# AIN311

Fundamentals of Machine Learning

Lecture 7:

Probability Review (cont'd.)

Maximum Likelihood Estimation (MLE)



#### Administrative

- Project proposal due November 7
- A half page description
  - problem to be investigated,
  - why it is interesting,
  - what data you will use,
  - related work.



# Today

- Probabilities
  - Dependence, Independence, Conditional Independence
- Parameter estimation
  - Maximum Likelihood Estimation (MLE)
  - Maximum a Posteriori (MAP)

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# Last time... Sample space

**Def**: A **sample space**  $\Omega$  is the set of all possible outcomes of a (conceptual or physical) random experiment. ( $\Omega$  can be finite or infinite.)

#### **Examples:**

- Ω may be the set of all possible outcomes of a dice roll (1,2,3,4,5,6)
- · Pages of a book opened randomly. (1-157)
- · Real numbers for temperature, location, time, etc

#### Last time... Events

We will ask the question:

What is the probability of a particular event?

**Def: Event** A is a **subset** of the sample space  $\Omega$ 

#### **Examples:**

What is the probability of

- the book is open at an odd number
- rolling a dice the number <4
- a random person's height X: a<X<b

slide by Barnabás Póczos & Alex Sm

# Last time... Probability

**Def:** *Probability P(A), the probability that event (subset) A happens*, is a function that maps the event A onto the interval [0, 1]. *P(A)* is also called the **probability measure** of A.

sample space  $\Omega$ 

1,3,5,6 outcomes in which A is true

2,4

#### **Example:**

What is the probability that the number on the dice is 2 or 4?

P(A) is the volume of the area.

### Last time... Kolmogorov Axioms

- (i) Nonnegativity:  $P(A) \ge 0$  for each A event.
- (ii)  $P(\Omega) = 1$ .
- (iii)  $\sigma$ -additivity: For disjoint sets (events)  $A_i$ , we have

$$P(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$$

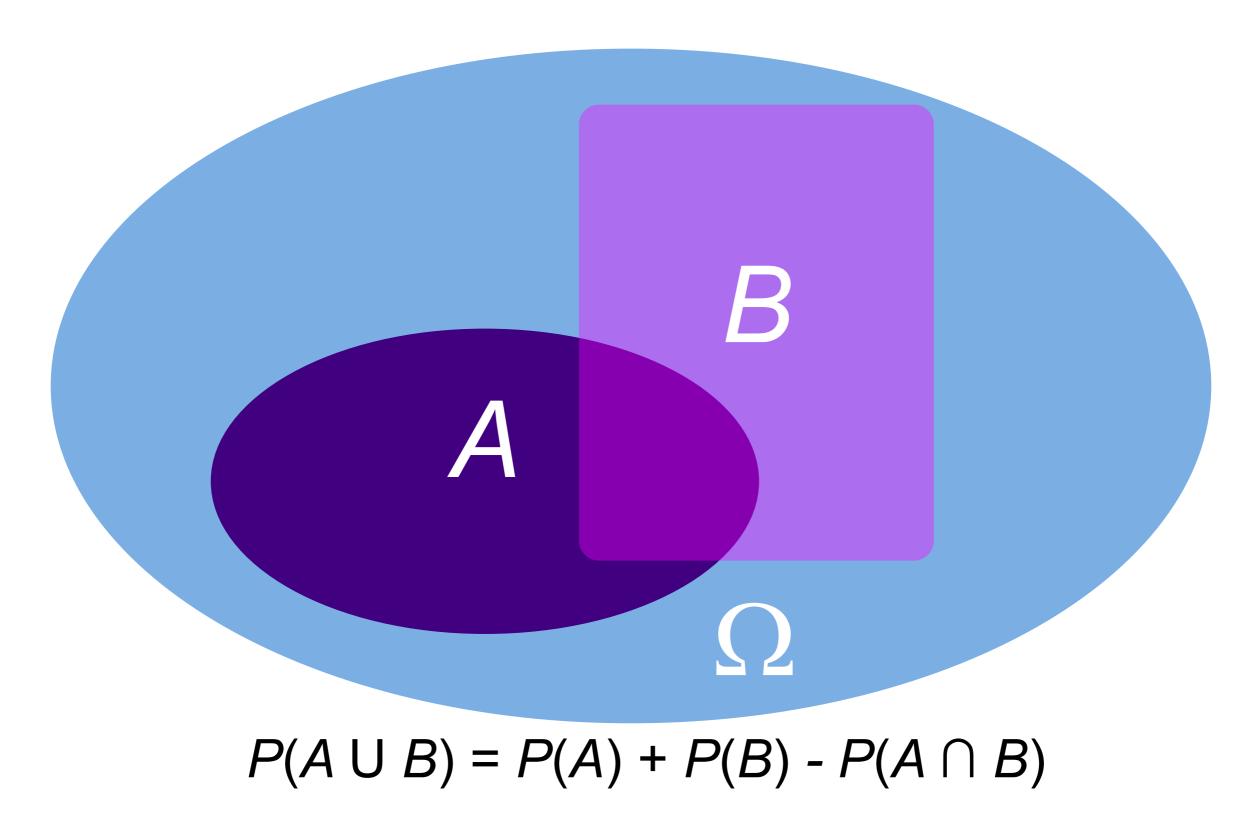
#### Consequences:

