2, \ldots, k\}$  s.t.

$$p(x=j;\boldsymbol{\theta})=\theta_j$$

where  $\boldsymbol{\theta}$  is a distribution over the k elements.

Size of  $\theta$  is independent of the size of the training set, so it's parametric.

#### **Parametric methods: estimation**

As usual, we can apply **MLE** to learn the parameters  $\theta$ :

$$\operatorname{argmax}_{\boldsymbol{\theta}} \sum_{i=1}^{n} \ln p(x_i ; \boldsymbol{\theta})$$

For some cases this is intractable and we can use algorithms such as EM to approximately solve the MLE problem (e.g. GMMs).

For some other cases this admits a simple closed-form solution (e.g. multinomial).

#### **MLE for multinomials**

The log-likelihood is

$$\sum_{i=1}^{n} \ln p(x = x_i; \theta) = \sum_{i=1}^{n} \ln \theta_{x_i} = \sum_{i=1}^{n} \sum_{j=1}^{k} \underbrace{\mathbf{1}(x_i = j) \ln \theta_j}_{\text{indication}}$$
$$= \sum_{j=1}^{k} \sum_{i:x_i = j} \ln \theta_j = \sum_{j=1}^{k} z_j \ln \theta_j$$

where  $z_j = |\{i : x_i = j\}|$  is the number of examples with value j.

The solution is simply

$$\theta_j = \frac{z_j}{n} \propto z_j,$$

i.e. the fraction of examples with value j. (See HW4 Q2.1)

# **Density estimation**

- Introduction
- Parametric methods
- Non-parametric methods

### **Nonparametric methods**

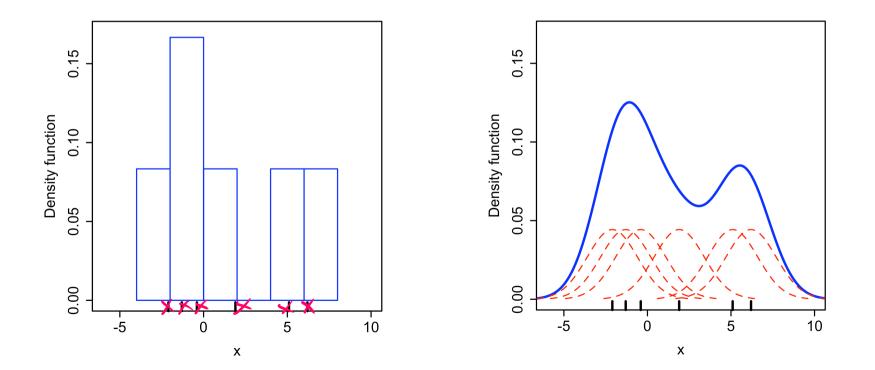
Can we estimate without assuming a fixed generative model?

Kernel density estimation (KDE) provides a solution.

- the approach is nonparametric: it keeps the entire training set
- we focus on the one-dimensional (continuous) case

# **High-level idea**

- Construct something similar to a histogram:
- For each data point, create a "bump" (via a Kernel)
- Sum up or average all the bumps

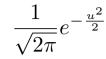


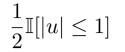
# Kernel

KDE with a kernel 
$$K: \mathbb{R} \to \mathbb{R}$$
:  
 $p(x) = \frac{1}{n} \sum_{i=1}^{n} K(x - x_i)$   
 $adding a two oround x$ ;  
e.g.  $K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{u^2}{2}}$ , the standard Gaussian density  
bump  
Kernel needs to satisfy:  
 $\int_{-\infty}^{\infty} K(u) du = 1$ , makes sure p is a density function.

