Prediction Mean Square Error Calculation based on PMSE Improvement

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 $\boldsymbol{\mu}^* = [\mu_0, \boldsymbol{\mu}']'$, and unknown covariance matrix $\boldsymbol{\Sigma}^* = \begin{bmatrix} \sigma_{00} & \boldsymbol{\sigma}' \\ \boldsymbol{\sigma} & \boldsymbol{\Sigma} \end{bmatrix}$. Let $\boldsymbol{z_1}, \boldsymbol{z_2}, ..., \boldsymbol{z_n}$ be n independent (k-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

$$\hat{m{y}} = ar{y} + \hat{m{eta}}_1(m{z}_1 - ar{z}_1) + \hat{m{eta}}_2(m{z}_2 - ar{z}_2) + ... + \hat{m{eta}}_k(m{z}_k - ar{z}_k) = ar{y} + m{X'}\hat{m{eta}}$$

$$\hat{y}_i = ar{y} + m{x}_i'\hat{m{eta}}$$

For any given z_i ,

$$E(y_i|z_i) = \alpha + \beta z_i$$

$$= \mu_0 - \sigma' \Sigma^{-1} \mu + \sigma' \Sigma^{-1} z_i$$

$$= \mu_0 + \sigma' \Sigma^{-1} (z_i - \mu)$$

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

$$E[(y_0 - \hat{y_0})^2 | \mathbf{z_0}] = E[(\alpha + (\mathbf{z_0} - \boldsymbol{\mu})'\boldsymbol{\beta} + \epsilon_0 - \bar{y} - \mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0})^2]$$

$$= E[(\alpha + (\mathbf{z_0} - \boldsymbol{\mu})'\boldsymbol{\beta} + \epsilon_0 - \alpha - (\bar{z} - \boldsymbol{\mu})'\boldsymbol{\beta} - \bar{\epsilon} - \mathbf{x_0'}\boldsymbol{\beta}|\mathbf{z_0})^2]$$

$$= E[(\mathbf{x_0'}\boldsymbol{\beta} - \bar{\mathbf{x}}'\boldsymbol{\beta} + \epsilon_0 - \bar{\epsilon} - \mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0})^2]$$

$$= E[(\mathbf{x_0'}\boldsymbol{\beta} + (\epsilon_0 - \bar{\epsilon}) - \mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0})^2]$$

$$= E[(\mathbf{x_0'}\boldsymbol{\beta} + (\epsilon_0 - \bar{\epsilon}))^2 + (\mathbf{x_0'}\boldsymbol{\hat{\beta}})^2 - 2(\mathbf{x_0'}\boldsymbol{\beta} + (\epsilon_0 - \bar{\epsilon}))\mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0}]$$

$$= E[(\mathbf{x_0'}\boldsymbol{\beta})^2 + (\epsilon_0 - \bar{\epsilon})^2 + (\mathbf{x_0'}\boldsymbol{\hat{\beta}})^2 - 2\mathbf{x_0'}\boldsymbol{\beta}\mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0}]$$

$$= \boldsymbol{\beta}' E(\mathbf{x_0}\mathbf{x_0'}|\mathbf{z_0})\boldsymbol{\beta} + E[(\epsilon_0 - \bar{\epsilon})^2 |\mathbf{z_0}] + E[(\mathbf{x_0'}\boldsymbol{\hat{\beta}})^2 |\mathbf{z_0}] - 2\boldsymbol{\beta}' E[\mathbf{x_0}\mathbf{x_0'}\boldsymbol{\hat{\beta}}|\mathbf{z_0}]$$

By Lemma A1, Lemma A3, Lemma A7

$$\begin{split} E(\tilde{\beta}_1|X_1) &= \beta_1 + \Sigma_{11}^{-1} \Sigma_{12} \beta_2 = \Phi_1 \\ E(x_{01}x_{01}'|z_0) &= (z_{01} - \mu_1)(z_{01} - \mu_1)' + \frac{\Sigma_{11}}{n} \\ E(x_0x_0'|z_0) &= (z_0 - \mu)(z_0 - \mu)' + \frac{\Sigma}{n} \\ E[(x_{01}'\tilde{\beta}_1)^2|z_0] &= \sigma_p^2 \left[(z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1) + \frac{p}{n} \right] \frac{1}{n - p - 2} \\ &+ \Phi_1' \Sigma_{11} \Phi_1 \frac{1}{n} + \Phi_1' (z_{01} - \mu_1)(z_{01} - \mu_1)' \Phi_1 \\ \sigma' \Sigma^{-1} \begin{bmatrix} \Sigma_{11} \\ \Sigma_{21} \end{bmatrix} &= \sigma_1' \end{split}$$

The conditional PMSE can be written as

$$E[(y_0 - \hat{y_0})^2 | \mathbf{z_0}] = \boldsymbol{\beta'} E(\mathbf{x_0} \mathbf{x_0'} | \mathbf{z_0}) \boldsymbol{\beta} + E[(\epsilon_0 - \bar{\epsilon})^2 | \mathbf{z_0}] + E[(\mathbf{x_0'} \hat{\boldsymbol{\beta}})^2 | \mathbf{z_0}] - 2\boldsymbol{\beta'} E[\mathbf{x_0} \mathbf{x_0'} \hat{\boldsymbol{\beta}} | \mathbf{z_0}]$$

$$= \boldsymbol{\beta'} \left[(\mathbf{z_0} - \boldsymbol{\mu})(\mathbf{z_0} - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \boldsymbol{\beta} + \sigma_k^2 \left(1 + \frac{1}{n} \right)$$

$$+ \sigma_k^2 \left[(\mathbf{z_0} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z_0} - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2}$$

$$+ \frac{1}{n} \boldsymbol{\Phi'} \boldsymbol{\Sigma} \boldsymbol{\Phi} + \boldsymbol{\Phi'} (\mathbf{z_0} - \boldsymbol{\mu}) (\mathbf{z_0} - \boldsymbol{\mu})' \boldsymbol{\Phi} - 2\boldsymbol{\beta'} \left[(\mathbf{z_0} - \boldsymbol{\mu})(\mathbf{z_0} - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \boldsymbol{\beta}$$

$$= \sigma_k^2 \left(1 + \frac{1}{n} \right) + \sigma_k^2 \left[(\mathbf{z_0} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z_0} - \boldsymbol{\mu}) + \frac{k}{n} \right] \frac{1}{n - k - 2}$$

Since Φ 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

$$E[(y_0 - \hat{y_0})^2] = E\{E[(y_0 - \hat{y_0})^2 | \mathbf{z_0}]\}$$

$$= E\left[\sigma_k^2 \left(1 + \frac{1}{n}\right) + \sigma_k^2 \left[(\mathbf{z_0} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z_0} - \boldsymbol{\mu}) + \frac{k}{n}\right] \frac{1}{n - k - 2}\right]$$

$$= \sigma_k^2 \left(1 + \frac{1}{n}\right) + \sigma_k^2 E\left[(\mathbf{z_0} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{z_0} - \boldsymbol{\mu}) + \frac{k}{n}\right] \frac{1}{n - k - 2}$$

$$= \sigma_k^2 \left(1 + \frac{1}{n}\right) + \sigma_k^2 \left(k + \frac{k}{n}\right) \frac{1}{n - k - 2}$$

$$= \sigma_k^2 \left(1 + \frac{1}{n}\right) \left(1 + \frac{1}{n - k - 2}\right)$$

$$= \sigma_k^2 \left(1 + \frac{1}{n}\right) \left(\frac{n - 2}{n - k - 2}\right)$$

For subset, we partition the k-component vector of predictor variables into two parts, $Z = [Z_1, Z_2], X = [X_1, X_2], x_1' = [x_{i1}', x_{i2}'], \mu' = [\mu_1', \mu_2'], \sigma' = [\sigma_1', \sigma_2'], s' = [s_1', s_2'],$ $\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}, S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$

$$\tilde{y}_i = \bar{y} + \boldsymbol{x_{i1}'} \tilde{\boldsymbol{\beta_1}}$$

where $\tilde{\beta}_1 = S_{11}^{-1} s_1$. By LemmaA1, LemmaA3, LemmaA7, $\Phi_1 = \beta_1 + \Sigma_{11}^{-1} \Sigma_{12} \beta_2$, the conditional PMSE at z_0 is given by

