目录

1 线性判别分析

1.1 问题定义

数据数学表示形式为:

$$
\begin{aligned}
& X = (x_1, x_2, ..., x_N)^T = \begin{pmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{pmatrix}_{N*P} \\
& Y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}_{N\times 1}
\end{aligned} \tag{1}
$$

$$
\begin{aligned}
& \{(x_i, y_i)\}_{i=1}^N, x_i \in \mathbb{R}^p, y_i \in \{+1, -1\} \\
& x_{c_1} = \{x_i | y_i = +1\}, \quad x_{c_2} = \{x_i | y_i = -1\} \\
& |x_{c_1}| = N_1, |x_{c_2}| = N_2, N_1 + N_2 = N
\end{aligned} \tag{2}
$$

其中 $c_1 = +1, c_2 = -1$, N, N_1, N_2 分别表示样本总数，正样本数量以及负样本数量，x_{c_1}, x_{c_2} 分布表示正样本集合与负样本集合。

1.2 核心思想

类内小，类间大 (高内聚，低耦合)

1.3 目标函数

1.3.1 目标函数的设计

为了实现”类内小，类间大”的目标。我们要使得，不同类别的均值之间的差值尽可能大，各个类别类内的方差尽可能小。单一类别的均值与方差可以表示为如下形式。

$$
\begin{aligned}
z_i &= w^\top x_i \\
\bar{z} &= \frac{1}{N}\sum_{i=1}^{N} z_i = \frac{1}{N}\sum_{i=1}^{N} w^\top x_i \\
S_z &= \frac{1}{N}\sum_{i=1}^{N} \left(z_i-\bar{z}\right)\left(z_i-\bar{z}\right)^\top \\
&= \frac{1}{N}\sum_{i=1}^{N} \left(w^\top x_i-\bar{z}\right)\left(w^\top x_i-\bar{z}\right)^\top
\end{aligned} \tag{3}
$$

因此更进一步，c_1, c_2 类别对应的均值与方差可以表示为如下形式:

$$
\begin{aligned}
C_1 : \bar{z}_1 &= \frac{1}{N_1}\sum_{i=1}^{N_1} w^\top x_i \\
S_1 &= \frac{1}{N_1}\sum_{i=1}^{N_1} \left(w^\top x_i-\bar{z}_1\right)\left(w^\top x_i-\bar{z}_1\right)^\top \\
C_2 : \bar{z}_2 &= \frac{1}{N_2}\sum_{i=1}^{N_2} w^\top x_i \\
S_2 &= \frac{1}{N_2}\sum_{i=1}^{N_2} \left(w^T x_i-\bar{z}_2\right)\left(w^\top x_i-\bar{z}_2\right)^\top
\end{aligned} \tag{4}
$$

类内距离可以表示为：$S_1 + S_2$ 类间距离可以表示为: $\left(\bar{z}_1-\bar{z}_2\right)^2$ 要达到类内小，类间大的效果，目标函数最终设计为:

$$
J(w) = \frac{\left(\bar{z}_1-\bar{z}_2\right)^2}{S_1+S_2} \tag{5}
$$

1.3.2 目标函数的推导

对目标函数 $J(w)=\frac{(\bar{z}_1-\bar{z}_2)^2}{S_1+S_2}$ 分子与分母进行进一步的展开。

$$
\begin{aligned}
molecule &= \left(\frac{1}{N_1}\sum_{i=1}^{N_1} w^\top x_i - \frac{1}{N_2}\sum_{j=1}^{N_2} w^\top x_i\right)^2 = \left[w^\top\left(\frac{1}{N_1}\sum_{i=1}^{n} x_i - \frac{1}{N_2}\sum_{i=1}^{n} x_i\right)\right]^2 \\
&= \left(w^\top\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)\right)^2 = w^\top\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)^\top \cdot w
\end{aligned} \tag{6}
$$

$$
\begin{aligned}
S_1 &= \frac{1}{N_1}\sum_{i=1}^{N_1}\left(w^\top x_i - \frac{1}{N_1}\sum_{j=1}^{N} w^\top x_j\right)\left(w^\top x_i - \frac{1}{N_1}\sum_{j=1}^{N_1} w^\top x_j\right)^\top \\
&= \frac{1}{N_1}\sum_{i=1}^{N_1} w^\top\left(x_i - \quad \bar{x}_{c_1}\right)\left(x_i-\bar{x}_{c_1}\right)^\top w \\
&= w^\top\left[\frac{1}{N_1}\sum_{i=1}^{N}\left(x_i-\overline{x_{c_1}}\right)\left(x_i-\bar{x}_{c_1}\right)^\top\right] w \\
&= w^T \cdot S_{c_1} \cdot w \\
&= w^\top S_{c_1} w
\end{aligned} \tag{7}
$$

$$
\begin{aligned}
Denominator &= S_1 + S_2 \\
&= w^T S_{c_1} w + w^T S_{c_2} w \\
&= W^T\left(S_{c_1}+S_{c_2}\right) w
\end{aligned} \tag{8}
$$

所以最终目标函数可以表示为

$$
J(w) = \frac{w^T\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)^T w}{w^T\left(S_{c_1}+S_{c_2}\right) w} \tag{9}
$$

1.4 参数求解

根据上一节我们推导出目标函数为如下形式

$$
J(w) = \frac{w^T\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)\left(\bar{x}_{c_1}-\bar{x}_{c_2}\right)^T w}{w^T\left(S_{c_1}+S_{c_2}\right) w} \tag{10}
$$

在此我们将会推导 w 。首先我们为了简化运算使得

$$\begin{aligned}
&S_b = \left(\bar{x}_{c_1} - \bar{x}_{c_2}\right)\left(\bar{x}_{c_1} - \bar{x}_{c_2}\right)^T \\
&S_w = S_{c_1} + S_{c_2} \\
&J\left(w\right) = \frac{w^T S_b w}{w^T S_w w} = w^T S_b w (w^T S_w w)^{-1}
\end{aligned} \tag{11}$$

进一步，我们使得 $\frac{\partial J(w)}{\delta w} = 0$ 以推导 w (这里假设 w 的最优解为导数为 0 的时候) 。

$$\begin{aligned}
\frac{\partial J\left(w\right)}{\partial w} &= 2S_b w \cdot \left(w^T S_w w\right)^{-1} + w^T S_b w \cdot (-1)\left(w^T S_w w\right)^{-2} \cdot 2S_w w = 0 \\
S_b w\left(w^T S_w w\right) &= \left(w^T S_b w\right) S_w w, \quad \left(w^T S_w w\right), \left(w^T s_w w\right) \in \mathbb{R} \\
S_w w &= \frac{w^T S_w w}{w^T S_b w} S_b w \\
w &= \frac{w^T S_w w}{w^T S_b w} S_w^{-1} S_b w \\
w &\propto S_w^{-1} S_b w \\
w &\propto S_w^{-1} (\bar{x}_{c_1} - \bar{x}_{c_2})(\bar{x}_{c_1} - \bar{x}_{c_2})^T w, \quad (\bar{x}_{c_1} - \bar{x}_{c_2})^T w \in \mathbb{R} \\
w &\propto S_w^{-1}\left(\bar{x}_{c_1} - \bar{x}_{c_2}\right)
\end{aligned} \tag{12}$$

当 S_w 对角且各项同性, $S_w^{-1} \propto I$

$$w \propto \left(\bar{x}_{c_1} - \bar{x}_{c_2}\right) \tag{13}$$