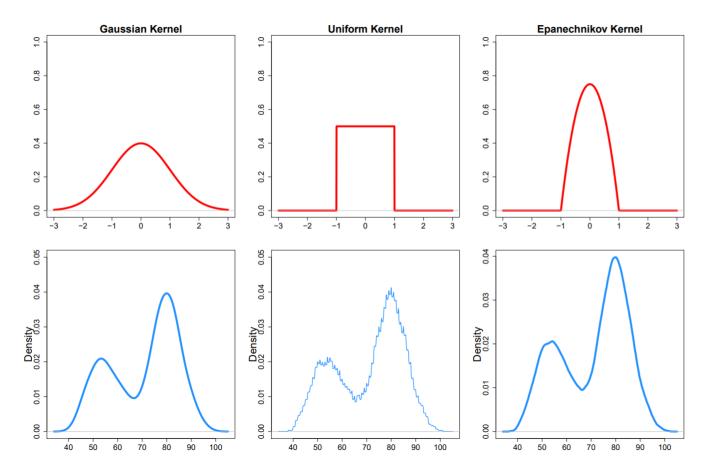
х

# **Different kernels**





$$\frac{3}{4}\max\{1-u^2,0\}$$





If K(u) is a kernel, then for any h > 0

$$K_h(u) := \frac{1}{h} K\left(\frac{u}{h}\right)$$

(stretching the kernel)

can be used as a kernel too (verify the two properties yourself)

So general KDE is determined by both the kernel K and the bandwidth h

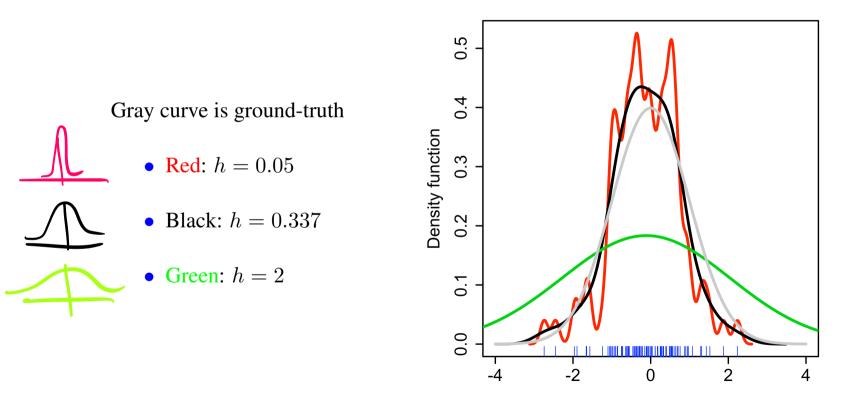
$$p(x) = \frac{1}{n} \sum_{i=1}^{n} K_h \left( x - x_i \right) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{x - x_i}{h} \right)$$

- $x_i$  controls the center of each bump
- *h* controls the width/variance of the bumps

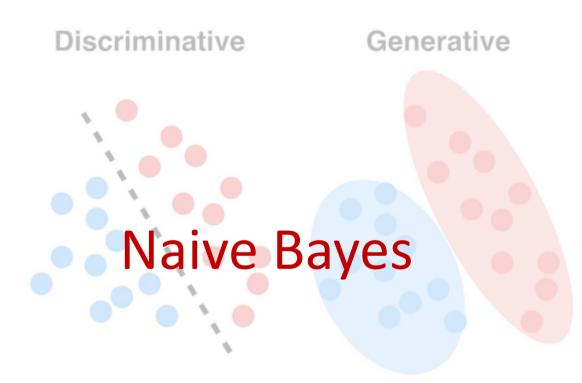
 $\int_{-\infty}^{\infty} \int_{h} \frac{1}{K} \left( \frac{y}{h} \right) du = 1$ 

# Bandwidth

#### Larger *h* means larger variance and smoother density

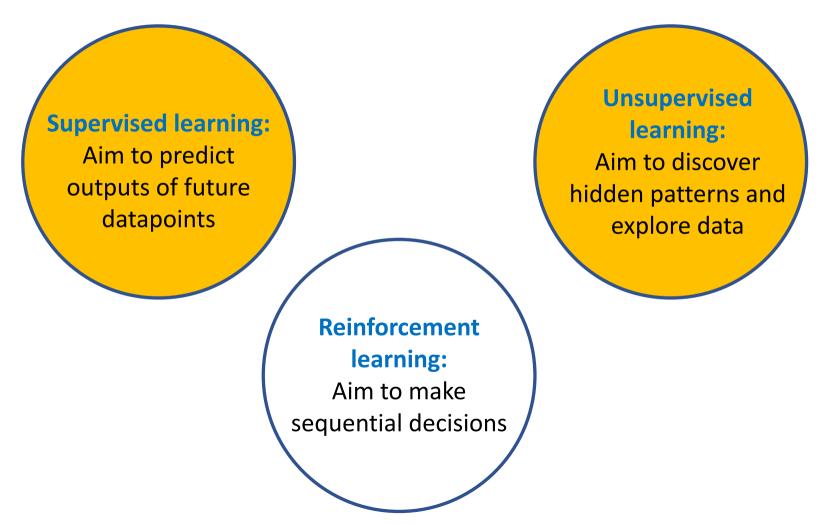


Х



**Image source** 

# A simplistic taxonomy of ML



#### **Naïve Bayes**

- Motivation & setup
- Prediction with Naïve Bayes, and some connections

# **Bayes optimal classifier**

Suppose (x, y) is drawn from a joint distribution p. The Bayes optimal classifier is

