Multiple Regression (II)

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Special Topics for Multiple Regression

- Extra Sums of Squares
- Standardized Version of the Multiple Regression Model
- Multicollinearity

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 the extra sum of squares as measuring the marginal increase in the regression sum of squares

Example

- Multiple regression
  – Output: Body fat percentage
  – Input:
  1. triceps skin fold thickness(X_1)
  2. thigh circumference (X_2)
  3. midarm circumference (X_3)
- Aim
  –Replace cumbersome and expensive immersion in water procedure with model.
- Goal
  – Determine which predictor variables 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

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

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

Regression of Y on X_1, X_2 and X_3.

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

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

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
- The difference is called *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 $SSR(X_2|X_1)$ measure the marginal effect of adding X_2 to the regression model when X_1 is already in the model

SSR increase and SSE decrease

The extra sum of squares $SSR(X_2|X_1)$ can equivalently be viewed as the marginal increase in the regression sum of squares.

$$\begin{aligned} SSR(X_2|X_1) &= SSR(X_1, X_2) - SSR(X_1) \\ &= 385.44 - 352.27 \\ &= 33.17 \end{aligned}$$

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

$$\begin{aligned} SSR(X_3|X_1, X_2) &= SSE(X_1, X_2) - SSE(X_1, X_2, X_3) \\ &= SSR(X_1, X_2, X_3) - SSR(X_1, X_2) \\ &= 11.54 \end{aligned}$$

or with multiple variables included at time

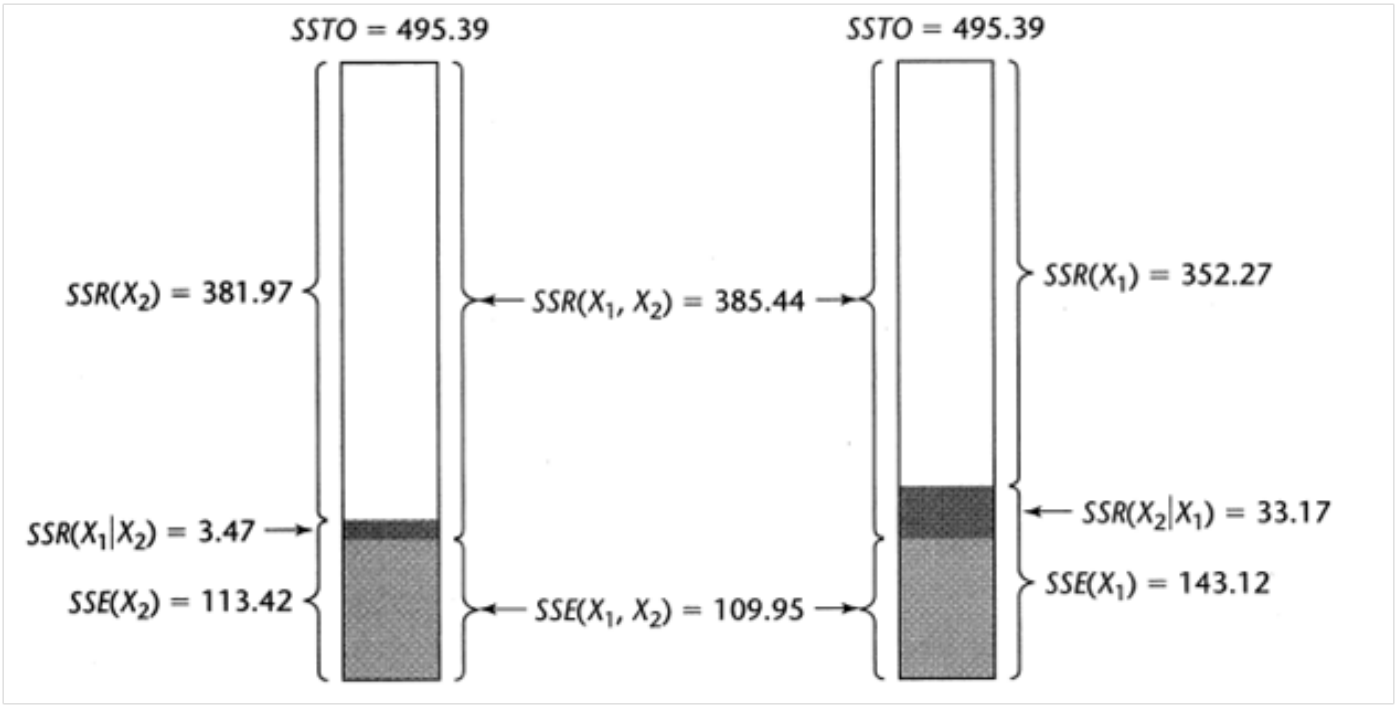
$$\begin{aligned} SSR(X_2, X_3|X_1) &= SSE(X_1) - SSE(X_1, X_2, X_3) \\ &= SSR(X_1, X_2, X_3) - SSR(X_1) \\ &= 44.71 \end{aligned}$$

