



NYC DATA SCIENCE  
**ACADEMY**

# Python Machine Learning Class 2: Classification Part I

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Data Science Bootcamp

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# Outline

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## ❖ Limitation of Linear Regression

- ❖ Logistic Regression
- ❖ Discriminant Analysis: Motivation
- ❖ Discriminant Analysis: Models
- ❖ Naive Bayes

# Classification Problems

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- ❖ *Categorical* (qualitative) variables: takes values in a finite set (usually unordered).
  - email: {spam, non-spam}
  - blood type: {A, B, AB, O}
  - tumor: {malignant, benign}
- ❖ *Classification*: given a feature (or a set of features), we want to predict categorical a output.
- ❖ Sometime people are also interested in estimating the probabilities that *an observation* belongs to each category.

## A Classification Example

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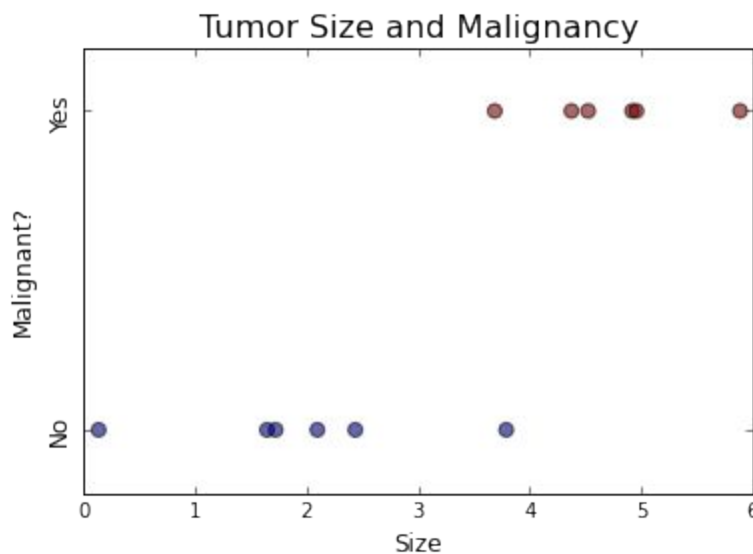
- ❖ Predict whether a tumor is malignant or benign based on the size
- ❖ The output is binary:
  - 0: benign
  - 1: malignant
- ❖ Here is a simulated data set:

	Size	Malignant
<b>0</b>	3.788628	0
<b>1</b>	2.436510	0
<b>2</b>	2.096497	0
<b>3</b>	0.136507	0
<b>4</b>	1.722612	0
<b>5</b>	1.645241	0

	Size	Malignant
<b>6</b>	4.917259	1
<b>7</b>	4.372999	1
<b>8</b>	4.956182	1
<b>9</b>	4.522782	1
<b>10</b>	3.686135	1
<b>11</b>	5.884622	1

## A Classification Example

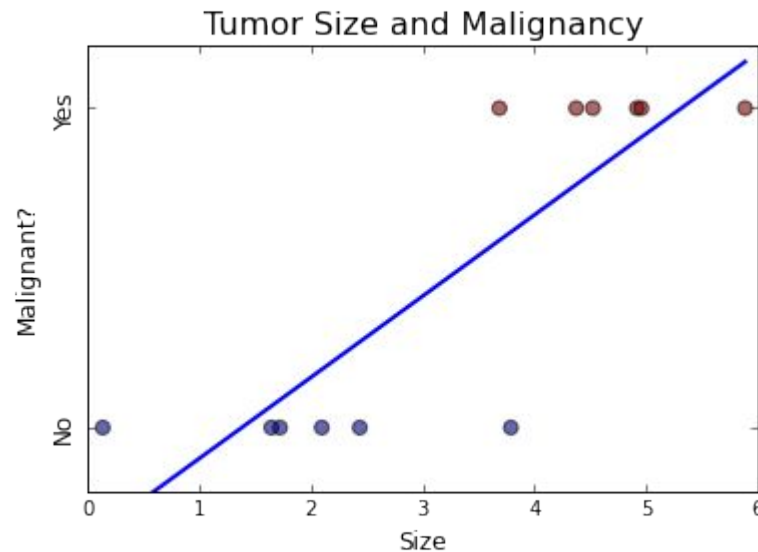
- ❖ By selecting the Size as feature and Malignant as output, we can visualize the data as:



- ❖ Question: can we use linear regression?

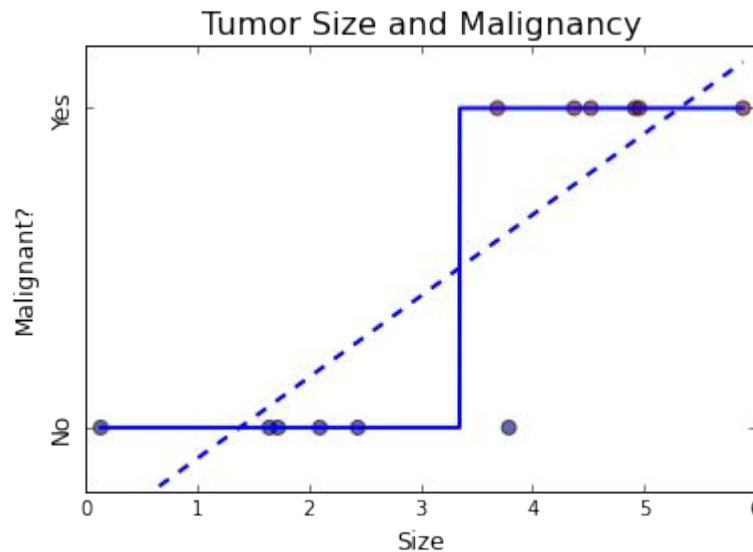
## Can We Use Linear Regression?

- ❖ Let's fit a linear regression model with the simulated tumor data:



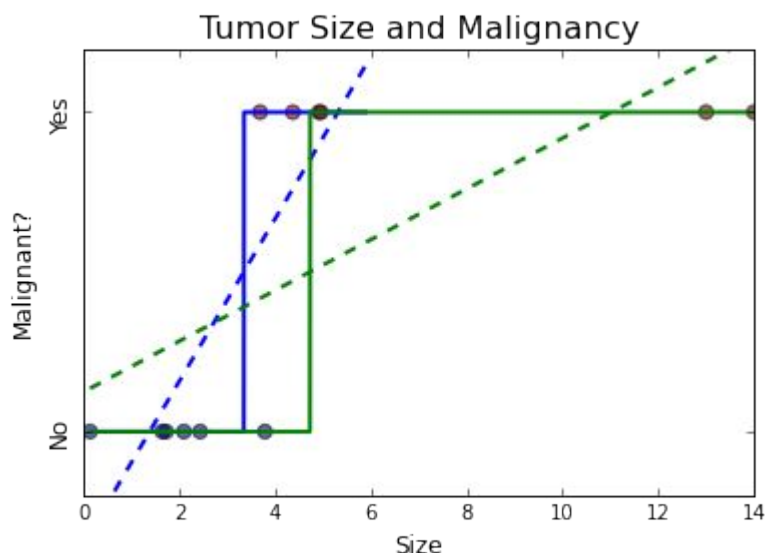
# Can We Use Linear Regression?

- ❖ We may then set a threshold
  - Predict 1 if  $\hat{y} \geq 0.5$
  - Predict 0 if  $\hat{y} < 0.5$
- ❖ The predicted values become binary:



## Issues with Linear Regression

- ❖ It looks like the binary prediction with linear regression is not so bad. However, we do have the following two problems:
  - the continuous output exceeds the interval  $[0, 1]$ . Therefore we cannot interpret it as [probability](#).
  - the prediction can be affected by outliers easily.





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- ❖ **Logistic Regression**
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- ❖ Discriminant Analysis: Models
- ❖ Naive Bayes

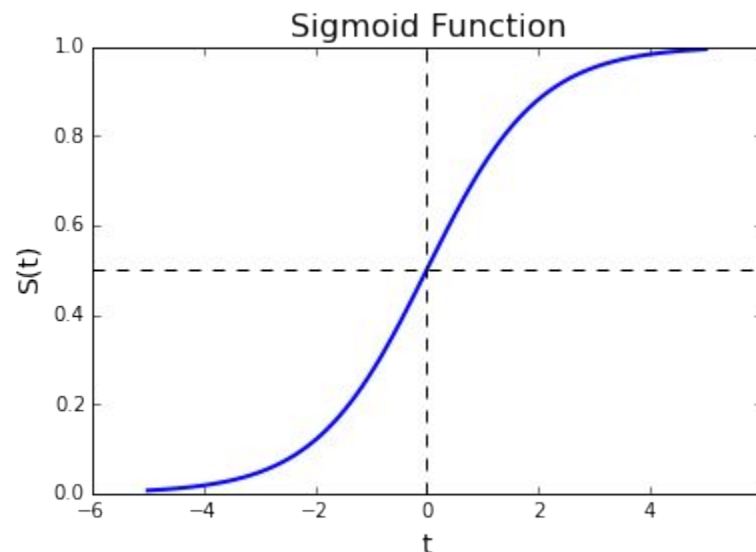
# Sigmoid Function

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- ❖ Sigmoid Function: a monotonically increasing function which maps a real value to a new value bounded between 0 and 1.

$$S(t) = \frac{e^t}{1 + e^t}$$

- ❖  $e = 2.718$  is a mathematical constant (Euler's number).



