## "EXTRA" Sums of Squares

These are values of SS attributable to adding some variable(s) to a model which already has some variable(s) in the model. Take for example the model,

$$
\mathrm{Y}_{i}=\mathrm{b}_{0}+\mathrm{b}_{k} \mathrm{X}_{k i}+\mathrm{b}_{l} \mathrm{X}_{l i}+\mathrm{b}_{m} \mathrm{X}_{m i}+\mathrm{e}_{i}
$$

where we may be interested in the contribution of a single variable to the model (eg X $\mathrm{X}_{m}$ ).

We wish to get $\operatorname{SSRX}_{m}$ given that $\mathrm{X}_{k}$ and $\mathrm{X}_{l}$ are already in the model. This measures the IMPROVEMENT in the model from entering another variable or variables $\left(\mathrm{X}_{m}\right)$ in this case.

This is EXACTLY the SSDifference one would get with the General Linear Test if the Model with $\mathrm{X}_{m}$ is viewed as the Full model and the model without $\mathrm{X}_{m}$ is taken as the Reduced model.

The textbook refers to this SS as the "EXTRA" Sums of Squares. This is a measure of the improvement in the model (or reduction in the Error) by one or more variables given that some other variable or variables are already in the model.
for example, the Full model is

$$
\mathrm{Y}_{i}=\mathrm{b}_{0}+\mathrm{b}_{k} \mathrm{X}_{k i}+\mathrm{b}_{l} \mathrm{X}_{l i}+\mathrm{b}_{m} \mathrm{X}_{m i}+\mathrm{b}_{n} \mathrm{X}_{n i}+\mathrm{e}_{i}
$$

the reduced model is (any combination of X variables can be removed)

$$
\mathrm{Y}_{i}=\mathrm{b}_{0}+\mathrm{b}_{k} \mathrm{X}_{k i}+\mathrm{b}_{l} \mathrm{X}_{l i}+\mathrm{e}_{i}
$$

The difference between these models is the EXTRA SS, and is calculated as

$$
\begin{aligned}
& \operatorname{SSR}\left(\mathrm{X}_{m}, \mathrm{X}_{n} \mid \mathrm{X}_{k}, \mathrm{X}_{l}\right)=\operatorname{SSR}\left(\mathrm{X}_{k}, \mathrm{X}_{l}, \mathrm{X}_{m}, \mathrm{X}_{n}\right)-\operatorname{SSR}\left(\mathrm{X}_{k}, \mathrm{X}_{l}\right)= \\
& \quad \operatorname{SSE}\left(\mathrm{X}_{k}, \mathrm{X}_{l}\right)-\operatorname{SSE}\left(\mathrm{X}_{k}, \mathrm{X}_{l}, \mathrm{X}_{m}, \mathrm{X}_{n}\right)
\end{aligned}
$$

I will continue using problem 7.20 as an example in class. You can follow a similar discussion of the material in your textbook, where they use Table 8.1. To assist in this endeavor, I have provided SAS output for this example as well.

Think about the ways the SSRegression can be partitioned between the various variables in a model. For the mathematician salary example

First look at the SSRegression for the various combinations of variables. These values are simply the SSReg for the fitted models.

SSCorrected Total $=689.26$

$$
\begin{array}{ll}
\operatorname{SSR}\left(X_{1}\right)=306.73233 & \mathrm{SSE}=382.52767 \\
\operatorname{SSR}\left(X_{2}\right)=508.06883 & \mathrm{SSE}=181.19117 \\
\operatorname{SSR}\left(X_{3}\right)=214.76157 & \mathrm{SSE}=474.49843 \\
\operatorname{SSR}\left(X_{1}, X_{2}\right)=570.52677 & \mathrm{SSE}=118.73323 \\
\operatorname{SSR}\left(X_{1}, X_{3}\right)=397.19152 & \mathrm{SSE}=292.06848 \\
\operatorname{SSR}\left(X_{2}, X_{3}\right)=593.39849 & \mathrm{SSE}=95.86151 \\
\operatorname{SSR}\left(X_{1}, X_{2}, X_{3}\right)=627.817 & \mathrm{SSE}=61.44300
\end{array}
$$

Now look at the gain from entering each $X_{k}$ after each of the others has been entered in the model.