Definitions

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

N! different partitions

Figure :



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

Figure :

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	$SSTO$	$n-1$	

Importance

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

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i$$

We want to answer the following hypothesis test

$$H_0 : \beta_3 = 0$$
$$H_1 : \beta_3 \neq 0$$

Test whether a single $\beta_k = 0$

- For the full model we have $SSE(F) = SSE(X_1, X_2, X_3)$
- The reduced model is $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i$
- 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 whether a single $\beta_k = 0$

The general linear test statistics is

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

which becomes

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

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

Test whether a single $\beta_k = 0$

The general linear test statistics is

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

Extra sum of squares has one associated degree of freedom.

Example

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

Figure :

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	

$$F^* = \frac{SSR(X_3|X_1,X_2)}{1} \Big/ \frac{SSE(X_1,X_2,X_3)}{n-4} = 1.88$$

Example Cont.

- For $\alpha = .01$ we require $F(.99; 1, 16) = 8.53$
- We observe $F^* = 1.88$
- We conclude $H_0 : \beta_3 = 0$

Test whether several $\beta_k = 0$

Another example

$H_0 : \beta_2 = \beta_3 = 0$

H_1 : not both β_2 and β_3 are zero

The general linear test can be used again

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

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

- General linear test can be used to determine whether or not a predictor variable(or sets of 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.

Summary of Tests Concerning Regression Coefficients

- Test whether all $\beta_k = 0$
- Test whether a single $\beta_k = 0$
- Test whether some $\beta_k = 0$
- Test involving relationships among coefficients, for example,
  - $H_0 : \beta_1 = \beta_2$ vs. $H_a : \beta_1 \neq \beta_2$
  - $H_0 : \beta_1 = 3, \beta_2 = 5$ vs. H_a : otherwise
- Key point in all tests: form the full model and the reduced model, then calculate the SSE(F) and SSE(R).

Coefficients of Partial Determination

- Recall "Coefficient of determination":
  R^2 measures the proportionate reduction in the variation of Y by introduction of the entire set of X.
- Partial Determination:
  measures the marginal contribution of one X variable when all others are already in the model.

Two predictor variables

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i$$

- Coefficient of partial determination between Y and X_1 given X_2 in the model is denoted as $R^2_{Y1|2}$:

$$R^2_{Y1|2} = \frac{SSE(X_2) - SSE(X_1, X_2)}{SSE(X_2)} = \frac{SSR(X_1|X_2)}{SSE(X_2)}$$

- Likewise:

$$R^2_{Y2|1} = \frac{SSE(X_1) - SSE(X_1, X_2)}{SSE(X_1)} = \frac{SSR(X_2|X_1)}{SSE(X_1)}$$

General case

- $$R^2_{Y1|23} = \frac{SSR(X_1|X_2, X_3)}{SSE(X_2, X_3)}$$
- $$R^2_{Y4|123} = \frac{SSR(X_4|X_1, X_2, X_3)}{SSE(X_1, X_2, X_3)}$$

Properties

- Value between 0 and 1
- Another way of getting $R^2_{Y1|2}$:
  1. Regress Y on X_2 and obtain the residuals $e_i(Y|X_2) = Y_i - \hat{Y}_i(X_2)$
  2. Regress X_1 on X_2 and obtain the residuals $e_i(X_1|X_2) = X_{i1} - \hat{X}_{i1}(X_2)$
  3. R^2 between $e_i(Y|X_2)$ and $e_i(X_1|X_2)$ will be the same as $R^2_{Y1|2}$.
- Followup, the scatter plot of $e_i(Y|X_2)$ and $e_i(X_1|X_2)$ provides a graphical representation of the strength of the relationship between Y and X_1, adjusted for X_2. Called "added variable pots" or "partial regression plots". More on Chapter 10.1.

Coefficients of Partial Correlation

- Coefficients of Partial Correlation:
  square root of a coefficient of partial determination, following the same sign with the regression coefficient.