# Logistic Regression

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Logistic regression, despite its name, is a linear model for classification rather than regression.

- ❖ Idea: if we transform the linear function  $\beta_0 + \beta_1 X$  using the sigmoid function  $S(t)$ , then no matter what values  $\beta_0$ ,  $\beta_1$  or  $X$  take,  $y$  will always have values between 0 and 1.
- ❖ *Logistic Regression models* use this form to estimate the probability that  $y = 1$  given its size  $X$ :

$$Pr(Y = 1 | X = x) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

- ❖ So different  $\beta_0$  and  $\beta_1$  will give different estimations Pr.

## Maximum Likelihood

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- ❖ Let's write the likelihood function

$$p(x_i, \beta_0, \beta_1) = \text{Pr}(Y = 1 | X = x_i)$$

to describe the probability of observed outcomes to be 1 given  $X = x_i$ .

- ❖ Then, given an input  $X$  with  $n$  observations, the likelihood gives the probability of having the same label for each observations:

$$L(\beta_0, \beta_1) = \prod_{i, y_i=1} p(x_i, \beta_0, \beta_1) \prod_{i, y_i=0} (1 - p(x_i, \beta_0, \beta_1))$$

where the first product gives the probability of successfully predicting the “1”s and the second product is the probability of successfully predicting the “0”s in the training data.

## Maximum Likelihood

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- ❖ The likelihood function  $L(\beta_0, \beta_1)$  gives the probability of making the same prediction as the observed data.
- ❖ We want to pick  $\beta_0$  and  $\beta_1$  to maximize the likelihood  $L(\beta_0, \beta_1)$ , i.e., to maximize the “agreement” of the selected model with the observed data.

## Log-Likelihood

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- ❖ In practice it is often more convenient to work with the logarithm of the likelihood function, called the **log-likelihood**:

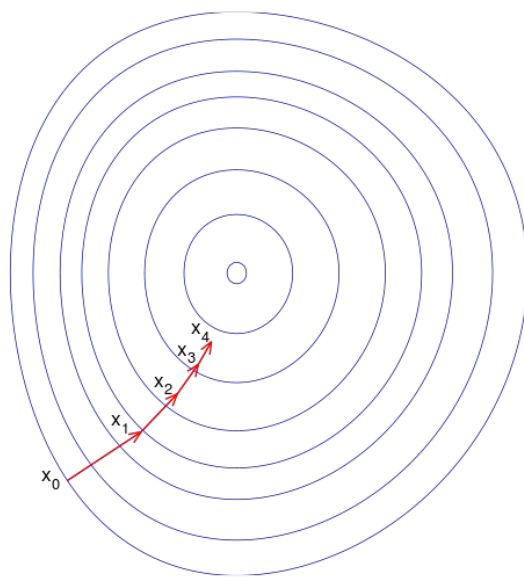
$$\begin{aligned}\log L(\beta_0, \beta_1) &= \sum_{i=1}^n \{y_i \log p(x_i, \beta_0, \beta_1) + (1 - y_i) \log(1 - p(x_i, \beta_0, \beta_1))\} \\ &= \sum_{i=1}^n \{y_i(\beta_0 + \beta_1 X) - \log(1 + e^{\beta_0 + \beta_1 X})\}\end{aligned}$$

- ❖ Logistic regression models are usually fit by maximum likelihood, i.e., to find  $\beta_0$  and  $\beta_1$  that maximize the function above.

# Gradient Descent

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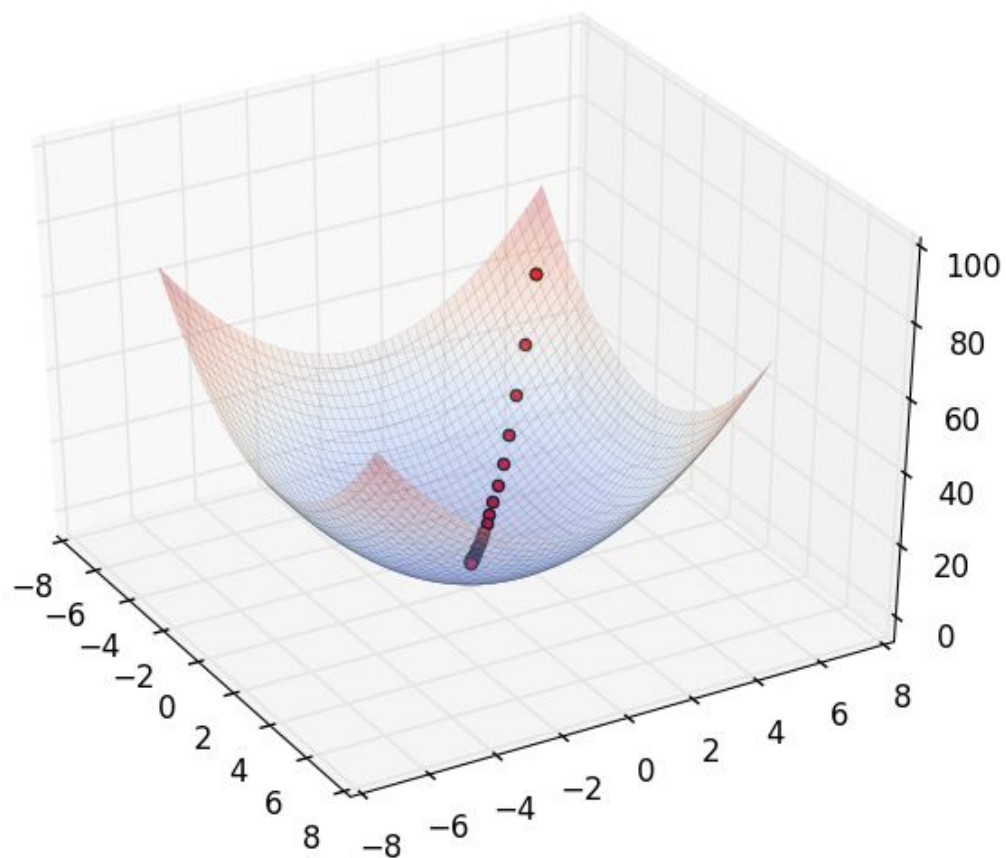
- ❖ To maximize the log-likelihood, most packages, including scikit-learn, use a numerical method called *gradient descent*, i.e., to find the maximum by search along a steepest path on the log-likelihood function.



source: [https://en.wikipedia.org/wiki/Gradient\\_descent](https://en.wikipedia.org/wiki/Gradient_descent)

# Gradient Descent

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## Making Predictions

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- ❖ After estimating the parameters, the likelihood function  $p(x, \beta_0, \beta_1)$  predicts the probability of output  $Y$  to be 1 given  $x$ . If we set a threshold, then we can predict binary outputs.
- ❖ Let's consider using tumor size to predict malignancy:
  - If the maximum likelihood gives  $Pr(Y=1 | X=x) = 0.2$ , then our prediction is 20% chance of tumor being malignant, or equivalently, 80% of change it's benign.
  - If we set the threshold, for example, to be 0.5, then we can predict the tumor is benign.

## Hands-on Session

- ❖ Please go to the "**Logistic Regression in Scikit-Learn**" in the lecture code.

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## Conditional Probability

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- ❖ Let  $Y$  be an event with probability  $P(Y) > 0$ , the *conditional probability* of observing  $X$  given that  $Y$  has occurred is defined as:

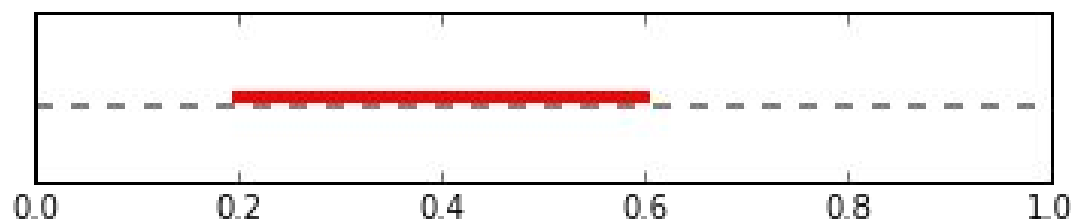
$$P(X|Y) = \frac{P(X, Y)}{P(Y)}$$

- $P(X, Y)$  refers to the probability that  $X$  and  $Y$  occur at the same time.
- $P(X|Y)$  is the probability of  $X$  after insuring  $Y$ 's occurrence.

