# BBM406 Fundamentals of Machine Learning

Lecture 7: Probability Review (cont'd.)

Maximum Likelihood Estimation (MLE)



### Administrative

- Project proposal due March 31
- 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)

# 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

## 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

1,4

#### **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

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

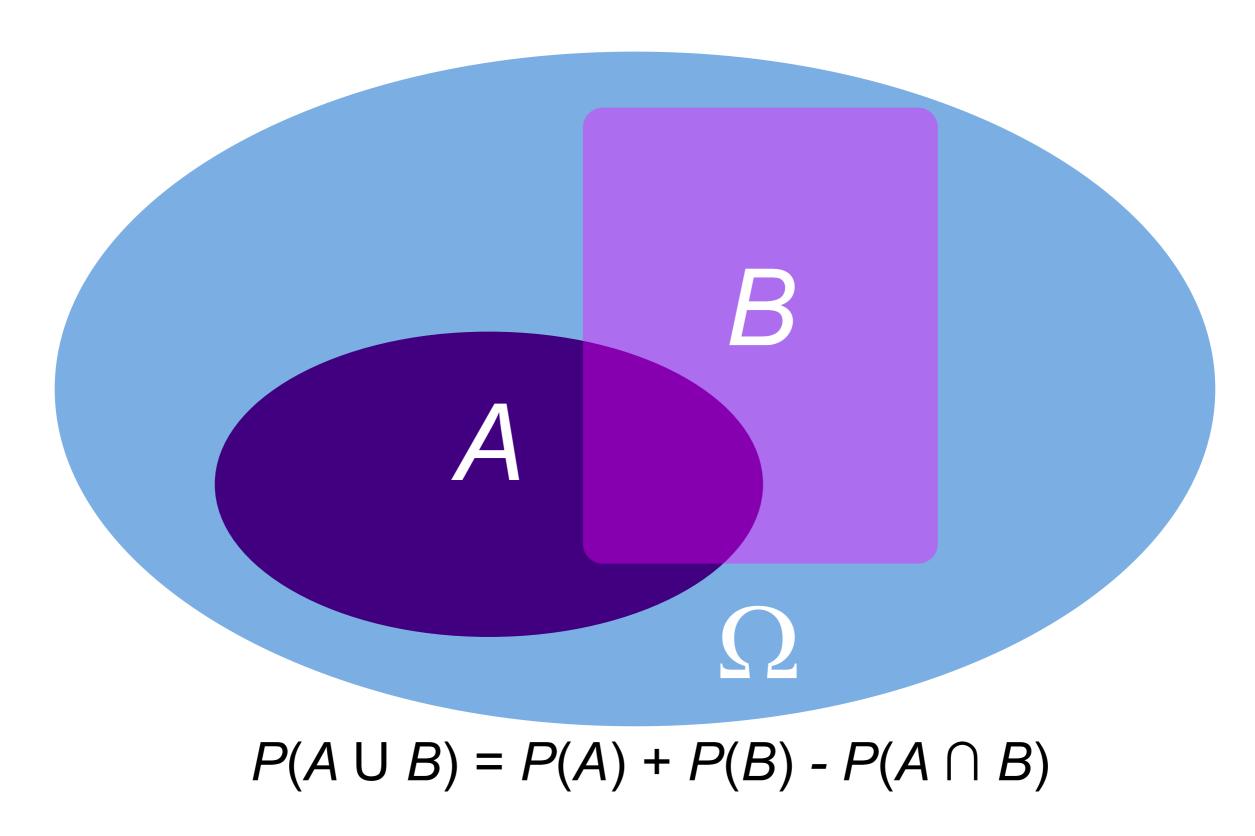
#### Consequences:

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

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

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

### 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):
- $X(\omega)$  = True if a randomly drawn person  $(\omega)$  from our class  $(\Omega)$  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
```

Bernoulli distribution: Ber(p)

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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.

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

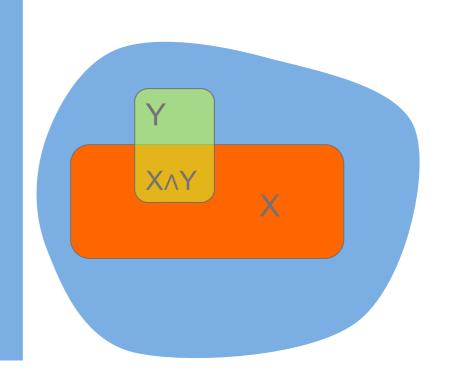
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$$P(\text{flu}|\text{headache}) = \frac{P(\text{flu, headache})}{P(\text{headache})} = \frac{1/80}{1/80 + 7/80}$$

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



# Independence

#### Independent random variables:

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

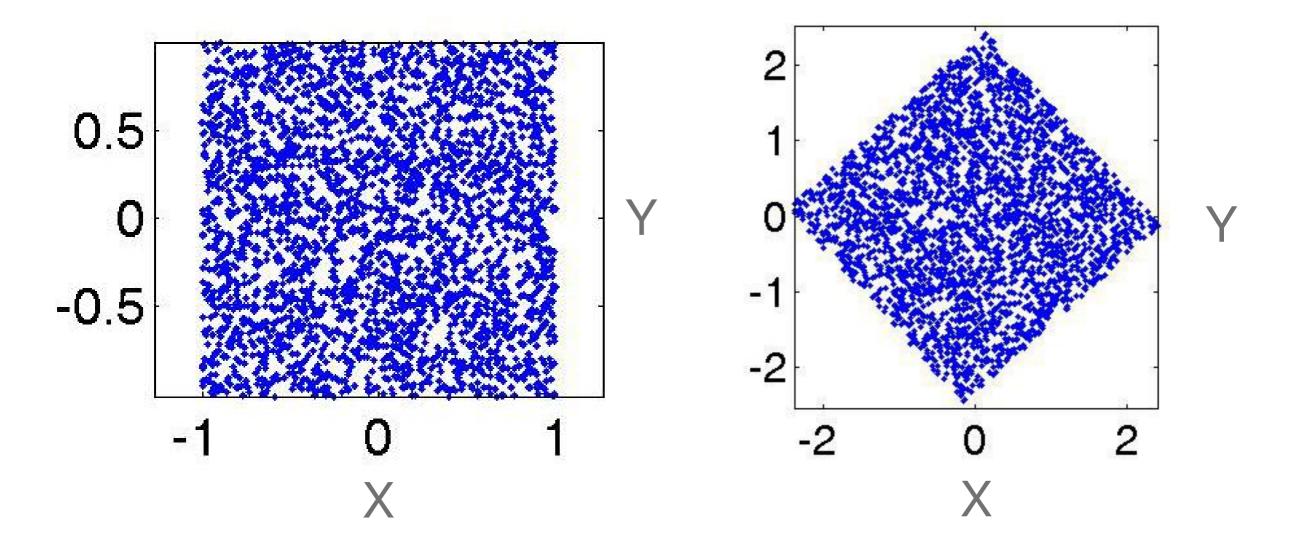
Y and X don't contain information about each other. Observing Y doesn't help predicting X. Observing X doesn't help predicting Y.

#### **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 skills given age

#### Stork deliver babies:

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

# Conditionally Independent

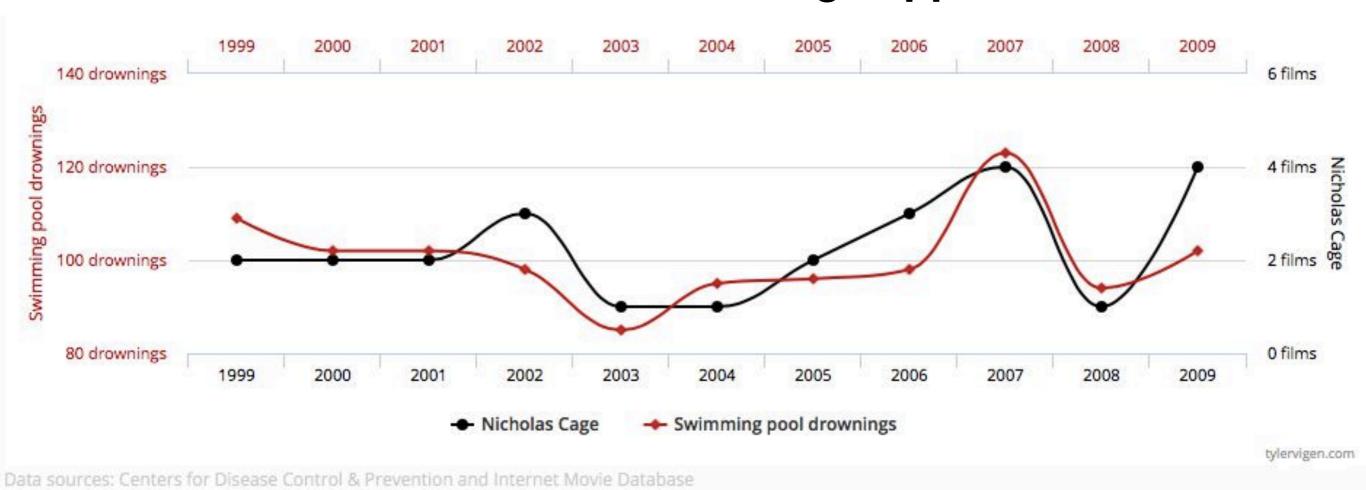
London taxi drivers: A survey has pointed out a positive and significant correlation between the number of accidents and wearing coats. They concluded that coats could hinder movements of drivers and be the cause of accidents. A new law was prepared to prohibit drivers from wearing coats when driving.

