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# Naive Bayes



## Lecture 8



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# Learning objective:

- Modern methods for classification problems

# Tasks

Input →  
real number →

Regressor  
→

Predict

Input →  
category

Classifier

Predict

Input

Density Estimator

Probability

# Types of classifiers

- Discriminative classifiers:
  - Directly estimate a decision rule/boundary
  - e.g. decision tree, SVM
- Instance based classifiers:
  - Use observation directly
  - e.g. K nearest neighborhood
- Generative classifiers:
  - Build a generative statistical model
  - e.g. Bayesian Network

# Classification

- Goal: Construct a predictor  $f: X \rightarrow Y$  to minimize the risk of misclassification!



**Features, X**



**Sports  
Science  
News**

**Labels, Y**

# Discriminative vs Generative Classifiers

Optimal Classifier:

$$\begin{aligned} f^*(x) &= \arg \max_{Y=y} P(Y = y|X = x) \\ &= \arg \max_{Y=y} P(X = x|Y = y)P(Y = y) \end{aligned}$$

**Generative (Model based) approach:** e.g. Naïve Bayes

- Assume some probability model for  $P(Y)$  and  $P(X|Y)$
- Estimate parameters of probability models from training data

**Discriminative (Model free) approach:** e.g. Logistic regression

**Why not learn  $P(Y|X)$  directly? Or better yet, why not learn the decision boundary directly?**

- Assume some functional form for  $P(Y|X)$  or for the decision boundary
- Estimate parameters of functional form directly from training data

# Optimal Classifier

**Bayes Rule:**  $P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$

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

**Optimal classifier:**

$$\begin{aligned} f^*(x) &= \arg \max_{Y=y} P(Y = y|X = x) \\ &= \arg \max_{Y=y} \underbrace{P(X = x|Y = y)}_{\text{Class conditional density}} \underbrace{P(Y = y)}_{\text{Class prior}} \end{aligned}$$

# Model-based approach

$$f^*(x) = \arg \max_{Y=y} \underbrace{P(X = x|Y = y)}_{\text{Class conditional distribution}} \underbrace{P(Y = y)}_{\text{Class probability}}$$

We therefore consider appropriate models for these 2 terms

Modeling Class probability  $P(Y=y) = \text{Bernoulli}(\theta)$

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

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

Like a coin flip

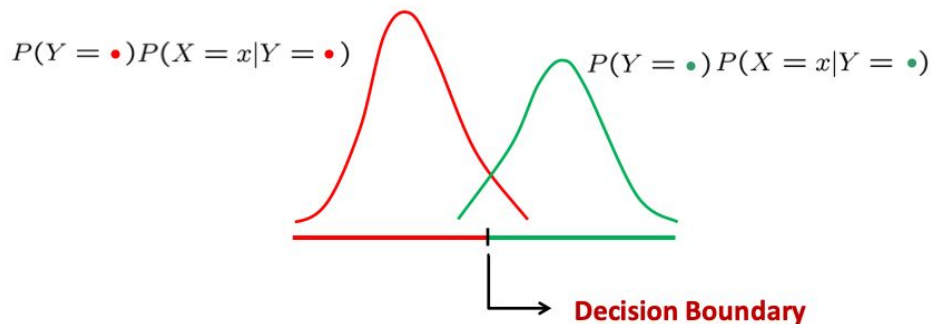




# More complicated models...

- We model the class conditional distribution of features
- One popular choice is Gaussian class conditional density (1-dim/feature)

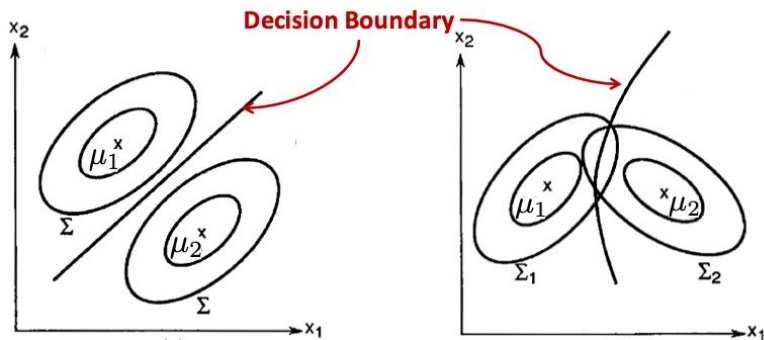
$$P(X = x|Y = y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x - \mu_y)^2}{2\sigma_y^2}\right)$$



# More complicated models...

- We model the class conditional distribution of features
- One popular choice is Gaussian class conditional density (1-dim/feature)