$$P(\emptyset) = 0.$$

$$P(A \cup B) = P(A) + P(B) - P(A \cap B).$$

$$P(A^c) = 1 - P(A).$$

## Last time... Venn Diagram



#### Last time... Random Variables

**Def:** Real valued **random variable** is a function of the outcome of a randomized experiment

$$X:\Omega\to\mathbb{R}$$

$$P(a < X < b) \stackrel{.}{=} P(\omega : a < X(\omega) < b)$$
  
 $P(X = a) \stackrel{.}{=} P(\omega : X(\omega) = a)$ 

#### **Examples:**

- **Discrete** random variable examples ( $\Omega$  is discrete):
- X(ω) = True if a randomly drawn person (ω) from our class (Ω) is female
- X(ω) = The hometown X(ω) of a randomly drawn person
   (ω) from our class (Ω)

Bernoulli distribution: Ber(p)

```
\Omega = \{\text{head, tail}\}\ X(head) = 1,\ X(tail) = 0.
```



Bernoulli distribution: Ber(p)

$$\Omega = \{\text{head, tail}\}\ X(head) = 1,\ X(tail) = 0.$$

$$P(X = a) = P(\omega : X(\omega) = a) = \begin{cases} p, & \text{for } a = 1\\ 1 - p, & \text{for } a = 0 \end{cases}$$



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Binomial distribution: Bin(n,p)

Suppose a coin with head prob. *p* is tossed *n* times. What is the probability of getting *k* heads and *n-k* tails?

$$\Omega = \{ \text{ possible } n \text{ long head/tail series} \}, |\Omega| = 2^n$$
  
 $K(\omega) = \text{ number of heads in } \omega = (\omega_1, \dots, \omega_n) \in \{\text{head, tail}\}^n = \Omega$ 

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$$P(K = k) = P(\omega : K(\omega) = k) = \sum_{\omega : K(\omega) = k} p^{k} (1-p)^{n-k} = {n \choose k} p^{k} (1-p)^{n-k}$$

#### Last time... Conditional Probability

P(X|Y) = Fraction of worlds in which X event is true given Y event is true.

$$P(X|Y) = \frac{P(X,Y)}{P(Y)}$$

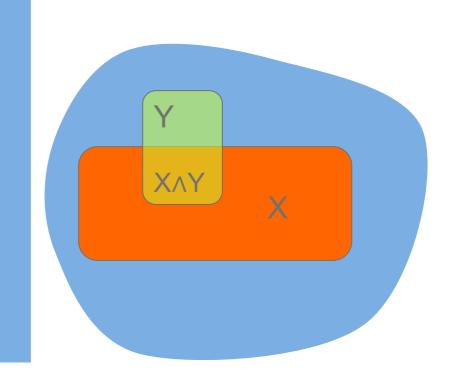
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$$P(\text{flu}|\text{headache}) = \frac{P(\text{flu, headache})}{P(\text{headache})} = \frac{1/80}{1/80 + 7/80}$$