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

### Correlation ≠ Causation

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

#### Number of films Nicolas Cage appeared in



Correlation: 0.666004

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

#### 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** 



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)

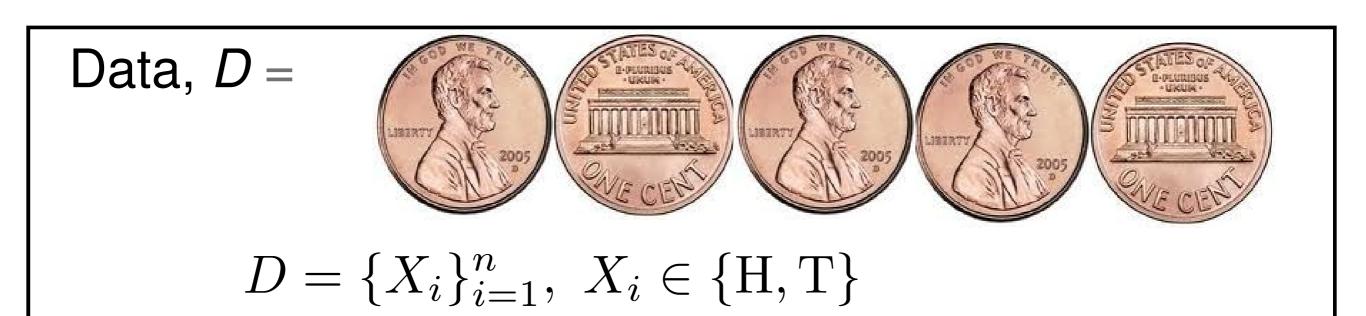


$$P(Heads) = \theta$$
,  $P(Tails) = 1-\theta$ 



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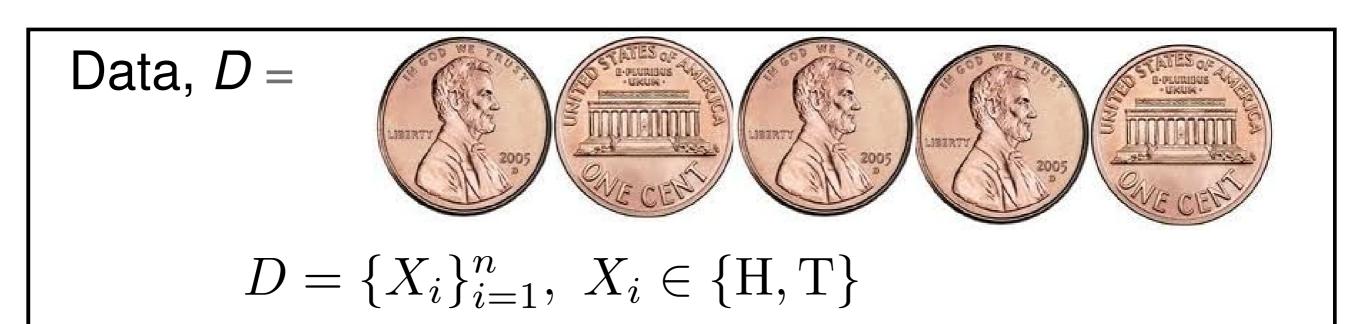
Flips are i.i.d.:



$$P(Heads) = \theta$$
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#### Flips are i.i.d.:

- Independent events
  - Identically distributed according to Bernoulli distribution



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MLE: Choose  $\theta$  that maximizes the probability of observed data

# slide by Barnabás Póczos & Alex Smo

# Maximum Likelihood Estimation

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

MLE: Choose θ that maximizes the probability of observed data

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

$$= \arg \max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$

independent draws

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

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$$egin{aligned} \widehat{ heta}_{MLE} &= rg \max_{ heta} P(D| heta) \ &= rg \max_{ heta} \prod_{i=1}^n P(X_i| heta) \quad & ext{independent draws} \ &= rg \max_{ heta} \prod_{i:X_i=H} heta \prod_{i:X_i=T} (1- heta) \quad & ext{identically distributed} \ &= rg \max_{ heta} heta^{lpha_H} (1- heta)^{lpha_T} \end{aligned}$$

