7. Extra Sums of Squares

Football Example:

 $Y_i = \#$ points scored by UF football team in game i $X_{i1} = \#$ games won by opponent in their last 10 games $X_{i2} = \#$ healthy starters for UF (out of 22) in game i

Suppose we fit the SLR

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

and plot the residuals e_i against X_{i2} :



Q: What do we conclude from this ?

A: The residuals appear to be linearly related to X_{i2} , thus, X_{i2} should be put into the model.

Another Example:

 Y_i = height of a person X_{i1} = length of left foot X_{i2} = length of right foot

Suppose we fit the SLR

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

and plot the residuals e_i against X_{i2} :



length of right foot

Q: Why no pattern?

A: X_{i2} is providing the same information about Y that X_{i1} does. Thus, even though X_{i2} is a good predictor of height, it is unnecessary if X_{i1} is already in the model. **Extra sums of squares** provide a means of formally testing whether one set of predictors is necessary **given** that another set is already in the model.

Recall that

$$SSTO = SSR + SSE$$

$$\sum_{i=1}^{n} (Y_i - \bar{Y})^2 = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 + \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$

$$R^2 = \frac{SSR}{SSTO}$$

Important Fact: R^2 will never decrease when a predictor is added to a regression model.

Consider the two different models:

$$E(Y_i) = \beta_0 + \beta_1 X_{i1}$$
$$E(Y_i) = \beta_0^* + \beta_1^* X_{i1} + \beta_2^* X_{i2}$$

Q: Is SSTO the same for both models?

A: Yes! Thus, SSR will never decrease when a predictor is added to a model.

Since SSE and SSR are different depending upon which predictors are in the model, we use the following notation:

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SSR(X_1): SSR for a model with only X_1
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 $SSR(X_1, X_2)$: SSR for a model with X_1 and X_2

 $\mathsf{SSE}(X_1)$ and $\mathsf{SSE}(X_1,X_2)$ have analogous def's

Note

 $SSTO = SSR(X_1) + SSE(X_1)$ $SSTO = SSR(X_1, X_2) + SSE(X_1, X_2)$

We also know $SSR(X_1, X_2) \ge SSR(X_1)$.

Thus $SSE(X_1, X_2) \leq SSE(X_1)$.

Conclusion: SSE never increases when a predictor is added to a model.

Reconsider the Example:

 Y_i = height of a person X_{i1} = length of left foot; X_{i2} = length of right foot

Q: What do you think about the quantity

$$\mathsf{SSR}(X_1, X_2) - \mathsf{SSR}(X_1)$$

A: Probably small because if we know the length of the left foot, knowing the length of the right won't help.

Notation: Extra Sum of Squares

$$\mathsf{SSR}(X_2|X_1) = \mathsf{SSR}(X_1, X_2) - \mathsf{SSR}(X_1)$$

 $SSR(X_2|X_1)$ tells us how much we gain by adding X_2 to the model **given** that X_1 is already in the model.

We define $SSR(X_1|X_2) = SSR(X_1, X_2) - SSR(X_2)$

We can do this with as many predictors as we like, e.g.

 $SSR(X_3, X_5 | X_1, X_2, X_4) = SSR(X_1, X_2, X_3, X_4, X_5) - SSR(X_1, X_2, X_4)$ = SSR(all predictors) - SSR(given predictors) Suppose our model is:

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3}$$

Consider tests involving β_1 , β_2 , and β_3 .

One Beta:
$$H_0: \beta_k = 0, \quad k = 1, 2, \text{ or } 3$$

 $H_A: \text{ not } H_0$

In words, this test says "Do we need X_k given that the other two predictors are in the model?"