## Conditional Probability

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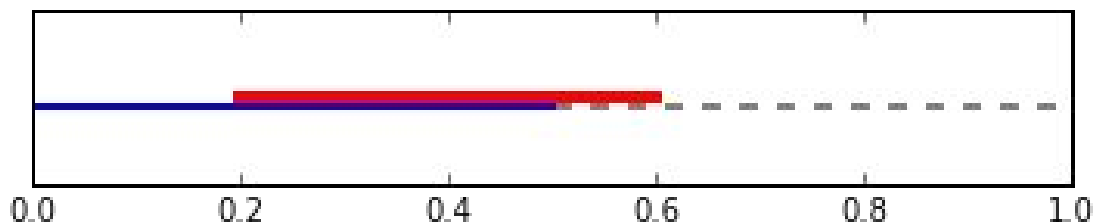
- ❖ How do we compute the probability of obtaining a number in the red region?



$$0.4 \div 1 = 0.4$$

## Conditional Probability

- ❖ How about the probability of obtaining a number in the red region when restricted in the blue region?



$$\frac{P(\text{red, blue})}{P(\text{blue})} = \frac{0.3}{0.5} = 0.6$$

## Conditional Probability

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❖ If  $X$  and  $Y$  are independent,  $P(X, Y) = P(X)P(Y)$ :

➤ Then the conditional probability is

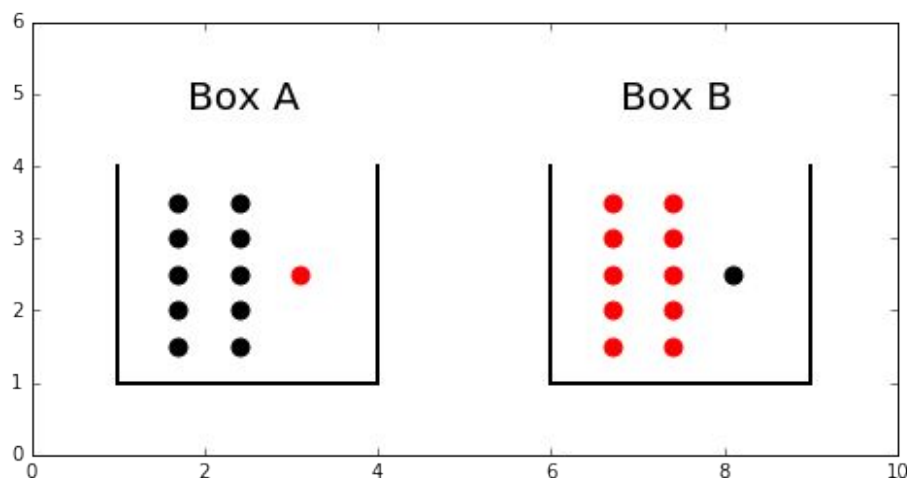
$$P(X|Y) = \frac{P(X, Y)}{P(Y)} = \frac{P(X)P(Y)}{P(Y)} = P(X)$$

➤ This implies that the occurrence of  $Y$  does not have any impact on  $X$ .

## Conditional Probability Example

Consider an experiment of picking balls of two colors, red and black, from two boxes labeled A and B.

1. There are 10 black balls and 1 red ball in box A, and 1 black ball and 10 red balls in box B.
2. We randomly choose a box and then pick a ball from it.
3. What is the probability that we get a red ball?





## Conditional Probability Example

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When choosing a box to pick, we have:

1.  $P(A) = P(B) = 0.5$ .
2. If we choose  $A$ ,  $P(\text{red}|A) = 1/11$ .
3. If we choose  $B$ ,  $P(\text{red}|B) = 10/11$ .

So the probability to get one red ball from either box A or box B is:

$$\begin{aligned} P(\text{red}) &= P(\text{red}|A) \cdot P(A) + P(\text{red}|B) \cdot P(B) \\ &= \frac{1}{11} \times 0.5 + \frac{10}{11} \times 0.5 \\ &= \frac{1}{2} \end{aligned}$$

# Bayes Theorem

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- ❖ Bayes theorem is named after Thomas Bayes.
- ❖ It describes the probability of an event, based on conditions that might be related to the event.
- ❖ Bayes theorem states:

$$\begin{aligned} Pr(Y|X) &= \frac{Pr(X|Y) \cdot Pr(Y)}{Pr(X)} \\ &= \frac{Pr(X|Y) \cdot Pr(Y)}{\sum_l Pr(X|Y = l) \cdot Pr(Y = l)} \end{aligned}$$

## Bayes Theorem Example

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- ❖ Consider the same experiment of picking balls from two boxes.
- ❖ If the ball we picked is red, then what is the probability that the ball was from box A?

According to Bayes' theorem, we have:

$$\begin{aligned} P(A|red) &= \frac{P(red|A) \cdot P(A)}{P(red)} \\ &= \frac{P(red|A) \cdot P(A)}{P(red|A)P(A) + P(red|B)P(B)} \\ &= \frac{\frac{1}{11} \times 0.5}{\left(\frac{1}{11} \times 0.5 + \frac{10}{11} \times 0.5\right)} \\ &= \frac{1}{11} \end{aligned}$$

## Bayes Theorem Example

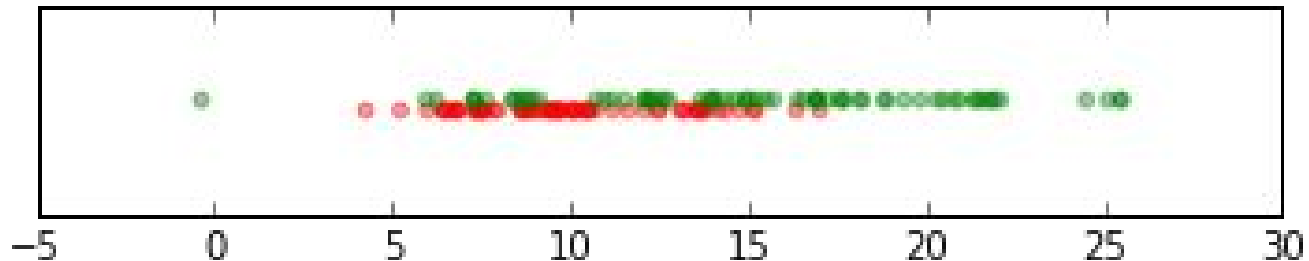
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- ❖ How does this relate to our classification problem? Consider from the **training set** we realize that for a red ball:
  - the probability that the red ball was from box A is  $1/11$
  - and the probability that the red ball was from box B is  $10/11$
- ❖ Next time if we get a red ball, shouldn't we be more confident that the ball was from box B?

# Discriminant Analysis

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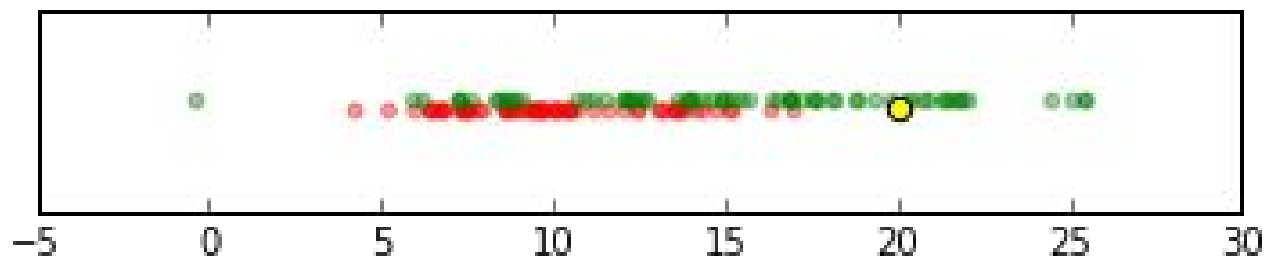
- ❖ *Discriminant analysis* is a statistical analysis technique which finds a set of prediction equations based on independent variables that are used to classify observations into classes.
- ❖ **Motivation:** To be more precisely, let's consider binary classification based on a numerical feature.



## Discriminant Analysis

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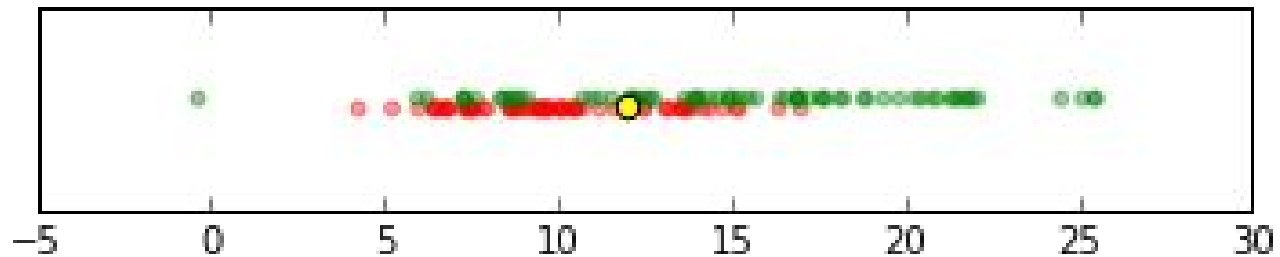
- ❖ If we found a new observation, which class do you think it belongs to?



