

Prediction Mean Square Error Calculation based on PMSE Improvement

The proof of Errors of Prediction in Multiple Regression with Stochastic Regressor Variables - D. Kerridge and Sample size and the accuracy predictions made from multiple regression equations - Richard Sawyer.

Consider p -dimensional vectors $\mathbf{x}_1, \dots, \mathbf{x}_n$ are given as a random sample from multivariate normal population $N(\mu, \Sigma)$, corresponding to observations y_1, y_2, \dots, y_n . We assume that for each y_i , we have

$$y_i = \beta + \mathbf{X}_i' \mathbf{A} + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$

β is the constant coefficient and \mathbf{A} is the coefficient matrix. Let $\bar{\mathbf{x}}$ be the mean over random sample $i = 1, 2, \dots, n$, and let

$$\mathbf{S} = \sum_{i,j} (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'$$

Let $(y^*, \mathbf{x}^{*'})$ be an additional independent observation and y^* to be predicted by

$$\hat{y} = \beta + \mathbf{x}^{*'} \hat{\mathbf{A}} = \bar{y} - \bar{\mathbf{x}}' \hat{\mathbf{A}} + \mathbf{x}^{*'} \hat{\mathbf{A}} = \bar{y} + (\mathbf{x}^* - \bar{\mathbf{x}})' \hat{\mathbf{A}}$$

where \mathbf{A} is estimated by least square estimation

$$\hat{\mathbf{A}} = \mathbf{S}^{-1} \sum_i y_i (\mathbf{x}_i - \bar{\mathbf{x}})$$

The prediction error is

$$\begin{aligned} y^* - \hat{y} &= \beta + \mathbf{X}^{*'} \mathbf{A} + \epsilon_* - \bar{y} - (\mathbf{x}^* - \bar{\mathbf{x}})' \hat{\mathbf{A}} \\ &= (\mathbf{x}^* - \bar{\mathbf{x}})' (\mathbf{A} - \hat{\mathbf{A}}) + \epsilon_* + \bar{\epsilon} \end{aligned} \tag{1}$$

We argue that the conditional distribution is $\mathbf{A} - \hat{\mathbf{A}} | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^* \sim N(0, \sigma^2 \mathbf{S}^{-1})$. Thus the unconditional distribution is like (the exact distribution of $y^* - \hat{y}$ cannot be obtained)

$$y^* - \hat{y} | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^* \sim N(0, [(\mathbf{x}^* - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}^* - \bar{\mathbf{x}}) + 1 + \frac{1}{n}] \sigma^2).$$

But $(1 + \frac{1}{n})^{-1}(n-1)(\mathbf{x}^* - \bar{\mathbf{x}})' \mathbf{S}^{-1}(\mathbf{x}^* - \bar{\mathbf{x}})$ is distributed like $Hotelling - T^2(p, n-1) = (n-1)\frac{p}{n-p}F_{p, n-p}$. Denote $T^2 = [\mathbf{x}^* - \bar{\mathbf{x}}]' \mathbf{S}^{-1}[\mathbf{x}^* - \bar{\mathbf{x}}]$, the expactation of PMSE is

$$\begin{aligned}
E[(y^* - \hat{y})^2] &= E\{E[(y^* - \hat{y})^2 | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*]\} \\
&= E\{E[z^2 \sigma^2 (T^2 + 1 + \frac{1}{n}) | T^2]\} \\
&= \sigma^2 E[(T^2 + 1 + \frac{1}{n})] \\
&= \sigma^2 [(1 + \frac{1}{n}) \frac{k}{n-p} E(F_{p, n-p}) + 1 + \frac{1}{n}] \\
&= \sigma^2 [(1 + \frac{1}{n}) (\frac{k}{n-p} \frac{n-p}{n-p-2} + 1)] \\
&= \sigma^2 (1 + \frac{1}{n}) (\frac{n-2}{n-p-2}) \\
&= \sigma^2 \frac{(n+1)(n-2)}{n(n-p-2)}
\end{aligned} \tag{2}$$

Proporsition: Let M be a positive integer. Then

$$E[(y^* - \hat{y})^{2M-1}] = 0$$

when $2M \leq n-p$;

$$E[(y^* - \hat{y})^{2M}] = \frac{\sigma^{2M} \frac{(2M)!}{M!} (\frac{n+1}{2n})^M \prod_{j=1}^M (n-2j)}{\prod_{j=1}^M (n-p-2j)}$$

when $2M \leq n-p-1$.