Can do this with a t-test:

$$t^* = b_k / \sqrt{\mathsf{MSE} \cdot [(\mathbf{X'X})^{-1}]_{k+1,k+1}}$$

Two Betas: (some of the Betas)

 $\begin{array}{rll} H_0: \beta_1 \!=\! \beta_2 \!=\! 0 & H_0: \beta_1 \!=\! \beta_3 \!=\! 0 & H_0: \beta_2 \!=\! \beta_3 \!=\! 0 \\ H_A: \text{not } H_0 & H_A: \text{not } H_0 & H_A: \text{not } H_0 \end{array}$

For example, the first of these asks "Do we need X_1 and X_2 given that X_3 is in the model?"

All Betas: $H_0: \beta_1 = \beta_2 = \beta_3 = 0$ $H_A: \text{not } H_0$

This is just the overall F-Test

We can do all of these tests using extra sum of squares.

Here is the ANOVA table corresponding to the model

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3}$$

ANOVA Table:

Source of variation	SS	$d\!f$
Regression	$SSR(X_1, X_2, X_3)$	p - 1 = 3
Error	$SSE(X_1, X_2, X_3)$	n-p=n-4
Total	SSTO	n - 1

Partition $SSR(X_1, X_2, X_3)$ into 3 one df extra sums of squares. One way to do it is:

 $\mathsf{SSR}(X_1, X_2, X_3) = \mathsf{SSR}(X_1) + \mathsf{SSR}(X_2 | X_1) + \mathsf{SSR}(X_3 | X_1, X_2)$

Modified ANOVA Table:

Source of variation	SS	df
Regression	$SSR(X_1, X_2, X_3)$	3
	$SSR(X_1)$	1
	$SSR(X_2 X_1)$	1
	$SSR(X_3 X_1,X_2)$	1
Error	$SSE(X_1, X_2, X_3)$	n-4
Total	SSTO	n-1

Note: there are 6 equivalent ways of partitioning $SSR(X_1, X_2, X_3)$.

Three Tests: (p = 4 in this example)

• One Beta: $H_0: \beta_2 = 0$ vs. $H_A:$ not H_0

Test statistic:
$$F^* = \frac{\mathsf{SSR}(X_2|X_1, X_3)/1}{\mathsf{SSE}(X_1, X_2, X_3)/(n-p)}$$

Rejection rule: Reject H_0 if $F^* > F(1-\alpha; 1, n-p)$

• Some Betas: $H_0: \beta_2 = \beta_3 = 0$ vs. $H_A: \text{not } H_0$

Test statistic:
$$F^* = \frac{\mathsf{SSR}(X_2, X_3 | X_1)/2}{\mathsf{SSE}(X_1, X_2, X_3)/(n-p)}$$

Rejection rule: Reject H_0 if $F^* > F(1-\alpha; 2, n-p)$

• All Betas: $H_0: \beta_1 = \beta_2 = \beta_3 = 0$ vs. $H_A:$ not H_0

Test statistic:
$$F^* = \frac{\mathsf{SSR}(X_1, X_2, X_3)/3}{\mathsf{SSE}(X_1, X_2, X_3)/(n-p)}$$

Rejection rule: Reject H_0 if $F^* > F(1-\alpha; p-1, n-p)$

Let's return to the model

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3}$$

and think about testing

$$H_0: \beta_2 = \beta_3 = 0$$
 vs. $H_A: \operatorname{not} H_0$

Test statistic:
$$F^* = \frac{\mathsf{SSR}(X_2, X_3 | X_1)/2}{\mathsf{MSE}(X_1, X_2, X_3)}$$

How do we get $SSR(X_2, X_3|X_1)$ if we have $SSR(X_1)$, $SSR(X_2|X_1)$, and $SSR(X_3|X_1, X_2)$?