## Discriminant Analysis

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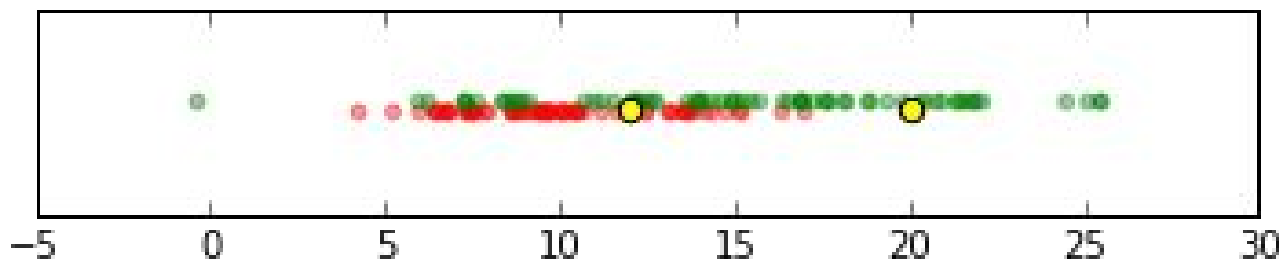
❖ What about this one?



# Discriminant Analysis

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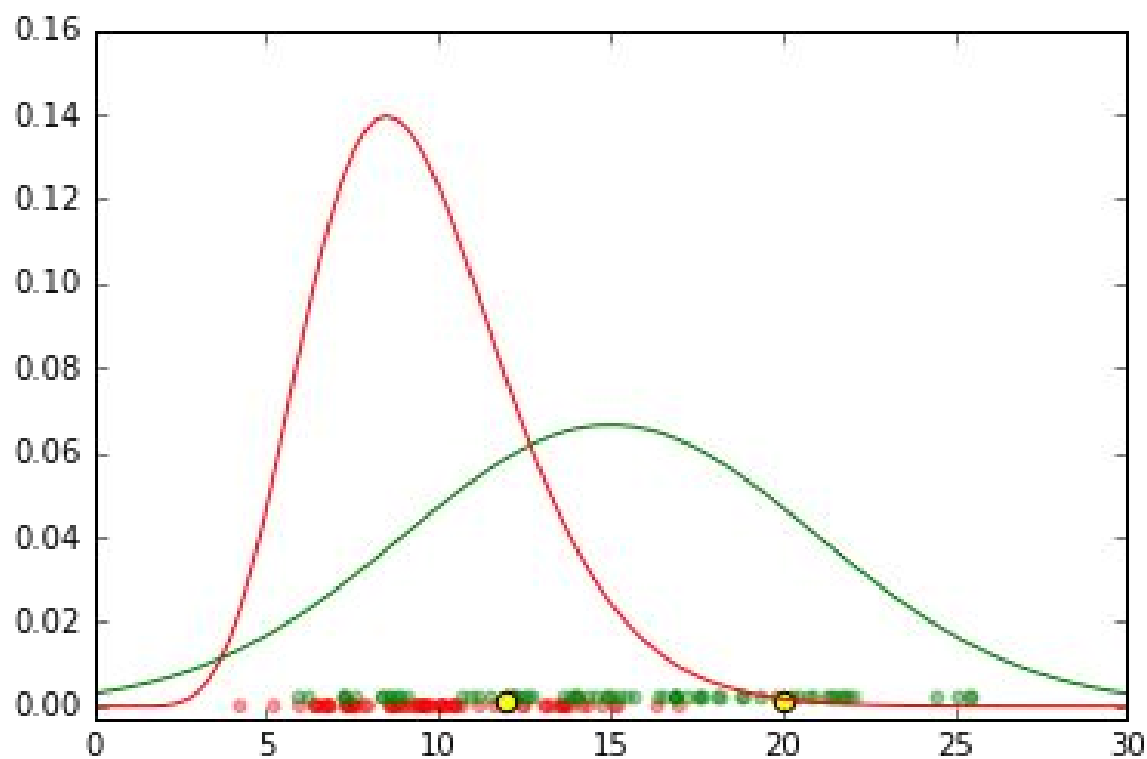
- ❖ What makes us feel differently?
  - If there is some other information tacitly guided us to the conclusion, can we somehow name it? Visualize it?





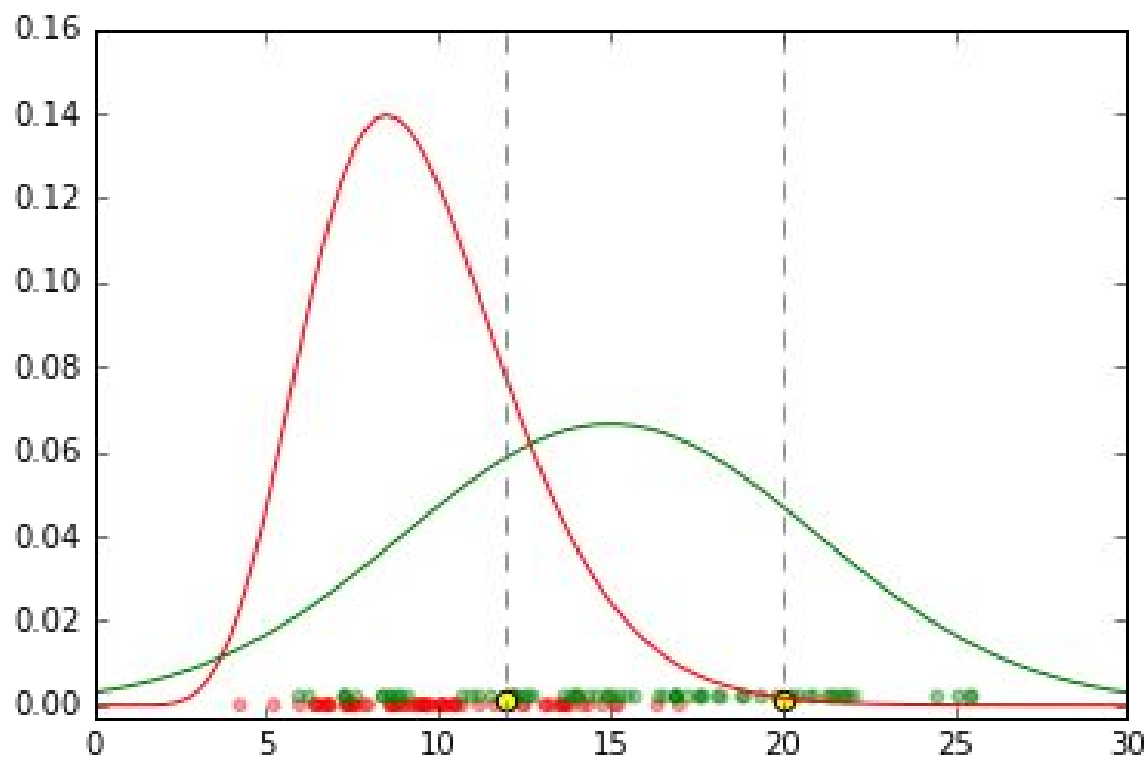
# Discriminant Analysis

- ❖ How about **density plot** for each class?



## Discriminant Analysis

- ❖ What happens to the density plots at the two yellow observations?



## Discriminant Analysis

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- ❖ Note the goal of classification is to compute

$$P(Y = k \mid X = x) \text{ for each class } k$$

- ❖ But we just found that

$$p(X = x \mid Y = k) \text{ for each class } k$$

Is helpful! How do we relate the two kinds of conditional probability?

# Discriminant Analysis and Bayes Theorem

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- ❖ Bayes theorem comes into play because we want to relate the two conditional probabilities above.

$$P(Y = k \mid X = x) = \frac{p(X = x \mid Y = k)P(Y = k)}{\sum_l p(X = x \mid Y = l)P(Y = l)}$$

- ❖ **Questions:**

- How do we model  $P(Y = k)$  (this is called the **prior probability** for class  $k$ )?
- How do we model  $p(X = x \mid Y = k)$ ?

# Discriminant Analysis and Bayes Theorem

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## ❖ Answers:

➤  $P(Y = k)$  is simply  $\frac{n_k}{n}$ .

Where:

- $n_k$  = the number of observations in class  $k$ .
  - $n$  = the total count of observations.
- Modeling  $p(X = x \mid Y = k)$  is nontrivial. Different models result in different classifiers as we will see.

