Extra Sums of Squares and Marginal Effect

Extra Sum of Squares

- Measures the marginal reduction in the error sum of square when one or several predictor variables are added to the regression model, given that other predictor variables are already in the model.
- Can view as measuring the marginal effect in the regression sum of squares when one or several predictor variables are added to the regression model.
- The body fat example: a study of the relation of amount of body fat (Y) to several possible predictor variables, based on a sample of n=20 healthy females 25-34 years old. The possible predictors are

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X1: The triceps skinfold thickness;
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X2: The thigh circumference;

X3: mid-arm circumference.

• We now construct 4 models, Y is regressed

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(model1) on X1 alone; lm(y\sim x1)
(model2) on X2 alone; lm(y\sim x2)
(model3) on X1 and X2 only; and lm(y\sim x1+x2)
(model4) on X1, X2 and X3. lm(y\sim x1+x2+x3)
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• There could be 2^3 ways to construct MLR (including the null set model).

The scatter plot

X1: The triceps skinfold thickness;

X2: The thigh circumference;

X3: mid-arm circumference;

Y: body fat



Model 1, Y~X1

	Df	SS	MS
x1	1	352	352
Residuals	18	143	7.9
Total	19	495	

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Reductions in error variance Extra sum of square of Error

Increase in regression variance Extra sum of square of Regression

$$R^2 = \frac{352}{495} = 71\%$$

Model 3, Y~X1+X2

	Df	SS	MS
x1	1	352	352
x2	1	33	33
Residuals	17	110	6.5
Total	19	495	

$$R^2 = \frac{385}{495} = 78\%$$

$$R^{2} = \frac{385}{495} = 78\%$$

$$SSE(X1) = 143$$

$$- SSE(X1, X2) = 110$$

$$SSE(X2 \mid X1) = 33$$

	Df	SS	MS
x1	1	352	352
x2	1	33	33
x 3	1	12	12
Residuals	16	98	6.1
Total	19	495	

$$R^2 = \frac{397}{495} = 80\%$$

$$SSE(X1, X2) = 110$$

$$- SSE(X1, X2, X3) = 98$$

$$SSE(X3 \mid X1, X2) = 12$$

Note that the extra sum of squares, SSR(A|B) notation is equivalent to SSE(A|B) But the SSR(A) notation is not equivalent to SSE(A).

	Df	SS	MS
x1	1	352	352
x2	1	33	33
x3	1	12	12
Residuals	16	98	6.1
Total	19	495	

Source of variation	Df	SS	MS
Regression	3	SSR(X1,X2, X3)=397	MSR(X1,X2, X3)=397/3=132.33
X1	1	SSR(X1) = 352	MSR(X1)=352
X2 X1	1	SSR(X2 X1)=SSE(X2 X1)=33	MSR(X2 X1)=MSE(X2 X1)=33
X3 X1, X2	1	SSR(X3 X1,X2)=SSE(X3 X1, X2)=12	MSR(X3 X1,X2)=MSE(X3 X1, X2)=12
Residuals	16	SSE(X1, X2, X3)=98	MSE(X1, X2, X3)=98/16=6.13
Total	19	SSTO=495	

Note that the extra sum of squares, SSR(A|B) notation is equivalent to SSE(A|B) But the SSR(A) notation is not equivalent to SSE(A).

	Df	SS	MS
x1	1	352	352
x2	1	33	33
x3	1	12	12
Residuals	16	98	6.1
Total	19	495	

	Df	SS	MS
X1	1	352	352
X2, X3 X1	2	45	22.5
Residuals	16	98	6.1
Total	19	495	

SSR(X2,X3|X1)= SSR(X2|X1)+SSR(X3|X1 X2)=33+12=45 OR = SSR(X1, X2, X3)-SSR(X1)= 397-352=45 OR = SSE(X1) - SSE(X1, X2, X3)=143-98=45 MSR(X2,X3|X1)=SSR(X2,X3|X1)/2 =22.5