 $SSR(X_2, X_3 | X_1) = SSR(X_2 | X_1) + SSR(X_3 | X_1, X_2)$

What if we would have $SSR(X_2)$, $SSR(X_1|X_2)$, and $SSR(X_3|X_1, X_2)$? Stuck!

lm(Y \sim X1+X2+X3)	lm(Y \sim X2+X1+X3)
$SSR(X_1)$	$SSR(X_2)$
$SSR(X_2 X_1)$	$SSR(X_1 X_2)$
$SSR(X_3 X_1,X_2)$	$SSR(X_3 X_1,X_2)$

Example: Patient Satisfaction

 Y_i = patient satisfaction (n = 23) X_{i1} = patient's age in years X_{i2} = severity of illness (index) X_{i3} = anxiety level (index)

Model 1: Consider the model with all 3 pairwise interactions included (p = 7)

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \beta_4 X_{i1} X_{i2} + \beta_5 X_{i1} X_{i3} + \beta_6 X_{i2} X_{i3}$$

and think about testing the 3 interaction terms:

$$H_0: \beta_4 = \beta_5 = \beta_6 = 0$$
 vs. $H_A: \operatorname{not} H_0$

Denote the interaction $X_j X_k$ by I_{jk} . Then

Test statistic:
$$F^* = \frac{\mathsf{SSR}(I_{12}, I_{13}, I_{23} | X_1, X_2, X_3)/3}{\mathsf{MSE}(X_1, X_2, X_3, I_{12}, I_{13}, I_{23})}$$

Rejection rule: Reject H_0 if $F^* > F(1 - \alpha; 3, n - p)$

How do we get this extra sum of squares?

Q: How many partitions of $SSR(X_1, X_2, X_3, I_{12}, I_{13}, I_{23})$ into 6 one df extra sums of squares are there?

A: $6 \times 5 \times 4 \times 3 \times 2 = 6! = 720$

Q: Which ones will allow us to compute F^* ? A: The ones with I_{12} , I_{13} , and I_{23} last.

$$SSR(\cdot) = SSR(X_1) + SSR(X_2|X_1) + SSR(X_3|X_1, X_2) +SSR(I_{12}|X_1, X_2, X_3) +SSR(I_{13}|X_1, X_2, X_3, I_{12}) +SSR(I_{23}|X_1, X_2, X_3, I_{12}, I_{13})$$

Add the last 3 (the interaction terms) to get $SSR(I_{12}, I_{13}, I_{23}|X_1, X_2, X_3)$

> summary(mod1 <- lm(sat ~ age + sev + anx + age:sev + age:anx + sev:anx))
Coefficients:</pre>

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	241.57104	169.91520	1.422	0.174
age	0.28112	4.65467	0.060	0.953
sev	-6.32700	5.40579	-1.170	0.259
anx	24.02586	101.65309	0.236	0.816
age:sev	0.06969	0.10910	0.639	0.532
age:anx	-2.20711	1.74936	-1.262	0.225
sev:anx	1.16347	1.98054	0.587	0.565

> anova(mod1) Analysis of Variance Table Response: sat Df Sum Sq Mean Sq F value Pr(>F) 1 3678.44 3678.44 32.20 3.45e-05 *** age 1 402.78 402.78 3.53 0.079 sev . anx 1 52.41 52.41 0.46 0.508 sev:age 1 0.02 0.02 0.00 0.989 sev:anx 1 1.81 1.81 0.02 0.901 age:anx 1 181.85 181.85 1.59 0.225 Residuals 16 1827.90 114.24 $F^* = \frac{(0.02+1.81+181.85)/3}{114.24} = 0.54$ is compared to F(0.95; 3, 16)> qf(0.95, 3, 16) [1] 3.238872 Because $F^* < F(0.95; 3, 16) = 3.24$ we fail to reject H_0 (Interactions are not

needed).

