Statistics 101C - Week 3 - Tuesday

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How can we construct classifier?

- **Discriminative models**
  - Discriminative modeling studies the $\mathbb{P}(Y|\boldsymbol{X})$ or when $\mathbb{P}(Y|\boldsymbol{X}) > 1/2$, does not care the distribution of $\mathbb{P}(\boldsymbol{X})$.
  - **Examples**: Logistic regression (LR) and KNN
- **Generative models**
  - Generative models studies the joint probability distribution $\mathbb{P}(\boldsymbol{X}, Y)$
  - **Examples**: linear discriminant analysis and quadratic discriminant analysis

Estimate the Bayes Classifier

- **Bayes Classifier**: Let $\eta(\boldsymbol{x}) = \mathbb{P}(Y = 1|\boldsymbol{X} = \boldsymbol{x})$

$$f^*(\boldsymbol{x}) = \text{sign}(\eta(\boldsymbol{x}) - 1/2)$$

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- **Implication**: If we know $\eta(\boldsymbol{x})$, we know the Best classifier.
- **Both Generative and Discriminative models** intend to estimate

$$\eta(\boldsymbol{x}) = \mathbb{P}(Y = 1|\boldsymbol{X} = \boldsymbol{x})$$

Recall: two main classes of classifiers

- **Discriminative models**
  - Discriminative modeling studies the $\mathbb{P}(Y|\boldsymbol{X})$
  - Examples: Logistic regression (LR)
- **General Steps of Discriminative models**:
  - Estimate the conditional probability

$$\widehat{\mathbb{P}}(Y=1|\boldsymbol{X})$$

  - The classifier can be constructed as

$$\mathrm{sign}(\widehat{\mathbb{P}}(Y=1|\boldsymbol{X})-1/2)$$

Generative models

- **Generative models**
  - Generative models studies the joint probability distribution $\mathbb{P}(\boldsymbol{X}, Y)$
  - Examples: linear discriminant analysis and quadratic discriminant analysis
- **General Steps of Generative models**:
  - Estimate the conditional probability $\widehat{\mathbb{P}}(\boldsymbol{X}|Y=1)$ and $\widehat{\mathbb{P}}(Y=1)$
  - The classifier can be constructed as

$$\widehat{P}(Y=1|\boldsymbol{X}) = \frac{\widehat{\mathbb{P}}(Y=1)\widehat{\mathbb{P}}(\boldsymbol{X}|Y=1)}{\widehat{\mathbb{P}}(Y=1)\widehat{\mathbb{P}}(\boldsymbol{X}|Y=1) + \widehat{\mathbb{P}}(Y=0)\widehat{\mathbb{P}}(\boldsymbol{X}|Y=0)}$$

Basics: $\boldsymbol{x}$ is p-dimensional vector

1. multivariate linear function

$$f(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0$$

2. linear equation

$$\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$$

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2. linear equation

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3. multivariate quadratic function

$$f(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0$$

4. multivariate quadratic equation

$$\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$$

Basics of Generative models

- LDA and QDA are **generative models**, we need to consider the structure of $\mathbb{P}(\boldsymbol{X}, Y)$
  - Model $\mathbb{P}(Y)$
  - Model $\mathbb{P}(\boldsymbol{X}|Y)$
- Once we obtain the estimated joint distribution $\widehat{\mathbb{P}}(Y)$ and $\widehat{\mathbb{P}}(\boldsymbol{X}|Y)$
  - We can compute the conditional probability

$$\widehat{\mathbb{P}}(Y = 1|\boldsymbol{X} = \boldsymbol{x})$$

  - Construct the classifier:

$$\text{sign}(\widehat{\mathbb{P}}(Y = 1|\boldsymbol{X} = \boldsymbol{x}) - 1/2)$$

An alternative look

Let $k \in \{0, 1\}$. We can develop an alternative formulation of $\mathbb{P}(Y = k|\boldsymbol{X} = \boldsymbol{x})$ from the definition of conditional probability.