$$\begin{split} E[(y_0 - \tilde{y_0})^2 | \boldsymbol{z_0}] &= E[(\boldsymbol{x_0'}\boldsymbol{\beta} + \epsilon_0 - \bar{\epsilon} - \boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}}|\boldsymbol{z_0})^2] \\ &= E[(\boldsymbol{x_0'}\boldsymbol{\beta})^2 + (\boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}})^2 - 2\boldsymbol{x_0'}\boldsymbol{\beta}\boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}} + (\epsilon_0 - \bar{\epsilon})^2 + 2(\boldsymbol{x_0'}\boldsymbol{\beta} - \boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}})(\epsilon_0 - \bar{\epsilon})|\boldsymbol{z_0}] \\ &= E[(\boldsymbol{x_0'}\boldsymbol{\beta})^2 | \boldsymbol{z_0}] + E[\boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}})^2 | \boldsymbol{z_0}] - 2E[\boldsymbol{x_0'}\boldsymbol{\beta}\boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}}|\boldsymbol{z_0}] + E[(\epsilon_0 - \bar{\epsilon})^2 | \boldsymbol{z_0}] \\ &+ 2E[(\boldsymbol{x_0'}\boldsymbol{\beta} - \boldsymbol{x_{01}'}\tilde{\boldsymbol{\beta_1}})(\epsilon_0 - \bar{\epsilon})|\boldsymbol{z_0}] \end{split}$$

where

$$E[(\mathbf{x_0'}\boldsymbol{\beta})^2|\mathbf{z_0}] = \boldsymbol{\beta} \left[(\mathbf{z_0} - \boldsymbol{\mu})(\mathbf{z_0} - \boldsymbol{\mu})' + \frac{\boldsymbol{\Sigma}}{n} \right] \boldsymbol{\beta}$$

$$E[(\mathbf{x_{01}'}\tilde{\boldsymbol{\beta_1}})^2|\mathbf{z_0}] = \sigma_p^2 \left[(\mathbf{z_{01}} - \boldsymbol{\mu_1})'\boldsymbol{\Sigma_{11}}^{-1}(\mathbf{z_{01}} - \boldsymbol{\mu_1}) + \frac{p}{n} \right] \frac{1}{n - p - 2}$$

$$+ \boldsymbol{\Phi_1'}\boldsymbol{\Sigma_{11}}\boldsymbol{\Phi_1} \frac{1}{n} + \boldsymbol{\Phi_1'}(\mathbf{z_{01}} - \boldsymbol{\mu_1})(\mathbf{z_{01}} - \boldsymbol{\mu_1})'\boldsymbol{\Phi_1},$$

$$E[(\epsilon_0 - \bar{\epsilon})^2|\mathbf{z_0}] = \sigma_k^2 + \frac{1}{n}\sigma_k^2,$$

$$E[(\boldsymbol{x_0'\beta} - \boldsymbol{x_{01}'\tilde{\beta_1}})(\epsilon_0 - \bar{\epsilon})|\boldsymbol{z_0}] = E[(\boldsymbol{x_0'\beta} - \boldsymbol{x_{01}'\tilde{\beta_1}})\epsilon_0|\boldsymbol{z_0}] - E[(\boldsymbol{x_0'\beta} - \boldsymbol{x_{01}'\tilde{\beta_1}})\bar{\epsilon}|\boldsymbol{z_0}] = 0$$