Model 2: Let's get rid of the interactions and consider

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3}$$

Do we need X_2 (severity of illness) and X_3 (anxiety level) if X_1 (age) is already in the model?

$$H_0: \beta_2 = \beta_3 = 0$$
 vs. $H_A:$ not H_0

Test statistic:
$$F^* = \frac{\mathsf{SSR}(X_2, X_3 | X_1)/2}{\mathsf{MSE}(X_1, X_2, X_3)}$$

Rejection rule: Reject H_0 if $F^* > F(1 - \alpha; 2, n - p)$

How do we get this extra sum of squares?

$$SSR(X_2, X_3 | X_1) = SSR(X_2 | X_1) + SSR(X_3 | X_1, X_2)$$

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> summary(mod2 <- lm(sat ~ age + sev + anx))
Coefficients:</pre>
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	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	162.8759	25.7757	6.319	4.59e-06	***
age	-1.2103	0.3015	-4.015	0.00074	***
sev	-0.6659	0.8210	-0.811	0.42736	
anx	-8.6130	12.2413	-0.704	0.49021	

$$F^* = \frac{(402.8 + 52.4)/2}{105.9} = 2.15$$
 is compared to > qf(0.95, 2, 19)
[1] 3.521893

Because $F^* < F(0.95; 2, 19) = 3.52$ we again fail to reject H_0 (X_2 and X_3 are not needed).

Model 3: Let's get rid of X_2 (severity of illness) and X_3 (anxiety level) and consider the SLR with X_1 (age)

 $\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1}$

Let's construct 95% CI's for β_1 and for $E(Y_h) = X'_h \beta$, where $X'_h = (1 \ 40 \ 50 \ 2)$, based on these 3 models.

> new <- data.frame(age=40, sev=50, anx=2)</pre>

Model 3: (p = 2) $b_1 \pm t(0.975; 21)\sqrt{\mathsf{MSE}/S_{XX}} = (-2.09, -0.96)$

Model 2: (p = 4) $b_1 \pm t(0.975; 19)\sqrt{\mathsf{MSE}[(\mathbf{X}'\mathbf{X})^{-1}]_{22}} = (-1.84, -0.58)$

Model 1: (p = 7) $b_1 \pm t(0.975; 16)\sqrt{\mathsf{MSE}[(\mathbf{X}'\mathbf{X})^{-1}]_{22}} = (-9.59, 10.15)$

Correlation of Predictors Multicollinearity

Recall the SLR situation: data (X_i, Y_i) , $i = 1, \ldots, n$

$$r^2 = SSR/SSTO$$

describes the amount of total variability in the Y_i 's explained by the linear relationship between X and Y.

Because of SSR = $b_1^2 S_{XX}$, where $b_1 = S_{XY}/S_{XX}$, and with $S_{YY} = SSTO$, the sample coefficient of correlation between X and Y is

$$r = \operatorname{sign}(b_1)\sqrt{r^2} = \frac{S_{XY}}{\sqrt{S_{XX}S_{YY}}}$$

and gives us information about the strength of the linear relationship between X and Y, as well as the sign of the slope $(-1 \le r \le 1)$.



Patient Satisfaction:

Correlation between X_{i2} = severity of illness X_{i3} = anxiety level r_{23} = 0.7945 (see below) For a multiple regression data set $(X_{i1}, \ldots, X_{i,p-1}, Y_i)$

 r_{jY} is the sample correlation coefficient between X_j and Y,

 r_{jk} is the sample correlation coefficient between X_j and X_k .

• If $r_{jk} = 0$ then X_j and X_k are **uncorrelated**.

When most of the r_{jk} 's are close to 1 or -1, we say we have **multicollinearity** among the predictors.

