第 3 章作业答案

1

1.1

$$
\begin{aligned}
L &= \prod_{i=1}^{n} p(y_i|\boldsymbol{x}_i;\boldsymbol{w},w_0) \\
&= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(y_i-\boldsymbol{w}^T\boldsymbol{x}_i-w_0)^2}{2\sigma^2}) \\
&= (2\pi\sigma^2)^{-\frac{n}{2}} \exp(-\sum_{i=1}^{n} \frac{(y_i-\boldsymbol{w}^T\boldsymbol{x}_i-w_0)^2}{2\sigma^2})
\end{aligned}
$$

1.2

记 $\boldsymbol{w}' = \begin{bmatrix} \boldsymbol{w} \\ w_0 \end{bmatrix}$, $\boldsymbol{x}_i' = \begin{bmatrix} \boldsymbol{x}_i \\ 1 \end{bmatrix}$, $\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1'^T \\ \boldsymbol{x}_2'^T \\ \dots \\ \boldsymbol{x}_n'^T \end{bmatrix}$, $\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$,

$$
\begin{aligned}
\log L(\boldsymbol{w},w_0) &= -\frac{n}{2}\log(2\pi\sigma^2) - \sum_{i=1}^{n}\frac{(y_i-\boldsymbol{w}^T\boldsymbol{x}_i-x_0)^2}{2\sigma^2} \\
&= -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}')^T(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}')
\end{aligned}
$$

$$
\frac{\partial \log L}{\partial \boldsymbol{w}'} = -\frac{1}{2\sigma^2}(-2\boldsymbol{X}^T\boldsymbol{y} + 2\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}') = 0
$$

$$
\boldsymbol{w}' = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}
$$

最大化对数似然 $logL$ 等价于最小化平方误差和 $(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})$，与最小二乘法的目标一致，解也相同。

2

2.1

对 $\forall \boldsymbol{x} \in \mathbb{R}^d$

$$\begin{aligned}
\boldsymbol{x}^T \boldsymbol{S}_i \boldsymbol{x} &= \boldsymbol{x}^T (\sum_{\boldsymbol{x}_j \in \mathcal{X}_i} (\boldsymbol{x}_j - \boldsymbol{m}_i)(\boldsymbol{x}_j - \boldsymbol{m}_i)^T) \boldsymbol{x} \\
&= \sum_{\boldsymbol{x}_j \in \mathcal{X}_i} \boldsymbol{x}^T (\boldsymbol{x}_j - \boldsymbol{m}_i)(\boldsymbol{x}_j - \boldsymbol{m}_i)^T \boldsymbol{x} \\
&= \sum_{\boldsymbol{x}_j \in \mathcal{X}_i} ((\boldsymbol{x}_j - \boldsymbol{m}_i)^T \boldsymbol{x})^T (\boldsymbol{x}_j - \boldsymbol{m}_i)^T \boldsymbol{x} \\
&\geq 0
\end{aligned}$$

$$\boldsymbol{x}^T \boldsymbol{S}_w \boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{S}_1 \boldsymbol{x} + \boldsymbol{x}^T \boldsymbol{S}_2 \boldsymbol{x} \geq 0$$

$$\begin{aligned}
\boldsymbol{x}^T \boldsymbol{S}_b \boldsymbol{x} &= \boldsymbol{x}^T ((\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T) \boldsymbol{x} \\
&= ((\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{x})^T (\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{x} \\
&\geq 0
\end{aligned}$$

所以，$\boldsymbol{S}_w, \boldsymbol{S}_b$ 半正定。

设 $\boldsymbol{S}_b$ 的特征值为 λ，则

$$\begin{aligned}
&\boldsymbol{S}_b(\boldsymbol{m}_1 - \boldsymbol{m}_2) = \lambda(\boldsymbol{m}_1 - \boldsymbol{m}_2) \\
&(\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T(\boldsymbol{m}_1 - \boldsymbol{m}_2) = \lambda(\boldsymbol{m}_1 - \boldsymbol{m}_2)
\end{aligned}$$

当 $\boldsymbol{m}_1 \neq \boldsymbol{m}_2$ 时，$(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)$ 是非零标量，$\boldsymbol{S}_b$ 只有一个非零特征值 $\lambda = (\boldsymbol{m}_1 - \boldsymbol{m}_2)^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)$，对应的特征向量为 $(\boldsymbol{m}_1 - \boldsymbol{m}_2)$。

2.2

$$\max_{\boldsymbol{w} \neq \boldsymbol{0}} \frac{\boldsymbol{w}^\top \boldsymbol{S}_b \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{S}_w \boldsymbol{w}}$$