$$egin{aligned} \widehat{ heta}_{MLE} &= rg \max_{m{ heta}} P(D|m{ heta}) \ &= rg \max_{m{ heta}} m{ heta}^{lpha_H} (1 - m{ heta})^{lpha_T} \ &= rg \max_{m{ heta}} m{ heta}^{lpha_H} (1 m{ heta})^{lpha_T} \ J(m{ heta})^{m{ heta}})^{lpha_T} \end{aligned}$$

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$$\frac{\partial J(\theta)}{\partial \theta} = \alpha_H \theta^{\alpha_H - 1} (1 - \theta)^{\alpha_T} - \alpha_T \theta^{\alpha_H} (1 - \theta)^{\alpha_T - 1} \Big|_{\theta = \hat{\theta}_{\text{MLE}}} = 0$$

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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???

#### 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:

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

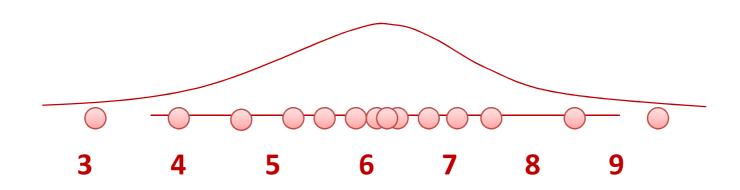
# Question (3)

#### 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)

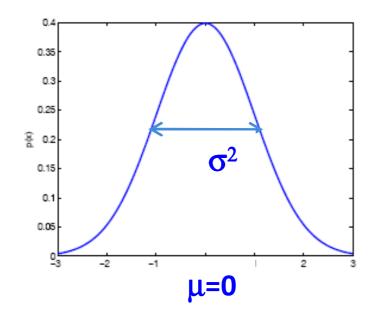
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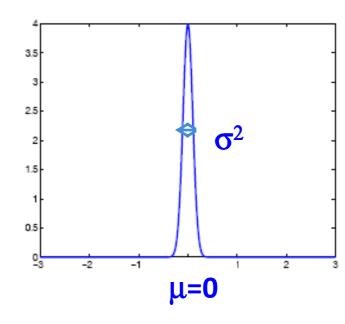
# What about continuous features?



#### 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

$$\widehat{ heta}_{MLE} = \arg\max_{ heta} P(D \mid heta)$$

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

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

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

$$J(\theta)$$

# 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:  $\hat{\sigma}_{unbiased}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \hat{\mu})^2$ 

# Next Class:

MAP estimation Naïve Bayes Classifier