	Df	SS	MS
X1, X2	2	385	192.5
X3 X1,X2	1	12	12
Residuals	16	98	6.1
Total	19	495	

SSR(X1,X2)= SSR(X1)+SSR(X2|X1)=352+33=385 OR =SSR(X1, X2, X3)-SSR(X3|X1 X2=397-12=385 OR=SST-SSE(X1, X2)=SST- (SSE(X1, X2, X3)+SSE(X3|X1, X2))=497-(98+12)=385

MSR(X1,X2) = SSR(X1,X2)/2 = 192.5

Comments:

- Note that the extra sum of squares can be denoted as either SSR(A|B) or SSE(A|B) and should not be confused with the usual sum of squares, including SSR(A), SSE(A), SSR(B), SSE(B), SSR(A, B) and SSE(A, B)
- The extra sum of squares can be decomposed in multiple ways in multiple steps.
 - \Leftrightarrow SSR(B, C|A)=SSR(B|A)+SSR(C|A, B)
- The order in which the variables are presented matters in the extra sum of square terms.
 - \Leftrightarrow SSR(A|B) is not usually the same as SSR(B|A).
 - \Leftrightarrow However, SSR(A,B) = SSR(B,A), and SSE(A, B)=SSE(B, A)
- The total sum of squares, $SST = \Sigma (Y_i \overline{Y})^2$ always remains the same.
 - \Leftrightarrow SST=SSR(A)+SSE(A)=SSR(B)+SSE(B)=SSR(A,B)+SSE(A, B)=SSR(B, A)+SSE(B, A)
 - \Leftrightarrow SST=SSR(A)+SSR(B|A)+SSE(A, B), or SST=SSR(B)+SSR(A|B)+SSE(B, A).

A GLT Test for all $\beta_k = 0$ (e.g., $\beta_1 = 1, \beta_2 = 0, \beta_3 = 0$)

 H_0 : $\beta_1=\beta_2=\beta_3=0$ (Reduced model) H_a : not all β_k equal 0 (Full model)

$$Y_i = \beta_0 + \epsilon_i$$
 (The null model)
$$dfE(Reduced) = n - p = n - 1$$
 $dfE(Full) = n - p = n - 4$

$$Y_{i} = \beta_{0} + \beta_{1} X_{i,1} + \beta_{2} X_{i,2} + \beta_{3} X_{i,3} + \epsilon_{i}$$

$$dfE(Full) = n - p = n - 4$$

Analysis of Variance Table

$$F_{S} = \frac{SSE(R) - SSE(F)}{df_{R} - df_{F}} = \frac{MSR}{MSE} \sim F (df_{R} - df_{F}, df_{F})$$

$$F_{s} = \frac{\frac{SSR(X1, X2, X3)}{p-1}}{\frac{SSE(X1, X2, X3)}{n-4}}$$

= 21.52

Residual standard error: 2.48 on 16 degrees of freedom Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641 F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

$$F_s = \frac{352.27 + 33.17 + 11.55}{3}$$

$$\frac{98.41}{16}$$

- The critical value F(0.95, 3, 16) = 3.24, we reject the Ho, not all betas are zero.
- This is the result shown in the R output.
- Since it is for all predictors, it is also known as the *global test*.

$$H_0\colon \beta_3=0 \text{ (Reduced model)} \qquad H_a\colon \beta_3\neq 0 \text{ (Full model)} \qquad \text{Analogy}$$

$$Y_i=\beta_0+\beta_1X_{i,1}+\beta_2X_{i,2}+\varepsilon_i \qquad Y_i=\beta_0+\beta_1X_{i,1}+\beta_2X_{i,2}+\beta_3X_{i,3}+\varepsilon_i \qquad \text{Resp}$$

$$dfE(Reduced)=n-p=n-3 \qquad dfE(Full)=n-p=n-4 \qquad \qquad \text{X1}$$

$$X_2 = \frac{SSE(R)-SSE(F)}{SSE(F)/df_F} = \frac{MSR}{MSE} \sim F\left(df_R-df_F,df_F\right) \qquad \qquad \text{X3}$$

$$Resp$$

$$F_S = \frac{SSR(X3|X1,X2)}{\frac{N-3-n+4}{SSE(X1,X2,X3)}} \qquad \text{Based on the critical value of } F\left(0.95, conclude that X3 can be removed from the control of the property o$$

- Based on the critical value of F(0.95, 1, 16) = 4.49, and a p-value of 0.19. We can conclude that X3 can be removed from the MLR that already includes X1 and X2.
- When determining the significance of a predictor in an MLR, it is assumed that all other predictors have already been considered, this this predictor being the last to be evaluated.
- This process is also a test of the predictor's marginal effect.
- By default, in an MLR, the significance of a predictor is evaluated based on its marginal effect.