These values are calculated as $\operatorname{SSR}\left(\mathrm{X}_{k} \mid \mathrm{X}_{l}\right)=\operatorname{SSR}\left(\mathrm{X}_{k}, \mathrm{X}_{l}\right)-\operatorname{SSR}\left(\mathrm{X}_{l}\right)$

$$
\begin{aligned}
& \operatorname{SSR}\left(X_{2} \mid X_{1}\right)=263.79444 \\
& \operatorname{SSR}\left(X_{3} \mid X_{1}\right)=90.45919 \\
& \operatorname{SSR}\left(X_{1} \mid X_{2}\right)=62.45794 \\
& \operatorname{SSR}\left(X_{3} \mid X_{2}\right)=85.32966 \\
& \operatorname{SSR}\left(X_{1} \mid X_{3}\right)=182.42995 \\
& \operatorname{SSR}\left(X_{2} \mid X_{3}\right)=378.63692
\end{aligned}
$$

Now look at the gain from entering each $\mathrm{X}_{k}$ after all of the others has been entered in the model.

These values are calculated as $\operatorname{SSR}\left(\mathrm{X}_{k} \mid \mathrm{X}_{l}, \mathrm{X}_{m}\right)=\operatorname{SSR}\left(\mathrm{X}_{k}, \mathrm{X}_{l}, \mathrm{X}_{m}\right)-\operatorname{SSR}\left(\mathrm{X}_{k}, \mathrm{X}_{l}\right)$

$$
\begin{aligned}
& \operatorname{SSR}\left(X_{1} \mid X_{2}, X_{3}\right)=34.41851 \\
& \operatorname{SSR}\left(X_{2} \mid X_{1}, X_{3}\right)=230.62548 \\
& \operatorname{SSR}\left(X_{3} \mid X_{1}, X_{2}\right)=57.29023
\end{aligned}
$$

Which of all of of these possible EXTRA SS are most likely to be of interest?
This will depend primarily on the hypotheses to be tested.
Also, how can we set up models to most easily estimate these with some computer package?

SAS provides two types of SS calculations to estimated EXTRA SS. SAS terms these TYPE I and TYPE II, TYPE III or TYPE IV (the last 3 are the same in regression, but not in Design).

TYPE I SS gives the contribution to the model of each variable entered in order. If we enter three variables $\mathrm{X}_{k}, \mathrm{X}_{l}$ and $\mathrm{X}_{m}$ in this order then we would get TYPE I SS which give
$\operatorname{SSR}\left(\mathrm{X}_{k}\right)=$
$\operatorname{SSR}\left(\mathrm{X}_{l} \mid \mathrm{X}_{k}\right)=$
$\operatorname{SSR}\left(\mathrm{X}_{m} \mid \mathrm{X}_{k}, \mathrm{X}_{l}\right)=$

These SS are also referred to as the Sequentially adjusted SS, and are entirely order dependent. If order is changed, the results will be different.

These can be obtained from PROC REG with the SS1 option on the MODEL statement. These are given by default by PROC GLM along with SS3.

PROC GLM will also give SS2 and SS4 upon request, while PROC REG gives only SS1 and SS2.

## Output from PROC REG



The Hypotheses of interest generally include one or more of the following
For the model

$$
\mathbf{Y}=\beta_{0}+\beta_{1} \mathbf{X}_{1 i}+\beta_{2} \mathbf{X}_{2 i}+\beta_{3} \mathbf{X}_{3 i}+\epsilon_{i}
$$

Common hypotheses to test

1) Test all $\beta_{k}$ jointly
$\mathrm{H}_{0}: \beta_{1}=\beta_{2}=\beta_{3}=0$
$\mathrm{H}_{1}$ : some $\beta_{k} \neq 0$
This test we have seen. It is a test of the whole model. The necessary SS is the $\operatorname{SSR}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right)$ tested with the $\operatorname{SSE}$ for the full model. This test is provided by most software.
2) Test some subset of $\beta_{k}$, jointly
$\mathrm{H}_{0}: \beta_{2}=\beta_{3}=0$
3) Test individual $\beta_{k}$
$\mathrm{H}_{0}: \beta_{2}=0$
4) Test relationships between 2 or more $\beta_{k}$
$\mathrm{H}_{0}: \beta_{2}=\beta_{3}$
5) Test all $\beta_{k}$ jointly

$$
\begin{aligned}
& \mathrm{H}_{0}: \beta_{1}=\beta_{2}=\beta_{3}=\ldots=\beta_{\mathrm{k}}=0 \\
& \mathrm{H}_{1}: \beta_{\mathrm{j}} \neq 0 \text { for at least one } \mathrm{j}
\end{aligned}
$$

The test is done as

$$
F=\frac{\operatorname{MSReg}\left(b_{1}, b_{2}, \ldots, b_{k}\right)}{\operatorname{MSE}}
$$

A different approach to this same test is given as
a) Full Model: $\quad \mathrm{Y}=\beta_{0}+\beta_{1} \mathrm{X}_{1 \mathrm{i}}+\ldots+\beta_{\mathrm{k}} \mathrm{X}_{\mathrm{ki}}$

$$
\operatorname{SSE}_{\text {Full }}=\mathrm{Y}^{\prime} \mathrm{Y}-\operatorname{SSReg}_{\left(\mathrm{b}_{0}, \mathrm{~b}_{1}, \ldots, b_{k}\right)}
$$

b) Reduced Model: $\quad \mathrm{Y}=\beta_{0}$

$$
\mathrm{SSE}_{\text {Reduced }}=\mathrm{Y}^{\prime} \mathrm{Y}-\mathrm{n} \overline{\mathrm{Y}}^{2}
$$

The test statistic is now - expressions using SSErrors
or expressions using SSRegressions
where; $\mathrm{n}=$ number of observations

$$
k=\text { number of parameters }
$$

" 1 " is for the intercept ( $\beta_{0}$ )

Analysis of Variance

|  | Sum of |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| Source | DF | Squares | Mean Square | F Value | Pr > F |
| Model | 3 | 627.8169964 | 209.2723321 | 68.12 | $<.0001$ |
| Error | 20 | 61.4430036 | 3.0721502 |  |  |
| Corrected Total | 23 | 689.2600000 |  |  |  |

## Utility of TYPE I SS

1) Some special types of models do have an order. eg. Polynomials and some cases of analysis of covariance. We will see both of these later.
2) This is also convenient to use to set up the General Linear Test, the reduced model variables are entered first, and the SSDifference is given by the sum of the remaining variables.

For example, suppose we wish to test to see of several $\beta^{\prime}$ s jointly $=0$

$$
\mathrm{H}_{0}: \beta_{2}=\beta_{3}=0
$$

$\mathrm{H}_{0}$ : both $\beta_{2}$ and $\beta_{3}$ do not $=0$
The SS for the reduced model will be $\operatorname{SSR}\left(\mathrm{X}_{1}\right)$
The SS for the full model will be $\operatorname{SSR}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right)$
The SS for the difference will be $\operatorname{SSR}\left(\mathrm{X}_{2}, \mathrm{X}_{3} \mid \mathrm{X}_{1}\right)$
The SS for the difference can be calculated as
$\operatorname{SSR}\left(\mathrm{X}_{2}, \mathrm{X}_{3} \mid \mathrm{X}_{1}\right)=\operatorname{SSR}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right)-\operatorname{SSR}\left(\mathrm{X}_{1}\right)$
or as

$$
\operatorname{SSR}\left(\mathrm{X}_{2} \mid \mathrm{X}_{1}\right)+\operatorname{SSR}\left(\mathrm{X}_{3} \mid \mathrm{X}_{1}, \mathrm{X}_{2}\right)
$$