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

Equation 3.6 could be written as

$$\begin{split} &= \sigma_{p}^{2} \left[(z_{01} - \mu_{1})' \Sigma_{11}^{-1} (z_{01} - \mu_{1}) + \frac{p}{n} \right] \frac{1}{n - p - 2} + \Phi_{1}' \Sigma_{11} \Phi_{1} \frac{1}{n} + \Phi_{1}' (z_{01} - \mu_{1}) (z_{01} - \mu_{1})' \Phi_{1} \\ &+ \beta (z_{0} - \mu) (z_{0} - \mu)' \beta + \beta' \Sigma \beta \frac{1}{n} - 2 \beta' E (x_{0} x'_{01} | z_{0}) \Phi_{1} + \sigma_{k}^{2} + \frac{1}{n} \sigma_{k}^{2} \\ &= \sigma_{k}^{2} + \frac{1}{n} (\sigma_{p}^{2} + \sigma_{1}' \Sigma_{11}^{-1} \sigma_{1} - \sigma' \Sigma^{-1} \sigma) + [(z_{0} - \mu)' \beta]^{2} + [(z_{01} - \mu_{1})' \Phi_{1}]^{2} \\ &+ \sigma_{p}^{2} \left[(z_{01} - \mu_{1})' \Sigma_{11}^{-1} (z_{01} - \mu_{1}) + \frac{p}{n} \right] \frac{1}{n - p - 2} \\ &+ \beta' \Sigma \beta \frac{1}{n} + \Phi_{1}' \Sigma_{11} \Phi_{1} \frac{1}{n} - 2 \beta' E (x_{0} x'_{01} | z_{0}) \Phi_{1} \\ &= \sigma_{k}^{2} + \frac{1}{n} \sigma_{p}^{2} + \sigma_{p}^{2} \left[(z_{01} - \mu_{1})' \Sigma_{11}^{-1} (z_{01} - \mu_{1}) + \frac{p}{n} \right] \frac{1}{n - p - 2} + [(z_{0} - \mu)' \beta]^{2} + [(z_{01} - \mu_{1})' \Phi_{1}]^{2} \\ &+ \frac{1}{n} \beta' \Sigma \beta + \frac{1}{n} \Phi_{1}' \Sigma_{11} \Phi_{1} + \frac{1}{n} \sigma_{1}' \Sigma_{11}^{-1} \sigma_{1} - \frac{1}{n} \sigma' \Sigma^{-1} \sigma - 2 \beta' E (x_{0} x'_{01} | z_{0}) \Phi_{1} \end{split}$$

where

$$E(x_0x'_{01}|z_0) = E\left[\begin{bmatrix} x_{01}x'_{01} \\ x_{02}x'_{01} \end{bmatrix}|z_0\right] = \begin{bmatrix} (z_{01} - \mu_1)(z_{01} - \mu_1)' + \Sigma_{11}/n \\ (z_{02} - \mu_2)(z_{01} - \mu_1)' + \Sigma_{21}/n \end{bmatrix}$$
$$\sigma'\Sigma^{-1}\sigma = \beta'\Sigma\beta, \sigma'_1\Sigma_{11}^{-1}\sigma_1 = \beta'_1\Sigma_{11}\beta_1$$

so

$$\beta' E(x_0 x_{01}' | z_0) \Phi_1 = [\beta_1' (z_{01} - \mu_1) (z_{01} - \mu_1)' + \beta_1' \Sigma_{11} / n + \beta_2' (z_{02} - \mu_2) (z_{01} - \mu_1)' + \beta_2' \Sigma_{21} / n] \Phi_1$$

$$= \beta_1' (z_{01} - \mu_1) (z_{01} - \mu_1)' \Phi_1 + \beta_2' (z_{02} - \mu_2) (z_{01} - \mu_1)' \Phi_1 + \sigma_1' \Phi_1 / n$$

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

$$\frac{1}{n}\beta'\Sigma\beta + \frac{1}{n}\Phi'_{1}\Sigma_{11}\Phi_{1} + \frac{1}{n}\sigma'_{1}\Sigma_{11}^{-1}\sigma_{1} - \frac{1}{n}\sigma'\Sigma^{-1}\sigma - \frac{2}{n}\sigma'_{1}\Phi_{1}$$

$$= \frac{1}{n}\Phi'_{1}\Sigma_{11}\Phi_{1} + \frac{1}{n}\sigma'_{1}\Sigma_{11}^{-1}\sigma_{1} - \frac{2}{n}\sigma'_{1}\Phi_{1}$$

$$= \frac{1}{n}\sigma'_{1}\Sigma_{11}^{-1}\sigma_{1} + \frac{1}{n}\sigma'_{1}\Sigma_{11}^{-1}\sigma_{1} - \frac{2}{n}\sigma'_{1}\Sigma_{11}^{-1}\sigma_{1} = 0$$