=1.88

 $F_s = \frac{1}{98.41}$

A GLT test for whether a single $\beta_k = 0$ (e.g., $\beta_2 = 0$)

$$H_0: \ \beta_2 = 0 \ (\text{Reduced model}) \qquad H_a: \ \beta_2 \neq 0 \ (\text{Full model})$$

$$Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_3 X_{i,2} + \varepsilon_i \qquad Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_3 X_{i,3} + \beta_2 X_{i,2} + \varepsilon_i$$

$$df E(Reduced) = n - p = n - 3 \qquad df E(Full) = n - p = n - 4$$

$$F_s = \frac{\underbrace{SSE(R) - SSE(F)}_{GSE(F)/df_F}}_{SSE(F)/df_F} = \underbrace{\frac{MSR}{MSE}}_{MSE} \sim F \ (df_R - df_F, df_F)$$

$$\underbrace{SSR(X2|X1, X3)}$$

- $F_s = \frac{\frac{7.53}{1}}{\frac{98.41}{16}}$
 - =1.22

- Need to refit the model as Y~X1+X3+X2, or Y~X3+X1+X2.
- It is important to note that $SSR(X2|X1, X3) \neq SSR(X2|X1)$, indicating that the effect of X2 is not independent of the other variable in the model.
- With a p-value of 0.28, we can conclude that X2 can be removed from the MLR that already includes X1 and X3.

$$H_0$$
: $\beta_2 = \beta_3 = 0$ (Reduced model)

 H_0 : $\beta_2 = \beta_3 = 0$ (Reduced model) H_a : not both β_2 and β_3 equal 0 (Full model)

$$Y_i = \beta_0 + \beta_1 X_{i,1} + \epsilon_i$$

$$Y_{i} = \beta_{0} + \beta_{1} X_{i,1} + \beta_{2} X_{i,2} + \beta_{3} X_{i,3} + \epsilon_{i}$$

$$dfE_R = n - 2$$

$$dfE_F = n - 4$$

$$F_{S} = \frac{\frac{SSE(R) - SSE(F)}{df_{R} - df_{F}}}{SSE(F)/df_{F}} = \frac{MSR}{MSE} \sim F (df_{R} - df_{F}, df_{F})$$

$$F_{S} = \frac{\frac{SSR(X2, X3|X1)}{2}}{\frac{SSE(X1, X2, X3)}{n-4}}$$

$$F_s = \frac{33.17 + 11.55}{2}$$

$$\frac{98.41}{16}$$

• The critical value of F(0.95, 2, 16) = 3.63, indicating that further analysis maybe required before deciding whether X2 and X3 should be dropped from the regression model that already includes X1.

=3.635

In R this can also be done with function *anova*(reduced model, full model)

```
Model 1: y \sim x1
Model 2: y \sim x1 + x2 + x3
             RSS Df Sum of Sq
      18 143.120
      16 98.405 2 44.715 3.6352 0.04995 *
```

```
Analysis of Variance Table

Response: y

Df Sum Sq Mean Sq F Value Pr(>F)

x1 1 352.27 352.27 44.305 3.024e-06 ***

Residuals 18 143.12 7.95
```

$$H_0$$
: $\beta_1 = 0$ H_a : $\beta_1 \neq 0$ $Y_i = \beta_0 + \varepsilon_i$ The null model $Y_i = \beta_0 + \beta_1 X_{i,1} + \varepsilon_i$ $F_S = \frac{MSR}{MSE(Full\ model)} = \frac{352.27}{7.95} = 44.305 \sim F(1, 18)$

- The F test is used to evaluate the overall significance of the regression model. It considers the joint effect of all predictors in the model. In SLR, F test for the predictor is testing the significance of the predictor.
- The F test is equivalent to the t test corresponding to the predictor