$$\mathbb{P}(Y = k|\boldsymbol{X} = \boldsymbol{x}) = \frac{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}, Y = k)}{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x})} = \frac{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k) \cdot \mathbb{P}(Y = k)}{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x})}$$
$$= \frac{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k) \cdot \mathbb{P}(Y = k)}{\sum_{k=0}^{1} \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k) \cdot \mathbb{P}(Y = k)}$$

- $\mathbb{P}(\boldsymbol{X} = \boldsymbol{x})$ the marginal distribution
- $\mathbb{P}(Y = k|\boldsymbol{X} = \boldsymbol{x})$: given $\boldsymbol{X} = \boldsymbol{x}$ the probability that outcome $Y = k$.

Banknote Dataset

conterfeit	Length	Left	Right	Bottom	Top	Diagonal
0	214.70000	129.70000	129.30000	8.60000	9.60000	141.60000
0	215.40000	130.00000	129.90000	8.50000	9.70000	141.40000
0	214.90000	129.40000	129.50000	8.20000	9.90000	141.50000
0	214.50000	129.50000	129.30000	7.40000	10.70000	141.50000
0	214.70000	129.60000	129.50000	8.30000	10.00000	142.00000
0	215.60000	129.90000	129.90000	9.00000	9.50000	141.70000
0	215.00000	130.40000	130.30000	9.10000	10.20000	141.10000
0	214.40000	129.70000	129.50000	8.00000	10.30000	141.20000
0	215.10000	130.00000	129.80000	9.10000	10.20000	141.50000
0	214.70000	130.00000	129.40000	7.80000	10.00000	141.20000
1	214.40000	130.10000	130.30000	9.70000	11.70000	139.80000
1	214.90000	130.50000	130.20000	11.00000	11.50000	139.50000
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Discriminant Analysis (DA)

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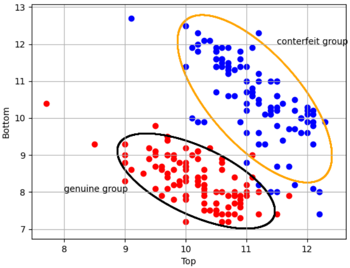

Figure: Black ellipsoid: covariance structure of genuine group. Green ellipsoid: covariance structure of the counterfeit group

Discriminant Analysis (DA)

- $\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k)$ is a multivariate normal distribution with mean $\boldsymbol{\mu}_k$ and covariance matrix $\boldsymbol{\Sigma}_k$.

$$\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}_k|^{1/2}} \exp\Big(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_k)\Big),$$

where

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{pmatrix}, \boldsymbol{\mu}_k = \begin{pmatrix} \mu_{1,k} \\ \mu_{2,k} \\ \vdots \\ \mu_{p,k} \end{pmatrix}, \boldsymbol{\Sigma}_k = \begin{pmatrix} \sigma^2_{1,1,k} & \sigma^2_{1,2,k} & \cdots & \sigma^2_{2,2,k} \\ \sigma^2_{2,1,k} & \sigma^2_{2,2,k} & \cdots & \sigma^2_{2,p,k} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma^2_{p,1,k} & \sigma^2_{p,2,k} & \cdots & \sigma^2_{p,p,k} \end{pmatrix}.$$

Discriminant Analysis (DA)

- Step 2: We use the Bayes' theorem to compute $\mathbb{P}(Y = k|\boldsymbol{X} = \boldsymbol{x}), k = 0, 1$.

$$\mathbb{P}(Y = k|\boldsymbol{X} = \boldsymbol{x}) = \frac{\pi_k \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = k)}{\pi_1 \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 1) + \pi_0 \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 0)}$$

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Question: What is the difference between Linear and Quadratic discriminant analyses?

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Question: What is the difference between Linear and Quadratic discriminant analyses?

- **Linear** Discriminant Analysis (LDA) assumes that the classes have a common covariance matrix. In other words, that is $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_0 = \boldsymbol{\Sigma}_1$
- **Quadratic** Discriminant Analysis (QDA) does not assumes this. So, we have a covariance matrix $\boldsymbol{\Sigma}_0$ for class 0 and $\boldsymbol{\Sigma}_1$ for class 1.

