University of Pittsburgh

ECE 2195: Special Topics – Computers Machine Learning

Classification – Multiple Classes, LDA & QDA

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Discriminant Analysis for Classification

- Linear Discriminant Analysis
- Quadratic Discriminant Analysis

Bayes Theorem

$$\Pr(Y = k|X = x) = \frac{\Pr(X = x|Y = k) \cdot \Pr(Y = k)}{\Pr(X = x)}$$

X contains Features (e.g., number of words in an email). Y is the class label (e.g. Y=0 means not spam, Y=1 means spam email).

- Another way to write the equation above is:

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

$K: number\ of\ classes$

$k: is\ a\ class\ label\ \{1,2, \ldots K\}$

$f_k(x) = \Pr(X = x|Y = k)$: is the density of x given that it is an observation from class k

$\pi_k = \Pr(Y = k)$: is the prior probability of class k

Discriminant Analysis

- **Approach**: Model the **distribution of each class** separately, then use Bayes Rule

- Recall Bayes Classifier: Assign a new observation with features x_0 to class k that has largest Pr $(Y = k | X = x_0)$

Pr( ) and P( ) both stands for probability; the sign "|" reflects conditional (information is given)

- Both Linear and Quadratic Discriminant analysis **use normal (Gaussian) distribution to model features in each class** ➔ P(X|y) is Gaussian

- More popular than logistic regression when there is more than 2 classes

Discriminant Analysis (LDA) with One Feature

- Assume multiple classes, and one feature (p=1)
- With one feature, the Gaussian density is given by:

$$f_k(x) = \Pr(X = x|Y = k) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma_k}\right)^2}$$

μ_k *is the* *mean* *of* x *in class* k *(class specific mean)* , σ_k^2 *is the* *variance* *of* x *in class* k

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

- Using training data, we estimate μ_k, σ_k, π_k for each class k

Linear Discriminant Analysis (LDA) assumes equal variance (or covariance) in all classes

Use Training Data for Estimation

- Prior of class k is estimated as the training observations n_k that belong to the kth class divided by the total number of observations *n*

$$\hat{\pi}_k = \frac{n_k}{n} \quad .$$

- The mean can be estimated by the average of all training observations from the kth class

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

- The variance can be estimated as weighted average of variances of all k classes

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

LDA - discriminant score

- Log (P(x|y=k) P(y=k)) when is is Gaussian with mean μ_k *and variance* σ_k^2

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

LDA - discriminant score

- **Build classifier:** have an estimation for $\Pr(Y = k|X = x)$

- **Prediction**: assign X to class k with largest $\Pr(Y = k|X = x)$

  - Equivalent to **finding the class** that gives the **largest discriminant score** given by:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

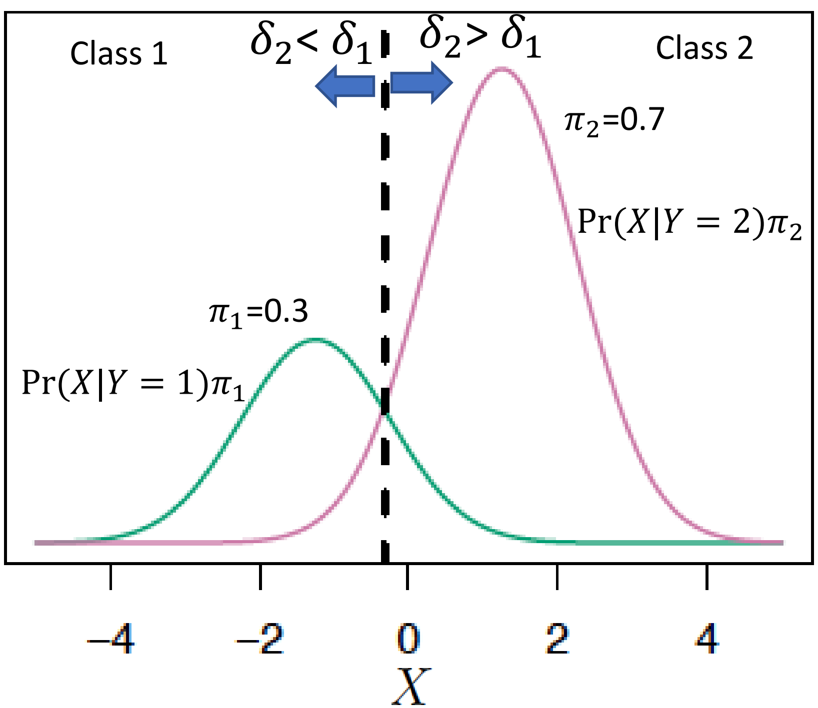
You can get this by taking log and discarding the terms that do not depend on k. Try it!