等价于

$$\begin{aligned}
&\max_{\boldsymbol{w} \neq \boldsymbol{0}} \boldsymbol{w}^\top \boldsymbol{S}_b \boldsymbol{w} \\
\text{s.t.} \quad &\boldsymbol{w}^\top \boldsymbol{S}_w \boldsymbol{w} = c
\end{aligned}$$

使用拉格朗日乘子法

$$
\begin{gathered}
L(\boldsymbol{w}, \lambda) = \boldsymbol{w}^\top \boldsymbol{S}_b \boldsymbol{w} - \lambda(\boldsymbol{w}^\top \boldsymbol{S}_w \boldsymbol{w} - c) \\
\frac{\partial L(\boldsymbol{w}, \lambda)}{\partial \boldsymbol{w} = 2\boldsymbol{S}_b \boldsymbol{w} - 2\lambda \boldsymbol{S}_w \boldsymbol{w} = 0}
\end{gathered}
$$

若 $\boldsymbol{S}_w$ 可逆，则

$$
\begin{aligned}
\boldsymbol{S}_w^{-1} \boldsymbol{S}_b \boldsymbol{w} &= \lambda \boldsymbol{w} \\
\boldsymbol{S}_w^{-1} (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{w} &= \lambda \boldsymbol{w}
\end{aligned}
$$

因为 $(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{w}$ 是标量，只考虑 $\boldsymbol{w}$ 的方向，取 $\boldsymbol{w} = \boldsymbol{S}_w^{-1}(\boldsymbol{m}_1 - \boldsymbol{m}_2)$，此时 J_F 取最大值。

课件和教材上均有答案。

2.3

$$
\begin{gathered}
\boldsymbol{m}_1 = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, \boldsymbol{m}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \\
\boldsymbol{S}_w = \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix} \\
\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w} = 0
\end{gathered}
$$

解得 $\boldsymbol{w} = \begin{bmatrix} 1 & 0 \end{bmatrix}$

此时所有样本的投影都为 1，对分类无效。

3

3.1

因为最小二乘法的目标是最小化 SSE

$$
\begin{aligned}
\mathrm{SSE} &= \sum_{i=1}^{n} (y_i - \hat{y})^2 \\
&= \sum_{i=1}^{n} (y_i - w x_i - w_0)^2
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathrm{SSE}}{\partial w} &= \sum_{i=1}^{n} 2(y_i - wx_i - w_0)x_i = -\sum_{i=1}^{n} 2(y_i - \hat{y})x_i = 0 \\
\frac{\partial \mathrm{SSE}}{\partial w_0} &= \sum_{i=1}^{n} 2(y_i - wx_i - w_0) = -\sum_{i=1}^{n} 2(y_i - \hat{y}) = 0
\end{aligned}
$$

所以

$$
\begin{aligned}
\mathrm{SST} &= \sum_{i=1}^{n} (y_i - \bar{y})^2 \\
&= \sum_{i=1}^{n} (y_i - \hat{y} + \hat{y} - \bar{y})^2 \\
&= \sum_{i=1}^{n} (y_i - \hat{y})^2 + \sum_{i=1}^{n} (y_i - \hat{y})^2 + \sum_{i=1}^{n} 2(y_i - \hat{y})(\hat{y} - \bar{y}) \\
&= \mathrm{SSE} + \mathrm{SSR} + 2\sum_{i=1}^{n} (y_i - \hat{y})(\hat{y} - \bar{y}) \\
&= \mathrm{SSE} + \mathrm{SSR} + 2\sum_{i=1}^{n} ((y_i - \hat{y})\hat{y} - (y_i - \hat{y})\bar{y}) \\
&= \mathrm{SSE} + \mathrm{SSR} + 2\sum_{i=1}^{n} ((y_i - \hat{y})(wx + w_0) - (y_i - \hat{y})\bar{y}) \\
&= \mathrm{SSE} + \mathrm{SSR}
\end{aligned}
$$

3.2

$$
\begin{aligned}
R^2 &= 1 - \frac{\mathrm{SSE}}{\mathrm{SST}} \\
&= \frac{\sum_{i=1}^{n} (\hat{y} - \bar{y})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \\
&= \frac{\sum_{i=1}^{n} (w(x - \bar{x}))^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \\
&= w^2 \frac{\sum_{i=1}^{n} (x - \bar{x})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}
\end{aligned}
$$

因为

$$
w = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}
$$

所以

$$\begin{aligned}
R^2 &= (\frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2})^2 \frac{\sum_{i=1}^n (x - \bar{x})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\
&= \frac{(\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}))^2}{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2} \\
&= r^2
\end{aligned}$$