

Linear Discriminant Analysis (LDA).

Data $\{(y_i, x_i)_{i=1}^n\}$

Assumptions: $X|Y=0 \sim N_p(\mu_0, \Sigma)$ $X|Y=1 \sim N_p(\mu_1, \Sigma)$

Optimal Bayes Classifier = $I\{P(Y=1|X) \geq P(Y=0|X)\}$.

more generally, $\hat{k} = \underset{k}{\operatorname{argmax}} P(Y=k|X)$

$$\log f_0 = \frac{1}{2} \log |\Sigma| + \frac{1}{2} (X - \mu_0)^T \Sigma^{-1} (X - \mu_0) \quad (X|Y=0)$$

$$\log f_1 = \frac{1}{2} \log |\Sigma| + \frac{1}{2} (X - \mu_1)^T \Sigma^{-1} (X - \mu_1) \quad (X|Y=1)$$

$$P(Y=0|X) = \frac{P(Y=0, X)}{P(X)} = \frac{P(X|Y=0)P(Y=0)}{P(X|Y=0)P(Y=0) + P(X|Y=1)P(Y=1)} \quad \text{Bayes' Formulae.}$$

$$P(Y=0) = \pi, \quad P(Y=1) = 1 - \pi, \quad \text{then,}$$

$$P(Y=0|X) = \frac{\pi f_0}{\pi f_0 + (1-\pi) f_1}, \quad P(Y=1|X) = \frac{(1-\pi) f_1}{\pi f_0 + (1-\pi) f_1}$$

$$P(Y=1|X) \geq P(Y=0|X) \Leftrightarrow \frac{(1-\pi) f_1}{\pi f_0 + (1-\pi) f_1} \geq \frac{1}{2}$$

$$\Leftrightarrow \frac{(1-\pi)}{\pi \cdot f_0 / f_1 + (1-\pi)} \geq \frac{1}{2} \Leftrightarrow (1-\pi) \geq \frac{1}{2} \pi \frac{f_0}{f_1} + \frac{1}{2} (1-\pi)$$

$$\Leftrightarrow \frac{1}{2} (1-\pi) \geq \frac{1}{2} \pi \cdot \frac{f_0}{f_1} \Leftrightarrow \frac{1-\pi}{\pi} \geq \frac{f_0}{f_1} \Leftrightarrow \log \frac{1-\pi}{\pi} \geq \log \frac{f_0}{f_1}$$

$$\log \frac{f_0}{f_1} = \log f_0 - \log f_1 = -|X - \mu_0|^T \Sigma^{-1} (X - \mu_0) + |X - \mu_1|^T \Sigma^{-1} (X - \mu_1)$$

$$= -(\mu_1 - \mu_0)^T \Sigma^{-1} X - \frac{1}{2} \mu_0^T \Sigma^{-1} \mu_0 + \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 \leq \log \frac{1-\pi}{\pi}$$

$$\Leftrightarrow (\mu_1 - \mu_0)^T \Sigma^{-1} X \leq C, \quad C = (*) - (**).$$

classify as class 1 if $(\hat{\mu}_1 - \hat{\mu}_0)^T \hat{\Sigma}^{-1} x \leq c$

$$c = \log\left(\frac{1-\pi}{\pi}\right) + \frac{1}{2} \hat{\mu}_1^T \hat{\Sigma}^{-1} \hat{\mu}_1 - \frac{1}{2} \hat{\mu}_0^T \hat{\Sigma}^{-1} \hat{\mu}_0$$

If we can obtain (from data): $X: (X_1, \dots, X_{n_0}, X_{n_0+1}, \dots, X_{n_0+n_1})$
 $Y: (0, \dots, 0, 1, \dots, 1)$

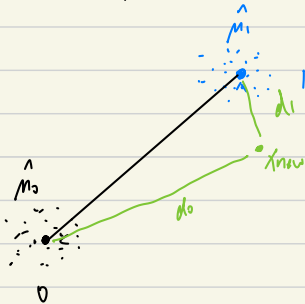
$$\hat{\mu}_0 = \frac{1}{n_0} \sum_{i=1}^{n_0} X_i \quad \hat{\mu}_1 = \frac{1}{n_1} \sum_{i=n_0+1}^{n_0+n_1} X_i \quad \hat{\pi} = \frac{n_1}{n}$$

Let $\begin{cases} X_{ij} = X_j & \text{if } i=0 \\ X_{ij} = X_{j+n_0} & \text{if } i=1 \end{cases} \quad \begin{pmatrix} X_1, \dots, X_{n_0} = X_{01}, \dots, X_{0n_0} \\ X_{n_0+1}, \dots, X_{n_0+n_1} = X_{11}, \dots, X_{1n_1} \end{pmatrix}$

$$\hat{\Sigma} = \frac{1}{n-2} \sum_{j=1}^2 \sum_{i=1}^{n_j} (X_{ji} - \bar{X}_j) (X_{ji} - \bar{X}_j)^T$$

We can classify new observation x_{new} by:

$$I\left((\hat{\mu}_1 - \hat{\mu}_0)^T \hat{\Sigma}^{-1} x_{new} \leq \hat{c}\right) = \text{guess}(x_{new})$$



$d_0 > d_1$
 $\Rightarrow x_{new}$ is "closer" to $\hat{\mu}_1$ than $\hat{\mu}_0$.
 \Rightarrow classify as class 1.

