

Deduction of PMSE in Predictive Mean Square Error and Stochastic Regressor Variables  
by SUBHASH C. NARULA

The response variable and the predictor variables follow a joint  $(k+1)$ -variate normal distribution with unknown mean vector  $\mu^* = [\mu_0, \mu']'$ , and unknown covariance matrix  $\Sigma^* = \begin{bmatrix} \sigma_{00} & \sigma' \\ \sigma & \Sigma \end{bmatrix}$ . Let  $z_1, z_2, \dots, z_n$  be  $n$  independent  $(k\text{-component vector})$  observations on the predictor variables,  $x_i = z_i - \bar{z}$ . Let  $S^* = \begin{bmatrix} s_{00} & s' \\ s & S \end{bmatrix}$  be sample covariance matrix, where

$$s_{00} = \sum \frac{(y_i - \bar{y})^2}{n-1}, s = \sum \frac{(y_i - \bar{y})x_i}{n-1}, S = \sum \frac{x_i x_i'}{n-1}$$

We assume the correct the model(1.1)

$$y = \alpha + \beta_1 z_1 + \beta_2 z_2 + \dots + \beta_k z_k + \epsilon$$

The LSE prediction equation

$$\hat{y} = \bar{y} + \hat{\beta}_1(z_1 - \bar{z}_1) + \hat{\beta}_2(z_2 - \bar{z}_2) + \dots + \hat{\beta}_k(z_k - \bar{z}_k) = \bar{y} + X'\hat{\beta}$$

$$\hat{y}_i = \bar{y} + x_i'\hat{\beta}$$

For any given  $z_i$ ,

$$\begin{aligned} E(y_i|z_i) &= \alpha + \beta z_i \\ &= \mu_0 - \sigma'\Sigma^{-1}\mu + \sigma'\Sigma^{-1}z_i \\ &= \mu_0 + \sigma'\Sigma^{-1}(z_i - \mu) \end{aligned}$$

where  $\alpha = \mu_0 - \sigma'\Sigma^{-1}\mu, \beta = \sigma'\Sigma^{-1}$ . Thus  $\hat{\alpha} = \bar{y} - s'S^{-1}\bar{x}, \hat{\beta} = S^{-1}s$ .

The conditional predictive mean square error by

$$\begin{aligned} E[(y_0 - \hat{y}_0)^2|z_0] &= E[(\alpha + (z_0 - \mu)'\beta + \epsilon_0 - \bar{y} - x_0'\hat{\beta}|z_0)^2] \\ &= E[(\alpha + (z_0 - \mu)'\beta + \epsilon_0 - \alpha - (\bar{z} - \mu)'\beta - \bar{\epsilon} - x_0'\beta|z_0)^2] \\ &= E[(x_0'\beta - \bar{x}'\beta + \epsilon_0 - \bar{\epsilon} - x_0'\hat{\beta}|z_0)^2] \\ &= E[(x_0'\beta + (\epsilon_0 - \bar{\epsilon}) - x_0'\hat{\beta}|z_0)^2] \\ &= E[(x_0'\beta + (\epsilon_0 - \bar{\epsilon}))^2 + (x_0'\hat{\beta})^2 - 2(x_0'\beta + (\epsilon_0 - \bar{\epsilon}))x_0'\hat{\beta}|z_0] \\ &= E[(x_0'\beta)^2 + (\epsilon_0 - \bar{\epsilon})^2 + (x_0'\hat{\beta})^2 - 2x_0'\beta x_0'\hat{\beta}|z_0] \\ &= \beta'E(x_0 x_0'|z_0)\beta + E[(\epsilon_0 - \bar{\epsilon})^2|z_0] + E[(x_0'\hat{\beta})^2|z_0] - 2\beta'E[x_0 x_0'\hat{\beta}|z_0] \end{aligned}$$

