

#### Prediction of a New Observation

$$\bullet \ \ Y_{h(new)} = \mathbf{X}_h' \boldsymbol{\beta} + \epsilon_h : \qquad \text{with the observations } Y_i \mathbf{s}.$$

$$\bullet \ \ \text{Predicted value: } \widehat{Y}_h := \qquad .$$

$$\bullet \ \ \sigma^2(pred_h) := \qquad .$$

$$\bullet \ \ \text{Standard error for prediction:}$$

$$s(pred_h) = \qquad .$$

$$\bullet \ \ (1 - \alpha) \text{-prediction interval for } Y_{h(new)} :$$

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#### Prediction of a New Observation

• 
$$Y_{h(new)} = X_h' \beta + \epsilon_h$$
: independent with the observations  $Y_i$ s.

• Predicted value:  $\widehat{Y}_h := \mathbf{X}'_h \hat{\boldsymbol{\beta}}$ 

$$\sigma^2(\mathsf{pred}_h) := \mathsf{Var}(\widehat{\mathsf{Y}}_h - \mathsf{Y}_{h(\mathsf{new})}) = \sigma^2(\widehat{\mathsf{Y}}_h) + \sigma^2(\mathsf{Y}_{h(\mathsf{new})}) = \sigma^2 \mathsf{X}_h'(\mathsf{X}'\mathsf{X})^{-1} \mathsf{X}_h + \sigma^2.$$

Standard error for prediction:

$$s(pred_h) = \sqrt{MSE[1 + \mathbf{X}'_h(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_h]}.$$

• 
$$(1 - \alpha)$$
-prediction interval for  $Y_{h(new)}$ :

$$Y_h \pm t(1-\alpha/2; n-p)s(pred_h).$$

# Multiple Regression: Example

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3								0.4															
 30					12			0.6															
30			1.4	۷.	12	-0.	. 6 -	<b>u</b> . 0.															
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# Example: Model 2

Nonadditive model with interaction between 
$$X_1$$
 and  $X_2$ :

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \beta_4 X_{i1} X_{i2} + \epsilon_i, \quad i = 1, \cdots, 30.$$

( $\rho = 5$ )
Call:
Im(formula = Y \(^{-1} X\_1 + X\_2 + X\_3 + X\_1 : X\_2, \text{ data} = \text{ data})

Coefficients:
Estimate Std. Error t value \(^{-1} Pr(>|t|) \)
(Intercept) 0.8832 0.2153 4.103 0.00038 \*\*\*
X1 1.5946 0.2421 6.587 6.69e-07 \*\*\*
X2 1.7091 0.2605 6.560 7.16e-07 \*\*\*
X3 2.1266 0.2687 7.916 2.85e-08 \*\*\*
X1:X2 1.0076 0.2467 4.084 0.00040 \*\*\*

X1:X2 1.0076 0.2467 4.084 0.00040 \*\*\*

Signif. codes: 0 \*\*\* 0.001 \*\* 0.01 \* 0.05 . 0.1 1

Residual standard error: 1.026 on 25 degrees of freedom Multiple R-squared: 0.933, Adjusted R-squared: 0.9223 F-statistic: 87.04 on 4 and 25 DF, p-value: 2.681e-14



- Predict a new observation when  $X_1 = 0.8, X_2 = 0.5, X_3 = +1$
- under Model 2. Standard error for prediction:
  - s(pred) =
  - A 99%-prediction interval for  $Y_{hnew}$ :
    - $1.290 \pm 2.787 \times 1.1098 = [-1.803, 4.383].$
  - R codes.
  - > newX=data.frame(X1=0.8, X2=0.5, X3=-1)
  - > predict.lm(fit2, newX, interval="confidence",
  - + level=0.99, se.fit=TRUE)
  - > predict.lm(fit2, newX, interval="prediction", + level=0.99, se.fit=TRUE)

Predict a new observation when  $X_1 = 0.8, X_2 = 0.5, X_3 = -1$ under Model 2.