Linear Discriminant Analysis (LDA)

Three Assumptions in LDA

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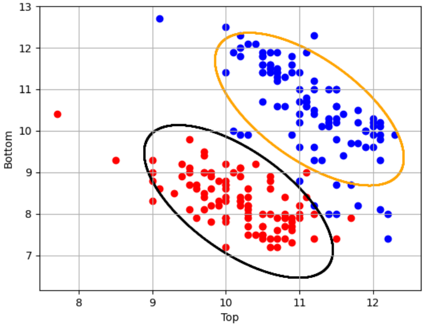
1. Multivariate normal distribution for each group, that $\mathbb{P}(\boldsymbol{X} = \boldsymbol{x} | Y = k)$ is multivariate normal
2. They have different mean vectors
3. **Same covariance matrices**



Use LDA for classification

We make predictions using LDA as follows:

$$f_{LDA}(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \frac{\pi_1 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=1)}{\pi_1 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=1)+\pi_0 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=0)} > 0.5 \\ 0, & \text{if } \frac{\pi_1 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=1)}{\pi_1 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=1)+\pi_0 \mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=0)} \leq 0.5 \end{cases}$$

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Conclusions we can make

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Conclusions we can make

1. Similar to the Bayes classifier, we classify to the most probable class using the posterior probability
2. The decision boundary can be easily derived as

$$\frac{\pi_1 \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 1)}{\pi_1 \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 1) + \pi_0 \mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 0)} = 1/2$$
$$\Leftrightarrow \log \frac{\pi_1}{\pi_0} + \log \frac{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 1)}{\mathbb{P}(\boldsymbol{X} = \boldsymbol{x}|Y = 0)} = 0.$$

Decision boundary in LDA

A closer look at the decision boundary.

$$\log\frac{\pi_1}{\pi_0}+\log\frac{\mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=1)}{\mathbb{P}(\boldsymbol{X}=\boldsymbol{x}|Y=0)}=0$$

$$\Updownarrow$$

$$\log\frac{\pi_1}{\pi_0}+\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)-\frac{1}{2}\boldsymbol{\mu}_{\mathbf{1}}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1+\frac{1}{2}\boldsymbol{\mu}_{\mathbf{0}}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0=0$$

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$$\Updownarrow$$

$$\log \frac{\pi_1}{\pi_0} + \boldsymbol{x}^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - \frac{1}{2}(\boldsymbol{\mu}_{\mathbf{1}} + \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathbf{1}} - \boldsymbol{\mu}_0) = 0.$$

The decision boundary can be written as (a linear equation)

$$\boldsymbol{x}^T C_1(\boldsymbol{\mu}_0, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) + C_2(\boldsymbol{\mu}_0, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) = 0,$$

where $C_1(\boldsymbol{\mu}_0, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$ and
$C_2(\boldsymbol{\mu}_0, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) = \log \frac{\pi_1}{\pi_0} - \frac{1}{2}(\boldsymbol{\mu}_{\mathbf{1}} + \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_{\mathbf{1}} - \boldsymbol{\mu}_0)$.

Parameter estimation in LDA

Thanks to the formulation of LDA, we can easily estimate its parameters.

- The prior probability π_0 and π_1.

$$\widehat{\pi}_0 = \frac{n_0}{n_0 + n_1} \text{ and } \widehat{\pi}_1 = \frac{n_1}{n_0 + n_1},$$

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  where n_k is the number of observations in the training data set that belong to class.