By Lemma A1, Lemma A3, Lemma A7

$$\begin{aligned} E(\tilde{\beta}_1|X_1) &= \beta_1 + \Sigma_{11}^{-1}\Sigma_{12}\beta_2 = \Phi_1 \\ E(x_{01}x_{01}'|z_0) &= (z_{01} - \mu_1)(z_{01} - \mu_1)' + \frac{\Sigma_{11}}{n} \\ E(x_0 x_0'|z_0) &= (z_0 - \mu)(z_0 - \mu)' + \frac{\Sigma}{n} \\ E[(x_{01}'\tilde{\beta}_1)^2|z_0] &= \sigma_p^2 \left[ (z_{01} - \mu_1)'\Sigma_{11}^{-1}(z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n-p-2} \\ &\quad + \Phi_1'\Sigma_{11}\Phi_1 \frac{1}{n} + \Phi_1'(z_{01} - \mu_1)(z_{01} - \mu_1)'\Phi_1 \\ \sigma'\Sigma^{-1} \begin{bmatrix} \Sigma_{11} \\ \Sigma_{21} \end{bmatrix} &= \sigma_1' \end{aligned}$$

The conditional PMSE can be written as

$$\begin{aligned}
E[(y_0 - \hat{y}_0)^2 | \mathbf{z}_0] &= \beta' E(\mathbf{x}_0 \mathbf{x}_0' | \mathbf{z}_0) \beta + E[(\epsilon_0 - \bar{\epsilon})^2 | \mathbf{z}_0] + E[(\mathbf{x}_0' \hat{\beta})^2 | \mathbf{z}_0] - 2\beta' E[\mathbf{x}_0 \mathbf{x}_0' \hat{\beta} | \mathbf{z}_0] \\
&= \beta' \left[ (\mathbf{z}_0 - \boldsymbol{\mu})(\mathbf{z}_0 - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \beta + \sigma_k^2 \left( 1 + \frac{1}{n} \right) \\
&\quad + \sigma_k^2 \left[ (\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z}_0 - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2} \\
&\quad + \frac{1}{n} \boldsymbol{\Phi}' \boldsymbol{\Sigma} \boldsymbol{\Phi} + \boldsymbol{\Phi}' (\mathbf{z}_0 - \boldsymbol{\mu})(\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\Phi} - 2\beta' \left[ (\mathbf{z}_0 - \boldsymbol{\mu})(\mathbf{z}_0 - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \beta \\
&= \sigma_k^2 \left( 1 + \frac{1}{n} \right) + \sigma_k^2 \left[ (\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z}_0 - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2}
\end{aligned}$$

Since  $\Phi$  is the notation of expectation of  $\tilde{\beta}_1$ , when we are using all predictors, the LSE is unbiased, which means  $\Phi = \beta$ .

The unconditional PMSE

$$\begin{aligned}
E[(y_0 - \hat{y}_0)^2] &= E\{E[(y_0 - \hat{y}_0)^2 | \mathbf{z}_0]\} \\
&= E \left[ \sigma_k^2 \left( 1 + \frac{1}{n} \right) + \sigma_k^2 \left[ (\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z}_0 - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2} \right] \\
&= \sigma_k^2 \left( 1 + \frac{1}{n} \right) + \sigma_k^2 E \left[ (\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z}_0 - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2} \\
&= \sigma_k^2 \left( 1 + \frac{1}{n} \right) + \sigma_k^2 \left( k + \frac{k}{n} \right) \frac{1}{n - k - 2} \\
&= \sigma_k^2 \left( 1 + \frac{1}{n} \right) \left( 1 + \frac{1}{n - k - 2} \right) \\
&= \sigma_k^2 \left( 1 + \frac{1}{n} \right) \left( \frac{n - 2}{n - k - 2} \right)
\end{aligned}$$

For subset, we partition the  $k$ -component vector of predictor variables into two parts,  $\mathbf{Z} = [\mathbf{Z}_1, \mathbf{Z}_2]$ ,  $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2]$ ,  $\mathbf{x}'_1 = [\mathbf{x}'_{i1}, \mathbf{x}'_{i2}]$ ,  $\boldsymbol{\mu}' = [\boldsymbol{\mu}'_1, \boldsymbol{\mu}'_2]$ ,  $\boldsymbol{\sigma}' = [\boldsymbol{\sigma}'_1, \boldsymbol{\sigma}'_2]$ ,  $\mathbf{s}' = [\mathbf{s}'_1, \mathbf{s}'_2]$ ,  $\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$ ,  $\mathbf{S} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix}$ , so the subset prediction equation is given by