 $f^*(\boldsymbol{x}) = \operatorname*{argmax}_{c \in [\mathsf{C}]} p(c \mid \boldsymbol{x})$ 

i.e. predict the class with the largest conditional probability.

p is of course unknown, but we can estimate it, which is *exactly a density estimation problem!* 

### **Estimation**

How to estimate a joint distribution? Observe we always have

 $p(\boldsymbol{x},y) = p(y)p(\boldsymbol{x} \mid y)$  $f(\boldsymbol{x},y) = p(y)p(\boldsymbol{x} \mid y)$ 

We know how to estimate p(y) by now.

To estimate p(x | y = c) for some  $c \in [C]$ , we are doing density estimation using data  $\{x_i : y_i = c\}$ .

This is *not a 1D problem* in general.

#### A naïve assumption

Naive Bayes assumption: conditioning on a label, features are independent, which means

$$p(\boldsymbol{x} \mid y = c) = \prod_{j=1}^{d} p(x_j \mid y = c)$$

Now for each j and c we have a simple 1D density estimation problem!

Is this a reasonable assumption? Sometimes yes, e.g.

- use  $\boldsymbol{x} = (\text{Height}, \text{Vocabulary})$  to predict y = Age
- Height and Vocabulary are dependent
- but conditioned on Age, they are independent!

More often this assumption is *unrealistic and "naive*", but still Naive Bayes can work very well even if the assumption is wrong.

#### **Example: Discrete features**

> 5possible ralies Height:  $\leq 3', 3'-4', 4'-5', 5'-6', \geq 6'$ Vocabulary: ≤5K, 5K-10K, 10K-15K, 15K-20K, >20K Age:  $\leq 5, 5-10, 10-15, 15-20, 20-25, \geq 25$  ~ ( values

MLE estimation: e.g.

 $p(Age = 10-15) = \frac{\text{#examples with age 10-15}}{\text{#examples}}$ 

 $p(\text{Height} = 5'-6' \mid \text{Age} = 10-15)$  $= \frac{\#\text{examples with height 5'-6' and age 10-15}}{\#\text{examples with age 10-15}} \rightarrow \text{conditional} = \frac{\text{joint}}{\text{monginal}}$ 

# **Discrete features: More formally**

For a label 
$$c \in [C]$$
,  

$$p(y = c) = \frac{|\{i : y_i = c\}|}{n}$$
For each possible value  $\ell$  of a discrete feature  $j$ ,  

$$p(x_j = \ell \mid y = c) = \frac{|\{i : x_{i,j} = \ell, y_i = c\}|}{|\{i : y_i = c\}|}$$
density for jth feature

#### **Continuous features**

If the feature is continuous, we can do

• parametric estimation, e.g. via a Gaussian

$$p(x_j = x \mid y = c) = \frac{1}{\sqrt{2\pi}\sigma_{c,j}} \exp\left(-\frac{(x - \mu_{c,j})^2}{2\sigma_{c,j}^2}\right)$$

where  $\mu_{c,j}$  and  $\sigma_{c,j}^2$  are the empirical mean and variance of feature *j* among all examples with label *c*.

• or nonparametric estimation, e.g. via a Kernel K and bandwidth h:

$$p(x_j = x \mid y = c) = \frac{1}{|\{i : y_i = c\}|} \sum_{i:y_i = c} K_h(x - x_{i,j})$$