> cor(patsat)

	sat	age	sev	anx
sat	1.0000	-0.7737	-0.5874	-0.6023
age	-0.7737	1.0000	0.4666	0.4977
sev	-0.5874	0.4666	1.0000	0.7945
anx	-0.6023	0.4977	0.7945	1.0000

Uncorrelated vs. correlated predictors

Consider the 3 models:

(1) $E(Y_i) = \beta_0 + \beta_1 X_{i1}$ (2) $E(Y_i) = \beta_0 + \beta_2 X_{i2}$ (3) $E(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}$

and the 2 cases:

• X_1 and X_2 are uncorrelated $(r_{12} \approx 0)$, then b_1 will be the same for models (1) and (3) b_2 will be the same for models (2) and (3) $SSR(X_1|X_2) = SSR(X_1)$ $SSR(X_2|X_1) = SSR(X_2)$ • X_1 and X_2 are correlated $(|r_{12}| \approx 1)$, then b_1 will be different for models (1) and (3) b_2 will be different for models (2) and (3) $SSR(X_1|X_2) < SSR(X_1)$ $SSR(X_2|X_1) < SSR(X_2)$

When $r_{12} \approx 0$, X_1 and X_2 contain no redundant information about Y.

Thus, X_1 explains the same amount of the SSTO when X_2 is in the model as it does when X_2 is not.

Overview of the Effect of Multicollinearity

The standard errors of the parameter estimates are inflated. Thus, CI's for the regression parameters may be to large to be useful.

Inferences about $E(Y_h) = \mathbf{X}'_h \boldsymbol{\beta}$, the mean of a response at \mathbf{X}'_h , and $Y_{h(new)}$, a new random variable observed at \mathbf{X}_h , are unaffected for the most part.

The idea of increasing X_1 , when X_2 is fixed, may not be reasonable.

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}$$

Interpretation: β_1 represents "the change in the mean of Y corresponding to a unit increase in X_1 holding X_2 fixed".

Polynomial Regression

Suppose we have SLR type data (X_i, Y_i) , i = 1, ..., n. If $Y_i = f(X_i) + \epsilon_i$, where $f(\cdot)$ is unknown, it may be reasonable to approximate $f(\cdot)$ using a polynomial

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 + \cdots$$

Usually, you wouldn't go beyond the 3rd power.

Standard Procedure:

- Start with a higher order model and try to simplify.
- If X^k is retained, so are the lower order terms X^{k-1} , X^{k-2} ,..., X.

Warning:

- The model $E(Y_i) = \beta_0 + \beta_1 X_i + \dots + \beta_{n-1} X_i^{n-1}$ always fits perfectly (p = n).
- Polynomials in X are highly correlated.

Polynomial Regression Example: Fish Data

 $Y_i = \log(\text{species richness} + 1)$ observed at lake i, i = 1, ..., 80, in NY's Adirondack State Park.

We consider the 3rd order model:

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 p H_i + \beta_2 p H_i^2 + \beta_3 p H_i^3$$

Residual standard error: 0.4577 on 76 df Multiple R-Squared: 0.447, Adjusted R-squared: 0.425 F-statistic: 20.45 on 3 and 76 df, p-value: 8.24e-10

Looks like pH^3 is not needed.

Let's see if we can get away with a SLR:

 $H_0: \beta_2 = \beta_3 = 0$ vs. $H_A: \operatorname{not} H_0$

Test statistic:

$$F^* = \frac{\mathsf{SSR}(pH^2, pH^3|pH)/2}{\mathsf{MSE}(pH, pH^2, pH^3)}$$
$$= \frac{(4.6180 + 0.2998)/2}{0.2095} = 11.74$$

Rejection rule: Reject H_0 if $F^* > F(0.95; 2, 76) = 3.1$

Thus, a higher order term is necessary.

Let's test

$$H_0: \beta_3 = 0$$
 vs. $H_A: \beta_3 \neq 0$

Test statistic: $F^* = \frac{\mathsf{SSR}(pH^3|pH, pH^2)/1}{\mathsf{MSE}(pH, pH^2, pH^3)} = 1.43$

Rejection rule: Reject H_0 if $F^* > F(0.95; 1, 76) = 4.0$

Conclusion: Can't throw away pH and pH^2 so the model we use is

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 p H_i + \beta_2 p H_i^2$$

```
Residual standard error: 0.459 on 77 df
Multiple R-Squared: 0.436, