Applied Regression

Dr. Frank Wood

Extra Sums of Squares

- A topic unique to multiple regression
- An "extra sum of squares" measures the marginal *decrease* in the error sum of squares when one or several predictor variables are added to the regression model, given that other variables are already in the model
- Equivalently – one can view an extra sum of squares as measuring the marginal *increase* in the regression sum of squares.

Example

- Multiple regression
  - Output : Body fat percentage
  - Input :
    - triceps skin fold thickness (X_1)
    - thigh circumference (X_2)
    - midarm circumference (X_3)
- Aim
  - Replace cumbersome immersion procedure with model.
- Goal
  - Determine which predictor variable(s) provide a good model

The Data

Subject i	Triceps Skinfold Thickness X_{i1}	Thigh Circumference X_{i2}	Midarm Circumference X_{i3}	Body Fat Y_i
1	19.5	43.1	29.1	11.9
2	24.7	49.8	28.2	22.8
3	30.7	51.9	37.0	18.7
...	...	...	...	...
18	30.2	58.6	24.6	25.4
19	22.7	48.2	27.1	14.8
20	25.2	51.0	27.5	21.1

Regression of Y on X_1

(a) Regression of Y on X_1

$$\hat{Y} = -1.496 + .8572X_1$$

Source of Variation	SS	df	MS
Regression	352.27	1	352.27
Error	143.12	18	7.95
Total	495.39	19	

Variable	Estimated Regression Coefficient	Estimated Standard Deviation	t^*
X_1	$b_1 = .8572$	$s\{b_1\} = .1288$	6.66

Regression of Y on X_2

(b) Regression of Y on X_2

$\hat{Y} = -23.634 + .8565 X_2$

Source of Variation	SS	df	MS
Regression	381.97	1	381.97
Error	113.42	18	6.30
Total	495.39	19	

Variable	Estimated Regression Coefficient	Estimated Standard Deviation	t^*
X_2	$b_2 = .8565$	$s\{b_2\} = .1100$	7.79

Regression of Y on X_1 and X_2

(c) Regression of Y on X_1 and X_2

$$\hat{Y} = -19.174 + .2224X_1 + .6594X_2$$

Source of Variation	SS	df	MS
Regression	385.44	2	192.72
Error	109.95	17	6.47
Total	495.39	19	

Variable	Estimated Regression Coefficient	Estimated Standard Deviation	t^*
X_1	$b_1 = .2224$	$s\{b_1\} = .3034$	.73
X_2	$b_2 = .6594$	$s\{b_2\} = .2912$	2.26

(d) Regression of Y on X_1, X_2, and X_3

$$\hat{Y} = 117.08 + 4.334X_1 - 2.857X_2 - 2.186X_3$$

Regression of Y on X_1 and X_2 cont.

Source of Variation	SS	df	MS
Regression	396.98	3	132.33
Error	98.41	16	6.15
Total	495.39	19	

Variable	Estimated Regression Coefficient	Estimated Standard Deviation	t^*
X_1	$b_1 = 4.334$	$s\{b_1\} = 3.016$	1.44
X_2	$b_2 = -2.857$	$s\{b_2\} = 2.582$	−1.11
X_3	$b_3 = -2.186$	$s\{b_3\} = 1.596$	−1.37

Notation

- SSR X_1 only denoted by
  - $SSR(X_1) = 352.27$
- SSE X_1 only denoted by
  - $SSE(X_1) = 143.12$

- Accordingly
  - $SSR(X_1, X_2) = 385.44$
  - $SSE(X_1, X_2) = 109.95$

More Powerful Model, Smaller SSE

- When X_1 and X_2 are in the model, $SSE(X_1,X_2) = 109.95$ is smaller than when the model contains only X_1
  - $SSE(X_1) = 143.12$
- The difference is called an extra sum of squares and will be denoted by
  - $SSR(X_2|X_1) = SSE(X_1) - SSE(X_1, X_2) = 33.17$
- The extra sum of squares $SSR(X_2|X_1)$ measures the marginal effect of adding X_2 to the regression model when X_1 is already in the model.

SSR increase <-> SSE decrease

- The extra sum of squares $SSR(X_1|X_1)$ can equivalently be viewed as the marginal increase in the regression sum of squares
  - $SSR(X_2|X_1) = SSR(X_1,X_2) - SSR(X_1)$
  - $= 385.44 - 352.27 = 33.17$

Why does this relationship exist?

- Remember

$$SSTO = SSR + SSE$$

- SSTO measures only the variability of the Y's and does not depend on the regression model fitted
- Any increase in SSR must be accompanied by a corresponding decrease in the SSE.

Example relations

- $SSR(X_3 \mid X_1, X_2) = SSE(X_1, X_2) - SSE(X_1,X_2,X_3)$
  - $= 109.95 - 98.41 = 11.54$
- or $SSR(X_3 \mid X_1, X_2) = SSR(X_1,X_2,X_3) - SSR(X_1, X_2)$
  - $= 396.98 - 385.44 = 11.54$

- or with multiple variables included at a time
  - $SSR(X_2,X_3 \mid X_1) = SSE(X_1) - SSE(X_1,X_2,X_3)$
    - $= 143.12 - 98.41 = 44.71$
  - or $SSR(X_2,X_3 \mid X_1) = SSR(X_1,X_2,X_3) - SSR(X_1)$
    - $= 396.98 - 352.27 = 44.71$

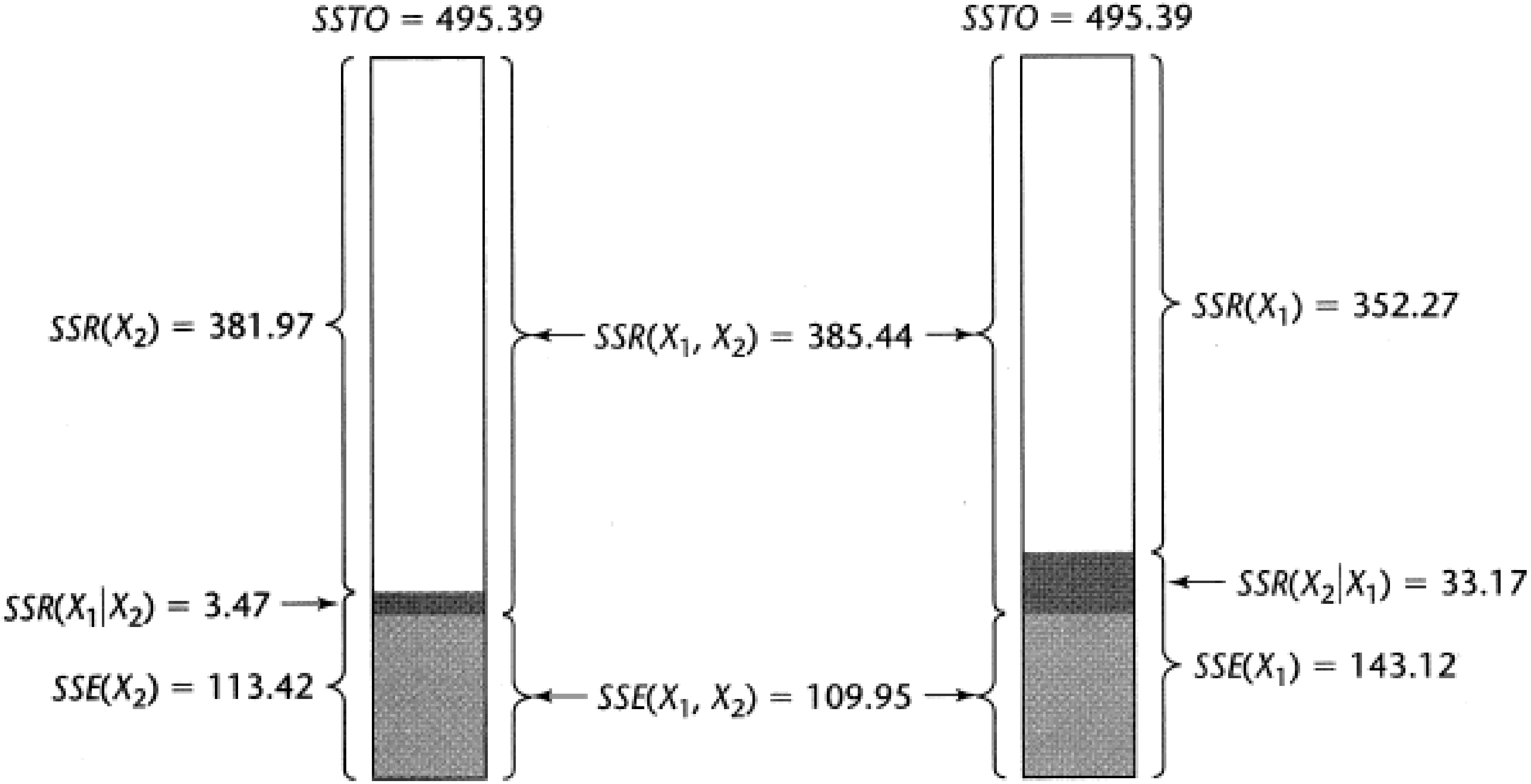
Extra sums of squares

- An extra sum of squares always involves the difference between the error sum of squares for the regression model containing the X variable(s) in the model already and the error sum of squares for the regression model containing both the original X variable(s) and the new X variable(s).

