

• 7.1

$$\begin{aligned}
\sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) &= \text{trace}(\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) \sigma_\epsilon^2 \\
&= \text{trace}((\mathbf{X}^T \mathbf{X})(\mathbf{X}^T \mathbf{X})^{-1}) \sigma_\epsilon^2 \\
&= \text{trace}(I) \sigma_\epsilon^2 \\
&= d \sigma_\epsilon^2
\end{aligned}$$

又因为

$$E_{\mathbf{y}}(\text{Err}_{\text{in}}) = E_{\mathbf{y}}(\overline{\text{err}}) + E(\text{op}) = E_{\mathbf{y}}(\overline{\text{err}}) + \frac{2}{N} \sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i)$$

所以

$$E_{\mathbf{y}}(\text{Err}_{\text{in}}) = E_{\mathbf{y}}(\overline{\text{err}}) + \frac{2}{N} d \sigma_\epsilon^2$$

也就是式(7.24)。

• 7.3

(1)

$$\begin{aligned}
\hat{f}^{-i}(x_i) &= x_i^T (\mathbf{X}_{-i}^T \mathbf{X}_{-i} + \lambda \mathbf{I})^{-1} \mathbf{X}_{-i}^T \mathbf{y}_{-i} \\
&= x_i^T (\mathbf{X}^T \mathbf{X} - x_i x_i^T + \lambda \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y} - x_i y_i)
\end{aligned}$$

由Woodbury矩阵恒等式

$$(\mathbf{A} + UCV)^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}U(C^{-1} + V\mathbf{A}^{-1}U)^{-1}V\mathbf{A}^{-1}$$

令 $U = x_i, C = 1, V = x_i^T, \mathbf{A} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})$ 。

$$\begin{aligned}
(\mathbf{A} - x_i x_i^T)^{-1} &= \mathbf{A}^{-1} + \mathbf{A}^{-1} x_i (1 - x_i^T \mathbf{A}^{-1} x_i)^{-1} x_i^T \mathbf{A}^{-1} \\
&= \mathbf{A}^{-1} + \frac{\mathbf{A}^{-1} x_i x_i^T \mathbf{A}^{-1}}{1 - x_i^T \mathbf{A}^{-1} x_i}
\end{aligned}$$

于是

$$\begin{aligned}
\hat{f}^{-i}(x_i) &= x_i^T \left(\mathbf{A}^{-1} + \frac{\mathbf{A}^{-1} x_i x_i^T \mathbf{A}^{-1}}{1 - x_i^T \mathbf{A}^{-1} x_i} \right) (\mathbf{X}^T \mathbf{y} - x_i y_i) \\
&= \left(x_i^T \mathbf{A}^{-1} + \frac{x_i^T \mathbf{A}^{-1} x_i x_i^T \mathbf{A}^{-1}}{1 - S_{ii}} \right) (\mathbf{X}^T \mathbf{y} - x_i y_i)
\end{aligned}$$

其中 $x_i^T \mathbf{A}^{-1} x_i = x_i^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} x_i = S_{ii}$,

$$\begin{aligned}
\hat{f}^{-i}(x_i) &= \left(x_i^T \mathbf{A}^{-1} + \frac{S_{ii} x_i^T \mathbf{A}^{-1}}{1 - S_{ii}} \right) (\mathbf{X}^T \mathbf{y} - x_i y_i) \\
&= x_i^T \mathbf{A}^{-1} \mathbf{X}^T \mathbf{y} - x_i^T \mathbf{A}^{-1} x_i y_i + \frac{S_{ii} x_i^T \mathbf{A}^{-1} \mathbf{X}^T \mathbf{y}}{1 - S_{ii}} - \frac{S_{ii} x_i^T \mathbf{A}^{-1} x_i y_i}{1 - S_{ii}}
\end{aligned}$$