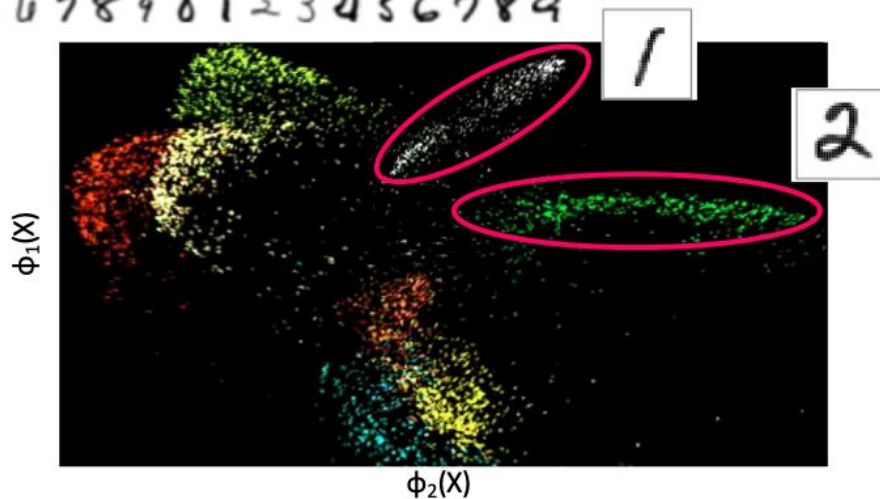
$$P(X = x|Y = y) = \frac{1}{\sqrt{2\pi|\Sigma_y|}} \exp\left(-\frac{(x - \mu_y)\Sigma_y^{-1}(x - \mu_y)'}{2}\right)$$



# Handwritten digit recognition (MNIST)

0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7  
8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5  
6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3  
4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1  
2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9

Multi-class  
classification



# Handwritten digit recognition (MNIST)

## Training Data:

Each image represented as  
a vector of **intensity values**  
at the **d pixels (features)**

Input, X



... n greyscale  
images

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \dots \\ X_d \end{bmatrix}$$

Label, Y

1

2

... n labels

## Gaussian Bayes model:

$P(Y = y) = p_y$  for all  $y$  in 0, 1, 2, ..., 9

$p_0, p_1, \dots, p_9$  (sum to 1)

$P(X=x|Y=y) \sim N(\mu_y, \Sigma_y)$  for each  $y$

$\mu_y$  - d-dim vector

$\Sigma_y$  - dxd matrix

# Gaussian Bayes Classifier

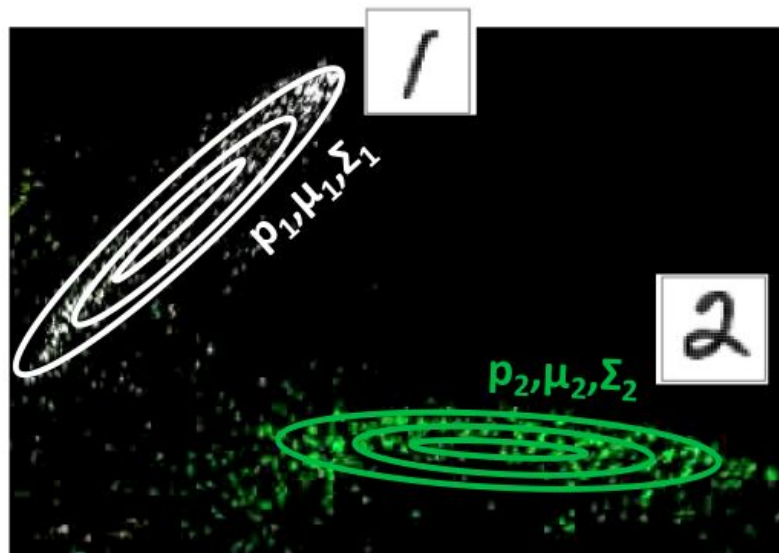
$p_0, p_1, \dots, p_9$  (sum to 1)

$\mu_y$  - d-dim vector

$\Sigma_y$  - dxd matrix

$P(Y = y) = p_y$  for all  $y$  in 0, 1, 2, ..., 9

$P(X=x|Y = y) \sim N(\mu_y, \Sigma_y)$  for each  $y$



# Gaussian Bayes Classifier

How to learn parameters  
 $p_y, \mu_y, \Sigma_y$  from data?