Standard error for prediction:

$$s(pred) = \sqrt{1.053 \times (1 + 0.170)} = 1.1098.$$

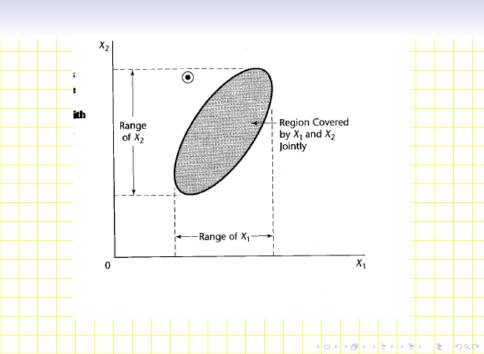
- A 99%-prediction interval for Y<sub>hnew</sub>:
  - $1.290 \pm 2.787 \times 1.1098 = [-1.803, 4.383].$
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- > newX=data.frame(X1=0.8, X2=0.5, X3=-1)
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  - + level=0.99, se.fit=TRUE)

## Hidden Extrapolations

- Recall that extrapolation occurs when predicting the response variable for values of the X variable(s) of the original data.
- It's possible that, the fitted model when extended outside the range of the observations.
- With more than one X variables, the levels of define the region of the observations. One can not merely look at the ranges of each X variable.
- With two X variables, we can look at their scatter plot.
- Procedure to identify hidden extrapolation for more than two X variables will be discussed later.

## Hidden Extrapolations

- Recall that extrapolation occurs when predicting the response variable for values of the X variable(s) lying outside the range of the original data.
- It's possible that, the fitted model does not hold when extended outside the range of the observations.
- With more than one X variables, the levels of all X variables jointly define the region of the observations. One can not merely look at the ranges of each X variable.
- With two X variables, we can look at their scatter plot.
- Procedure to identify hidden extrapolation for more than two X variables will be discussed later.



#### Extra Sum of Squares

$$I$$
 and  $\mathcal J$  are two **non-overlapping** index sets.

• Extra sum of squares (ESS):

$$SSR(X_{\mathcal J}|X_I) :=$$
• It indicates the

• Degrees of freedom:  $d.f.(SSR(X_{\mathcal J}|X_I)) =$ 

• Mean squares:  $MSR(X_{\mathcal{J}}|X_I) :=$ 

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#### Extra Sum of Squares

$$I$$
 and  $\mathcal J$  are two **non-overlapping** index sets.

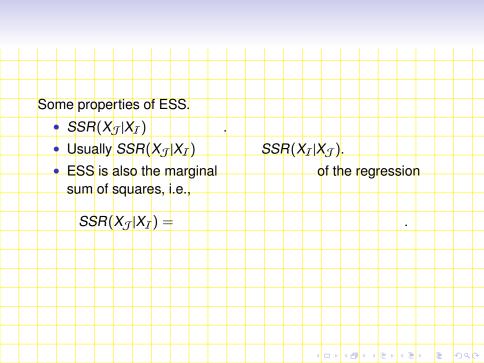
Extra sum of squares (ESS):

$$SSR(X_{\mathcal{I}}|X_{\mathcal{I}}) := SSE(X_{\mathcal{I}}) - SSE(X_{\mathcal{I}}, X_{\mathcal{I}}).$$

- It indicates the reduction in error sum of squares by adding  $X_{\mathcal{J}}$  to the model where  $X_{\mathcal{I}}$  is the set of X variables.
- Degrees of freedom:  $d_i f_i(SSR(X_{\mathcal{J}}|X_{\mathcal{I}})) = |\mathcal{J}|$ .
- Mean squares:  $MSR(X_{\mathcal{J}}|X_I) := \frac{SSR(X_{\mathcal{J}}|X_I)}{d.f.(SSR(X_{\mathcal{J}}|X_I))}$ .