## Test of a subset of coefficients

$$
\mathbf{Y}_{i}=\beta_{0}+\beta_{1} \mathbf{X}_{1 \mathrm{i}}+\beta_{2} \mathbf{X}_{2 \mathrm{i}}+\beta_{3} \mathbf{X}_{3 \mathrm{i}}+\epsilon_{i}
$$

versus

$$
\mathrm{Y}_{i}=\beta_{0}+\beta_{1} \mathrm{X}_{1 \mathrm{i}}+\epsilon_{i}
$$

The hypotheses are

$$
\mathrm{H}_{0}: \beta_{2}=\beta_{3}=0
$$

versus
$\mathrm{H}_{1}$ : at least one of either $\beta_{2}$ or $\beta_{3}$ does not equal 0
The test is done as

The computations are

$$
\begin{aligned}
\text { SSE }_{\text {Full }} & =\mathrm{Y}^{\prime} \mathrm{Y}-\mathrm{b}^{\prime} \mathrm{X}^{\prime} \mathrm{Y} \quad \text { where, } \mathrm{X}=\left(1, \mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right) \\
\mathrm{b} & =\left(\mathrm{X}^{\prime} \mathrm{X}\right)^{-1} \mathrm{X}^{\prime} \mathrm{Y} \\
\mathrm{SSE}_{\text {Red }} & =\mathrm{Y}^{\prime} \mathrm{Y}-\mathrm{b}_{\mathrm{R}}^{\prime} \mathrm{X}_{\mathrm{R}}^{\prime} \mathrm{Y} \quad \text { where, } \mathrm{X}_{\mathrm{R}}=\left(1, \mathrm{X}_{1}\right) \\
\mathrm{b}_{\mathrm{R}} & =\left(\mathrm{X}^{\prime} \mathrm{X}\right)^{-1} \mathrm{X}_{\mathrm{R}}^{\prime} \mathrm{Y} \\
\mathrm{~F}_{\mathrm{o}}= & \frac{\frac{b^{\prime} \mathrm{X}^{\prime} \mathrm{Y}-\mathrm{b}_{\mathrm{R}}^{\prime} \mathrm{X}_{\mathrm{R}}^{\prime} \mathrm{Y}}{\text { difterene in inumbor praneers }=\gamma}}{\text { MSE }}
\end{aligned}
$$

If $\mathrm{F}_{\mathrm{o}} \geq \mathrm{F}_{\alpha, \gamma, \mathrm{n}-\mathrm{p}}$ then we reject $\mathrm{H}_{0}$; otherwise accept

If the variables to be tested are entered last in the model, all of the necessary SS are available in SAS from a single run of PROC GLM or PROC REG with the SS1 option.

Output from PROC GLM with tests of TYPE I SS

| Sum of |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Source |  | DF | Squa |  |  | Mean | n Squar |  |  |  | Val | Pr > F |
| Model |  | 3 | 627.8169 |  |  | 209. | . 2723321 |  |  |  | 68. | <. 0001 |
| Error |  | 20 | 61.4430 |  |  |  | . 072150 |  |  |  |  |  |
| Corrected | Total | 23 | 689.2600 |  |  |  |  |  |  |  |  |  |
| Source | DF |  | ype I SS |  |  | an S | Square | F |  |  | lue | Pr > F |
| X1 | 1 | 30 | . 7323285 |  |  | 6.73 | 323285 |  |  |  | . 84 | <. 0001 |
| X2 | 1 | 26 | . 7944455 |  |  | 63.79 | 944455 |  |  |  | . 87 | <. 0001 |
| X3 | 1 |  | . 2902224 |  |  | 57.29 | 902224 |  |  |  | . 65 | 0.0003 |