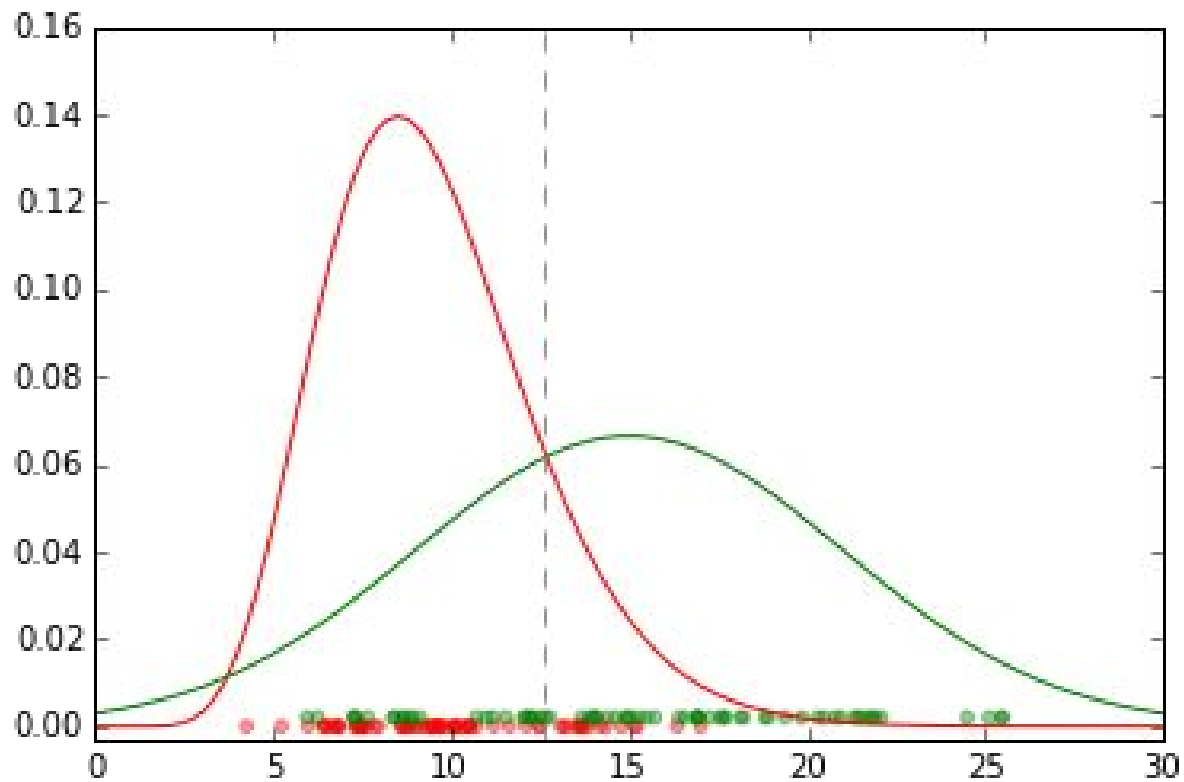
# Bayes Classifier

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- ❖ Now that we can predict the probability of belonging to a particular class, we can then classify the observation to the class with the highest probability.
  - This is known as **Bayes classifier**. It minimises the probability of misclassification.
  - The boundary of classification is simply where the probability of different classes happen to be the same.

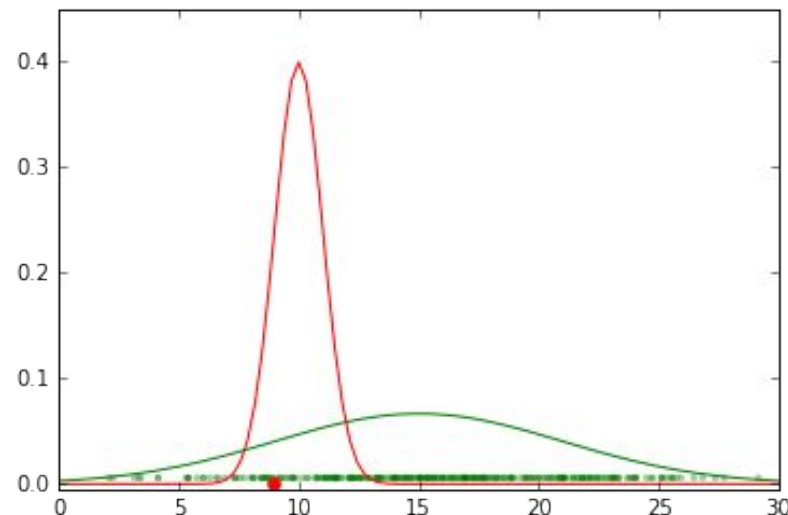
# Bayes Classifier

❖ So is this how we classify?



# Bayes Classifier

- ❖ **Observation:** There are prior probabilities in discriminant analysis, but the boundary above did **NOT** consider them.
- To emphasize the effect of the density within each class, we intentionally created two classes with the **same size**. When the sizes are different, **missing the prior would cause a big trouble**.
- Below is an extreme case:





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## ❖ Limitation of Linear Regression

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## ❖ Discriminant Analysis: Models

- ❖ Naive Bayes

## Discriminant Analysis: Models

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- ❖ To build a Bayes classifier, the only thing we miss is

$$p(X = x \mid Y = k)$$

- ❖ Since this is a continuous distribution, the **Gaussian** distribution is widely used to model it. Different kinds of Gaussian distribution result in different kind of classifiers. The following three are most common:
  - **Linear Discriminant Analysis (LDA)**
  - **Quadratic Discriminant Analysis (QDA)**
  - **Gaussian Naive Bayes** (This is the same as QDA in a one dimensional case)

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# Outline

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- One Dimensional Cases

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## One Dimensional Cases

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- ❖ When we have only one feature, we use one dimensional Gaussian distribution.

$$N(\mu, \sigma)(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x - \mu}{\sigma}\right)^2\right]$$

- Note that it is sufficient to specify the **mean** and the **standard deviation** to specify a Gaussian distribution.

## One Dimensional Cases

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- ❖ We always allow **different means** among different classes, but....

## Linear Discriminant Analysis

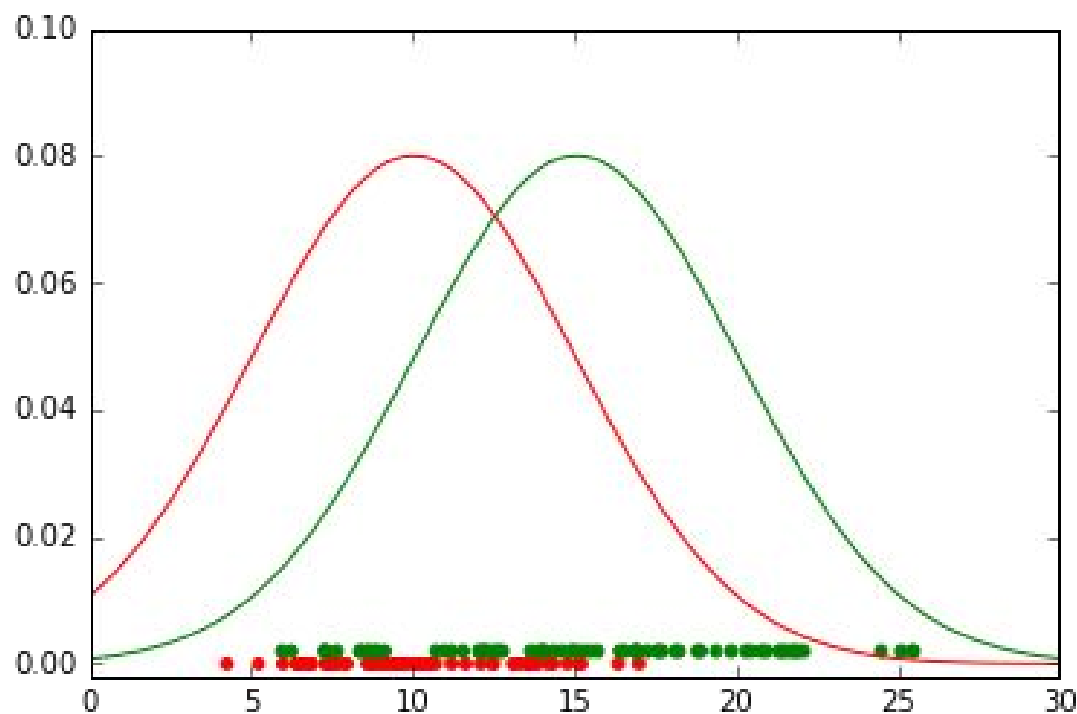
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- ❖ For LDA, we assume that the standard deviation is the **same** for every class. In one dimensional case, this means that the distribution for each class  $k$  is:

$$p(X = x \mid Y = k) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_k}{\sigma}\right)^2\right]$$

# Linear Discriminant Analysis

- ❖ With visualization, this means the **width** of the distribution for every class is unchanged.



## Linear Discriminant Analysis

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❖ **Question:** Now we know that with LDA the distribution for each class  $k$  is:

$$p(X = x \mid Y = k) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_k}{\sigma}\right)^2\right]$$

➤ How do we decide  $\mu_k$  and  $\sigma$ ?