- The discriminant score is **linear function of x** → thus called **Linear Discriminant** Analysis

- Decision boundary is linear

One Feature and Two Classes Example

Classification: new observation is assigned to class with highest $\Pr(Y = k|X = x)$



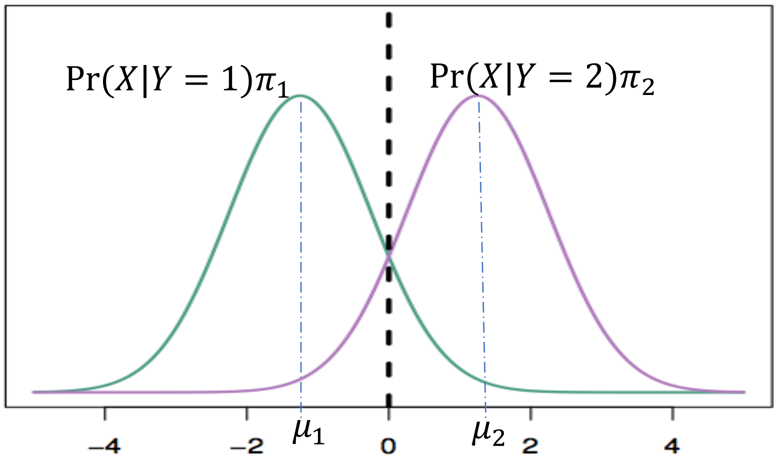
$$\pi_k = \Pr(Y = k)$$

The priors can be estimated by finding the fraction of training samples that belong to each class

Special Case: Two classes (K=1,2), equal priors, one feature

- Assume equal priors $\pi_1 = \pi_2$=0.5, we can get a decision boundary as follows:

Maximize $\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$ Try it! $\Rightarrow$ $x = \frac{\mu_1 + \mu_2}{2}$



This means that, for $\mu_2 > \mu_1$:

$$X \underset{\text{Class 1}}{\overset{\text{Class 2}}{\gtrless}} \frac{\mu_1+\mu_2}{2}$$

i.e.,

choose class 1 if X $< \frac{\mu_1+\mu_2}{2}$

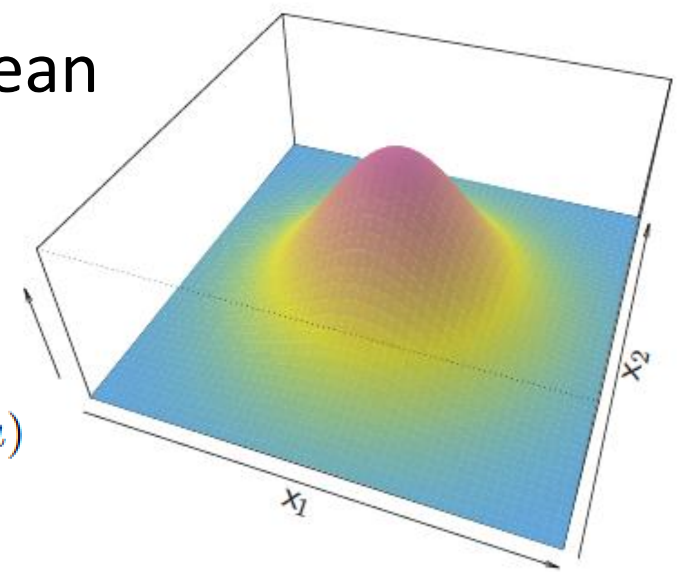
and class 2 if X $> \frac{\mu_1+\mu_2}{2}$

Linear Discriminant Analysis When P>1

- If X contains multiple features(p > 1), same approach is used except that the density function *f(x)* is modeled using the **multivariate normal density**, i.e.,

