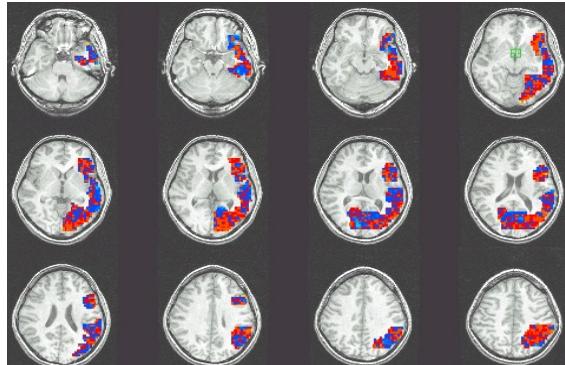


# Announcements

- Recitation on Friday Jan 28 – Convexity review
- QnA1 due TODAY
- HW1 to be released TODAY

# Recap – Bayes classifier



High Stress  
Moderate Stress  
Low Stress

$(X, Y)$  - random variables with joint distribution  $P_{XY}$

**Input feature vector,  $X$**

**Label,  $Y$**

If  $P_{XY}$  known, **Bayes classifier** – optimal for 0/1 loss

$$f(x) = \arg \max_{Y=y} P(Y = y | X = x)$$

$$= \arg \max_{Y=y} P(X = x | Y = y) P(Y = y)$$

Class conditional

Distribution of features

Class distribution

# Recap – Gaussian Bayes classifier

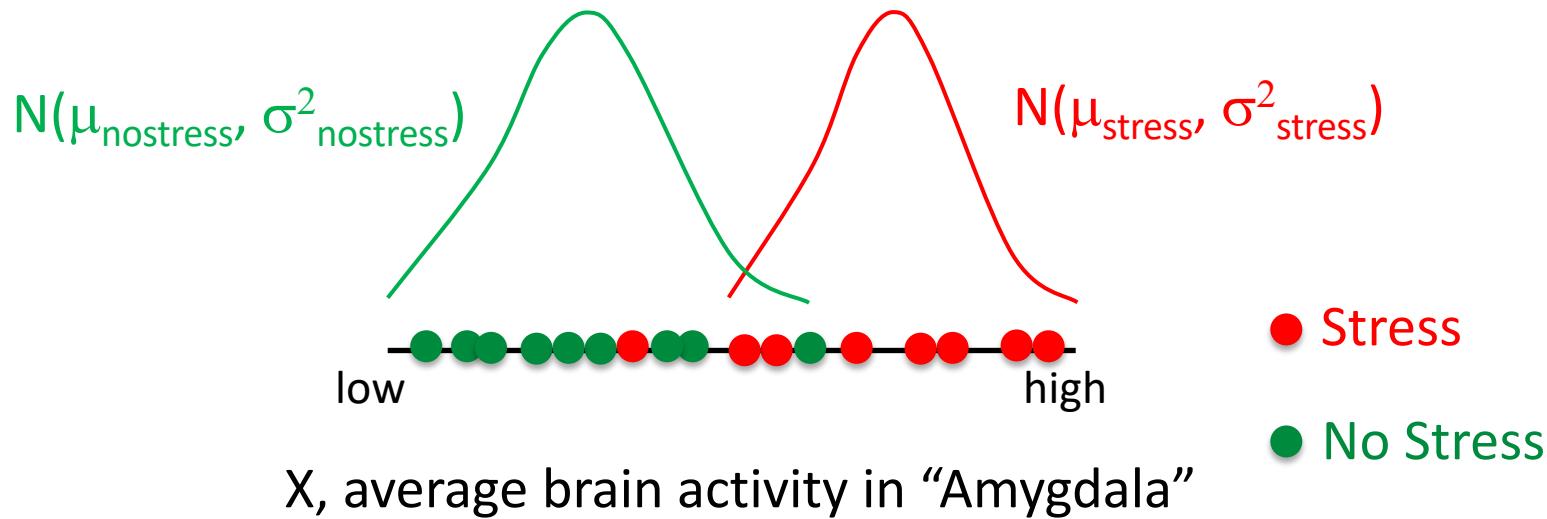
In practice  $P_{XY}$  unknown, use a distribution model to approximate