# Linear Discriminant Analysis

❖ **Answer:**

$$\begin{aligned}\hat{\mu}_k &= \frac{1}{n_k} \sum_{i; y_i=k} x_i \\ \hat{\sigma}^2 &= \frac{1}{n - K} \sum_{k=1}^K \sum_{i; y_i=k} (x_i - \hat{\mu}_k)^2 \\ &= \sum_{k=1}^K \frac{n_k - 1}{n - K} \cdot \hat{\sigma}_k^2\end{aligned}$$

where

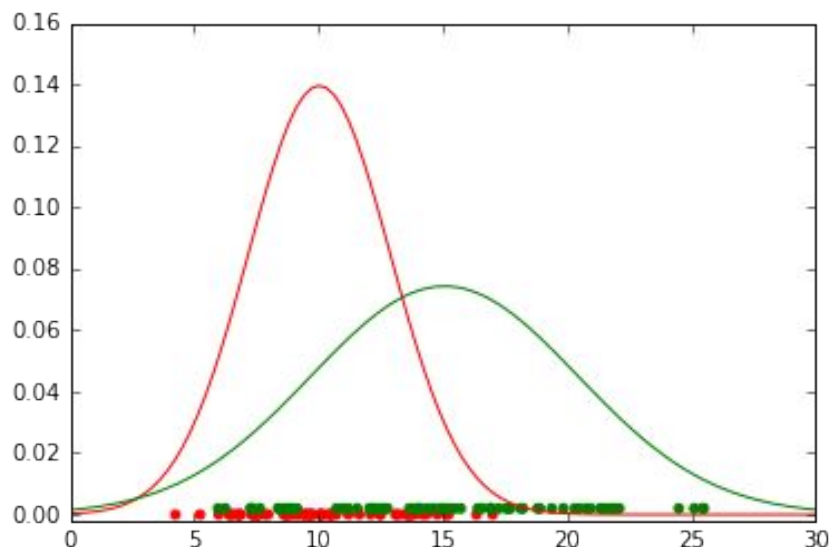
➤ K is the total number of classes.

➤  $\hat{\sigma}_k^2 = \frac{1}{n_k - 1} \sum_{i; y_i=k} (x_i - \hat{\mu}_k)^2$  is the sample variance of class k.

## Quadratic Discriminant Analysis

- ❖ For QDA, the standard deviation can vary among the classes. In one dimensional case, this means the width of the distribution for every class can be different. Therefore:

$$p(X = x \mid Y = k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_k}{\sigma_k}\right)^2\right]$$



## Quadratic Discriminant Analysis

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❖ **Question:** Now we know that with LDA the distribution for each class  $k$  is:

$$p(X = x \mid Y = k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_k}{\sigma_k}\right)^2\right]$$

➤ How do we estimate  $\hat{\mu}_k$  and  $\hat{\sigma}_k$ ?

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  - One Dimensional Cases

  - Higher Dimensional Cases

- ❖ Naive Bayes

## Higher Dimensional Cases

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- ❖ We start with the discussion on higher dimensional Gaussian distribution. This is essentially the only difference in higher dimensional discriminant analysis.

## Higher Dimensional Gaussian Distribution

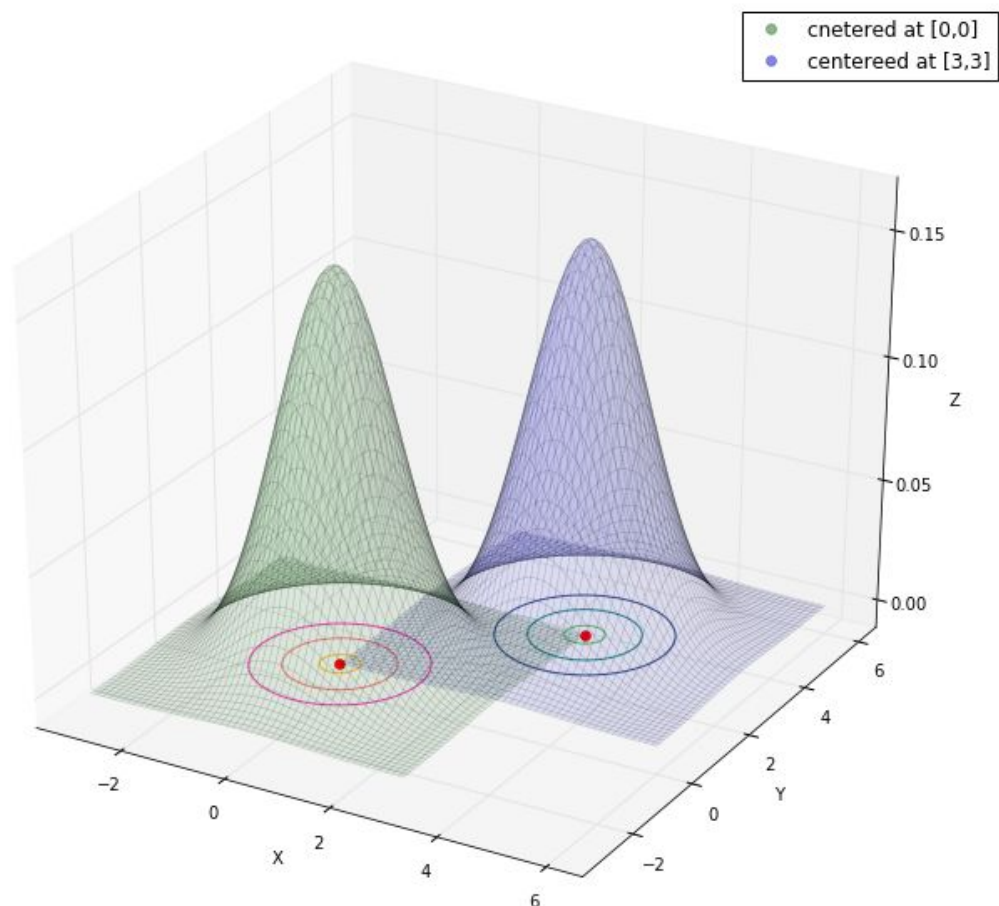
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- ❖ We still need only "two" parameters to specify higher dimensional Gaussian distribution: the **mean** and the **covariance**. However, for a  $p$  dimensional case (with  $p$  features):
  - the mean is a  $p$ -dimensional vector.
  - the covariance is a  $p \times p$  matrix.
- ❖ The distribution becomes:

$$N(\mu, \Sigma)(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right]$$

# Higher Dimensional Gaussian Distribution

- ◆ **mean:** The mean still decides where the "bell" centered at.



## Higher Dimensional Gaussian Distribution

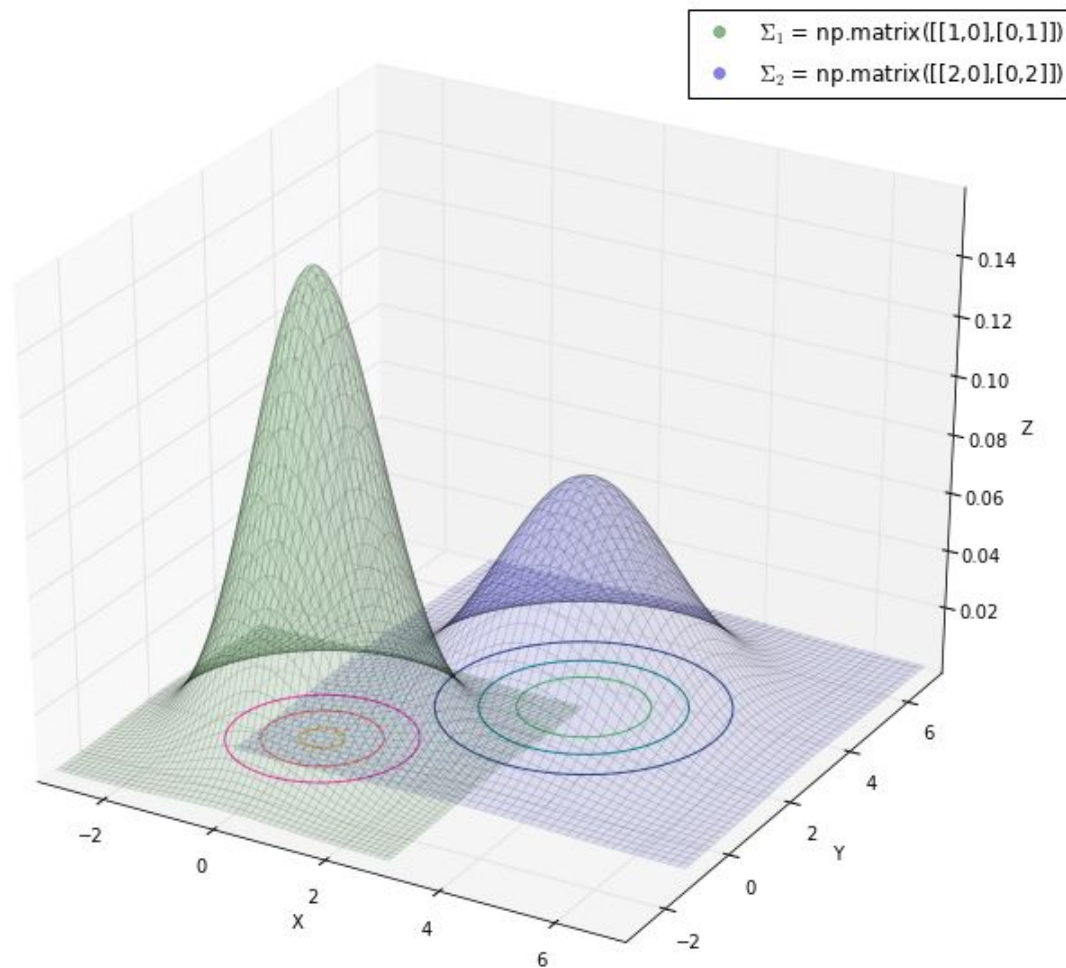
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- ❖ **Covariance Matrix:** The covariance matrix is a  $p \times p$  matrix. The covariance matrix, one of whose special cases is the square of standard deviation in one dimensional space, decide the **shape** of the "bell". However, the shape means more than just the width in a higher dimensional space.
- ❖ **Width:** Let's compare two Gaussian distribution with different covariance matrices in a two dimensional space.