	Flu	No Flu
Headache	1/80	7/80
No Headache	1/80	71/80



# Independence

#### Independent random variables:

$$P(X,Y) = P(X)P(Y)$$
$$P(X|Y) = P(X)$$

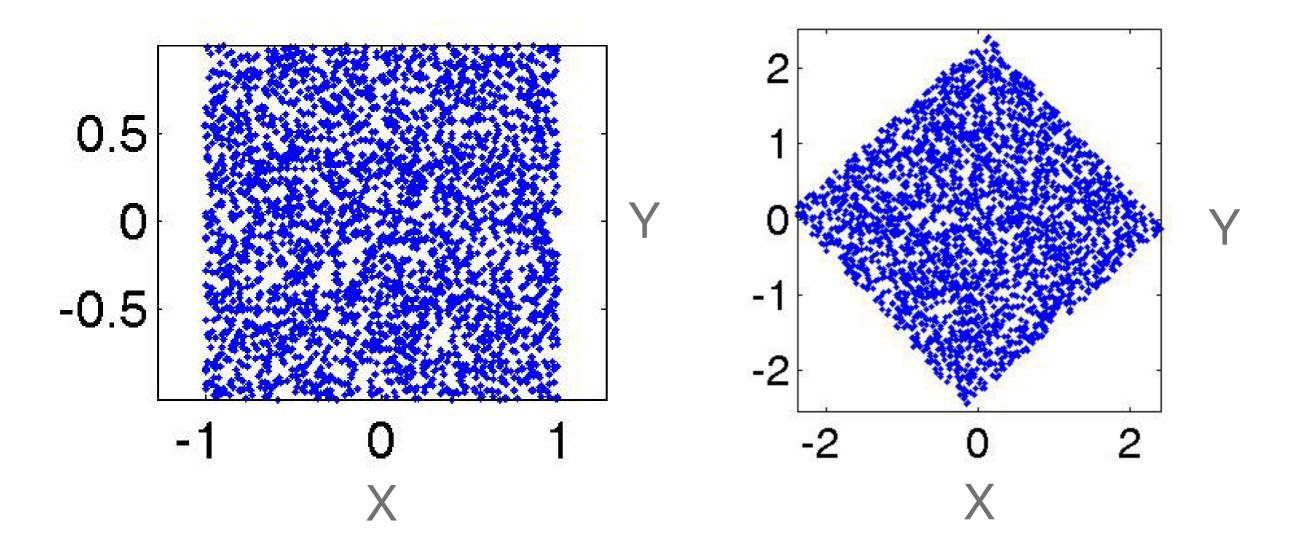
Y and X don't contain information about each other. Observing Y doesn't help predicting X. Observing X doesn't help predicting Y.

#### **Examples:**

Independent: Winning on roulette this week and next week.

Dependent: Russian roulette

# Dependent / Independent



Independent X,Y

Dependent X,Y

# Conditionally Independent

#### **Conditionally independent:**

$$P(X,Y|Z) = P(X|Z)P(Y|Z)$$

Knowing Z makes X and Y independent

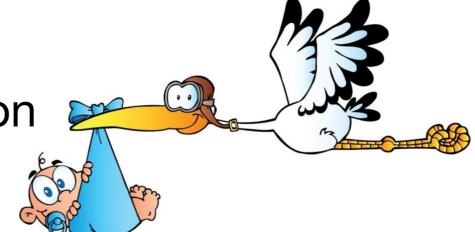
#### Examples:

Dependent: shoe size of children and reading skills

Conditionally independent: shoe size of children and reading

#### Stork deliver babies:

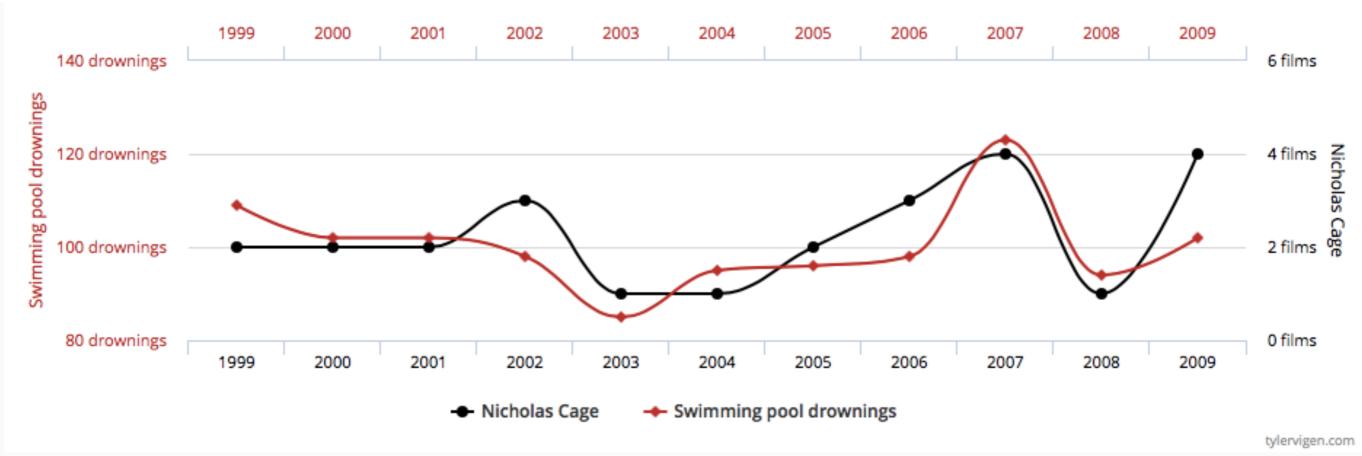
Highly statistically significant correlation exists between stork populations and human birth rates across Europe.



#### Correlation # Causation

## Number people who drowned by falling into a swimming-pool correlates with

#### Number of films Nicolas Cage appeared in



Data sources: Centers for Disease Control & Prevention and Internet Movie Database

Correlation: 0.666004

# Conditionally Independent

London taxi drivers: A survey has pointed out a positive and significant correlation between the number of accidents and wearing coats. They concluded that coats could hinder movements of drivers and be the cause of accidents. A new law was prepared to prohibit drivers from wearing coats when driving.

Finally, another study pointed out that people wear coats when it rains...

# Conditional Independence

Formally: X is conditionally independent of Y given Z

$$P(X,Y|Z) = P(X|Z)P(Y|Z)$$

P(Accidents, Coats | Rain) = P(Accidents | Rain)P(Coats | Rain)

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#### Equivalent to:

$$(\forall x, y, z) P(X = x | Y = y, Z = z) = P(X = x | Z = z)$$

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#### Equivalent to:

$$(\forall x, y, z)P(X = x | Y = y, Z = z) = P(X = x | Z = z)$$

P(Thunder|Rain, Lightning) = P(Thunder|Lightning)

Note: does NOT mean Thunder is independent of Rain But given Lightning knowing Rain doesn't give more info about Thunder

# Parameter estimation: MLE, MAP

**Estimating Probabilities** 



# slide by Barnabás Póczos & Alex Smola

# Flipping a Coin

I have a coin, if I flip it, what's the probability that it will fall with the head up?

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Let us flip it a few times to estimate the probability:

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The estimated probability is: 3/5 "Frequency of heads"



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#### **Questions:**

- (1) Why frequency of heads???
- (2) How good is this estimation???
  (3) Why is this a machine learning p (3) Why is this a machine learning problem???