**Gaussian Bayes classifier** – assumes

Class distribution  $P(Y)$  is Bernoulli( $\theta$ )

[Categorical if multiple classes]

Class conditional distribution of features  $P(X|Y)$  is Gaussian



# d-dim Gaussian Bayes classifier

$$f(x) = \arg \max_{Y=y} P(X = x|Y = y)P(Y = y)$$

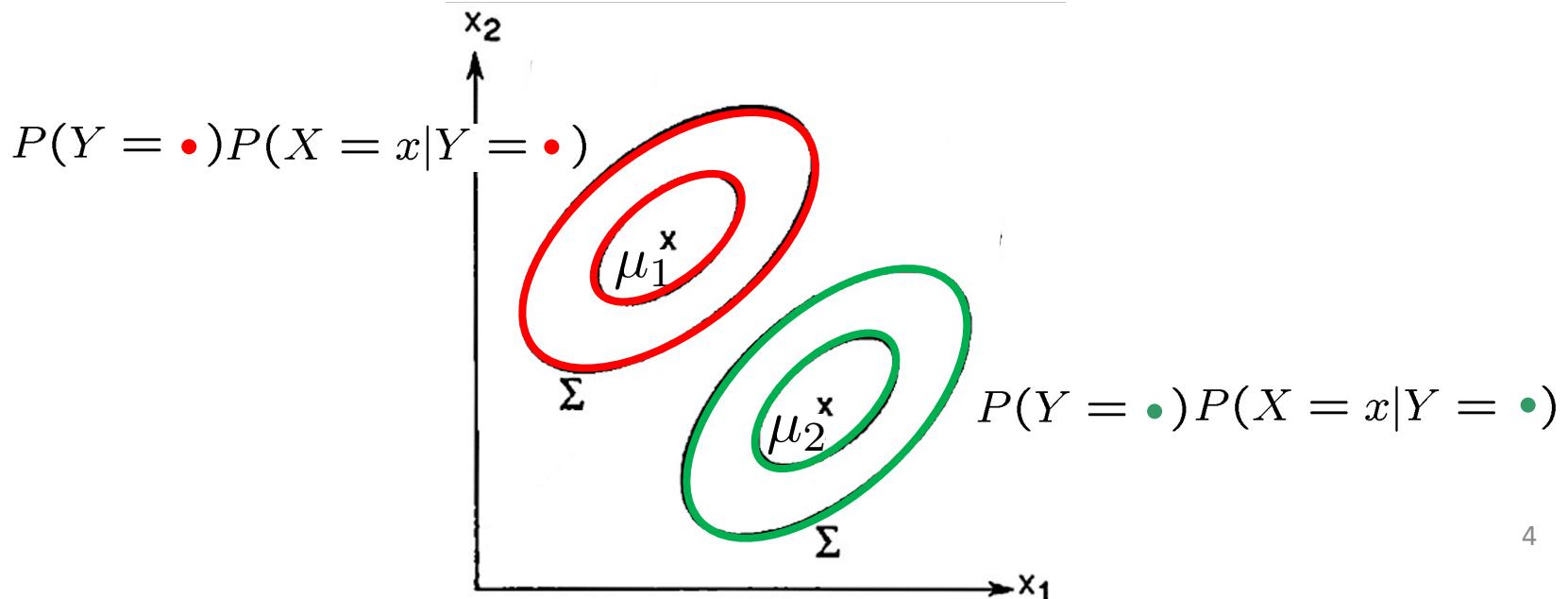
Learn parameters  $\theta, \mu_y, \Sigma_y$  from data

Class conditional  
Distribution of inputs

Class distribution

Gaussian( $\mu_y, \Sigma_y$ )

Bernoulli( $\theta$ )