其中 $x_i^T \mathbf{A}^{-1} \mathbf{X}^T \mathbf{y} = x_i^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y} = \hat{f}(x_i)$ 。

$$\begin{aligned}
\hat{f}^{-i}(x_i) &= \hat{f}(x_i) - S_{ii} y_i + \frac{S_{ii} \hat{f}(x_i)}{1 - S_{ii}} - \frac{S_{ii}^2 y_i}{1 - S_{ii}} \\
&= \frac{\hat{f}(x_i) - S_{ii} y_i}{1 - S_{ii}}
\end{aligned}$$

所以

$$y_i - \hat{f}^{-i}(x_i) = \frac{y_i - \hat{f}(x_i)}{1 - S_{ii}}$$

(2)

由于 \mathbf{S} 是实对称矩阵且 $\mathbf{S}\mathbf{S} \preceq \mathbf{S}$ ，所以

$$S_{ii} \geq \sum_k S_{ik} S_{ki} = \sum_k S_{ik}^2 \geq S_{ii}^2$$

有 $0 \leq S_{ii} \leq 1$ ，结合上一问的结论

$$\begin{aligned} |y_i - \hat{f}^{-i}(x_i)| &= \left| \frac{y_i - \hat{f}(x_i)}{1 - S_{ii}} \right| \\ &= |y_i - \hat{f}(x_i)| \cdot \frac{1}{|1 - S_{ii}|} \\ &\geq |y_i - \hat{f}(x_i)| \end{aligned}$$

(3)

只需要 \mathbf{S} 与 \mathbf{y} 无关，第一问中的结论就依然成立。

把平滑矩阵的一般形式写成 $\mathbf{S} = \mathbf{N}(\mathbf{N}^T \mathbf{N} + \lambda \mathbf{\Omega})^{-1} \mathbf{N}^T$ 。 \mathbf{N} 是一个与 \mathbf{X} 有关的同尺寸矩阵，且 \mathbf{N} 的第 i 列只与 \mathbf{x}_i 有关。那么我们可以将第一问中所有的 \mathbf{X} 用 \mathbf{N} 替换， \mathbf{x}_i 用 N_i 替换，第一问中的推导依然成立。

• 7.4

$$\begin{aligned} E(\text{op}) &= E[\text{Err}_{\text{in}} - \overline{\text{err}}] \\ &= E \left[\frac{1}{N} \sum_{i=1}^N E_{Y^0} (Y^0 - \hat{f}(x_i))^2 - \frac{1}{N} \sum_{i=1}^N (y_i - \hat{f}(x_i))^2 \right] \\ &= \frac{1}{N} E \left[\sum_{i=1}^N -y_i^2 - y_i E_{Y^0} Y^0 + 2\hat{f}(x_i) y_i + E_{Y^0} Y^0 y_i + E_{Y^0} Y^{0^2} - 2E_{Y^0} Y^0 \hat{f}(x_i) \right] \end{aligned}$$

上式中

$$E \sum_{i=1}^N -y_i^2 E_{Y^0} Y^{0^2} + E_{Y^0} Y^{0^2} = \sum_{i=1}^N E(E_{Y^0} Y^{0^2} - y_i^2 E_{Y^0} Y^{0^2}) = 0$$

$$E \sum_{i=1}^N -y_i E_{Y^0} Y^0 + E_{Y^0} Y^0 y_i = 0$$

所以

$$\begin{aligned} E(\text{op}) &= \frac{1}{N} E \sum_{i=1}^N 2\hat{f}(x_i) y_i - 2E_{Y^0} Y^0 \hat{f}(x_i) \\ &= \frac{2}{N} \sum_{i=1}^N \text{Cov}(\hat{f}(x_i), y_i) \end{aligned}$$

• 7.5

$$\begin{aligned} \sum_{i=1}^N \text{Cov}(\hat{y}_i, y_i) &= \text{trace}(\text{Cov}(\mathbf{S}\mathbf{y}, \mathbf{y})) \\ &= \text{trace}(\mathbf{S}\text{Var}(\mathbf{y})) \\ &= \text{trace}(\mathbf{S})\sigma_\epsilon^2 \end{aligned}$$