We are going to answer these questions

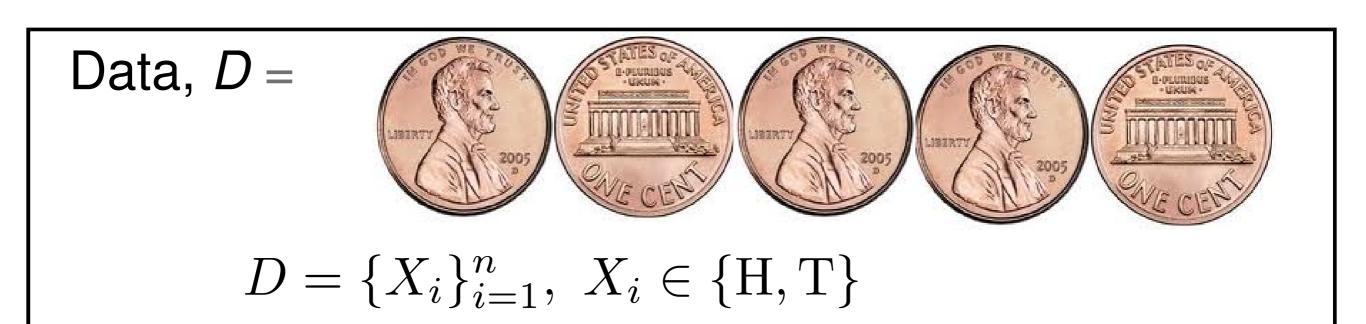
# Question (1)

#### Why frequency of heads???

- Frequency of heads is exactly the maximum likelihood estimator for this problem
- MLE has nice properties (interpretation, statistical guarantees, simple)

