理论题 1

- 令 $\boldsymbol{X}_s$ 表示经标准化后的特征，即 $\boldsymbol{X}_s = (\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_p)$ 中 $n^{-1}\sum_{i=1}^{n} x_{ij} = 0$ 而 $\sum_{i=1}^{n} x_{ij}^2 = 1$。$\boldsymbol{X}_s$ 的相关系数矩阵为 $(\boldsymbol{X}_s'\boldsymbol{X}_s)$，其逆矩阵为 $(\boldsymbol{X}_s'\boldsymbol{X}_s)^{-1} = \boldsymbol{C} = \{c_{ij}\}$。我们将 x_j 作为因变量，而将剩余的特征作为自变量，建立多元线性回归模型，即

$$x_j = \beta_1^j x_1 + \cdots + \beta_{j-1}^j x_{j-1} + \beta_{j+1}^j x_{j+1} + \cdots + \beta_p^j x_p + \varepsilon^j.$$

令 R_j^2 为该回归模型的复决定系数。证明:

$$c_{jj} = \frac{1}{1 - R_j^2}.$$

证明：对任意 $j \in \{1, 2, \dots, p\}$，设

$$T_j = \begin{bmatrix} & 1 & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ 1 & & & & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix}$$

则

$$T_j^{-1} = \begin{bmatrix} & & & 1 & & & \\ 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix} = T_j^T.$$

若令 $X_t = (x_j, X_0)$，其中 $X_0 = (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_p)$

则 $X_t = X_s T_j$. $\therefore X_s = X_t T_j^T$.

$$
\begin{aligned}
\therefore C &= (X_s^T X_s)^{-1} \\
&= ((X_t T_j^T)^T (X_t T_j^T))^{-1} \\
&= (T_j X_t^T X_t T_j^T)^{-1} \\
&= T_j (X_t^T X_t)^{-1} T_j^T .
\end{aligned}
$$

$$\because X_t^T X_t = \begin{pmatrix} x_j^T \\ X_0^T \end{pmatrix} (x_j \quad X_0) = \begin{pmatrix} x_j^T x_j & x_j^T X_0 \\ X_0^T x_j & X_0^T X_0 \end{pmatrix}$$

$$\therefore (X_t^T X_t)^{-1} = \begin{pmatrix} X_{11}^* & X_{12}^* \\ X_{21}^* & X_{22}^* \end{pmatrix}.$$

其中，$X_{11}^* = (x_j^T x_j - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1}$.

$X_{12}^* = -(x_j^T x_j - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1} x_j^T X_0 (X_0^T X_0)^{-1}$

$X_{21}^* = -(X_0^T X_0)^{-1} X_0^T x_j (x_j^T x_j - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1}$

$X_{22}^* = (X_0^T X_0)^{-1} + (X_0^T X_0)^{-1} X_0^T x_j (x_j^T x_j - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1} x_j^T X_0 (X_0^T X_0)^{-1}$.

$x_j^T x_j = 1$.

$$
\begin{aligned}
\therefore C_{jj} = X_{11}^* &= (x_j^T x_j - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1} \\
&= (1 - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1}.
\end{aligned}
$$

$$\because \bar{x}_j = \frac{1}{n} \sum_{k=1}^{n} x_{jk} = 0.$$

$$
\begin{aligned}
\therefore SS_R^j &= \sum_{k=1}^{n} (\hat{x}_{jk} - \bar{x}_j)^2 = \sum_{k=1}^{n} \hat{x}_{jk}^2 = \hat{x}_j^T \hat{x}_j \\
&= (X_0 \hat{\beta})^T X_0 \hat{\beta} \\
&= x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j ;
\end{aligned}
$$

$$\therefore SS_T^j = \sum_{k=1}^{n} (x_{jk} - \bar{x}_j)^2 = \sum_{k=1}^{n} x_{jk}^2 = 1.$$

$$\therefore R^2 = \frac{SS_R^j}{SS_T^j} = x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j$$

$$\therefore C_{jj} = (1 - x_j^T X_0 (X_0^T X_0)^{-1} X_0^T x_j)^{-1}$$

$$= \frac{1}{1 - R^2}.$$

理论题 2

- 经中心化后因变量 $\boldsymbol{y}$ 以及经标准化后的自变量 $\boldsymbol{X}$。我们建立多元线性回归模型，其最小二乘估计为

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}.$$

请计算

$$\mathrm{MSE}(\hat{\boldsymbol{\beta}}) = E(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})'(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}),$$

需要写出推导过程。

解： $\because E(\hat{\beta}) = \beta.$

$Cov(\hat{\beta}) = \sigma^2 (X^T X)^{-1}.$

$\therefore MSE(\hat{\beta}) = E[(\hat{\beta}-\beta)^T(\hat{\beta}-\beta)]$

$= E[(\hat{\beta} - E(\hat{\beta}) + E(\hat{\beta}) - \beta)^T(\hat{\beta} - E(\hat{\beta}) + E(\hat{\beta}) - \beta)]$

$= E[(\hat{\beta} - E(\hat{\beta}))^T(\hat{\beta} - E(\hat{\beta}))]$

$= tr(Cov(\hat{\beta}))$

$= \sigma^2 tr((X^T X)^{-1}).$

令 $X^T X$ 的特征值为 $\lambda_1, \lambda_2, \ldots, \lambda_{p+1}$，则 $(X^T X)^{-1}$ 的特征值为 $\frac{1}{\lambda_1}, \frac{1}{\lambda_2}, \ldots, \frac{1}{\lambda_{p+1}}$.

$\therefore MSE(\hat{\beta}) = \sigma^2 tr[(X^T X)^{-1}]$

$= \sigma^2 \sum_{i=1}^{N} \frac{1}{\lambda_i}.$