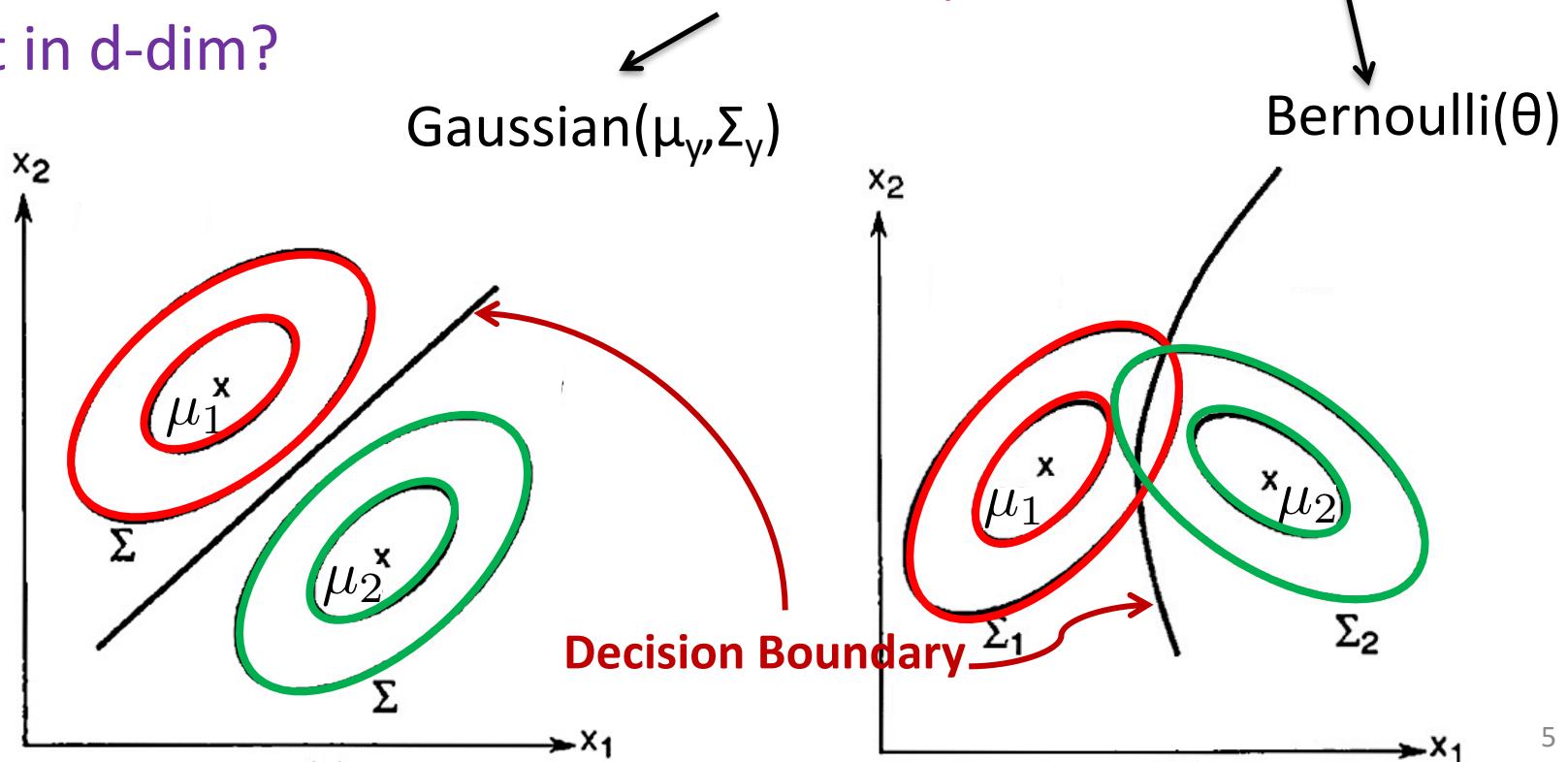
# d-dim Gaussian Bayes classifier

$$f(X) = \arg \max_{Y=y} P(X = x|Y = y)P(Y = y)$$

- What decision boundaries can we get in d-dim?

