

16: MULTIPLE REGRESSION

Rice 14.4

Prof Amanda Luby

1 The Hat Matrix

$$\begin{bmatrix} \hat{\epsilon}_1 \\ \hat{\epsilon}_2 \\ \vdots \\ \hat{\epsilon}_n \end{bmatrix}$$

$$\begin{aligned} \hat{\epsilon} &= Y - \hat{Y} \\ &= Y - X\hat{\beta} \\ &= Y - X(X^T X)^{-1} X^T Y \\ &= Y - HY \end{aligned}$$

$$H = X(X^T X)^{-1} X^T$$

$$\hat{Y} = HY$$

↑
puts a "hat" on Y

$$\begin{aligned} H^T &= X(X^T X)^{-1T} X^T \\ &= X(X^T X)^{-1} X^T \\ &= H \end{aligned}$$

H = constant, only a function of X's

Note: The "hat matrix" has some nice properties: $H = H^T = H^2$ and $(I - H) = (I - H)^T = (I - H)^2$.

2 Estimation of σ^2

$$Y = X\beta + \epsilon$$

$$\epsilon_i \sim N(0, \sigma^2)$$

$$\text{var}(\epsilon_i) = \sigma^2$$

In Notes 15, two of the properties that we worked with were:

$$\begin{aligned} (1) \quad \frac{n\hat{\sigma}^2}{\sigma^2} &\sim \chi_{n-2}^2 \\ (2) \quad S^2 &= \frac{n}{n-2} \hat{\sigma}^2 \end{aligned}$$

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n} \sum (Y_i - \hat{Y}_i)^2 \\ S^2 &= \frac{1}{n-2} \sum (Y_i - \hat{Y}_i)^2 \end{aligned}$$

$$E(S^2) = \sigma^2 \text{ (unbiased)} \quad \text{MLE: } \hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \dots + \hat{\beta}_p X_{ip}$$

In matrix notation, we can write:

$$\begin{aligned} \sum \hat{\epsilon}_i^2 &= \sum (Y_i - \hat{Y}_i)^2 = \|Y - HY\|^2 \\ &= \|(I - H)Y\|^2 \\ &= ((I - H)Y)^T (I - H)Y \\ &= Y^T (I - H)^T (I - H)Y \\ &= Y^T (I - H)(I - H)Y \\ &= Y^T (I - H)Y \end{aligned}$$

random vector \nearrow constant matrix \nwarrow random vector

$$\frac{n\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-p}^2$$

where p is # of columns in X (includes β_0)

Note: $\|z\|^2 = z^T z$

Then, using some nice properties for finding means of matrices (see Rice 14.4), we can show that $E(\|Y - \hat{Y}\|^2) = (n - p)\sigma^2$. This leads to the unbiased estimate for σ^2 for the multiple regression case:

$$\hat{\sigma}^2 = \frac{\|Y - \hat{Y}\|^2}{n - p} = \frac{1}{n - p} \sum (y_i - \hat{y}_i)^2$$

Errors vs Residuals:

Population Model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \epsilon$

Fitted Model: $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \dots + \hat{\beta}_k x_k$

Population / True error: $\epsilon_i \sim N(0, \sigma^2)$

Residuals: $\hat{\epsilon}_i = y_i - \hat{y}_i$

Covariance matrix of the residuals:

$$\hat{\epsilon} = Y - \hat{Y} = (I - H)Y$$

$$\Sigma_{\hat{\epsilon}} = (I - H) \Sigma_Y (I - H)^T$$

$$= (I - H) \Sigma_{\epsilon} (I - H)^T$$

$$= (I - H) \sigma^2 I (I - H)^T$$

$$= \sigma^2 (I - H) (I - H)^T$$

$$= \sigma^2 (I - H) \leftarrow \text{correlation between } \hat{\epsilon}_i, \hat{\epsilon}_j \text{ depends on } H = X(X^T X)^{-1} X^T$$

β_j 's are pop. parameters
(constant but unknown)
 $\epsilon \sim N(0, \sigma^2)$

