Supplementary Material

Mathematical working of LDA

• Problem and data

The problem demonstrated is a binary classification problem (K = 2).

In this problem, we want to classify an observation containing two predictor variables **minorAL** (X_1) and **ecc** (X_2) into two classes.

So, the response variable *Y* can takes two distinct values Kecimen and Besni.

Let the data distribution $f_i(x) \sim N(\mu_i, \Sigma)$,

where $E(X) = \mu_i$ is a mean vector of i^{th} class with two components and $Cov(X) = \Sigma$ is a 2x2 covariance matrix.

By homogeneity assumption, the covariance matrices for LDA are assumed to be equal.

• Constructing LDA decision boundary

Let π_i be the (prior) probability that a randomly selected observation belongs to i^{th} class.

$$P(Y = i) = \pi_i, i = 1,2.$$

For every observation x, and predictor variable $X = (X_1, X_2)$, $P(X = x | Y = i) = f_i(x), i = 1,2$

We are interested in finding the posterior probability for any observation belonging to i^{th} class given $X \approx x$.

Using Bayes Theorem,

$$P(Y = i | X = x) = \frac{\pi_i f_i(x)}{\pi_1 f_1(x) + \pi_2 f_2(x)}, \quad i = 1, 2 \quad \dots (i)$$

Any observation x is classified into a class with higher posterior probability. Therefore if,

$$P(Y = 1 | X = x) > P(Y = 2 | X = x)$$

then x is assigned to class 1. Implying,

$$\frac{P(Y = 1 | X = x)}{P(Y = 2 | X = x)} > 1 \qquad \dots (ii)$$

Note: The ratio given in (ii) is the probability (odds) of an event occurring over another event and is referred to as odds-ratio.

Formally the multivariate Gaussian density is defined as,

$$f_i(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{\left(-\frac{1}{2}(x-\mu_i)^T \Sigma^{-1}(x-\mu_i)\right)} \dots (iii)$$

Plugging the equation (iii) in (i) and calculating the odds ratio (eqn ii), we get,

$$\frac{P(Y = 1 | X = x)}{P(Y = 2 | X = x)} = \frac{\pi_1 e^{\left(-\frac{1}{2}(x-\mu_1)^T \Sigma^{-1}(x-\mu_1)\right)}}{\pi_2 e^{\left(-\frac{1}{2}(x-\mu_2)^T \Sigma^{-1}(x-\mu_2)\right)}}$$

Taking logarithm (a monotone increasing function) in both sides and calculating the log-odds ratio, we get,

$$\log\left(\frac{P(Y = 1 | X = x)}{P(Y = 2 | X = x)}\right)$$

= $\log\left(\frac{\pi_1}{\pi_2}\right) - \frac{1}{2}(\mu_1 + \mu_2)^T \Sigma^{-1}(\mu_1 - \mu_2) + x^T(\mu_1 - \mu_2)\Sigma^{-1}...(iii)$

The above equation can be expressed in the form,

$$\log\left(\frac{P(Y = 1 | X = x)}{P(Y = 2 | X = x)}\right) = \beta^{T}x + \beta_{0},$$

$$\beta = (\mu_{1} - \mu_{2})\Sigma^{-1}$$

$$\beta_{0} = -\frac{1}{2}(\mu_{1} + \mu_{2})^{T}\Sigma^{-1}(\mu_{1} - \mu_{2}) + \log\left(\frac{\pi_{1}}{\pi_{2}}\right)$$

The log-odds function is linear in x and describes a line.

Note: The decision boundary of the two classes is the set of points where,

$$P(Y = 1 | X = x) = P(Y = 2 | X = x)$$

or,
$$\log\left(\frac{P(Y = 1 | X = x)}{P(Y = 2 | X = x)}\right) = 0$$

The linear log-odds function implies that LDA is a linear classifier.

Equivalently, from equation (iii) the decision rule of LDA can be described as, $G(x) = argmax_k \delta_k(x),$ $\delta_k(x) = \log(\pi_k) - \frac{1}{2}\mu_k^T \Sigma^{-1} \mu_k + x^T \Sigma^{-1} \mu_k$

Estimating the parameters of LDA classifier

- In a real-world dataset, we cannot determine the parameters of the Gaussian distribution.
- The implementation of the algorithm includes the estimation of the parameters of the decision rule.
- The parameters are calculated and estimated using the following rule,
 - **Proportion of observations** belonging to kth class:

$$\hat{\pi}_k = \frac{N_k}{N}, \qquad k = 1,2$$

• Mean of the observations belonging to that class:

$$\hat{\mu}_k = \frac{\sum_{i=1}^{N_k} x_i}{N_k}, \qquad k = 1,2$$

• Covariance matrix:

$$\hat{\Sigma} = \frac{\sum_{k=1}^{K} \sum_{i=1}^{N_k} (x_i - \hat{\mu}_k) (x_i - \hat{\mu}_k)^T}{(N - K)}, \ K = 2$$

The LDA rule classifies to class 1 if

$$x^{T}(\widehat{\mu}_{1}-\widehat{\mu}_{2})\widehat{\Sigma}^{-1} > \frac{1}{2}(\widehat{\mu}_{1}+\widehat{\mu}_{2})^{T}\widehat{\Sigma}^{-1}(\widehat{\mu}_{1}-\widehat{\mu}) - \log\left(\frac{N_{2}}{N_{1}}\right)$$

References

- The Elements of Statistical Learning
- An Introduction to Statistical Learning with Applications in R
- Modern Multivariate Statistical Techniques