$$\tilde{y}_i = \bar{y} + \mathbf{x}'_{i1} \tilde{\beta}_1$$

where  $\tilde{\beta}_1 = \mathbf{S}_{11}^{-1} \mathbf{s}_1$ . By LemmaA1, LemmaA3, LemmaA7,  $\boldsymbol{\Phi}_1 = \beta_1 + \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\Sigma}_{12} \beta_2$ , the conditional PMSE at  $\mathbf{z}_0$  is given by

$$\begin{aligned}
E[(y_0 - \tilde{y}_0)^2 | \mathbf{z}_0] &= E[(\mathbf{x}'_0 \beta + \epsilon_0 - \bar{\epsilon} - \mathbf{x}'_{01} \tilde{\beta}_1 | \mathbf{z}_0)^2] \\
&= E[(\mathbf{x}'_0 \beta)^2 + (\mathbf{x}'_{01} \tilde{\beta}_1)^2 - 2\mathbf{x}'_0 \beta \mathbf{x}'_{01} \tilde{\beta}_1 + (\epsilon_0 - \bar{\epsilon})^2 + 2(\mathbf{x}'_0 \beta - \mathbf{x}'_{01} \tilde{\beta}_1)(\epsilon_0 - \bar{\epsilon}) | \mathbf{z}_0] \\
&= E[(\mathbf{x}'_0 \beta)^2 | \mathbf{z}_0] + E[(\mathbf{x}'_{01} \tilde{\beta}_1)^2 | \mathbf{z}_0] - 2E[\mathbf{x}'_0 \beta \mathbf{x}'_{01} \tilde{\beta}_1 | \mathbf{z}_0] + E[(\epsilon_0 - \bar{\epsilon})^2 | \mathbf{z}_0] \\
&\quad + 2E[(\mathbf{x}'_0 \beta - \mathbf{x}'_{01} \tilde{\beta}_1)(\epsilon_0 - \bar{\epsilon}) | \mathbf{z}_0]
\end{aligned}$$

where

$$E[(\mathbf{x}'_0 \beta)^2 | \mathbf{z}_0] = \beta' \left[ (\mathbf{z}_0 - \boldsymbol{\mu})(\mathbf{z}_0 - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \beta$$

$$\begin{aligned}
E[(x'_{01}\tilde{\beta}_1)^2|z_0] &= \sigma_p^2 \left[ (z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n-p-2} \\
&\quad + \Phi_1' \Sigma_{11} \Phi_1 \frac{1}{n} + \Phi_1' (z_{01} - \mu_1) (z_{01} - \mu_1)' \Phi_1, \\
E[(\epsilon_0 - \bar{\epsilon})^2|z_0] &= \sigma_k^2 + \frac{1}{n} \sigma_k^2,
\end{aligned}$$

$$E[(x'_0\beta - x'_{01}\tilde{\beta}_1)(\epsilon_0 - \bar{\epsilon})|z_0] = E[(x'_0\beta - x'_{01}\tilde{\beta}_1)\epsilon_0|z_0] - E[(x'_0\beta - x'_{01}\tilde{\beta}_1)\bar{\epsilon}|z_0] = 0$$

(but  $\bar{\epsilon} = 0$  is not necessary)