- The means are estimated as

$$\widehat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i: y_i = k} \boldsymbol{x}_i, k = 0, 1$$

- The covariance matrices are estimated as

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-2} \sum_{k=0}^{1} \sum_{i: y_i = k} (\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)^T$$

Quadratic Discriminant Analysis (QDA)

Three Assumptions in QDA

1. Multivariate normal distribution for each group, that $\mathbb{P}(\boldsymbol{X} = \boldsymbol{x} | Y = k)$ is multivariate normal
2. They have different mean vectors
3. **Different covariance matrices**

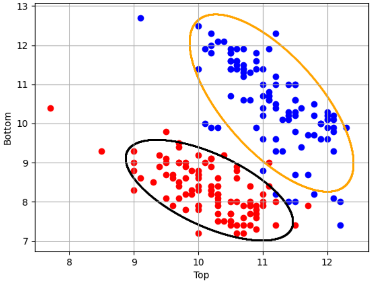

Figure: Different covariance structures

Decision boundary in QDA

We follow a similar analysis of QDA as with LDA. After some algebra, we arrive to the following (interesting) equation:

$$\log \frac{\pi_1}{\pi_0} - \frac{1}{2}\boldsymbol{x}^T(\boldsymbol{\Sigma}_1^{-1} - \boldsymbol{\Sigma}_0^{-1})\boldsymbol{x} + \boldsymbol{x}^T(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}_0^{-1}\boldsymbol{\mu}_0) + \cdots = 0$$

Conclusion

- The decision boundary in QDA is a quadratic function

LDA vs QDA

The difference between LDA and QDA can be summarized as

- LDA is simpler than QDA. (LDA is a special case of QDA)
- QDA needs to estimate more parameters. One covariance matrix for each class.
- LDA is much less flexible than QDA, but this also means that it has low variance
- If the assumptions of LDA do not hold, then it can lead to poor estimates and so, a high bias.

Exercise: Prediction of counterfeit banknotes

conterfeit	Length	Left	Right	Bottom	Top	Diagonal
0	214.70000	129.70000	129.30000	8.60000	9.60000	141.60000
0	215.40000	130.00000	129.90000	8.50000	9.70000	141.40000
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1	215.00000	130.20000	130.20000	10.60000	10.70000	139.90000
1	215.30000	130.30000	130.10000	9.30000	12.10000	140.20000

- Length: length of banknote (mm)
- Left: length of left edge (mm)
- Right: length of right edge (mm)
- Top: distance from the image to top edge
- Bottom: distance from image to bottom
- Diagonal: length of diagonal (mm)
- counterfeit: 1 means counterfeit and 0 means genuine

Exercise: Prediction of counterfeit banknotes using R

- Step 1: Loading the dataset and split the dataset into training set and testing set:

```
library(mclust)
# Load the data set.
data(banknote)
banknote$Status<-factor(banknote$Status,levels=c("genuine", "counterfeit"))
# Split into training and test data.
set.seed(123) # Set seed to reproduce results.
i <- 1:dim(banknote)[1]
# Generate a random sample.
i.train <- sample(i, 130, replace = F) # 130 samples are used for training
bn.train <- banknote[i.train,] # training dataset
bn.test <- banknote[-i.train,] # testing dataset
```

- Step 2: Implement LDA and make prediction by LDA

```
library(MASS)
lda.mod <- lda(Status~Length + Right + Left + Top, data = bn.train) # Fit a LD
pred.lda.test <- predict(lda.mod,bn.test[,-1])

table('Reference' = bn.test[,1], "Predicted" =
       pred.lda.test$class)
```

Exercise: Prediction of counterfeit banknotes using R

- Result:

```
> table('Reference' = bn.test[,1], "Predicted" =
+          pred.lda.test$class)
              Predicted
Reference      genuine counterfeit
  genuine           30           3
  counterfeit        4          33
```

- Conclusion: The prediction accuracy of LDA is $(30+33)/70=0.9$.

Exercise: Prediction of counterfeit banknotes using R

- Implementation of QDA

```
qda.mod <- qda(Status~Length + Right + Left + Top, data = bn.train)
pred.qda.test <- predict(qda.mod, bn.test[,-1])
table('Reference' = bn.test[,1],
      "Predicted" = pred.qda.test$class)
```

- Result:

```
> table('Reference' = bn.test[,1],
+       "Predicted" = pred.qda.test$class)
             Predicted
Reference     genuine counterfeit
  genuine          29           4
  counterfeit       3          34
```

- Conclusion: The prediction accuracy of LDA is $(29+34)/70=0.9$. No improvement is observed.