  $X \sim \mathcal{N}(\mu_k, \Sigma)$,
  - μ_k is the px1 mean vector
  - Σ is the pxp covariance matrix (LDA assume same for all classes)
- The multivariate normal density of mean μ *and covariance* Σ is given by

$$f(x) = \frac{1}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \mathbf{\Sigma}^{-1}(x-\mu)}$$



Linear Discriminant Analysis When P>1

- In this case, the discriminant functions will take the form

$$\delta_k(x) = x^T \boldsymbol{\Sigma}^{-1} \mu_k - \frac{1}{2} \mu_k^T \boldsymbol{\Sigma}^{-1} \mu_k + \log \pi_k$$

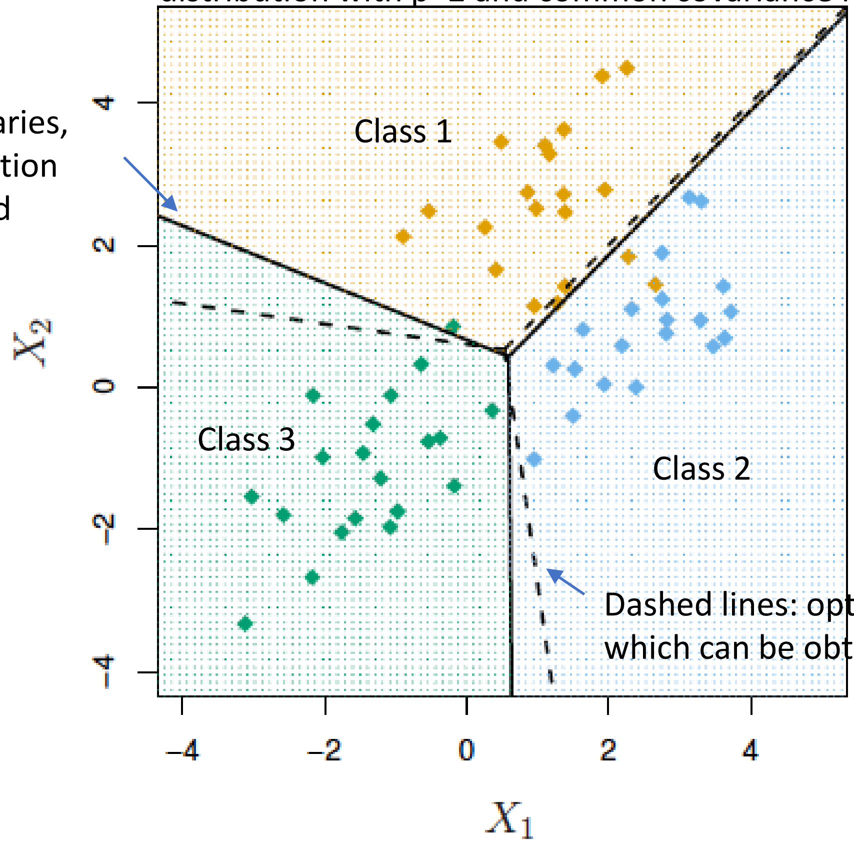
- Still LINEAR with feature vector x

Example: classify Iris flower to one of three possible species (K=3):
Setosa (Y=1), Versicolor (Y=2), Virginica (Y=3)
Using features: X=[sepal length, sepal width, petal length, petal width]
Build classifier: From the training data, we estimate mean and covariance matrix of this feature vector when Y=1, 2 and 3 = > find discriminant functions / decision boundaries
Classify: Apply the discriminant function to classify new observations

Illustration: Assume 3 classes (K=3), and 2 features

Observations drawn from multivariate Gaussian distribution with p=2 and common covariance matrix

Solid lines: LDA decision boundaries, obtained with Gaussian distribution with estimated priors, mean and covariance



Dashed lines: optimal Bayes decision boundary, which can be obtained if actual distributions are known

Observation points are drawn from multivariate Gaussian distribution with p=2 and common covariance matrix

Quadratic Discriminant Analysis (QDA)

- In QDA, the density $f_k(x)$ is assumed to also be Gaussian for each class, but each **class has a different covariance matrix $\boldsymbol{\Sigma_k}$**

- In this case we get discriminate functions that are **quadratic** with x (hence the name)