$$\Sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ and } \Sigma_2 = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$



# Higher Dimensional Gaussian Distribution



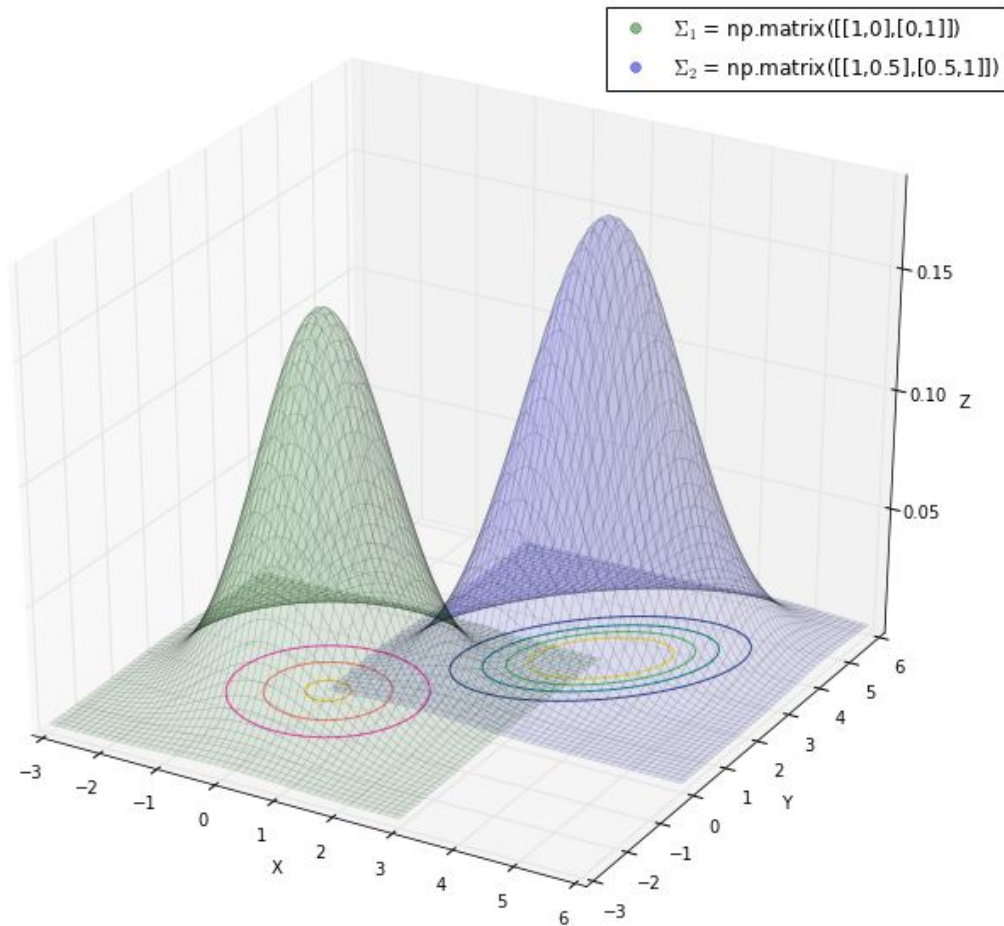
## Higher Dimensional Gaussian Distribution

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- ❖ **Correlation:** Let's compare two Gaussian distribution with different covariance matrices in a two dimensional space.

$$\Sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ and } \Sigma_2 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

# Higher Dimensional Gaussian Distribution



## Models in Higher Dimension

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- ❖ Recall what we have learned so far:
  - The purpose is to classify based on numerical features, so we want to compute the probability of class  $k$  under the condition that  $X = x$ :

$$P(Y = k \mid X = x)$$

- By Bayes theorem we can switch the condition as below:

$$P(Y = k \mid X = x) = \frac{p(X = x \mid Y = k)P(Y = k)}{\sum_l p(X = x \mid Y = l)P(Y = l)}$$

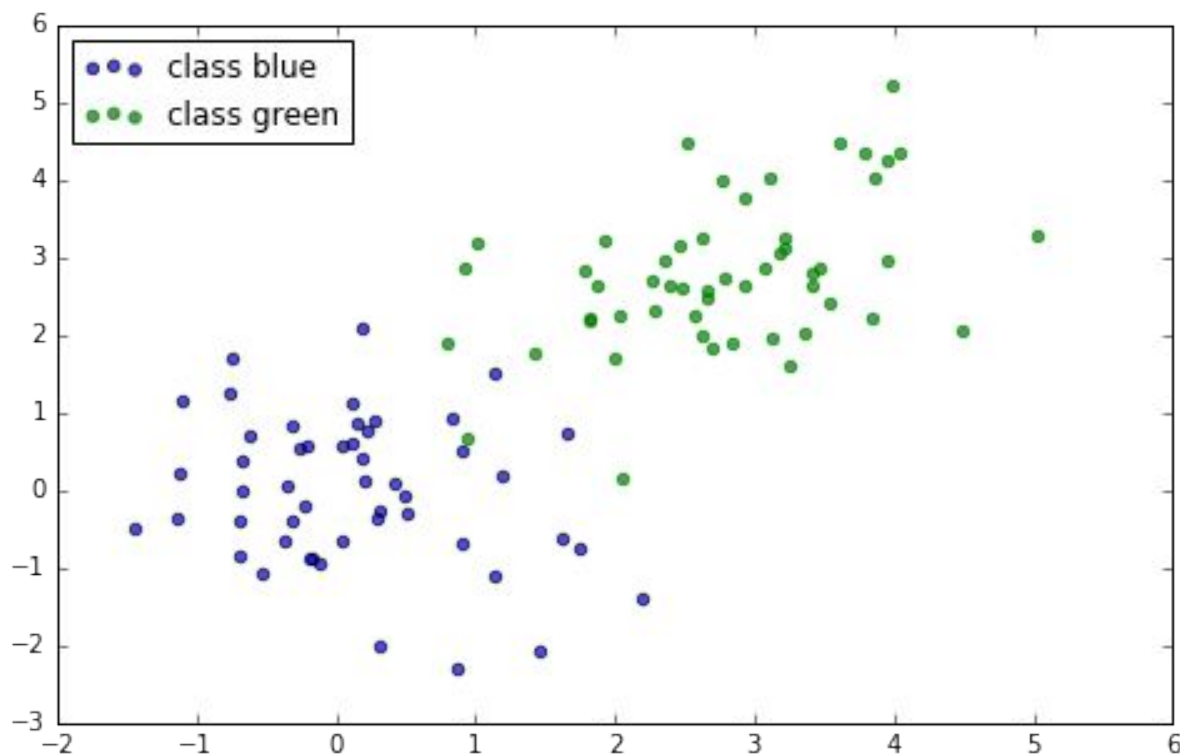
## Models in Higher Dimension

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- ❖ So we only need to decide:
  - prior probability.
  - distribution of the feature in each class.
- ❖ While estimating **prior** is easy; estimating the distribution in each class is hard.