To test $\beta_{2}$ and $\beta_{3}$ jointly, we use
Full Model $=\operatorname{SSR}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right)=627.8169964$
Reduced model is given by "X1" in the TYPE I SS $=\operatorname{SSR}\left(\mathrm{X}_{1}\right)=$ 306.7323285

The difference can be calculated as either
Full Model - Reduced model $=\operatorname{SSR}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \mathrm{X}_{3}\right)-\operatorname{SSR}\left(\mathrm{X}_{1}\right)$

$$
=627.8169964-306.7323285=321.08467
$$

or as the sum of "X2" and "X3" from the TYPE I SS

$$
\operatorname{SSR}\left(X_{2} \mid X_{1}\right)+\operatorname{SSR}\left(X_{3} \mid X_{1}, X_{2}\right)=263.7944455+57.2902224=321.08467
$$

Then, for either case, the F test for the General Linear Test is

$$
F=\frac{\text { MSDifference }}{\text { MSError }}=\frac{\frac{321.0467}{3.0721502}}{3.25732305}
$$

The Tabular F values are

$$
\mathrm{F}_{a=0.05: 1,20}=4.35 \quad \mathbf{F}_{a=0.05: 2,20}=\mathbf{3 . 4 9} \mathrm{F}_{a=0.05: 3,20}=3.10
$$

TYPE II SS gives the contribution to the model of each variable entered after the model has been adjusted for all other variables.
$\operatorname{SSR}\left(\mathrm{X}_{l} \mid \mathrm{X}_{m}, \mathrm{X}_{n}\right)=$
$\operatorname{SSR}\left(\mathrm{X}_{n} \mid \mathrm{X}_{l}, \mathrm{X}_{m}\right)=$
$\operatorname{SSR}\left(\mathrm{X}_{m} \mid \mathrm{X}_{l}, \mathrm{X}_{n}\right)=$
These SS are also referred to as the Partial SS or the fully adjusted SS. These SS are NOT order dependent. If order is changed, the results will not change

## Utility of TYPE II SS

1) These are the statistics generally examined to determine the "unique" contribution of each variable.

The test done by this type of SS is the test of individual $\beta_{k}$, given that all other variables are already in the model.

$$
\begin{aligned}
& \mathrm{H}_{0}: \beta_{2}=0 \\
& \mathrm{H}_{1}: \beta_{2} \neq 0
\end{aligned}
$$

This can also be tested by the $t$-test of the regression coefficient. These two tests (ie. F test of TYPE II SS and t -test of $\beta_{k}$ are identical).

NOTE that this implies that the $\mathrm{b}_{k}$ are fully adjusted. The $\mathrm{b}_{k}$ in Multiple Regression are also referred to as the Partial Regression Coefficient.

Test of individual coefficients - $\beta_{\mathrm{j}}$ against an hypothesized $\beta_{\mathrm{jo}}$

$$
t_{o}=\frac{\mathrm{b}_{\mathrm{j}}-\beta_{\mathrm{jo}}}{\sqrt{\hat{\sigma}^{2} \mathrm{c}_{\mathrm{jj}}}} \sim \mathrm{t}_{(\mathrm{n}-\mathrm{p})}
$$

Special tests

$$
\mathrm{H}_{0}: \beta_{1}=\beta_{3}
$$

$\mathrm{H}_{1}: \beta_{1} \neq \beta_{3}$
This can be tested with the full model

$$
\begin{aligned}
& \mathrm{Y}=\beta_{0}+\beta_{1} \mathrm{X}_{1 i}+\beta_{2} \mathrm{X}_{2 i}+\beta_{3} \mathrm{X}_{3 i}+\epsilon_{i} \\
& \mathrm{Y}=\beta_{0}+\beta_{1} \mathrm{X}_{2 i}+\beta_{2}\left(\mathrm{X}_{1 i}+\mathrm{X}_{3 i}\right)+\epsilon_{i}
\end{aligned}
$$

To test this, create a variable $\mathrm{X} 1 \mathrm{X} 2 \mathrm{SUM}=\mathrm{X} 1+\mathrm{X} 2$; , and fit this as a reduced model.