Response: y

Residuals 16 98.40

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
x1	1	352.27	352.27	57.2768	1.131e-06	***
x2	1	33.17	33.17	5.3931	0.03373	×
x3	1	11.55	11.55	1.8773	0.18956	
Residuals	16	98.40	6.15			

6.15

1. The first predictor, e.g. X1, in the model X1+X2+X3

$$F_s = \frac{SSR(X1)/1}{MSE(full\ model)} = \frac{352.27}{6.15} = 57.28 \sim F(1, 16)$$

- A significant F-value for the first predictor indicates that the inclusion X1 contributes significantly to explaining the variance in Y, after accounting for the other predictors in the model, in this specific order, X1, X2 and X3.
- Note that is not a test for the marginal effect of X1, which is testable in the model where X1 is last predictor in the model, e.g, Y~X2+X3+X1:

$$H_0: \ \beta_1 = 0$$
 $H_a: \ \beta_1 \neq 0$
$$Y_i = \beta_0 + \beta_2 X_{i,2} + \beta_3 X_{i,3} + \varepsilon_i \qquad Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \beta_3 X_{i,3} + \varepsilon_i$$

$$F_s = \frac{SSR(X1|X2,X3)/1}{MSE(full\ model)} = \frac{12.7}{6.15} = 2.065 \sim F(1,16)$$

```
Response: y

Df Sum Sq Mean Sq F value Pr(>F)

X1 1 352.27 352.27 57.2768 1.131e-06 ***

X2 1 33.17 33.17 5.3931 0.03373 *

X3 1 11.55 11.55 1.8773 0.18956

Residuals 16 98.40 6.15
```


2. The middle predictor, e.g. X2, in the model X1+X2+X3

$$F_S = \frac{SSR(X2|X1)/1}{MSE(full\ model)} = \frac{33.17}{6.15} = 5.3921 \sim F(1, 16)$$

- A significant F-value for the middle predictor indicates that the inclusion X2 contributes significantly to explaining the variance in Y, after accounting for the other predictors in the model, in this specific order, X1, X2 and X3.
- Note that is not a test for the marginal effect of X2, which is testable in the model where X1 is last predictor in the model, e.g, Y~X1+X3+X2:

$$H_0$$
: $\beta_2 = 0$ H_a : $\beta_2 \neq 0$
$$Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_3 X_{i,3} + \varepsilon_i \qquad Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \beta_3 X_{i,3} + \varepsilon$$

$$F_s = \frac{SSR(X2|X1,X3)/1}{MSE(full\ model)} = \frac{7.53}{6.15} = 1.2242 \sim F(1,16)$$

3. last predictor, e.g. X3, in the model X1+X2+X3

$$F_s = \frac{SSR(X3|X1,X2)/1}{MSE(full\ model)} = \frac{11.55}{6.15} = 1.8773 \sim F(1,16)$$

• Note that is the test for the marginal effect of X3 in a full model that Consists of X1, X2 and X3.

$$H_0$$
: $\beta_3 = 0$ H_a : $\beta_3 \neq 0$
$$Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \varepsilon_i \qquad Y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \beta_3 X_{i,3} + \varepsilon$$

$$F_S = \frac{SSR(X3|X1,X2)/1}{MSE(full\ model)} = \frac{11.55}{6.15} = 1.8773 \sim F(1,16)$$

Understanding the T tests and P-values in an MLR Model Summary Table

```
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 117.085
                        99.782
                                 1.173
                                           0.258
х1
              4.334
                         3.016
                                 1.437
                                          0.170
x2
              -2.857
                         2.582 -1.106
                                          0.285
              -2.186
                         1.595 -1.370
х3
                                          0.190
Residual standard error: 2.48 on 16 degrees of freedom
Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641
```

 Order doesn't matter for the T test of a predictor because it is for the marginal effect of a single predictor.