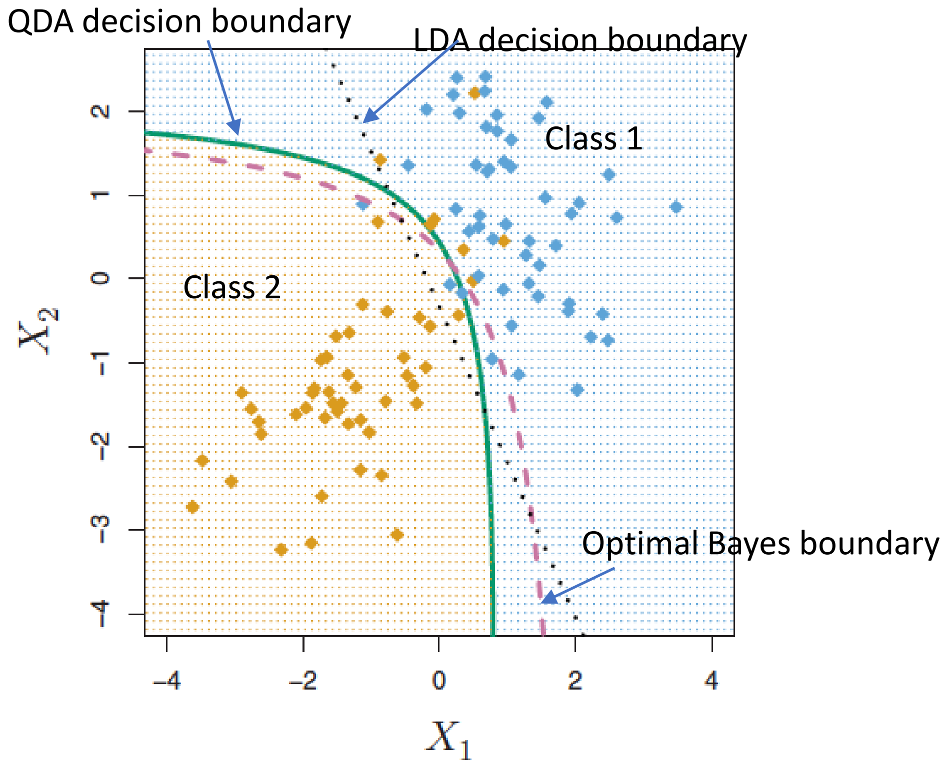
$$
\begin{aligned}
\delta_k(x) &= -\frac{1}{2}(x-\mu_k)^T \boldsymbol{\Sigma}_k^{-1}(x-\mu_k) - \frac{1}{2}\log|\boldsymbol{\Sigma}_k| + \log\pi_k \\
&= -\frac{1}{2}x^T \boldsymbol{\Sigma}_k^{-1} x + x^T \boldsymbol{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\log|\boldsymbol{\Sigma}_k| + \log\pi_k
\end{aligned}
$$

Quadratic Discriminant Analysis – Quadratic Decision Boundary

- Here, 2 features, and 2 classes
  - Two classes have different covariance in this example, hence QDA is better
- QDA, the covariance matrix is estimated for each class
  - Each matrix has p.(p+1)/2 parameters
  - Need large training data to avoid overfitting (high variance)

Bias-variance trade-off!

- LDA is simpler, but could lead to high bias
  - Estimate single covariance matrix



Naïve Bayes Classifier

- Assumes:
  - Gaussian densities (same as LDA and QDA)
  - Each class has its **own covariance** (same as QDA),
  - Covariance matrix of each class is diagonal matrix (<u>features are statistically independent</u>)
    - Now we need to estimate only p parameters for each covariance matrix

$$\begin{aligned}
\delta_k(x) &= -\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}_k^{-1}(x-\mu_k) - \frac{1}{2}\log|\mathbf{\Sigma}_k| + \log \pi_k \\
&= -\frac{1}{2}x^T \mathbf{\Sigma}_k^{-1} x + x^T \mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\log|\mathbf{\Sigma}_k| + \log \pi_k
\end{aligned}$$

LDA and QDA in Python

- Linear Discriminant Analysis (LDA)

from **sklearn.discriminant_analysis** import **LinearDiscriminantAnalysis**

LDAmodelFitted = LinearDiscriminantAnalysis().fit(X_train, Y_train)

- Quadratic Discriminant Analysis

from **sklearn.discriminant_analysis** import **QuadraticDiscriminantAnalysis**

QDAmodelFitted = **QuadraticDiscriminantAnalysis().**fit(X_train, Y_train)