The original estimates were $\beta_{1}=\mathbf{1 . 1 0 3 1 3}$ and $\beta_{3}=\mathbf{1 . 2 8 8 9 4}$.
The hypotheses are $\quad \mathrm{H}_{0}: \beta_{1}=\beta_{3} \mathrm{H}_{1}: \beta_{1} \neq \beta_{3}$
The variable X 1 X 2 Sum was created as $=\mathrm{X} 1+\mathrm{X} 3$; and run as the reduced model.

## Analysis of Variance

|  | Sum of |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Source | DF | Squares | Square | F Value | Pr > F |
| Model | 2 | 627.38353 | 313.69176 | 106.46 | $<.0001$ |
| Error | 21 | 61.87647 | 2.94650 |  |  |
| Corrected Total | 23 | 689.26000 |  |  |  |


| Parameter Estimates |  |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: |
|  | Parameter | Standard |  |  |  |
| Variable | DF | Estimate | Error | t Value | Pr |
| Intercept | 1 | 17.89290 | 1.95684 | 9.14 | $<.0001$ |
| X2 | 1 | 0.31865 | 0.03556 | 8.96 | $<.0001$ |
| X2X3SUM | 1 | 1.20345 | 0.18912 | 6.36 | $<.0001$ |

The full model error was $\mathbf{3 . 0 7 2 1 5 0 2}$ with 20 df
The F test is

$$
\begin{aligned}
& \mathrm{F}=\frac{\text { MSDifference }}{\text { MSError }}=\frac{61.87647-61.4430036}{3.0721502}=\frac{0.4334664}{3.0721502}=0.1410954 \\
& \mathbf{F}_{a=0.05: 1,20}=\mathbf{4 . 3 5} \mathrm{F}_{a=0.05: 2,20}=3.49 \quad \mathrm{~F}_{a=0.05: 3,20}=3.10
\end{aligned}
$$

See the test results for the second SAS technique below.

This test is facilitated in PROC REG several ways;
Using the "RESTRICT $\mathrm{x} 1=\mathrm{x} 3 ;$ " statement the results are:

Analysis of Variance

|  |  | Sum of | Mean |  | Fr Value |
| :--- | ---: | ---: | ---: | ---: | ---: | Pr > F


| Parameter | Estimates |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: |
|  |  | Parameter | Standard |  |  |
| Variable | DF | Estimate | Error | t Value | Pr $\quad$ \|t| |
| Intercept | 1 | 17.89290 | 1.95684 | 9.14 | $<.0001$ |
| X1 | 1 | 1.20345 | 0.18912 | 6.36 | $<.0001$ |
| X2 | 1 | 0.31865 | 0.03556 | 8.96 | $<.0001$ |
| X3 | 1 | 1.20345 | 0.18912 | 6.36 | $<.0001$ |
| RESTRICT | -1 | -2.33286 | 6.08223 | -0.38 | $0.7111 *$ |

Using the "TEST $x 1=x 3$;" statement the results are:
The results of the test were

| Test 1 Results for | DependentVariable <br> Mean |  |  |  |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Source | DF | Square | F Value | Pr > F |
| Numerator | 1 | 0.43347 | 0.14 | 0.7111 |
| Denominator | 20 | 3.07215 |  |  |

NOTE that the F value is the same. The difference is not significant, implying that the reduced model is as good as the full model, so we can conclude that the data is consistent with the Null hypothesis, $\mathrm{H}_{0}: \beta_{1}=\beta_{3}$
NOTE: that one results in the full model ANOVA and testing with the full model error, the other the reduced model ANOVA. Full model error is still used in testing.