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) -1.4961 3.3192 -0.451 0.658

x1 0.8572 0.1288 6.656 3.02e-06 ***
```

F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) -19.1742  8.3606 -2.293  0.0348 *

x1  0.2224  0.3034  0.733  0.4737

x2  0.6594  0.2912  2.265  0.0369 *
```

```
Coefficients:

Estimate Std. Error t value Pr(>|t|)

(Intercept) 6.7916 4.4883 1.513 0.1486

x1 1.0006 0.1282 7.803 5.12e-07 ***

x3 -0.4314 0.1766 -2.443 0.0258 *
```

Estimate Std. Error t value Pr(>|t|)

1.595 -1.370

2.582 -1.106

1.173

1.437

0.258

0.170

0.190

0.285

99.782

3.016

Coefficients:

x1

x3

x2

(Intercept) 117.085

4.334

-2.186

-2.857

Ha:
$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i$$
 (Full model)

Case 1.
$$H_o$$
: $\beta_1 = \beta_2 = \beta_{new}$ Not zero Ha : $\beta_1 \neq \beta_2$

Case 2.
$$H_o$$
: $\beta_1 = 3$, $\beta_2 = 5$
 Ha : not both equalities in H_o hold

$$Y_i = \beta_0 + \beta_{new}(X_{i1} + X_{i2}) + \beta_3 X_{i3} + \epsilon_i \quad \text{(Reduced model)}$$

$$Y_i = \beta_0 + 3X_{i1} + 5X_{i2} + \beta_3 X_{i3} + \epsilon_i$$
 , or
$$(Y_i - 3X_{i1} - 5X_{i2}) = \beta_0 + \beta_3 X_{i3} + \epsilon_i$$
 (Reduced model)

- The matrix form (Y and/or the design matrix) needs to be modified.
- In case 1, where the full and reduced models have the same response variable (Y), the anova(reduced model, full model)
- can be used in this scenario to evaluate the hypothesis.
- In case 2, where the response variable changes, direct comparison of the two models is not possible. However, the GLT test can still be performed By calculating the test statistics.

$$F_{S} = \frac{\frac{SSE(R) - SSE(F)}{df_{R} - df_{F}}}{SSE(F)/df_{F}} = \frac{MSR}{MSE} \sim F (df_{R} - df_{F}, df_{F})$$

A Simulated Case 1. H_o : $\beta_1 = \beta_2 = \beta_{new}$ Ha: $\beta_1 \neq \beta_2$

```
fr { r }
n = 30
set.seed(123)
X1 = runif(n)
X2 = runif(n, max=5)
X3 = runif(n, max=10)
```

```
set.seed(123)
b0 = 1
b1 = 2
b2 = 2
b3 = 5
Y = b0 + b1*X1 + b2*X2 + b3*X3 + rnorm(n)
m1 = lm(Y~X1+X2+X3)
m1_reduced = lm(Y~I(X1+X2)+X3)
anova(m1_reduced, m1)
```

Analysis of Variance Table

```
Model 1: Y ~ I(X1 + X2) + X3

Model 2: Y ~ X1 + X2 + X3

Res.Df RSS Df Sum of Sq F Pr(>F)

1 27 27.081

2 26 26.878 1 0.20344 0.1968 0.661
```

A Simulated Case 2. H_0 : $\beta_1 = 3$, $\beta_2 = 5$ Ha: not both equalities in H_0 hold

```
fr set.seed(123)
b0 = 1
b1 = 3
b2 = 5
b3 = 8
Y = b0 + b1*x1 + b2*x2 + b3*x3 + rnorm(n)

m2 = lm(Y~x1+x2+x3)
Y_new = Y-3*x1-5*x2
m2_reduced = lm(Y_new~x3)
```

In this case you may not directly use anova function because in R it requires the response to be the same. Therefore, we need to compute the F statistics.

{r}

MSR = (sum(m2_reduced\$residuals^2)-sum(m2\$residuals^2))/(m2_reduced\$df.residual-m2\$df.residual)

MSE = sum(m2\$residual)

MSE = sum(m2\$residuals^2)/m2\$df.residual

Fs = MSR/MSE

Fs

[1] 0.3404

The .95 quantile for F distribution in this case:

f(0.95, m2_reduced\$df.residual-m2\$df.residual, m2\$df.residual)

[1] 3.369016

The F statistics is smaller than the threshold, so we do not reject the null hypothesis.

Or we can use the p-value as well.

pf(Fs, m2_reduced\$df.residual-m2\$df.residual, m2\$df.residual)

[1] 0.2853909

The p-value is large.