Equation 3.6 could be written as

$$\begin{aligned}
&= \sigma_p^2 \left[ (z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n-p-2} + \Phi_1' \Sigma_{11} \Phi_1 \frac{1}{n} + \Phi_1' (z_{01} - \mu_1) (z_{01} - \mu_1)' \Phi_1 \\
&\quad + \beta(z_0 - \mu)(z_0 - \mu)' \beta + \beta' \Sigma \beta \frac{1}{n} - 2\beta' E(x_0 x'_{01}|z_0) \Phi_1 + \sigma_k^2 + \frac{1}{n} \sigma_k^2 \\
&= \sigma_k^2 + \frac{1}{n} (\sigma_p^2 + \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \sigma' \Sigma^{-1} \sigma) + [(z_0 - \mu)' \beta]^2 + [(z_{01} - \mu_1)' \Phi_1]^2 \\
&\quad + \sigma_p^2 \left[ (z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n-p-2} \\
&\quad + \beta' \Sigma \beta \frac{1}{n} + \Phi_1' \Sigma_{11} \Phi_1 \frac{1}{n} - 2\beta' E(x_0 x'_{01}|z_0) \Phi_1 \\
&= \sigma_k^2 + \frac{1}{n} \sigma_p^2 + \sigma_p^2 \left[ (z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n-p-2} + [(z_0 - \mu)' \beta]^2 + [(z_{01} - \mu_1)' \Phi_1]^2 \\
&\quad + \frac{1}{n} \beta' \Sigma \beta + \frac{1}{n} \Phi_1' \Sigma_{11} \Phi_1 + \frac{1}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \frac{1}{n} \sigma' \Sigma^{-1} \sigma - 2\beta' E(x_0 x'_{01}|z_0) \Phi_1
\end{aligned}$$

where

$$\begin{aligned}
E(x_0 x'_{01}|z_0) &= E \left[ \begin{bmatrix} x_{01} x'_{01} \\ x_{02} x'_{01} \end{bmatrix} | z_0 \right] = \begin{bmatrix} (z_{01} - \mu_1)(z_{01} - \mu_1)' + \Sigma_{11}/n \\ (z_{02} - \mu_2)(z_{01} - \mu_1)' + \Sigma_{21}/n \end{bmatrix} \\
\sigma' \Sigma^{-1} \sigma &= \beta' \Sigma \beta, \sigma_1' \Sigma_{11}^{-1} \sigma_1 = \beta_1' \Sigma_{11} \beta_1
\end{aligned}$$

so

$$\begin{aligned}
\beta' E(x_0 x'_{01}|z_0) \Phi_1 &= [\beta_1' (z_{01} - \mu_1)(z_{01} - \mu_1)' + \beta_1' \Sigma_{11}/n + \beta_2' (z_{02} - \mu_2)(z_{01} - \mu_1)' + \beta_2' \Sigma_{21}/n] \Phi_1 \\
&= \beta_1' (z_{01} - \mu_1)(z_{01} - \mu_1)' \Phi_1 + \beta_2' (z_{02} - \mu_2)(z_{01} - \mu_1)' \Phi_1 + \sigma_1' \Phi_1/n
\end{aligned}$$

In addition to a few terms appearing in 3.6a, other terms would be equal to

$$\begin{aligned}
&\frac{1}{n} \beta' \Sigma \beta + \frac{1}{n} \Phi_1' \Sigma_{11} \Phi_1 + \frac{1}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \frac{1}{n} \sigma' \Sigma^{-1} \sigma - \frac{2}{n} \sigma_1' \Phi_1 \\
&= \frac{1}{n} \Phi_1' \Sigma_{11} \Phi_1 + \frac{1}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \frac{2}{n} \sigma_1' \Phi_1 \\
&= \frac{1}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 + \frac{1}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \frac{2}{n} \sigma_1' \Sigma_{11}^{-1} \sigma_1 = 0
\end{aligned}$$

in which  $\Phi_1 = \Sigma_{11}^{-1} \sigma_1$

The conditional PMSE is equal to (3.6a)

$$\begin{aligned}
E[(y_0 - \tilde{y}_0)^2 | \mathbf{z}_0] &= \sigma_k^2 + \frac{\sigma_p^2}{n} + \sigma_p^2 \left[ (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Sigma}_{11}^{-1} (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' + \frac{p}{n} \right] \frac{1}{n-p-2} \\
&\quad + [(\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\beta} - (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Phi}_1]^2 \\
&= \sigma_k^2 + \frac{\sigma_p^2}{n} + \sigma_p^2 \left[ (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Sigma}_{11}^{-1} (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' + \frac{p}{n} \right] \frac{1}{n-p-2} \\
&\quad + [(\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\beta}_1 + (\mathbf{z}_{02} - \boldsymbol{\mu}_2)' - (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' (\boldsymbol{\beta}_1 + \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\Sigma}_{12} \boldsymbol{\beta}_2)]^2 \\
&= \sigma_k^2 + \frac{\sigma_p^2}{n} + \sigma_p^2 \left[ (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Sigma}_{11}^{-1} (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' + \frac{p}{n} \right] \frac{1}{n-p-2} \\
&\quad + [(\mathbf{z}_{02} - \boldsymbol{\mu}_2)' - (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\Sigma}_{12} \boldsymbol{\beta}_2]^2
\end{aligned}$$