#### **Naïve Bayes**

- Motivation & setup
- Prediction with Naïve Bayes, and some connections

# **Naïve Bayes: Prediction**

After learning the model

$$p(\boldsymbol{x}, y) = p(y) \prod_{j=1}^{d} p(x_j \mid y)$$

# **Example: Discrete features**

For **discrete features**, plugging in previous MLE estimation gives

$$\begin{aligned} \underset{c \in [\mathsf{C}]}{\operatorname{argmax}} & p(y = c \mid \boldsymbol{x}) \\ = \underset{c \in [\mathsf{C}]}{\operatorname{argmax}} & \left( \ln p(y = c) + \sum_{j=1}^{d} \ln p(x_j \mid y = c) \right) \\ = \underset{c \in [\mathsf{C}]}{\operatorname{argmax}} & \left( \ln |\{i : y_i = c\}| + \sum_{j=1}^{d} \ln \frac{|\{i : x_{i,j} = x_j, y_i = c\}|}{|\{i : y_i = c\}|} \right) \end{aligned}$$

#### What is Naïve Bayes learning?

Observe again for the case of continuous features with a Gaussian model, if we fix the variance for each feature to be  $\sigma$  (i.e. not a parameter of the model any more), then the prediction becomes

# **Connection to logistic regression**

Moreover, by a similar calculation you can verify

 $p(y = c \mid \boldsymbol{x}) \propto e^{\boldsymbol{w}_c^{\mathrm{T}} \boldsymbol{x}}$ 

This the softmax function, the same model we used for the probabilistic interpretation of logistic regression!

So what is different then? They learn the parameters in different ways:

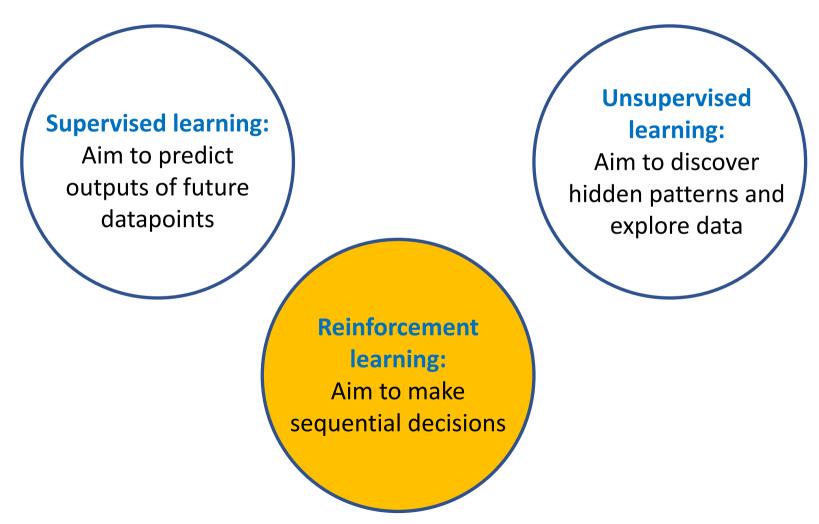
- both via MLE, one on  $p(y = c \mid \boldsymbol{x})$ , the other on  $p(\boldsymbol{x}, y)$
- solutions are different: logistic regression has no closed-form, naive Bayes admits a simple closed-form

# **Connection to logistic regression**

	Logistic regression	Naive Bayes
Model	conditional $p(y \mid \boldsymbol{x})$	joint $p(\boldsymbol{x}, y)$
Learning	MLE (can also be viewed as minimizing logistic loss)	MLE
Accuracy	usually better for large $n$	usually better for small $n$
$\int P(y=c x)  fog  c= \{\pm,j\}$ $= -(y, y^Tx)$		
	Discriminative models	Generative models



# A simplistic taxonomy of ML



# **Multi-armed bandits**

- Motivation & setup
- Exploration vs. Exploitation

# **Decision making**

Problems we have discussed so far:

- start with a fixed training dataset
- learn a predictor from the data or discover some patterns in the data

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/Instagram recommendation systems:

- a user visits the website (or views a post etc.)
- the system recommends some products/movies/posts
- 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...

# **Multiarmed 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 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 (Netflix employs a variant of bandit algorithm)
- game playing, each possible move is an arm (AlphaGo 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 usually referred to as bandit feedback

#### **Evaluating performance**

What should be the goal here?