Class conditional  
Distribution of inputs

Class distribution



# Decision Boundary of Gaussian Bayes

- Decision boundary is set of points  $x: P(Y=1|X=x) = P(Y=0|X=x)$

Compute the ratio

$$1 = \frac{P(Y=1|X=x)}{P(Y=0|X=x)} = \frac{P(X=x|Y=1)P(Y=1)}{P(X=x|Y=0)P(Y=0)}$$

$$= \sqrt{\frac{|\Sigma_0|}{|\Sigma_1|}} \exp \left( -\frac{(x - \mu_1)^\top \Sigma_1^{-1} (x - \mu_1)}{2} + \frac{(x - \mu_0)^\top \Sigma_0^{-1} (x - \mu_0)}{2} \right) \frac{\theta}{1 - \theta}$$

In general, this implies a quadratic equation in  $x$ . But if  $\Sigma_1 = \Sigma_0$ , then quadratic part cancels out and decision boundary is linear.

# d-dim Gaussian Bayes classifier

$$f(x) = \arg \max_{Y=y} P(X = x|Y = y)P(Y = y)$$

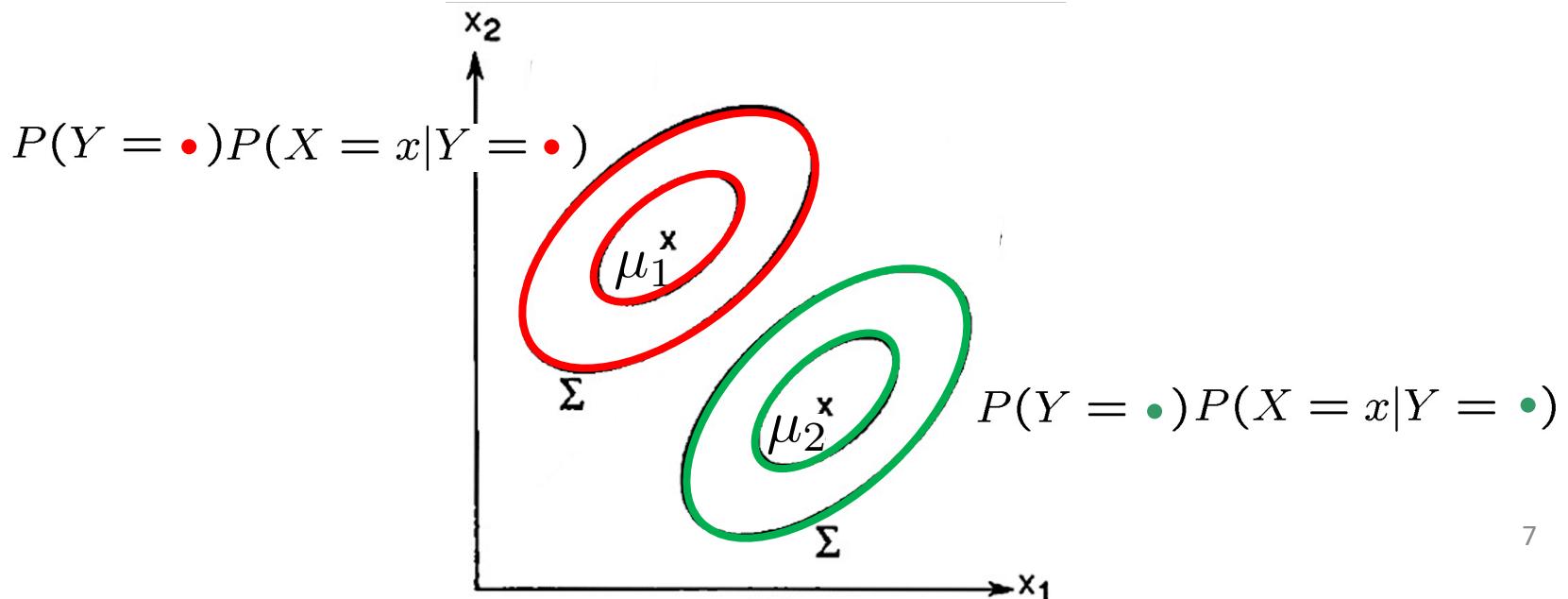
Learn parameters  $\theta, \mu_y, \Sigma_y$  from data