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 $X'X$ matrix for the transformed variables fall between -1 and 1 inclusive
- Lack of comparability of regression coefficients
  $\hat{Y} = 200 + 20000X_1 + .2X_2$
  Y in dollars, X_1 in thousand dollars, X_2 in cents
  – Which is most important predictor?

Correlation Transformation

- Makes all entries in $X'X$ matrix for the transformed variables fall between -1 and 1 inclusive
- Lack of comparability of regression coefficients
  $\hat{Y} = 200 + 20000X_1 + .2X_2$
  Y in dollars, X_1 in thousand dollars, X_2 in cents
  – Which is most important predictor?
  X_1 increase 1,000 dollars$\rightarrow$ Y increase $20,000$ dollars
  X_2 increase 1,000 dollars$\rightarrow$ Y also increase $20,000$ dollars

Correlation Transformation

Centering and scaling

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

$$\frac{X_{ik} - \bar{X}_k}{s_k}, k = 1, ..., p-1$$

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

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

Correlation Transformation

Transformed variables

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

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

Standardized Regression Model

Define the matrix consisting of the transformed X variables

$$X^* = \begin{pmatrix} X^*_{11} & \cdots & X^*_{1,p-1} \\ X^*_{21} & \cdots & X^*_{2,p-1} \\ \cdots & & \\ X^*_{n1} & \cdots & X^*_{n,p-1} \end{pmatrix}$$

And define $(X^*)'X^* = r_{XX}$

Correlation matrix of the X variables

Can show that

$$r_{XX} = \begin{pmatrix} 1 & r_{12} & \dots & r_{1,p-1} \\ r_{21} & 1 & \dots & r_{2,p-1} \\ \dots & & & \\ r_{p-1,1} & r_{p-1,2} & \dots & 1 \end{pmatrix}$$

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

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

Standardized Regression Model

- The regression model using the transformed variables:

$$Y_i^* = \beta_1^* X_{i1}^* + \cdots + \beta_{p-1}^* X_{i,p-1}^* + \epsilon_i^*$$

- Notice that there is no need for intercept
- If we define in a similar way $(X^*)'Y^* = r_{XY}$, where r_{XY} is the coefficient of simple correlations between X_j and Y
- Then we can set up a standard linear regression problem

$$r_{XX}\, b = r_{XY}$$

Standardized Regression Model

The solution

$$\mathbf{b}^* = \begin{pmatrix} b_1^* \\ b_2^* \\ . \\ . \\ . \\ b_{p-1}^* \end{pmatrix}$$

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

$$b_k = (\frac{s_y}{s_k}) b_k^*, k = 1, ..., p-1$$
$$b_0 = \bar{Y} - b_1 \bar{X}_1 - ... - b_{p-1} \bar{X}_{p-1}$$

Multicollinearity

When the predictor variables are correlated among themselves, *intercorrelation or multicollinearity* among them is said to exist.

- Uncorrelated Predictor Variables
- Perfectly Correlated Predictor Variables
- Effects of Multicollinearity

Uncorrelated Predictor Variables

Suppose we have the following three regression

- Regress Y on X_1. (Estimator b_1)
- Regress Y on X_2. (Estimator b_2)
- Regress Y on both X_1 and X_2 (Estimator b_1^* and b_2^*)

If X_1 and X_2 are uncorrelated, then we have

1. $b_1 = b_1^*$, $b_2 = b_2^*$
2. $SSR(X_1|X_2) = SSR(X_1)$, $SSR(X_2|X_1) = SSR(X_2)$

Perfectly Correlated Predictor Variables

Regress Y on both X_1 and X_2. If X_1 and X_2 are perfectly correlated (say $X_2 = 5 + .5X_1$), then

- We have infinitely many possible solutions which fits the model equally well (have the same SSE).
- The perfect relation between X_1 and X_2 does not inhibit our ability to obtain a good fit.
- The magnitude of the regression coefficients can not be interpreted as reflecting the effects of different predictor variables.

General Effects of Multicollinearity

- Usually, we still have good fit of the data, in addition, we still have good prediction.
- The estimated regression coefficients tends to have large sampling variability when the predictor variables are highly correlated. Some of the regression coefficients maybe statistically not significant even though a definite statistical relation exists.
- The common interpretation of a regression coefficient is NOT fully applicable any more.
- Regress Y on both X_1 and X_2. It is possible that when individual t-tests are performed, neither β_1 or β_2 is significant. However, when the F-test is performed for both β_1 and β_2, the results may still be significant.