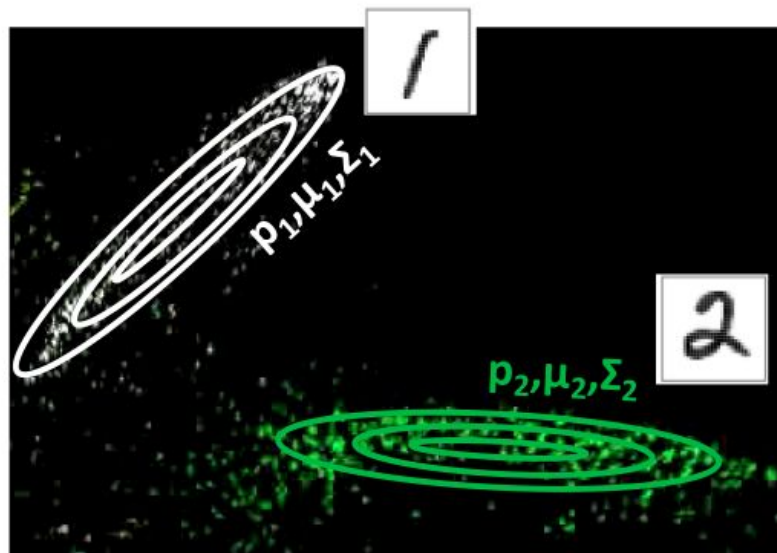
$p_0, p_1, \dots, p_9$  (sum to 1)

$\mu_y$  - d-dim vector

$\Sigma_y$  - dxd matrix

$P(Y = y) = p_y$  for all  $y$  in 0, 1, 2, ..., 9

$P(X=x|Y = y) \sim N(\mu_y, \Sigma_y)$  for each  $y$

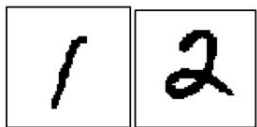


# How many parameters do we have to learn?

## Training Data:

Each image represented as a  
vector of **d binary features**  
(black 1 or white 0)

Input, X



... n **black-white**  
images

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \dots \\ X_d \end{bmatrix}$$

Label, Y

1

2

... n labels

## Discrete Bayes model:

$P(Y = y) = p_y$  for all  $y$  in 0, 1, 2, ..., 9

$p_0, p_1, \dots, p_9$  (sum to 1)

$P(X=x|Y=y) \sim$  For each label  $y$ , maintain probability table with  
 $2^d - 1$  entries

# How many parameters do we have to learn?

Class probability:

$$P(Y = y) = p_y \text{ for all } y \text{ in } 0, 1, 2, \dots, 9 \quad p_0, p_1, \dots, p_9 \text{ (sum to 1)}$$

Class conditional distribution of features:

$$P(X=x|Y = y) \sim N(\mu_y, \Sigma_y) \text{ for each } y$$

$\mu_y$  – d-dim vector  
 $\Sigma_y$  – dxd matrix



# How many parameters do we have to learn?

Class probability:

$P(Y = y) = p_y$  for all  $y$  in  $0, 1, 2, \dots, 9$

$p_0, p_1, \dots, p_9$  (sum to 1)

**K-1 if K labels**

Class conditional distribution of features:

$P(X=x|Y = y) \sim N(\mu_y, \Sigma_y)$  for each  $y$

$\mu_y$  – d-dim vector

$\Sigma_y$  – dxd matrix

**$Kd + Kd(d+1)/2 = O(Kd^2)$  if d features**

**Quadratic in dimension d! If  $d = 256 \times 256$  pixels, ~ 21.5 billion parameters!**

# Naive Bayes Classifier

If conditional independence holds, Naive Bayes classifier is the best classifier!

Bayes Classifier with additional “naïve” assumption:

- Features are independent given class:

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

$$\begin{aligned} P(X_1, X_2|Y) &= P(X_1|X_2, Y)P(X_2|Y) \\ &= P(X_1|Y)P(X_2|Y) \end{aligned}$$

- More generally:

$$P(X_1 \dots X_d|Y) = \prod_{i=1}^d P(X_i|Y)$$

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \dots \\ X_d \end{bmatrix}$$

# Recall conditional independence

- X is conditionally independent of Y given Z:

$$P[X = x \mid Y=y, Z=z] = P[X = x \mid Z=z]$$

- Or equivalently,

$$P[X=x, Y=y \mid Z=z] = P[X=x \mid Z=z] P[Y=y \mid Z=z]$$

$$P(\textit{Thunder} \mid \textit{Rain}, \textit{Lightning}) = P(\textit{Thunder} \mid \textit{Lightning})$$

**Note:** does NOT mean Thunder is independent of Rain

# Naive Bayes Classifier

- Bayes classifier with additional naive assumption:
  - features are independent given class:

$$P(X_1 \dots X_d | Y) = \prod_{i=1}^d P(X_i | Y)$$

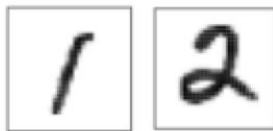
$$\begin{aligned} f_{NB}(\mathbf{x}) &= \arg \max_y P(x_1, \dots, x_d | y) P(y) \\ &= \arg \max_y \prod_{i=1}^d P(x_i | y) P(y) \end{aligned}$$

- How many parameters we have now?

# Naive Bayes Classifier

**Training Data:**

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \dots \\ X_d \end{bmatrix}$$



... n greyscale  
images with  
d pixels

Y

1

2

... n labels

**How many parameters?**

Class probability  $P(Y = y) = p_y$  for all y **K-1 if K labels**

May not  
hold

Class conditional distribution of features (using Naïve Bayes assumption)

$P(X_i = x_i | Y = y) \sim N(\mu_i^{(y)}, \sigma_i^{2(y)})$  for each y and each pixel i **2Kd**

# Naive Bayes Classifier

- Bayes classifier with additional naive assumption:
  - features are independent given class:

$$P(X_1 \dots X_d | Y) = \prod_{i=1}^d P(X_i | Y)$$

$$\begin{aligned} f_{NB}(\mathbf{x}) &= \arg \max_y P(x_1, \dots, x_d | y) P(y) \\ &= \arg \max_y \prod_{i=1}^d P(x_i | y) P(y) \end{aligned}$$

- Fewer parameters and hence requires fewer training data, even though the conditional independence assumptions might be violated in practice.

# What if the features are continuous

Gaussian Naïve Bayes (GNB):

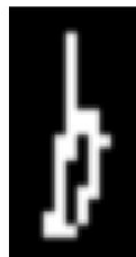
$$P(X_i = x \mid Y = y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}} e^{-\frac{(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

Different mean and variance for each class  $k$  and each pixel  $i$ .

Sometimes assume variance

- is independent of  $Y$  (i.e.,  $\sigma_i$ ),
- or independent of  $X_i$  (i.e.,  $\sigma_k$ )
- or both (i.e.,  $\sigma$ )

character recognition:  $X_i$  is intensity at  $i^{\text{th}}$  pixel



# Naive Bayes Classifier - Algorithm

- Training Data  $\{(X^{(j)}, Y^{(j)})\}_{j=1}^n$        $X^{(j)} = (X_1^{(j)}, \dots, X_d^{(j)})$

- Maximum Likelihood Estimates

- For Class probability

$$\hat{P}(y) = \frac{\{\#j : Y^{(j)} = y\}}{n}$$

- For class conditional distribution

$$\frac{\hat{P}(x_i, y)}{\hat{P}(y)} = \frac{\{\#j : X_i^{(j)} = x_i, Y^{(j)} = y\}/n}{\{\#j : Y^{(j)} = y\}/n}$$

- NB Prediction for test data       $X = (x_1, \dots, x_d)$

$$Y = \arg \max_y \hat{P}(y) \prod_{i=1}^d \frac{\hat{P}(x_i, y)}{\hat{P}(y)}$$



# Issues with Naive Bayes

- **Issue 1:** Usually, features are not conditionally independent:

$$P(X_1 \dots X_d | Y) \neq \prod_i P(X_i | Y)$$

Nonetheless, NB is the single most used classifier particularly when data is limited, works well

- **Issue 2:** Typically use MAP estimates instead of MLE since insufficient data may cause MLE to be zero.

# Naive Bayes Classifier - Algorithm

- Training Data  $\{(X^{(j)}, Y^{(j)})\}_{j=1}^n$   $X^{(j)} = (X_1^{(j)}, \dots, X_d^{(j)})$
- Maximum A Posteriori (MAP) Estimates – add  $m$  “virtual” datapts

Assume given some prior distribution (typically uniform):

$$Q(Y = b)$$

$$Q(X_i = a, Y = b)$$

$$\hat{P}(X_i = a|Y = b) = \frac{\{\#j : X_i^{(j)} = a, Y^{(j)} = b\} + mQ(X_i = a, Y = b)}{\{\#j : Y^{(j)} = b\} + \underbrace{mQ(Y = b)}_{\text{\# virtual examples with Y = b}}}$$

# virtual examples  
with Y = b

# Takeaways

- Optimal decision using Bayes Classifier
- Naïve Bayes classifier – What's the assumption
  - Why we use it
  - How do we learn it
  - Why is MAP estimation important
- Gaussian Naive Bayes
  - Features are still conditionally independent
  - Each feature has a Gaussian distribution given class