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

The conditional PMSE is equal to (3.6a)

$$E[(y_{0} - \tilde{y_{0}})^{2} | \boldsymbol{z_{0}}] = \sigma_{k}^{2} + \frac{\sigma_{p}^{2}}{n} + \sigma_{p}^{2} \left[(\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\Sigma_{11}^{-1}} (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' + \frac{p}{n} \right] \frac{1}{n - p - 2}$$

$$+ [(\boldsymbol{z_{0}} - \boldsymbol{\mu})' \boldsymbol{\beta} - (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\Phi_{1}}]^{2}$$

$$= \sigma_{k}^{2} + \frac{\sigma_{p}^{2}}{n} + \sigma_{p}^{2} \left[(\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\Sigma_{11}^{-1}} (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' + \frac{p}{n} \right] \frac{1}{n - p - 2}$$

$$+ [(\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\beta_{1}} + (\boldsymbol{z_{02}} - \boldsymbol{\mu_{2}})' - (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' (\boldsymbol{\beta_{1}} + \boldsymbol{\Sigma_{11}^{-1}} \boldsymbol{\Sigma_{12}} \boldsymbol{\beta_{2}})]^{2}$$

$$= \sigma_{k}^{2} + \frac{\sigma_{p}^{2}}{n} + \sigma_{p}^{2} \left[(\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\Sigma_{11}^{-1}} (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' + \frac{p}{n} \right] \frac{1}{n - p - 2}$$

$$+ [(\boldsymbol{z_{02}} - \boldsymbol{\mu_{2}})' - (\boldsymbol{z_{01}} - \boldsymbol{\mu_{1}})' \boldsymbol{\Sigma_{11}^{-1}} \boldsymbol{\Sigma_{12}} \boldsymbol{\beta_{2}}]^{2}$$

Take expectation

$$E[(y_0 - \tilde{y_0})^2] = E[E(y_0 - \tilde{y_0})^2 | z_0]$$

$$= E\{\sigma_k^2 + \frac{\sigma_p^2}{n} + \sigma_p^2 \left[(z_{01} - \mu_1)' \Sigma_{11}^{-1} (z_{01} - \mu_1)' + \frac{p}{n} \right] \frac{1}{n - p - 2}$$

$$+ \left[(z_0 - \mu)' \beta - (z_{01} - \mu_1)' \Phi_1 \right]^2 \}$$

$$= \sigma_p^2 + \frac{\sigma_p^2}{n} + \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \sigma' \Sigma^{-1} \sigma + \sigma_p^2 \left(p + \frac{p}{n} \right) \frac{1}{n - p - 2}$$

$$+ E[\beta'(z_0 - \mu)(z_0 - \mu)' \beta + \Phi_1'(z_{01} - \mu_1)(z_{01} - \mu_1)' \Phi_1$$

$$- 2\beta'(z_0 - \mu)(z_{01} - \mu_1)' \Phi_1$$

The expectation term is equal to

$$eta'\Sigmaeta+\Phi_1'\Sigma_{11}\Phi_1-2eta'egin{bmatrix}\Sigma_{11}\\Sigma_{21}\end{bmatrix}\Phi_1$$

The unconditional PMSE

$$\begin{split} E[(y_0 - \tilde{y_0})^2] &= \sigma_p^2 (1 + \frac{1}{n})(n - 2) / (n - p - 2) \\ &+ \sigma_1' \Sigma_{11}^{-1} \sigma_1 - \sigma' \Sigma^{-1} \sigma + \beta' \Sigma \beta + \Phi_1' \Sigma_{11} \Phi_1 - 2 \beta' \begin{bmatrix} \Sigma_{11} \\ \Sigma_{21} \end{bmatrix} \Phi_1 \\ &= \sigma_p^2 (1 + \frac{1}{n})(n - 2) / (n - p - 2) \\ &+ \Phi_1' \Sigma_{11} \Phi_1 - \beta' \Sigma \beta + \beta' \Sigma \beta + \Phi_1' \Sigma_{11} \Phi_1 - 2 \beta' \begin{bmatrix} \Sigma_{11} \\ \Sigma_{21} \end{bmatrix} \Phi_1 \\ &= \sigma_p^2 (1 + \frac{1}{n})(n - 2) / (n - p - 2) \end{split}$$

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