Class conditional  
Distribution of inputs

Class distribution

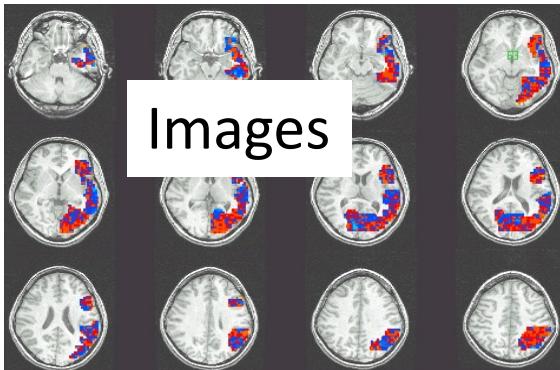
Gaussian( $\mu_y, \Sigma_y$ )

Bernoulli( $\theta$ )



# Notion of “Features aka Attributes”

**Input**  $X \in \mathcal{X}$



**Input**  $X \in \mathcal{X}$



# How to represent inputs mathematically?

- Image X = intensity/value at each pixel, fourier transform values, SIFT etc.
- Market information X = daily/monthly? price of share for past 10 years

# Notion of “Features aka Attributes”

Input  $X \in \mathcal{X}$



Document/Article

remember to wake up when class ends  
=   
wake ends to class remember up when

## How to represent inputs mathematically?

- Document vector  $X$  ➤ Ideas?
  - list of words (different length for each document)
  - frequency of words (length of each document = size of vocabulary), also known as **Bag-of-words** approach ➤ Why might this be limited?  
Misses out context!!
  - list of n-grams (n-tuples of words)

# Text classification

Raw input → Features → Model for input features



word1	5	$P(X=x   Y=y)$
word2	2	$= P(\text{word1} = 5, \text{word2} = 2,$
word3	10	$\text{word3} = 10, \dots   Y=y)$
word4	20	
word5	12	
word6	5	
word7	8	
word8	4	
.	.	
.	.	
.	.	

HW1!

# Glossary of Machine Learning

- Task
- Supervised learning
  - Classification
  - Regression
- Unsupervised learning
  - Learning distribution
  - Clustering
  - Dimensionality reduction/Embedding
- Input,  $X$
- Label,  $Y$
- Prediction,  $f(X)$
- Experience = Training data
- Test data
- Overfitting
- Generalization
- Performance measure/loss – 0/1, squared
- iid
- Class conditional distribution of inputs
- Bayes rule
- Bayes Optimal classifier
- Decision boundary
- Feature/Attribute

# Maximum Likelihood Estimation (MLE)

Aarti Singh

Machine Learning 10-315  
Jan 26, 2022



MACHINE LEARNING DEPARTMENT



# How to learn parameters from data?

## MLE

### (Discrete case)

# Learning parameters in distributions

$$P(Y = \text{Red}) = \theta$$

$$P(Y = \text{Green}) = 1 - \theta$$

Learning  $\theta$  is equivalent to learning probability of head in coin flip.

➤ How do you learn that?

Data =



Answer: 3/5

➤ Why??

# Bernoulli distribution

Data,  $D =$



- Parameter  $\theta$  :  $P(\text{Heads}) = \theta$ ,  $P(\text{Tails}) = 1-\theta$
- Flips are **i.i.d.**:
  - **Independent** events
  - **Identically distributed** according to Bernoulli distribution

Choose  $\theta$  that maximizes the probability of observed data  
aka Likelihood

# Maximum Likelihood Estimation (MLE)

Choose  $\theta$  that maximizes the probability of observed data (aka likelihood)