Proof: The conditional distribution of $y^* - \hat{y}$ given $\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*$ is

$$N(0, \sigma^2(1 + \frac{1}{n})[1 + (\frac{p}{n-p} F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))])$$

by KERRIDGE(1967).

The unconditional distribution of $y^* - \hat{y}$ is asymptotically normal with mean 0 and variance σ^2 . By symmetry of normal distribution, the odd moments in the unconditional distribution of $y^* - \hat{y}$ are 0. The unconditional even moments,

$$E[(y^* - \hat{y})^{2M}] = E\{E[(y^* - \hat{y})^{2M} | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*]\}$$

By properties of the normal distribution, for any non-negative integer M , $E[(x - \mu)^{2M}] = \sigma^{2M} (2M-1)!!$,

$$\begin{aligned}
& E\{E[(y^* - \hat{y})^{2M} | \mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*]\} \\
&= E\{[\sigma^2(1 + \frac{1}{n})(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M (2M-1)!!]\} \\
&= \sigma^{2M}(1 + \frac{1}{n})^M (2M-1)!! E[(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M] \\
&= \sigma^{2M}(1 + \frac{1}{n})^M \frac{(2M-1)!}{2^{M-1}(M-1)!} E[(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M] \\
&= \sigma^{2M}(\frac{n+1}{2n})^M \frac{2(2M-1)!}{(M-1)!} E[(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M] \\
&= \sigma^{2M}(\frac{n+1}{2n})^M \frac{2M(2M-1)\dots M(M-1)\dots 1}{M(M-1)\dots 1} E[(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M] \\
&= \sigma^{2M}(\frac{n+1}{2n})^M \frac{(2M)!}{M!} E[(1 + \frac{p}{n-p}F(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}^*))^M]
\end{aligned} \tag{3}$$

By binomial theorem, the latter expected value is equal to

$$\begin{aligned}
& \sum_{j=0}^M \binom{M}{j} (\frac{p}{n-p})^j E(F^j) \\
&= \sum_{j=0}^M \binom{M}{j} \frac{\Gamma(\frac{p}{2} + j) \Gamma(\frac{n-p}{2} - j)}{\Gamma(\frac{p}{2}) \Gamma(\frac{n-p}{2})} \\
&= \sum_{j=0}^M \binom{M}{j} \frac{(\frac{p}{2} + j - 1)! (\frac{n-p}{2} - j - 1)!}{(\frac{p}{2} - 1)! (\frac{n-p}{2} - 1)!} \\
&= \sum_{j=0}^M \binom{M}{j} \frac{(\frac{p}{2} + j - 1) \dots (\frac{p}{2} + j - j) (\frac{p}{2} - 1) \dots 1}{(\frac{p}{2} - 1) (\frac{p}{2} - 2) \dots 1} \frac{(\frac{n-p}{2} - j - 1) (\frac{n-p}{2} - j - 2) \dots 1}{(\frac{n-p}{2} - 1) \dots (\frac{n-p}{2} - j) (\frac{n-p}{2} - j - 1) \dots 1} \\
&= \sum_{j=0}^M \binom{M}{j} \frac{\prod_{k=1}^j (\frac{p}{2} + k - 1)}{\prod_{k=1}^j (\frac{n-p}{2} - k)} \\
&= \sum_{j=0}^M \binom{M}{j} \frac{\prod_{k=1}^j p + 2(k-1)}{\prod_{k=1}^j (n-p-2k)} \\
&= 1 + \sum_{j=1}^M \binom{M}{j} \frac{\prod_{k=1}^j p + 2(k-1)}{\prod_{k=1}^j (n-p-2k)}
\end{aligned} \tag{4}$$

Take $M = 1$, it follows that

$$MSE = E[(y^* - \hat{y})^2] = \sigma^2 \frac{(n+1)(n-2)}{n(n-p-2)}$$

same as Kerridge paper.