Definition(s)

- Definition
  - $SSR(X_1 \mid X_2) = SSE(X_2) - SSE(X_1, X_2)$
- Equivalently
  - $SSR(X_1 \mid X_2) = SSR(X_1, X_2) - SSR(X_2)$
- We can switch the order of X_1 and X_2 in these expressions
- We can easily generalize these definitions for more than two variable
  - $SSR(X_3 \mid X_1, X_2) = SSE(X_1, X_2) - SSE(X_1, X_2, X_3)$
  - $SSR(X_3 \mid X_1, X_2) = SSR(X_1, X_2, X_3) - SSR(X_1, X_2)$

N! Different Partitions



ANOVA Table

- Various software packages can provide extra sums of squares for regression analysis
- These are usually provided in the order in which the input variables are provided to the system, for instance

Source of Variation	SS	df	MS
Regression	$SSR(X_1, X_2, X_3)$	3	$MSR(X_1, X_2, X_3)$
X_1	$SSR(X_1)$	1	$MSR(X_1)$
$X_2 \mid X_1$	$SSR(X_2 \mid X_1)$	1	$MSR(X_2 \mid X_1)$
$X_3 \mid X_1, X_2$	$SSR(X_3 \mid X_1, X_2)$	1	$MSR(X_3 \mid X_1, X_2)$
Error	$SSE(X_1, X_2, X_3)$	$n-4$	$MSE(X_1, X_2, X_3)$
Total	$SSTO$	$n-1$	

Why? Who cares?

- Extra sums of squares are of interest because they occur in a variety of tests about regression coefficients where the question of concern is whether certain X variables can be dropped from the regression model.

Test whether a single $\beta_k = 0$

- Does X_k provide statistically significant improvement to the regression model fit?
- We can use the general linear test approach
- Example
  - First order model with three predictor variables

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \varepsilon_i \qquad \text{Full model}$$

  - We want to answer the following hypothesis test

$$H_0\colon \beta_3 = 0$$
$$H_a\colon \beta_3 \neq 0$$

Test for single $\beta_k = 0$

- For the full model we have

$$SSE(F) = SSE(X_1, X_2, X_3)$$

- The reduced model ($\beta_3 = 0$) is

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i \qquad \text{Reduced model}$$

- And for this model we have

$$SSE(R) = SSE(X_1, X_2)$$

- Where there are df_r = n-3 degrees of freedom associated with the reduced model

Test for single $\beta_k = 0$

- The general linear test statistic is

$$F^* = \frac{SSE(R) - SSE(F)}{df_R - df_F} \div \frac{SSE(F)}{df_F}$$

- which becomes

$$F^* = \frac{SSE(X_1, X_2) - SSE(X_1, X_2, X_3)}{(n-3) - (n-4)} \div \frac{SSE(X_1, X_2, X_3)}{n-4}$$

- but

$$SSE(X_1, X_2) - SSE(X_1, X_2, X_3) = SSR(X_3 | X_1, X_2)$$

Test for single $\beta_k = 0$

- The general linear test statistic is

$$F^* = \frac{SSR(X_3|X_1, X_2)}{1} \div \frac{SSE(X_1, X_2, X_3)}{n-4} = \frac{MSR(X_3|X_1, X_2)}{MSE(X_1, X_2, X_3)}$$

- Extra sum of squares has one associated degree of freedom

Example

- Body fat : Can X_3 (midarm circumference) be dropped from the model?

Source of Variation	*SS*	*df*	*MS*
Regression	396.98	3	132.33
X_1	352.27	1	352.27
$X_2 \mid X_1$	33.17	1	33.17
$X_3 \mid X_1, X_2$	11.54	1	11.54
Error	98.41	16	6.15
Total	495.39	19	

$$F^* = \frac{SSR(X_3|X_1, X_2)}{1} \div \frac{SSE(X_1, X_2, X_3)}{n-4}$$

$$= \frac{11.54}{1} \div \frac{98.41}{16} = 1.88$$

Example Cont.

- For α = .01 we require F(.99; 1, 16) = 8.53
- We observe F^* = 1.88
- We conclude H_0, β_3 = 0

Test whether several $\beta_k = 0$

- Another example

$$H_0\colon \beta_2 = \beta_3 = 0$$

$$H_a\colon \text{not both } \beta_2 \text{ and } \beta_3 \text{ equal zero}$$

- The general linear test can be used again

$$F^* = \frac{SSE(X_1) - SSE(X_1, X_2, X_3)}{(n-2) - (n-4)} \div \frac{SSE(X_1, X_2, X_3)}{n-4}$$

- But

$$SSE(X_1) - SSE(X_1, X_2, X_3) = SSR(X_2, X_3 | X_1)$$

- so the expression can be simplified

Tests concerning regression coefficients

- Summary
  - General linear test can be used to determine whether or not a predictor variable (or sets of predictor variables) should be included in the model
  - The ANOVA SSE's can be used to compute F^* test statistics
  - Some more general tests require fitting the model more than once unlike the examples given.