Quadratic Discriminant Analysis (QDA).

$$X|Y=0 \sim N_p(\mu_0, \Sigma_0), \quad X|Y=1 \sim N_p(\mu_1, \Sigma_1).$$

$$\log f_0 = \frac{1}{2} \log |\Sigma_0| + \frac{1}{2} (X - \mu_0)^T \Sigma_0^{-1} (X - \mu_0)$$

$$\log f_1 = \frac{1}{2} \log |\Sigma_1| + \frac{1}{2} (X - \mu_1)^T \Sigma_1^{-1} (X - \mu_1)$$

$$\log f_0 - \log f_1 = \text{const.} + \frac{1}{2} (X - \mu_0)^T \Sigma_0^{-1} (X - \mu_0) - \frac{1}{2} (X - \mu_1)^T \Sigma_1^{-1} (X - \mu_1)$$

$$= \text{const.} + \frac{1}{2} X^T (\Sigma_0^{-1} - \Sigma_1^{-1}) X - X^T \Sigma_0^{-1} \mu_0 + \frac{1}{2} \mu_0^T \Sigma_0^{-1} \mu_0$$

$$+ X^T \Sigma_1^{-1} \mu_1 - \frac{1}{2} \mu_1^T \Sigma_1^{-1} \mu_1.$$

$$= \text{const.} + \frac{1}{2} X^T (\Sigma_0^{-1} - \Sigma_1^{-1}) X - X^T (\Sigma_0^{-1} \mu_0 - \Sigma_1^{-1} \mu_1) \geq \underbrace{\left(\log \frac{1 - \pi}{\pi} \right)}$$

classify as class 1 if $\frac{1}{2} X^T (\Sigma_0^{-1} - \Sigma_1^{-1}) X - X^T (\Sigma_0^{-1} \mu_0 - \Sigma_1^{-1} \mu_1) \geq c$.

$$c = \log \left(\frac{1 - \pi}{\pi} \right) - \frac{1}{2} \mu_0^T \Sigma_0^{-1} \mu_0 + \frac{1}{2} \mu_1^T \Sigma_1^{-1} \mu_1 - \frac{1}{2} \log |\Sigma_0| + \frac{1}{2} \log |\Sigma_1|$$

For a new observation X_{new} ,

$$g_{\text{bayes}}(X_{\text{new}}) = \mathbb{I}(h(X_{\text{new}}) \geq c)$$

$$I \left(\log \frac{f_0}{f_1} \geq \frac{1-\pi}{\pi} \right)$$

Nonparametric Estimation of f_0, f_1 .

LDA, QDA are restrictive in the way that we have to assume a $N_p(\dots)$.
A more flexible approach is to estimate f_0, f_1 using nonparametric estimation.

HW3 Q2, Q3.

- KDE (Kernel Density Estimation).
- Smoothing Spline.

Idea: optimal bayes classifier

$$g_{\text{bayes}}(x) = I \left\{ \log \left(\frac{f_0(x)}{f_1(x)} \right) \geq \log \frac{1-\pi}{\pi} \right\}$$

1. Obtain $\hat{f}_0, \hat{f}_1, \hat{\pi} = \frac{n_0}{n}$.

2. $\hat{g}_{\text{bayes}}(x_{\text{new}}) = I \left\{ \log \left(\frac{\hat{f}_0(x_{\text{new}})}{\hat{f}_1(x_{\text{new}})} \right) \geq \log \left(\frac{1-\hat{\pi}}{\hat{\pi}} \right) \right\}$

KDE: $f(x) \approx \frac{1}{n} \sum_{i=1}^n K_h(x_i - x)$, $K_h(u) = \frac{1}{h} K\left(\frac{u}{h}\right)$, $K(\cdot)$ predetermined.

Popular choice of $K(\cdot) = \Phi(\cdot)$ standard normal cdf.

Best choice of $K(\cdot) = E\text{-kernel} = K(u) = (1-u)^2 I(|u| \leq 1)$

Idea: $f(x) = \frac{d}{dx} F(x) = \lim_{h \rightarrow 0} \frac{F(x+h) - F(x-h)}{2h} = \lim_{h \rightarrow 0} \frac{P(x-h \leq X \leq x+h)}{2h}$

Let $P = F_n$ empirical measure, $F_n(x) = \frac{1}{n} \sum_{i=1}^n I(X_i \leq x)$, then,

$$f(x) = \lim_{h \rightarrow 0} \frac{1}{2h} \frac{1}{n} \sum_{i=1}^n I(x-h \leq X_i \leq x+h)$$

When h is small, then,

$$f(x) \approx \frac{1}{2nh} \sum_{i=1}^n I(-h \leq X_i - x \leq h) = \frac{1}{n} \sum_{i=1}^n \frac{1}{2h} I(|X_i - x| \leq h)$$

$$K_h(\cdot) = \frac{1}{2h} I(|X_i - x| \leq h) \quad K(\cdot) = \frac{1}{2} I(|X_i - x| \leq 1)$$

\Rightarrow numerical stability: $K(\cdot) = \frac{1}{2} I(\cdot)$.

$$\hat{f}_0(x) = \frac{1}{n_0} \sum_{i=1}^{n_0} K_h(X_{0i} - x)$$

$$\hat{f}_1(x) = \frac{1}{n_1} \sum_{i=1}^{n_1} K_h(X_{1i} - x).$$

What is our h ? Hyperparameter selection.

$$\hat{h} = \arg \min_h CV(h)$$