# Notations. • I: an index set; $X_I := \{X_i : i \in I\}$ . • E.g. $I = \{2, 3\}, X_T = \{X_2, X_3\}.$ $SSE(X_T)$ and $SSR(X_T)$ denote the error sum of squares and regression sum of squares, respectively, under the regression model with $X_{\mathcal{I}} := \{X_i : i \in \mathcal{I}\}$ being the X variables. • E.g., $SSE(X_2, X_3)$ is the error sum of squares of the model with $X_2$ and $X_3$ .

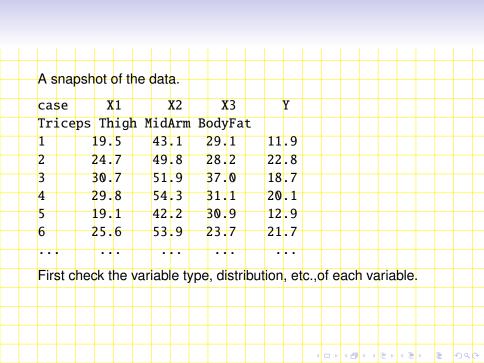
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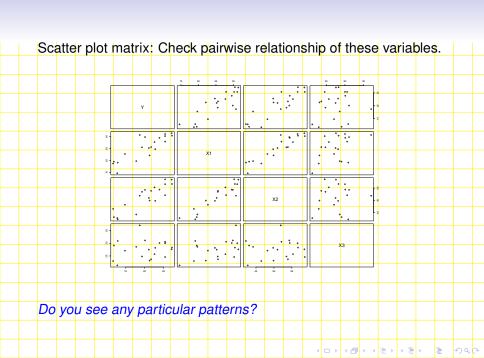


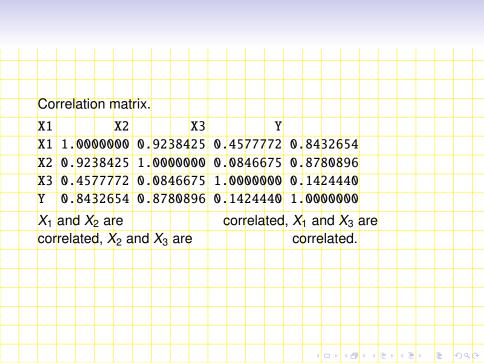
Some properties of ESS. •  $SSR(X_T|X_T) \geq 0$ . Usually  $SSR(X_T|X_T) \neq SSR(X_T|X_T)$ . ESS is also the marginal increase of the regression sum of squares, i.e.,  $SSR(X_T|X_T) = SSR(X_T, X_T) - SSR(X_T).$ 4 D > 4 B > 4 E > 4 E > E 900

# **Body Fat**

A researcher measured the amount of body fat (Y) of 20 healthy females 25 to 34 years old, together with three (potential) predictor variables, triceps skinfolds thickness  $(X_1)$ , thigh circumference  $(X_2)$ , and midarm circumference  $(X_3)$ . The amount of body fat was obtained by a cumbersome and expensive procedure requiring immersion of the person in water. Thus it would be helpful if a regression model with some or all of these predictors could provide reliable estimates of body fat as these predictors are easy to measure.







Consider the following 4 models.

$$Y_i = \beta_0 + \beta_1 X_{i1} + \epsilon_i, \quad i = 1, \cdots, 20.$$

 $Y_i = \beta_0 + \beta_2 X_{i2} + \epsilon_i, i = 1, \dots, 20.$ 

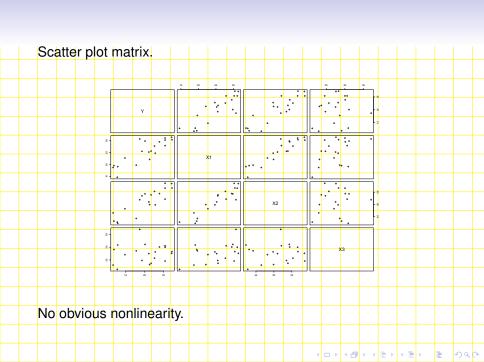
 $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i, i = 1, \dots, 20.$ 