Standardized Multiple Regression

- Numerical precision errors can occur when
  - $(X'X)^{-1}$ is poorly conditioned (near singular)
    - colinearity
  - And when the predictor variables have substantially different magnitudes
- Solution
  - Regularization
  - Standardized multiple regression
- First, transformed variables

Correlation Transformation

- Makes all entries in the X'X matrix for the transformed variables fall between -1 and 1 inclusive.
- Another motivation
  - Lack of comparability of regression coefficients

$$\hat{Y} = 200 + 20{,}000X_1 + .2X_2$$

Y in dollars
X_1 in thousand dollars
X_2 in cents

  - Which is most important predictor?

Correlation Transformation

- Centering

$$\frac{Y_i - \bar{Y}}{s_Y}$$

$$\frac{X_{ik} - \bar{X}_k}{s_k} \qquad (k = 1, \ldots, p-1)$$

- Scaling

$$s_Y = \sqrt{\frac{\sum_i (Y_i - \bar{Y})^2}{n-1}}$$

$$s_k = \sqrt{\frac{\sum_i (X_{ik} - \bar{X}_k)^2}{n-1}} \qquad (k = 1, \ldots, p-1)$$

Correlation Transformation

- Transformed variables

$$Y_i^* = \frac{1}{\sqrt{n-1}} \left(\frac{Y_i - \bar{Y}}{s_Y} \right)$$

$$X_{ik}^* = \frac{1}{\sqrt{n-1}} \left(\frac{X_{ik} - \bar{X}_k}{s_k} \right) \qquad (k = 1, \ldots, p-1)$$

Standardized Regression Model

- Define the matrix consisting of the transformed X variables

$$\underset{n\times(p-1)}{\mathbf{X}} = \begin{bmatrix} X_{11}^* & \cdots & X_{1,p-1}^* \\ X_{21}^* & \cdots & X_{2,p-1}^* \\ \vdots & & \vdots \\ X_{n1}^* & \cdots & X_{n,p-1}^* \end{bmatrix}$$

- And define

$$\underset{(p-1)\times(p-1)}{\mathbf{X}'\mathbf{X}} = \mathbf{r}_{XX}$$

Correlation matrix of the X variables

- Can show that

$$\underset{(p-1)\times(p-1)}{\mathbf{r}_{XX}} = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1,p-1} \\ r_{21} & 1 & \cdots & r_{2,p-1} \\ \vdots & \vdots & & \vdots \\ r_{p-1,1} & r_{p-1,2} & \cdots & 1 \end{bmatrix}$$

- where each entry is just the coefficient of correlation between X_i and X_j

$$\begin{aligned} \sum X_{i1}^* X_{i2}^* &= \sum \left(\frac{X_{i1} - \bar{X}_1}{\sqrt{n-1}\, s_1} \right) \left(\frac{X_{i2} - \bar{X}_2}{\sqrt{n-1}\, s_2} \right) \\ &= \frac{1}{n-1} \frac{\sum (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2)}{s_1 s_2} \\ &= \frac{\sum (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2)}{\left[\sum (X_{i1} - \bar{X}_1)^2 \sum (X_{i2} - \bar{X}_2)^2 \right]^{1/2}} \end{aligned}$$

Standardized Regression Model

- If we define in a similar way

$$\underset{(p-1)\times 1}{\mathbf{X}'\mathbf{Y}} = \mathbf{r}_{YX}$$

  where r_{Yj} is the coefficient of simple correlations between the response variable Y and X_j
- Then we can set up a standard linear regression problem

$$\mathbf{r}_{XX}\mathbf{b} = \mathbf{r}_{YX}$$

Standardized Regression Model

- The solution

$$\underset{(p-1)\times 1}{\mathbf{b}} = \begin{bmatrix} b_1^* \\ b_2^* \\ \vdots \\ b_{p-1}^* \end{bmatrix}$$

can be related to the solution to the untransformed regression problem through the relationship

$$b_k = \left(\frac{s_Y}{s_k}\right) b_k^* \qquad (k = 1, \ldots, p-1)$$

$$b_0 = \bar{Y} - b_1 \bar{X}_1 - \cdots - b_{p-1} \bar{X}_{p-1}$$

Multi-colinearity

- Brief comments
- (X'X)^{-1} must be full rank to compute regression solution
  - rank(AB) <= min(rank(A), rank(B))
- Multi-colinearity means that rows of X are linearly dependent
- Regression solution is degenerate
- High degrees of colinearity produce numerical instability
- Very important to consider in real world applications