In population model:

$$Y = X\beta + \epsilon$$

$$\Sigma_{\epsilon} = \begin{bmatrix} \sigma^2 & 0 & \dots & 0 \\ 0 & \sigma^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma^2 \end{bmatrix}$$

$$= \sigma^2 I$$

Cross-covariance matrix

Let X be a random vector of length n with covariance matrix Σ_X . If $Y = AX$ and $Z = BX$, where $A = p \times n$ and $B = m \times n$, then the cross-covariance matrix of Y and Z is given by:

$$\Sigma_{YZ} = A \Sigma_X B^T$$

$$(p \times n)(n \times n)(n \times m) \quad \Sigma_{YZ} = p \times m$$

$$\Sigma_{YZ} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \dots & \sigma_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \dots & \sigma_{pm} \end{bmatrix}$$

$\text{Cov}(Y_1, Z_1)$
 $\text{Cov}(Y_1, Z_2)$

If the errors have covariance matrix $\sigma^2 I$, the residuals are uncorrelated with the predicted values

Proof: $\hat{\epsilon} = (I - H)Y$ $\hat{Y} = HY$ $\Sigma_{\epsilon} = \sigma^2 I$, $\Sigma_Y = \sigma^2 I$

$$\Sigma_{\hat{\epsilon}\hat{Y}} = (I - H) \Sigma_Y H^T$$

$$= (I - H) \sigma^2 I H^T$$

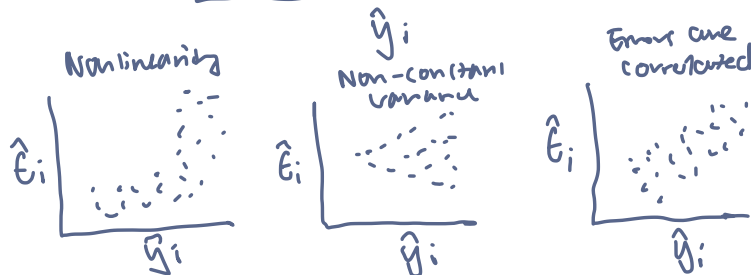
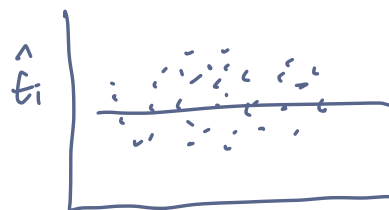
$$= \sigma^2 [(I - H) H^T]$$

$$= \sigma^2 [I H^T - H H^T]$$

$$= \sigma^2 [H - H^2]$$

$$= \sigma^2 [H - H]$$

$$= \mathbf{0}$$



3 CI's for β

Sampling distribution for $\hat{\beta}$

$\hat{\beta} \sim \text{MVN}(\beta, \sigma^2 (X^T X)^{-1})$ ← fun fact about MVN: each component has a marginal normal distribution

Each $\hat{\beta}_j \sim N(\beta_j, \sigma^2 c_{jj})$ $C = (X^T X)^{-1}$

$$S^2/\sigma^2 \sim \chi^2_{n-p}$$

$$u_j = \frac{\left(\frac{\hat{\beta}_j - \beta_j}{\sigma \sqrt{c_{jj}}} \right)}{\sqrt{S^2/\sigma^2 (n-p)}} = \frac{\hat{\beta}_j - \beta_j}{S \sqrt{c_{jj}}} \sim t_{n-p}$$

In the simple LR case:

$$(X^T X)^{-1} = \frac{1}{n \sum x_i^2 - (\sum x_i)^2} \begin{bmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{bmatrix}$$

$$\hat{\beta}_1 \sim N(\beta_1, \sigma^2 \cdot \frac{n}{n \sum x_i^2 - (\sum x_i)^2})$$

$$N(\beta_1, \sigma^2 \cdot \frac{n}{n \sum (x_i - \bar{x})^2})$$

→ same as SLR derivation

4 CI's and PI's for predictions

Let $x^T = (1, x_1, \dots, x_p)$ be a vector of predictors for a new observation Y .