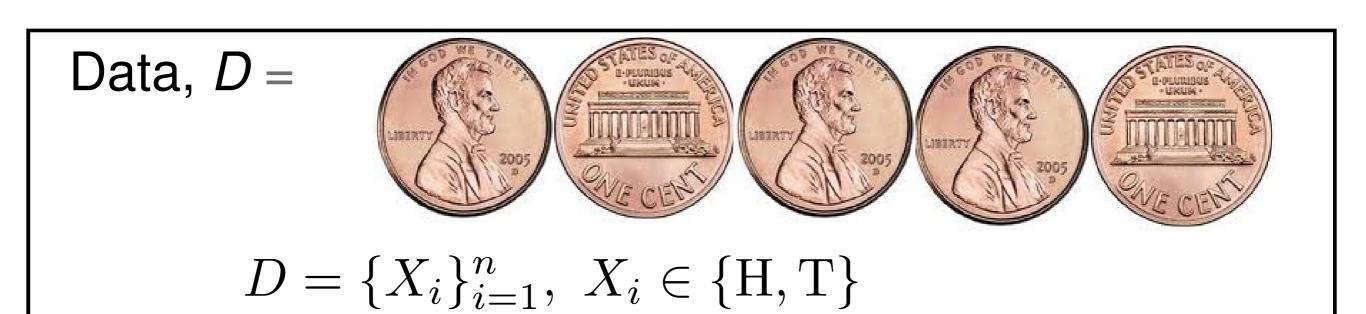
#### Maximum Likelihood Estimation

#### MLE for Bernoulli distribution



$$P(Heads) = \theta, P(Tails) = 1-\theta$$

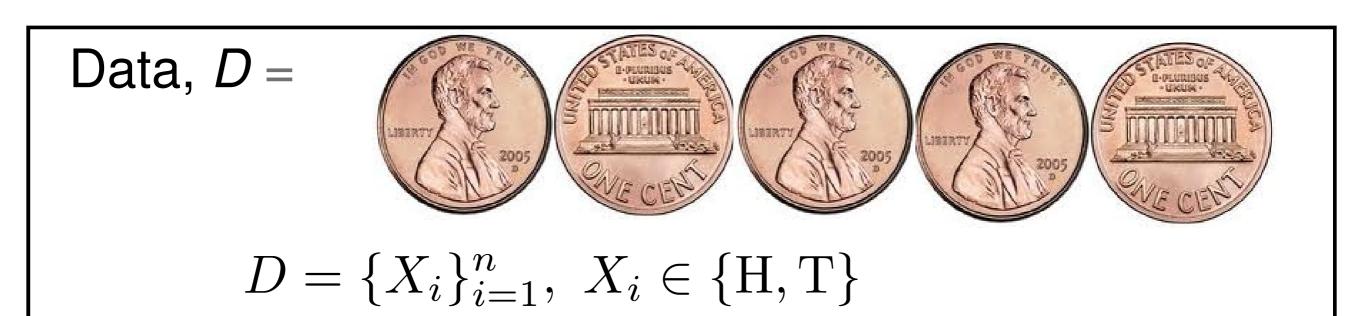
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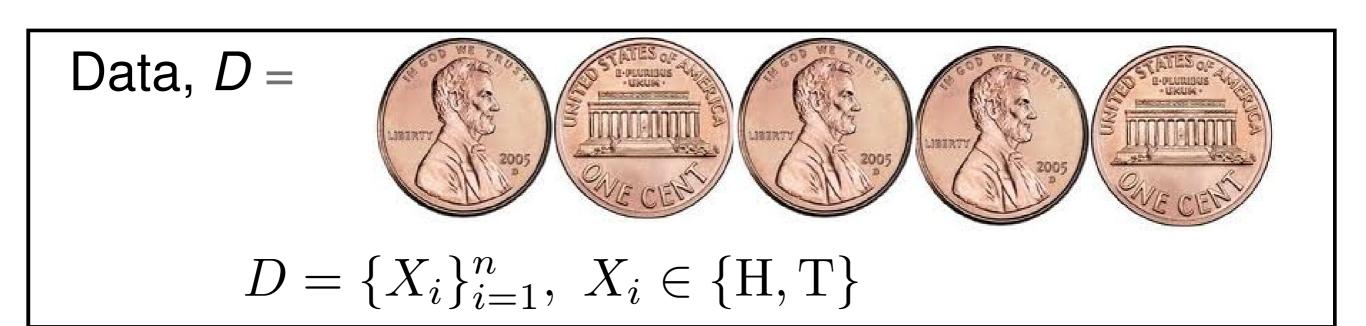


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#### Flips are i.i.d.:

- Independent events
  - Identically distributed according to Bernoulli distribution

## MLE for Bernoulli distribution



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## Maximum Likelihood Estimation

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$

$$\begin{split} \widehat{\theta}_{MLE} &= \arg\max_{\theta} P(D|\theta) \\ &= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta) \quad \text{ independent draws} \end{split}$$

$$\widehat{ heta}_{MLE} = rg \max_{ heta} P(D| heta)$$

$$= rg \max_{ heta} \prod_{i=1}^{n} P(X_i| heta) \qquad \text{independent draws}$$

$$= \arg\max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta) \quad \text{ identically distributed}$$

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$$= \arg \max_{\theta} \theta^{\alpha_H} (1 - \theta)^{\alpha_T}$$

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$$= \arg\max_{ heta} heta^{lpha_H} (1- heta)^{lpha_T}$$
 $J( heta)$ 

$$\widehat{\theta}_{MLE} = \underset{\theta}{\operatorname{arg\,max}} P(D|\theta) \\
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$$\frac{\partial J(\theta)}{\partial \theta} = \alpha_H \theta^{\alpha_H - 1} (1 - \theta)^{\alpha_T} - \alpha_T \theta^{\alpha_H} (1 - \theta)^{\alpha_T - 1} \Big|_{\theta = \hat{\theta}_{\text{MLE}}} = 0$$

$$\widehat{\theta}_{MLE} = \arg \max_{\theta} \frac{B(D|\theta)}{P(D|\theta)} \\
= \arg \max_{\theta} \theta^{\alpha_H} (1 - \theta)^{\alpha_T} \\
= \arg \max_{\theta} \frac{B(D|\theta)}{A(D|\theta)} \alpha_T$$

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$$\alpha_H H(1 \theta) \theta \alpha_T \theta_T \Big|_{\theta = \hat{\theta}_{\text{MLE}}} = 0$$

## Question (2)

How good is this MLE estimation???