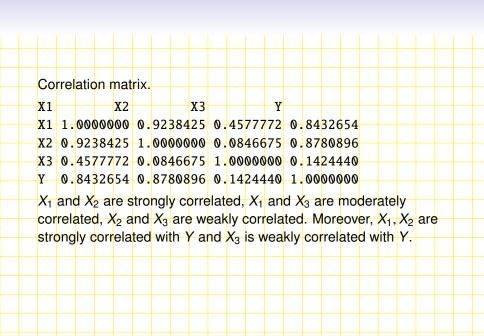
Model 2: regression of Y on 
$$X_2$$

Model 3: regression of Y on 
$$X_1$$
 and  $X_2$ 

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i, \quad i = 1, \dots, 20.$$







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Consider the following 4 models.

$$Y_i = \beta_0 + \beta_1 X_{i1} + \epsilon_i, \quad i = 1, \cdots, 20.$$

 $Y_i = \beta_0 + \beta_2 X_{i2} + \epsilon_i, i = 1, \dots, 20.$ 

 $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i, i = 1, \dots, 20.$ 

Model 2: regression of Y on 
$$X_2$$

Model 3: regression of Y on 
$$X_1$$
 and  $X_2$ 

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i, \quad i = 1, \dots, 20.$$



> summary(fit1)	
Call: lm(formula = Y ~ X1, data = fat)	
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 ***	
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1	
Residual standard error: 2.82 on 18 degrees of freedom	
Multiple R-squared: 0.7111, Adjusted R-squared: 0.695	
F-statistic: 44.3 on 1 and 18 DF, p-value: 3.024e-06	
> anova(fit1) Analysis of Variance Table	
marysis of variance rable	
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	
(GLT)	

> summar	y(fit	2)															
Call: lm(formu	15 - 1	v ~ v	o 4.	a+a -	fat.												
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Coeffici	ents:																
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X2				0.													
Signif.	codes	. 0	*** (	0.001	** (	0.01	* 0.	95.	0.1	1							
Residual																	
Multiple											7583						
F-statis	tic: (	50.62	on :	1 and	18	DF,	p-va	lue:	3.6e	-07							
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marysis	01 11	ii iun	CC 10	ubic													
Response	: Y																
Df Sum S																	
X2				81.97		617	3.6e	-07 *	**								
Residual	s 18	113.4	2	6.30													

> summary(fit	:3)							
Call:								
lm(formula =	Y ~ X1 + X2,	data = fat	:)					
Coefficients:								
Estimate Std.								
(Intercept) -	-19.17 <mark>42 {</mark>							
X1		0. <mark>3034</mark> 0.						
X2 	0.6594							
Signif. codes	s: 0 *** 0.00	01 ** 0.01	* 0.05 .	0.1 1				
Residual star								
Multiple R-so								
F-statistic:	29.8 on 2 at	id 17 DF,	p-value:	2.774e-06				
> anova(fit3)	<del>)</del>							
Analysis of V	/arian <mark>ce Ta</mark> ble	2						
Response: Y								
Df S <mark>u</mark> m Sq Mea								
	352.2 <mark>7 352.2</mark>							
	33.17 33.3		0.0369	*				
Residuals 17	109.95 6.4	17						
							<b>∢</b> GLT	

	\ e111	nmary	(fi+	1)															
	Call	: ´	-	-		<b>v</b> o .	vo .		fai	,									
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	X2					33.17													
	Х3					11.55													
	Resid	duals	16	98.4	:0	6.15													
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# Body Fat: ESS

From the R outputs, we can derive a number of extra sums of squares. For example:

$$SSR(X_2|X_1) =$$

$$SSR(X_1|X_2) =$$

- Both extra sums of squares have degrees of freedom , so  $MSR(X_2|X_1) =$  and  $MSR(X_1|X_2) =$
- The reduction of SSE by adding with is much more than the reduction of SSE by adding to a model with

to a model

# Body Fat: ESS

From the R outputs, we can derive a number of extra sums of squares. For example:

- From Model 1,  $SSE(X_1) = 143.12$  and from Model 3,  $SSE(X_1, X_2) = 109.95. So$ 
  - $SSR(X_2|X_1) = SSE(X_1) SSE(X_1, X_2) = 143.12 109.95 = 33.17.$
- From Model 2, SSE(X<sub>2</sub>) = 113.42, so

$$SSR(X_1|X_2) = SSE(X_2) - SSE(X_1, X_2) = 113.42 - 109.95 = 3.47.$$

- Both extra sums of squares have degrees of freedom 1, so  $MSR(X_2|X_1) = 33.17$  and  $MSR(X_1|X_2) = 3.47$ .
- The reduction of SSE by adding  $X_2$  to a model with  $X_1$  is much more than the reduction of SSE by adding  $X_1$  to a model with  $X_2$ .

 $SSR(X_3|X_1,X_2) =$ This extra sum of squares has degrees of freedom so  $MSR(X_3|X_1,X_2) =$  $SSR(X_2, X_3|X_1) =$ This extra sums of squares has degrees of freedom so  $MSR(X_2, X_3|X_1) =$ Are there other ESS that can be derived from the R outputs? 4 D > 4 B > 4 E > 4 E > E 900 • From Model 4,  $SSE(X_1, X_2, X_3) = 98.40$ , so

$$SSR(X_3|X_1, X_2) = SSE(X_1, X_2) - SSE(X_1, X_2, X_3)$$
  
= 109.95 - 98.40 = 11.55.

This extra sum of squares has degrees of freedom 1, so  $MSR(X_3|X_1,X_2) = 11.55$ .

• Moreover.

$$SSR(X_2, X_3|X_1) = SSE(X_1) - SSE(X_1, X_2, X_3) = 143.12 - 98.40 = 44.72,$$
  
 $SSR(X_1, X_3|X_2) = SSE(X_2) - SSE(X_1, X_2, X_3) = 113.42 - 98.40 = 15.02.$ 

 $SSR(X_1, X_3|X_2) = SSE(X_2) - SSE(X_1, X_2, X_3) = 113.42 - 98.40 = 15.02.$ These two extra sums of squares have degrees of freedom 2, so  $MSR(X_2, X_3|X_1) = 44.72/2 = 22.36$ .

 $MSR(X_1, X_3|X_2) = 15.02/2 = 7.51.$ 

Are there other ESS that can be derived from the R outputs?



# Decomposition of SSR into ESS

For a model with multiple X variables, the regression sum of squares (SSR) can be expressed as the of several extra sums of squares.

For example:

$$SSR(X_1, X_2) =$$

 $X_1$  is already in the model.

 $SSR(X_1)$  measures the contribution by in the model, whereas  $SSR(X_2|X_1)$  measures the contribution when , given that

However, such decomposition is usually not unique. For example,

$$SSR(X_1, X_2) =$$

## Decomposition of SSR into ESS

For a model with multiple X variables, the regression sum of squares (SSR) can be expressed as the sum of several extra sums of squares.

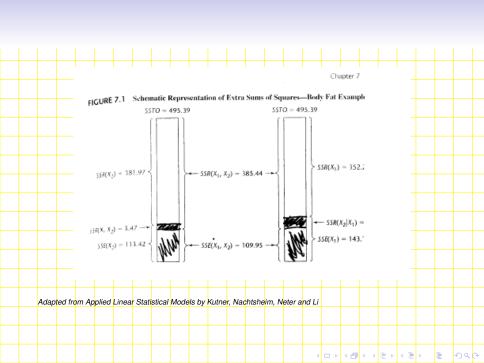
For example:

$$SSR(X_1, X_2) = SSR(X_1) + SSR(X_2|X_1).$$

 $SSR(X_1)$  measures the contribution by having  $X_1$  alone in the model, whereas  $SSR(X_2|X_1)$  measures the additional contribution when  $X_2$  is added, given that  $X_1$  is already in the model.