5 Multiple R^2

In the simple regression case, recall that

$$R^2 =$$

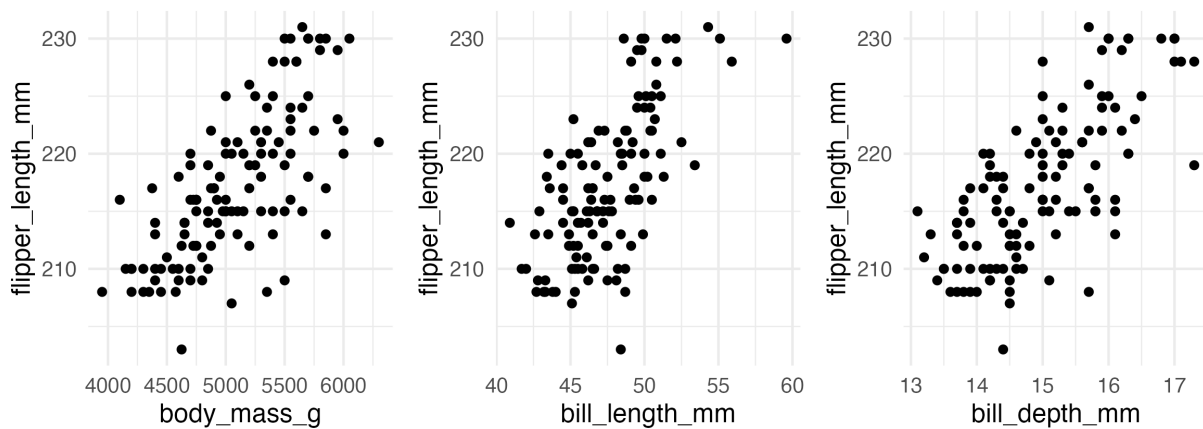
In simple linear regression, $R^2 = r^2$, where r is the sample correlation between X and Y . In the multiple regression case, we define $R = \text{Cor}(\hat{y}, y)$.

In multiple regression, whenever we add another predictor variable, R^2 *never gets worse*. The *Adjusted R^2* is more often used in practice:

$$\text{Adjusted } R^2 =$$

as the number of predictors increase, what happens to the adjusted R^2 ?

6 Interpretation of β_i in Multiple Regression



Call:

```
lm(formula = flipper_length_mm ~ body_mass_g, data = gentoo)
```

Coefficients:

```
(Intercept)  body_mass_g
 1.713e+02    9.039e-03
```

Call:

```
lm(formula = flipper_length_mm ~ bill_length_mm, data = gentoo)
```

Coefficients:

```
(Intercept)  bill_length_mm
 151.096      1.391
```

```
Call:
lm(formula = flipper_length_mm ~ bill_depth_mm, data = gentoo)
```

```
Coefficients:
  (Intercept)  bill_depth_mm
      147.22         4.67
```

```
Call:
lm(formula = flipper_length_mm ~ body_mass_g + bill_length_mm +
  bill_depth_mm, data = gentoo)
```

```
Coefficients:
  (Intercept)    body_mass_g  bill_length_mm  bill_depth_mm
    139.99254      0.00382      0.52150      2.20463
```

```
Call:
lm(formula = flipper_length_mm ~ body_mass_g + bill_length_mm +
  bill_depth_mm, data = gentoo)
```

```
Residuals:
    Min       1Q   Median       3Q      Max
-12.440  -2.492   0.023   2.829   8.322
```

```
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.400e+02  6.527e+00  21.448  < 2e-16 ***
body_mass_g   3.820e-03  1.153e-03   3.314  0.001217 **
bill_length_mm 5.215e-01  1.711e-01   3.047  0.002846 **
bill_depth_mm 2.205e+00  5.748e-01   3.836  0.000202 ***
```

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 4.11 on 119 degrees of freedom
(1 observation deleted due to missingness)
Multiple R-squared:  0.6082,    Adjusted R-squared:  0.5983
F-statistic: 61.58 on 3 and 119 DF,  p-value: < 2.2e-16
```