Take expectation

$$\begin{aligned}
E[(y_0 - \tilde{y}_0)^2] &= E[E(y_0 - \tilde{y}_0)^2 | \mathbf{z}_0] \\
&= E \left\{ \sigma_k^2 + \frac{\sigma_p^2}{n} + \sigma_p^2 \left[ (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Sigma}_{11}^{-1} (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' + \frac{p}{n} \right] \frac{1}{n-p-2} \right. \\
&\quad \left. + [(\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\beta} - (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Phi}_1]^2 \right\} \\
&= \sigma_p^2 + \frac{\sigma_p^2}{n} + \boldsymbol{\sigma}'_1 \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1} \boldsymbol{\sigma} + \sigma_p^2 \left( p + \frac{p}{n} \right) \frac{1}{n-p-2} \\
&\quad + E[\boldsymbol{\beta}' (\mathbf{z}_0 - \boldsymbol{\mu}) (\mathbf{z}_0 - \boldsymbol{\mu})' \boldsymbol{\beta} + \boldsymbol{\Phi}'_1 (\mathbf{z}_{01} - \boldsymbol{\mu}_1) (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Phi}_1 \\
&\quad - 2\boldsymbol{\beta}' (\mathbf{z}_0 - \boldsymbol{\mu}) (\mathbf{z}_{01} - \boldsymbol{\mu}_1)' \boldsymbol{\Phi}_1]
\end{aligned}$$

The expectation term is equal to

$$\boldsymbol{\beta}' \boldsymbol{\Sigma} \boldsymbol{\beta} + \boldsymbol{\Phi}'_1 \boldsymbol{\Sigma}_{11} \boldsymbol{\Phi}_1 - 2\boldsymbol{\beta}' \begin{bmatrix} \boldsymbol{\Sigma}_{11} \\ \boldsymbol{\Sigma}_{21} \end{bmatrix} \boldsymbol{\Phi}_1$$

The unconditional PMSE

$$\begin{aligned}
E[(y_0 - \tilde{y}_0)^2] &= \sigma_p^2 \left( 1 + \frac{1}{n} \right) (n-2) / (n-p-2) \\
&\quad + \boldsymbol{\sigma}'_1 \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1} \boldsymbol{\sigma} + \boldsymbol{\beta}' \boldsymbol{\Sigma} \boldsymbol{\beta} + \boldsymbol{\Phi}'_1 \boldsymbol{\Sigma}_{11} \boldsymbol{\Phi}_1 - 2\boldsymbol{\beta}' \begin{bmatrix} \boldsymbol{\Sigma}_{11} \\ \boldsymbol{\Sigma}_{21} \end{bmatrix} \boldsymbol{\Phi}_1 \\
&= \sigma_p^2 \left( 1 + \frac{1}{n} \right) (n-2) / (n-p-2) \\
&\quad + \boldsymbol{\Phi}'_1 \boldsymbol{\Sigma}_{11} \boldsymbol{\Phi}_1 - \boldsymbol{\beta}' \boldsymbol{\Sigma} \boldsymbol{\beta} + \boldsymbol{\beta}' \boldsymbol{\Sigma} \boldsymbol{\beta} + \boldsymbol{\Phi}'_1 \boldsymbol{\Sigma}_{11} \boldsymbol{\Phi}_1 - 2\boldsymbol{\beta}' \begin{bmatrix} \boldsymbol{\Sigma}_{11} \\ \boldsymbol{\Sigma}_{21} \end{bmatrix} \boldsymbol{\Phi}_1 \\
&= \sigma_p^2 \left( 1 + \frac{1}{n} \right) (n-2) / (n-p-2)
\end{aligned}$$

Thus, the unconditional PMSE =  $\sigma_p^2 (1 + \frac{1}{n}) (n-2) / (n-p-2)$