## Models in Higher Dimension

- ❖ To illustrate the difference, let's consider the two-dimensional sample below:



## Models in Higher Dimension: QDA

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- ❖ We start with QDA. For this particular example, we need to compute:

$$p(X = x \mid Y = b) = \frac{1}{(2\pi)^{|\Sigma_b|^{1/2}}} \exp\left[-\frac{1}{2}(x - \mu_b)^T \Sigma_b^{-1}(x - \mu_b)\right]$$

and

$$p(X = x \mid Y = g) = \frac{1}{(2\pi)^{|\Sigma_g|^{1/2}}} \exp\left[-\frac{1}{2}(x - \mu_g)^T \Sigma_g^{-1}(x - \mu_g)\right]$$

## Models in Higher Dimension: QDA

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- ❖ With the training data:

$$\text{class blue} = \begin{bmatrix} (x_1^b, y_1^b) \\ (x_2^b, y_2^b) \\ \vdots \\ (x_{50}^b, y_{50}^b) \end{bmatrix} \quad \text{and} \quad \text{class green} = \begin{bmatrix} (x_1^g, y_1^g) \\ (x_2^g, y_2^g) \\ \vdots \\ (x_{53}^g, y_{53}^g) \end{bmatrix}$$

- ❖ How do we compute  $\hat{\mu}_b$  and  $\hat{\mu}_g$ ?



## Models in Higher Dimension: QDA

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- ❖ The covariance matrices are given by:

$$\hat{\Sigma}_b = \begin{bmatrix} V_x^b & cov_{x,y}^b \\ cov_{y,x}^b & V_y^b \end{bmatrix}$$

What do the parameters in the matrix mean? How do we compute these parameters?

- ❖ What about

$$\hat{\Sigma}_g = \begin{bmatrix} V_x^g & cov_{x,y}^g \\ cov_{y,x}^g & V_y^g \end{bmatrix}$$

## Models in Higher Dimension: LDA

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- ❖ We turn to LDA. We need to compute, for each  $k$ :

$$p(X = x \mid Y = k) = \frac{1}{(2\pi)^{|\Sigma|^{1/2}}} \exp\left[-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)\right]$$

- ❖ **Estimation**

- We estimate the mean in the same way.
- We have

$$\hat{\Sigma}^2 = \sum_{k=b,g} \frac{n_k - 1}{n - K} \cdot \hat{\Sigma}_k^2$$

## Models in Higher Dimension: GNB

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- ❖ For GNB, while the mean can be estimated in the same way, we need to estimate the covariance matrix for each  $k$ :

$$p(X = x \mid Y = k) = \frac{1}{(2\pi)^{|\Sigma|^{1/2}}} \exp\left[-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)\right]$$

- ❖ We still have

$$\hat{\Sigma}_b = \begin{bmatrix} V_x^b & cov_{x,y}^b \\ cov_{y,x}^b & V_y^b \end{bmatrix} \quad \hat{\Sigma}_g = \begin{bmatrix} V_x^g & cov_{x,y}^g \\ cov_{y,x}^g & V_y^g \end{bmatrix}$$

**What's the difference (simplification) from QDA?**

## Models in Higher Dimension: GNB

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- ❖ GNB assumes

$$\Sigma_b = \begin{bmatrix} V_x^b & 0 \\ 0 & V_y^b \end{bmatrix} \text{ and } \Sigma_g = \begin{bmatrix} V_x^g & 0 \\ 0 & V_y^g \end{bmatrix}$$

- ❖ Recall that GNB stands for **Gaussian Naive Bayes** classifier. The name indicates a **Bayes classifier** with **Gaussian distribution**. The assumption of Gaussian distribution, together with uncorrelated features, imply that features are **mutually independent**. This is what **Naive** stands for.

## Hands-on Session

- ❖ Please go to the "[Discriminant Analysis in Scikit-Learn](#)" in the lecture code.

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# Outline

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- ❖ **Limitation of Linear Regression**
- ❖ **Logistic Regression**
- ❖ **Discriminant Analysis**
  - Linear Discriminant Analysis
  - Quadratic Discriminant Analysis
- ❖ **Naive Bayes**

## Naive Bayes

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- ❖ Recall that Bayes theorem assumes the probability that the output is in class  $K$  given  $X = x$  can be estimated by:

$$Pr(Y = k|X = x) = \frac{f_k(x)\pi_k}{\sum_l f_l(x)\pi_l}$$

- ❖ LDA and QDA use multivariate Gaussian densities (but with different assumptions on the covariance matrix). These do not work well when the number of features is large.
- ❖ *Naive Bayes* models assume that the inputs are conditionally independent in each class so can work with dataset of large number of features.

# Naive Bayes

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- ❖ The naive Bayes classifier is based on Bayes theorem with independence assumptions between predictors.
- ❖ The assumption of conditional independence requires:

$$f_k(x) = \prod_{j=1}^p f_{jk}(x)$$

where  $f_{jk}(x)$  is the probability density for the  $j^{\text{th}}$  feature  $X_j$  in class  $k$ .

- ❖ We will introduce three kinds of Naive Bayesian models:
  - Gaussian Naive Bayes
  - Multinomial Naive Bayes
  - Bernoulli Naive Bayes



# Gaussian Naive Bayes

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- ❖ Gaussian Naive Bayes assumes each feature follows a gaussian distribution ( $\Sigma_k$  is diagonal):

$$f_{jk}(x) = \frac{1}{\sqrt{2\pi}\sigma_{jk}} \exp\left[-\frac{(x_j - \mu_{jk})^2}{2\sigma_{jk}^2}\right]$$

where:

- $\mu_{jk}$ : the mean of the  $j^{\text{th}}$  feature  $X_j$  in class  $k$ ;
- $\sigma_{jk}^2$ : the variance of the  $j^{\text{th}}$  feature  $X_j$  in class  $k$ .
- ❖ Since we assume gaussian densities, Gaussian Naive Bayes is best used for continuous features.
- ❖ GaussianNB implements the Gaussian Naive Bayes algorithm for classification.

## Hands-on Session

- ❖ Please go to the **"Gaussian Naive Bayes in Scikit-Learn"** in the lecture code.

# Multinomial Naive Bayes

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- ❖ If all the features are categorical, then we can parameterize the distribution by vectors  $\theta_k = (\theta_{k1}, \theta_{k2}, \dots, \theta_{kn})$  for each class  $k$ , where:
  - $n$ : the number of features.
  - $\theta_{ki}$ : probability  $P(x_i|k)$  of feature  $i$  appearing in a sample belonging to class  $k$ .
- ❖ MultinomialNB implements the naive Bayes algorithm for multinomially distributed data, and is widely used in text classification.

## Multinomial Naive Bayes Example

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- ❖ In our training data, we choose three words to build the model: "sale", "money", "work", denoted by  $x_1, x_2, x_3$ .
  - In the spams, "sale" appears 48 times, "money" appears 50 times, "work" 2 times. 100 in total.

Thus we have:

- $\theta_1 = \{0.48, 0.50, 0.02\}$

- In the non-spams, the frequency of  $x_1, x_2, x_3$  are 5, 10, 85.

Thus we have:

- $\theta_0 = \{0.50, 0.10, 0.85\}$

## Hands-on Session

- ❖ Please go to the "**Multinomial Naive Bayes in Scikit-Learn**" in the lecture code.

## Bernoulli Naive Bayes

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- ❖ Bernoulli Naive Bayes is used for data that:
  - is distributed according to a multivariate Bernoulli distribution;
  - each feature is assumed to be a binary-valued variable.
- ❖ `BernoulliNB` implements the naive Bayes training and classification algorithms.

## Bernoulli Naive Bayes

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- ❖ Consider the spam filter problem. In Bernoulli naive Bayes we do not care about the frequency of a feature. We are just interested in the whether it appears or not.
- ❖ Given a feature  $x_k$  which denotes a word, does it appears in an email or not? What is the probability of its appearance?

## Bernoulli Naive Bayes Example

- ❖ Suppose we have 80 non-spams, and the word "sale" (denoted by  $x_k$ ) appears in 10 of them; we also have 20 spams, and  $x_k$  appears in 16 of them. We use  $y = 1$  to denote that an email is a spam. Then:

$$\begin{aligned} p(x_k = 1|y = 1) &= \frac{16}{20} = \frac{4}{5}, & p(x_k = 0|y = 1) &= \frac{1}{5} \\ p(x_k = 1|y = 0) &= \frac{10}{80} = \frac{1}{8}, & p(x_k = 0|y = 0) &= \frac{7}{8} \end{aligned}$$

- ❖ Given a new email which contains the word "sale", we have class = 1. If we use only this feature to predict:

$$\begin{aligned} p(y = 1|x_k = 1) &= \frac{p(y = 1)p(x_k = 1|y = 1)}{p(x_k = 1)} = \frac{\frac{20}{100} \times \frac{4}{5}}{p(x_k = 1)} = \frac{0.16}{p(x_k = 1)} \\ p(y = 0|x_k = 1) &= \frac{p(y = 0)p(x_k = 1|y = 0)}{p(x_k = 1)} = \frac{\frac{80}{100} \times \frac{1}{8}}{p(x_k = 1)} = \frac{0.1}{p(x_k = 1)} \end{aligned}$$

then we will predict this email to be spam.



## Hands-on Session

- ❖ Please go to the "**Bernoulli Naive Bayes in Scikit-Learn**" in the lecture code.