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 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:

> { 0113

- rewards of arm a are i.i.d. samples of  $\text{Ber}(\mu_a)$ , that is,  $r_{t,a}$  is 1 with prob.  $\mu_a$ , and 0 with prob.  $1 - \mu_a$ , independent of anything else. (indep. across all owns, across timesteps)
- 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*:

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

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  $\mu_a$  if  $n_{t,a}$  is large

## **Multi-armed bandits**

- Motivation & setup
- Exploration vs. Exploitation

# **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 algorithm first picks arm 1 and sees reward 0, then picks arm 2 and sees reward 1 (this happens with decent probability)
   ( 0.4 + 0.5 = 0.2)
- 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 \operatorname{argmax}_a \hat{\mu}_{T_0,a}
```

Parameter  $T_0$  clearly controls the exploration/exploitation trade-off

#### **Explore-then-Exploit: Issues**

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  $T_0/K$  times
- clearly it won't work if the environment is changing

# A slightly better algorithm

 $\epsilon$ -Greedy Pick each arm once for the first K rounds.

For t = K + 1, ..., T,

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

#### Pros

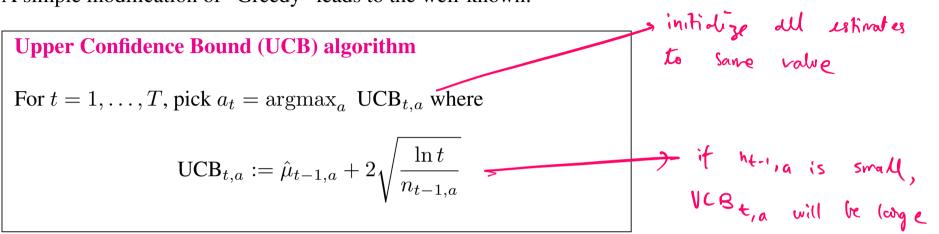
- always exploring and exploiting
- applicable to many other problems
- first thing to try usually

#### Cons

- need to tune  $\epsilon$
- same uniform exploration

Is there a more adaptive way to explore?

# More adaptive exploration



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

- the first term in  $UCB_{t,a}$  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,

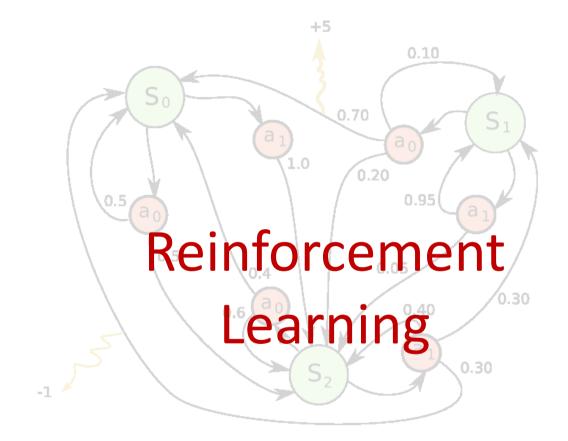
 $\mu_a \leq \text{UCB}_{t,a}$ 

so  $UCB_{t,a}$  is indeed an upper bound on the true mean.

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

- true environment (best mean) is unknown due to randomness (**uncertainty**)
- have an upper bound (optimistic guess) on the expected reward of each environment, and pick best one according to upper bound (**optimism**)

This principle is useful for many other bandit problems.



# **Reinforcement Learning**

- Motivation
- Markov Decision Process (MDP)
- Learning MDPs

# **Motivation**

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



Often, it can be too simple to capture real-life problems. One important aspect 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

• Video games, AlphaGo, Reinforcement Learning from Human Feedback (RLHF) for Chatbots, self-driving cars, etc.

The foundation of RL is **Markov Decision Process (MDP)**, a combination of Markov models and multi-armed bandits.

# **Reinforcement Learning**

- Motivation
- Markov Decision Process (MDP)
- Learning MDPs

#### **Markov Decision Process**

An MDP is parameterized by five elements

- S: a set of possible states
- *A*: a set of possible actions
- P: transition probability, P<sub>a</sub>(s, s') is the probability of transiting from state s to state s' after taking action a (Markov property) -> Conditioned on present state, future stated do not depend on post states
- r: reward function,  $r_a(s)$  is (expected) reward of action a at state s

Difference from Markov models, the state transition is influenced by the taken action. Difference from Multi-armed bandit, the reward depends on the state.

# **Measuring reward**

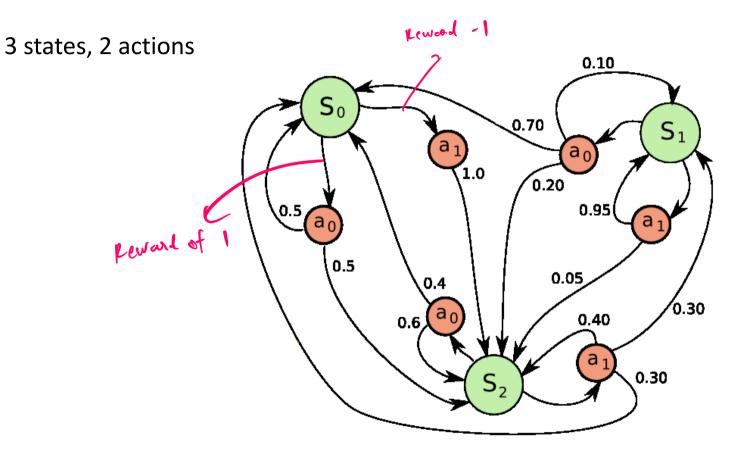
There can be different ways of measuring reward, for example:

- Fix some finite horizon (say 100 time steps) and sum total the rewards obtained in this horizon.
- Discount future rewards by discount factor  $\gamma \in (0, 1)$ . Reward of 1 from tomorrow is only counted as  $\gamma$  for today, more generally reward n time steps away is discounted by  $\gamma^n$ .

Discounting is most popular and well-studied.

- It models the fact that the process could stop at any time step
- It has a preference for solutions which are rewarding over short time scales
- It is like a smoothed version of a fixed horizon.

## Example



# Policy

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

If we start from state  $s_0 \in S$  and act according to a policy  $\pi$ , the discounted rewards for time  $0, 1, 2, \ldots$  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

#### **Optimal policy and Bellman equation**

First goal: knowing all parameters, how do we find the optimal policy

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

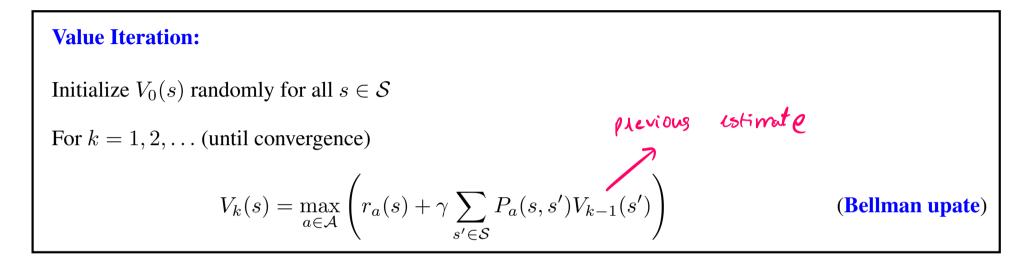
We first answer a related question: *what is the maximum reward one can achieve starting from an arbitrary state s?* 

$$V(s) = \max_{\pi} \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^{t} r_{\pi(s_{t})}(s_{t}) \mid s_{0} = s \right]$$
$$= \max_{a \in \mathcal{A}} \left( r_{a}(s) + \gamma \sum_{s' \in \mathcal{S}} P_{a}(s, s') V(s') \right)$$

V is called the (optimal) value function.

It satisfies the above **Bellman equation**: |S| nonlinear equations with |S| unknowns, *how do we solve it?* 

#### **Value iteration**



Knowing V, the optimal policy  $\pi^*$  is simply

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

#### **Convergence of value iteration**

Does Value Iteration always find the true value function V? Yes! f(m) $|V_k(s) - V(s)| = \left| \max_{a \in \mathcal{A}} \left( r_a(s) + \gamma \sum_{s' \in \mathcal{S}} P_a(s, s') V_{k-1}(s') \right) \right|$  $\leq \gamma \max_{a \in \mathcal{A}} \left| \sum_{s' \in \mathcal{S}} P_a(s, s') \left( V_{k-1}(s') - V(s') \right) \right|$  $\leq \gamma \max_{a \in \mathcal{A}} \sum_{s \in \mathcal{S}} P_a(s, s') \left| V_{k-1}(s') - V(s') \right|$  $\leq \gamma \max |V_{k-1}(s') - V(s')| \leq \cdots \leq \gamma^k \max |V_0(s') - V(s')|$ 

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

# **Reinforcement Learning**

- Motivation
- Markov Decision Process (MDP)
- Learning MDPs ---- Next fime !