However, such decomposition is usually not unique. For example,

$$SSR(X_1, X_2) = SSR(X_2) + SSR(X_1|X_2).$$



```
    More X variables.

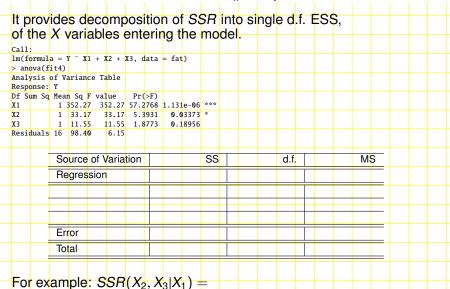
                                       decompositions. For
  example, with three X variables:
   SSR(X_1, X_2, X_3) =
                         SSR(X_1) + SSR(X_2|X_1) + SSR(X_3|X_1, X_2)
   SSR(X_1, X_2, X_3) = SSR(X_2) + SSR(X_1|X_2) + SSR(X_3|X_1, X_2)
   SSR(X_1, X_2, X_3) = SSR(X_1) + SSR(X_2, X_3|X_1), \dots, \dots

    Body Fat.

     • From Model 1, SSR(X_1) = 352.27; Also SSR(X_2|X_1) = 33.17
       and SSR(X_3|X_1, X_2) = 11.55. So
             SSR(X_1, X_2, X_3) =
     • From Model 2, SSR(X_2) = 381.97; Also SSR(X_1|X_2) = 3.47.
       So
             SSR(X_1, X_2, X_3) =
```

- More X variables, more decompositions. For example, with three X variables:
- $SSR(X_1, X_2, X_3) = SSR(X_1) + SSR(X_2|X_1) + SSR(X_3|X_1, X_2)$  $SSR(X_1, X_2, X_3) = SSR(X_2) + SSR(X_1|X_2) + SSR(X_3|X_1, X_2)$
- $SSR(X_1, X_2, X_3) = SSR(X_1) + SSR(X_2, X_3|X_1), \cdots, \cdots$
- Body Fat. • From Model 1,  $SSR(X_1) = 352.27$ ; Also  $SSR(X_2|X_1) = 33.17$ 
  - and  $SSR(X_3|X_1, X_2) = 11.55$ . So
- $SSR(X_1, X_2, X_3) = 352.27 + 33.17 + 11.55 = 396.99.$ • From Model 2,  $SSR(X_2) = 381.97$ ; Also  $SSR(X_1|X_2) = 3.47$ .
  - So  $SSR(X_1, X_2, X_3) = 381.97 + 3.47 + 11.55 = 396.99$

# Read anova() output



# Read anova() output

It provides decomposition of SSR into single d.f. ESS, in the order of the X variables entering the model.

```
Ca11 ·
lm(formula = Y ~ X1 + X2 + X3, data = fat)
> anova(fit4)
Analysis of Variance Table
Response: Y
Df Sum Sq Mean Sq F value
                          Pr(>F)
Х1
          1 352.27 352.27 57.2768 1.131e-06 ***
X2
          1 33.17 33.17 5.3931
                                    0.03373 *
          1 11.55 11.55 1.8773
                                    0.18956
Residuals 16 98.40
                      6 15
```

	So	urce	of V	'aria	tion		SS		d.f.		MS	
	Re	gres	sion				96.9		3		32.3	_
	$X_1$					3	52.2	7	1	3	52.2	7
	^1					1 -			' '	1 -		-
	$X_2$	$X_1$				3	3.17	7	1	3	33.17	7
	<i>X</i> <sub>3</sub>	$X_1, X_2$	$X_2$			1	1.55	5	1	1	11.55	5
_	Err	or					8.40		16		6.15	
		OI				=	10.40	,	10		0.15	
-	Tot	اد				1	a5 3	a	10			

For example:  $SSR(X_2, X_3|X_1) = SSR(X_2|X_1) + SSR(X_3|X_1, X_2) = 33.17 + 11.55 = 44.72.$ 