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

## How many flips do I need?

I flipped the coins 5 times: 3 heads, 2 tails

$$\widehat{ heta}_{MLE} = rac{3}{5}$$

What if I flipped 30 heads and 20 tails?

$$\widehat{\theta}_{MLE} = \frac{30}{50}$$

- Which estimator should we trust more?
- The more the merrier???

## Simple Bound

Let  $\theta^*$  be the true parameter.

For 
$$n = \alpha_H + \alpha_T$$
, and  $\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$ 

For any  $\varepsilon > 0$ :

#### Hoeffding's inequality:

$$P(|\hat{\theta} - \theta^*| \ge \epsilon) \le 2e^{-2n\epsilon^2}$$

## Probably Approximate Correct (PAC) Learning

I want to know the coin parameter  $\theta$ , within  $\epsilon = 0.1$  error with probability at least  $1-\delta = 0.95$ .

#### How many flips do I need?

$$P(|\hat{\theta} - \theta^*| \ge \epsilon) \le 2e^{-2n\epsilon^2}$$

Sample complexity:

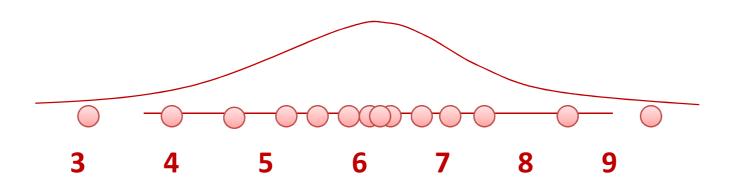
$$n \ge \frac{\ln(2/\delta)}{2\epsilon^2}$$

## Question (3)

### Why is this a machine learning problem???

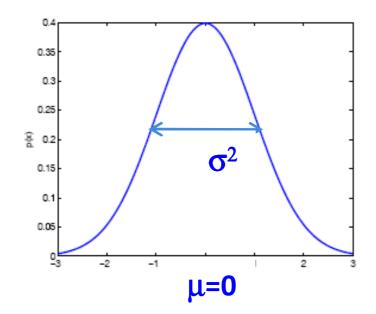
- improve their performance (accuracy of the predicted prob.)
- at some task (predicting the probability of heads)
- with experience (the more coins we flip the better we are)

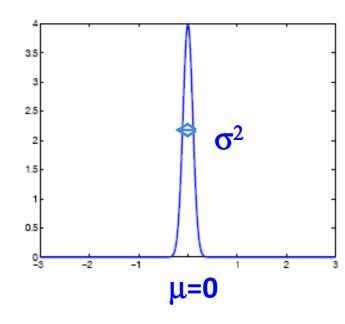
## What about continuous features?



### Let us try Gaussians...

$$p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(x-\mu)^2}{2\sigma^2}) = \mathcal{N}_x(\mu, \sigma)$$





## MLE for Gaussian mean and variance

Choose  $\theta$ = ( $\mu$ , $\sigma$ <sup>2</sup>) that maximizes the probability of observed data

$$\widehat{ heta}_{MLE} = \arg\max_{ heta} \ P(D \mid heta)$$
 
$$= \arg\max_{ heta} \prod_{i=1}^n P(X_i | heta) \qquad \text{Independent draws}$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} \frac{1}{2\sigma^2} e^{-(X_i - \mu)^2/2\sigma^2} \quad \begin{array}{l} \text{Identically} \\ \text{distributed} \end{array}$$

$$= \arg \max_{\theta = (\mu, \sigma^2)} \frac{1}{2\sigma^2} e^{-\sum_{i=1}^n (X_i - \mu)^2 / 2\sigma^2}$$

$$J(\theta)$$

## MLE for Gaussian mean and variance

$$\widehat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\widehat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \widehat{\mu})^2$$

#### Note: MLE for the variance of a Gaussian is biased

[Expected result of estimation is not the true parameter!]

Unbiased variance estimator:  $\widehat{\sigma}_{unbiased}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \widehat{\mu})^2$