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

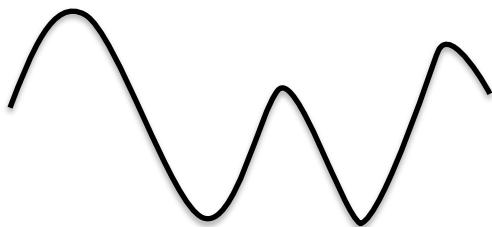
MLE of probability of head:

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T} = 3/5$$

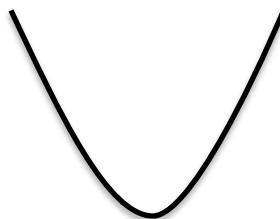
“Frequency of heads”

# Short detour - Optimization

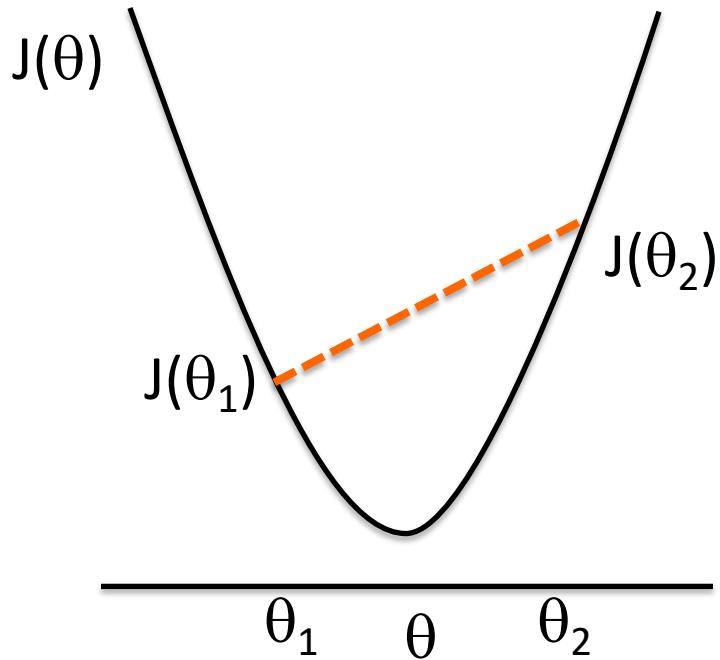
- Optimization objective  $J(\theta)$
- Minimum value  $J^* = \min_{\theta} J(\theta)$
- Minima (points at which minimum value is achieved) may not be unique



- If function is strictly convex, then minimum is unique

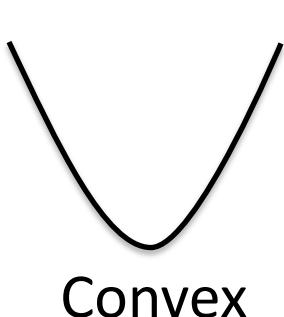


# Convex functions

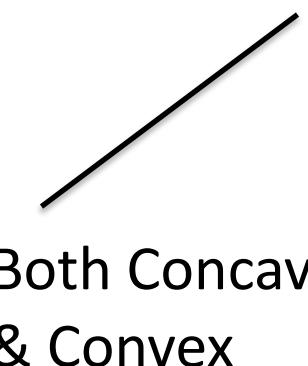


A function  $J(\theta)$  is called **convex** if the line joining two points  $J(\theta_1), J(\theta_2)$  on the function does not go below the function on the interval  $[\theta_1, \theta_2]$

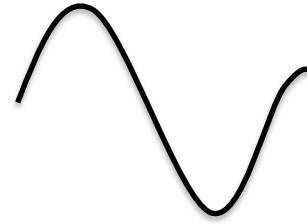
*(Strictly) Convex functions have a unique minimum!*



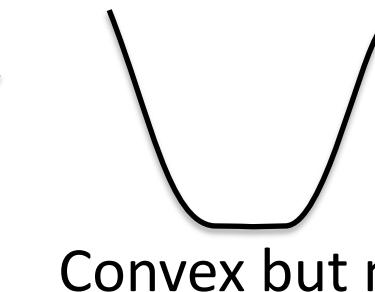
Convex



Both Concave & Convex



Neither



Convex but not strictly convex

# Optimizing convex (concave) functions

- Derivative of a function
- Derivative is zero at minimum of a convex function
- Second derivative is positive at minimum of a convex function

# Bernoulli MLE Derivation

$$\hat{\theta}_{MLE} = \arg \max_{\theta} P(D \mid \theta)$$

# Categorical distribution

Data,  $D$  = rolls of a dice



- $P(1) = p_1, P(2) = p_2, \dots, P(6) = p_6 \quad p_1 + \dots + p_6 = 1$
- Rolls are **i.i.d.:**
  - **Independent** events
  - **Identically distributed** according to Categorical( $\theta$ ) distribution where
$$\theta = \{p_1, p_2, \dots, p_6\}$$

Choose  $\theta$  that maximizes the probability of observed data  
aka “Likelihood”

# Maximum Likelihood Estimation (MLE)

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

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

MLE of probability of rolls:

$$\hat{\theta}_{MLE} = \hat{p}_{1,MLE}, \dots, \hat{p}_{6,MLE}$$

$$\hat{p}_{y,MLE} = \frac{\alpha_y}{\sum_y \alpha_y}$$

$\alpha_y$  ← Rolls that turn up y  
 $\sum_y \alpha_y$  ← Total number of rolls

“Frequency of roll y”

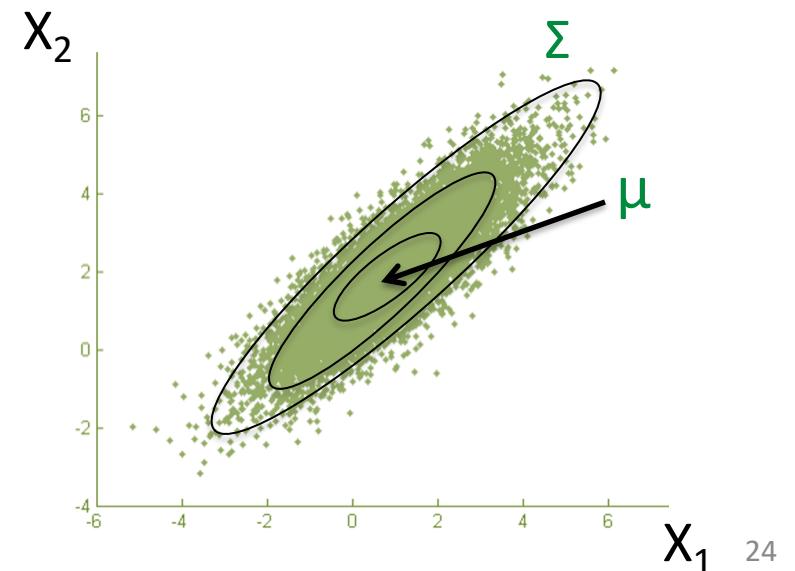
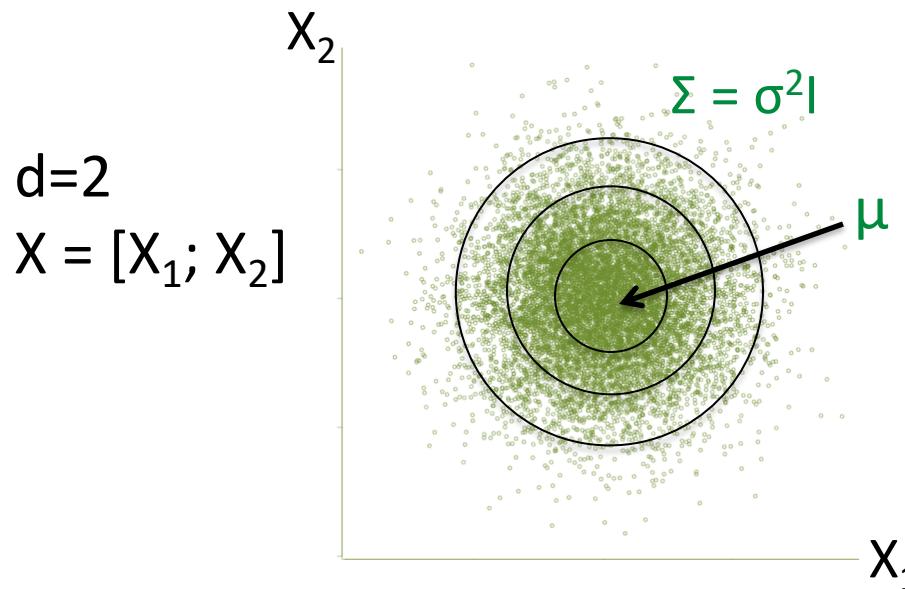
# How to learn parameters from data? MLE (Continuous case)

# d-dim Gaussian distribution

$X$  is Gaussian  $N(\mu, \Sigma)$

$\mu$  is d-dim vector,  $\Sigma$  is  $d \times d$  dim matrix

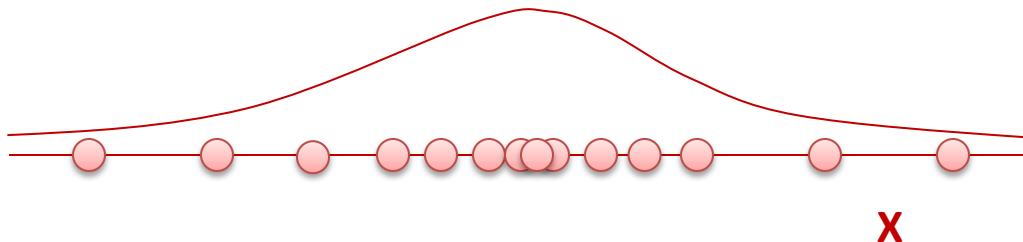
$$P(X = x | \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right),$$



# How to learn parameters from data? MLE (Continuous case)

# Gaussian distribution

Data,  $D =$



- Parameters:  $\mu$  – mean,  $\sigma^2$  - variance
- Data are **i.i.d.:**
  - **Independent** events
  - **Identically distributed** according to Gaussian distribution

# Maximum Likelihood Estimation (MLE)

Choose  $\theta = (\mu, \sigma^2)$  that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D \mid \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^n P(X_i \mid \theta) \quad \text{Independent draws}\end{aligned}$$

# Maximum Likelihood Estimation (MLE)

Choose  $\theta = (\mu, \sigma^2)$  that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D | \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^n P(X_i | \theta) \quad \text{Independent draws} \\ &= \arg \max_{\theta} \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(X_i - \mu)^2 / 2\sigma^2} \quad \text{Identically distributed}\end{aligned}$$

# Maximum Likelihood Estimation (MLE)

Choose  $\theta = (\mu, \sigma^2)$  that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D | \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^n P(X_i | \theta) \quad \text{Independent draws} \\ &= \arg \max_{\theta} \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(X_i - \mu)^2 / 2\sigma^2} \quad \text{Identically distributed} \\ &= \arg \max_{\theta=(\mu,\sigma^2)} \underbrace{\frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\sum_{i=1}^n (X_i - \mu)^2 / 2\sigma^2}}_{J(\theta)}\end{aligned}$$

# MLE for Gaussian mean

➤ Poll

$$P(D | \theta) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\sum_{i=1}^n (X_i - \mu)^2 / 2\sigma^2}$$

A.  $\max_{\mu} \sum_{i=1}^n (X_i - \mu)^2$

B.  $\min_{\mu} \sum_{i=1}^n (X_i - \mu)^2$

C.  $\max_{\mu} \mu^2 - 2\mu \sum_{i=1}^n X_i$

D.  $\max_{\mu} n\mu^2 - 2\mu \sum_{i=1}^n X_i$

# MLE for Gaussian mean and variance

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

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

Self exercise:

Derive MLE of variance?

d-dimensional versions?

MLE for uniform or  
exponential  
distribution?

More coming up in HW1