

Recall:

- $\vec{\varepsilon} \sim MVN(\vec{0}, \sigma^2 I)$
- $\vec{y} \sim MVN(\vec{\mu} = X\vec{\beta}, \sigma^2 I)$
- $\vec{\beta} \sim MVN(\vec{\beta}_0, \sigma^2 (X^T X)^{-1})$

Related Quantities: $\hat{\mu} = X\hat{\beta}$ and $\vec{e} = \vec{y} - \hat{\mu} = \vec{y} - X\hat{\beta}$

\uparrow fitted values \uparrow residuals

We want to derive the distributions of $\hat{\mu}$ and \vec{e} . It will become useful to define the "hat" matrix $H = X(X^T X)^{-1}X^T$.

$$\hat{\mu} = X\hat{\beta} = X(X^T X)^{-1}X^T \vec{y} = H\vec{y}$$

$$\vec{e} = \vec{y} - X\hat{\beta} = \vec{y} - H\vec{y} = (I - H)\vec{y}$$

Notice that $\hat{\mu}$ and \vec{e} can both be written as a matrix multiple of the response vector \vec{y} , which MVN distribution. Therefore, we know $\hat{\mu}$ and \vec{e} both follow MVN distributions also.

Let's derive the mean vector and variance-covariance matrices for both of these distributions. It will be useful to recognize that both H and $I - H$ are symmetric ($A^T = A$) and idempotent ($AA = A$).

$$\bullet E[\hat{\mu}] = E[H\vec{y}] = H E[\vec{y}] = X \underline{(X^T X)^{-1}} \underline{X^T} X\vec{\beta} = X\vec{\beta} = \hat{\mu}$$

$$\begin{aligned} \bullet \text{Var}[\hat{\mu}] &= \text{Var}[H\vec{y}] = H \text{Var}[\vec{y}] H^T = H \sigma^2 I H^T \\ &= \sigma^2 H H^T \\ &= \sigma^2 H \\ \therefore \hat{\mu} &\sim MVN(\hat{\mu}, \sigma^2 H) \end{aligned}$$

$$\begin{aligned} \bullet E[\vec{e}] &= E[(I - H)\vec{y}] = (I - H) E[\vec{y}] = (I - H) X\vec{\beta} \\ &= X\vec{\beta} - H X\vec{\beta} \\ &= \vec{\mu} - \hat{\mu} \\ &= \vec{0} \end{aligned}$$

$$\therefore \vec{e} \sim MVN(\vec{0}, \sigma^2 (I - H))$$

* One consequence of this result for the residuals is that $\frac{\sigma^2(n-p-1)}{\sigma^2} \sim \chi^2_{n-p-1}$.

Confidence intervals for μ_0 and Prediction intervals for y_0

Given a set of values for the explanatory variables, we wish to estimate μ and predict y . We typically want to accompany these point estimates and point predictions with the appropriate interval estimate.

We organize the relevant explanatory variable values as follows:

$$\vec{x}_0 = [1 \ x_{01} \ x_{02} \ x_{03} \ \dots \ x_{0p}]^{1 \times (p+1)}$$

where x_{0j} is the particular value of x_j that we care about.

The corresponding estimate of μ_0 (equivalently, the prediction y_0) is:

$$\hat{\mu}_0 = \hat{y}_0 = \vec{x}_0 \hat{\beta} = \hat{\beta}_0 + \hat{\beta}_1 x_{01} + \hat{\beta}_2 x_{02} + \dots + \hat{\beta}_p x_{0p}$$

This estimator $\hat{\mu}_0$ has the following normal distribution

$$\hat{\mu}_0 \sim N(\vec{x}_0 \vec{\beta}, \sigma^2 \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T)$$

$$\Rightarrow \frac{\hat{\mu}_0 - \mu_0}{\sigma \sqrt{\vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}} \sim N(0, 1)$$

$$\Rightarrow \frac{\hat{\mu}_0 - \mu_0}{\hat{\sigma} \sqrt{1 + \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}} \sim t_{(n-p-1)}$$

And so a $(1-\alpha) \times 100\%$ CI for μ_0 is:

$$\hat{\mu}_0 \pm t_{(n-p-1)}(1-\alpha/2) \hat{\sigma} \sqrt{\vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}$$

est. critical value st.-error

When we're interested in predicting y at \vec{x}_0 our point prediction is $\hat{y}_0 = \hat{\mu}_0 = \vec{x}_0 \hat{\beta} \in \mathbb{R}$. To derive the PI for y_0 we must consider the prediction error:

$$y_0 - \hat{y}_0 = (\mu_0 + \varepsilon_0) - \hat{\mu}_0$$

$$= (\mu_0 - \hat{\mu}_0) + \varepsilon_0$$

Since $\hat{y}_0 = \hat{\mu}_0 \sim N(\mu_0, \sigma^2 \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T)$ then

$$y_0 - \hat{y}_0 \sim N(0, \sigma^2 (1 + \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T))$$

$$\Rightarrow \frac{y_0 - \hat{y}_0}{\sigma \sqrt{1 + \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}} \sim N(0, 1)$$

$$\Rightarrow \frac{y_0 - \hat{y}_0}{\hat{\sigma} \sqrt{1 + \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}} \sim t_{(n-p-1)}$$

And so a $(1-\alpha) \times 100\%$ PI for y_0 is

$$\hat{y}_0 \pm t_{(n-p-1)}(1-\alpha/2) \hat{\sigma} \sqrt{1 + \vec{x}_0 (X^T X)^{-1} \vec{x}_0^T}$$

est. c.v. s.e.

* Notice that since $\hat{\mu}_0 = \hat{y}_0$ that the CI for μ_0 and PI for y_0 are centered at the same value, but their widths differ. In particular the PI will always be wider than the CI.

Example (Sales)

Let's estimate the expected response and calculate the predicted response when:

$$x_1 = 3 \quad (\$3000 \text{ in promotional expenditures})$$

$$x_2 = 45 \quad (45 \text{ stores in the district})$$

$$x_3 = 10 \quad (10 \text{ competitors in the district})$$

$$x_4 = 10 \quad (\text{district potential score is 10})$$

The estimate of μ_0 / prediction of y_0 is given by

$$\hat{\mu}_0 = \hat{y}_0 = \hat{\beta}_0 + \hat{\beta}_1 x_{01} + \hat{\beta}_2 x_{02} + \hat{\beta}_3 x_{03} + \hat{\beta}_4 x_{04}$$

$$= \vec{x}_0 \hat{\beta} = [1 \ 3 \ 45 \ 10] \begin{bmatrix} 177.23 \\ 2.17 \\ 3.54 \\ -22.16 \\ 0.20 \end{bmatrix}$$

$$= (1)(177.23) + (3)(2.17) + (45)(3.54) + (10)(-22.16) + (10)(0.20)$$

$$= 123,401.8$$

So the estimated expected sales / predicted sales is $\$12,340,180$

The corresponding CI is $(118,798.6, 128,005.1)$. So we're 95% confident that the true expected sales is between $\$11,879,860$ and $\$12,800,510$.

The corresponding PI is $(111,101.5, 135,702.2)$. So we're 95% confident that the true sales is between $\$11,110,150$ and $\$13,570,220$.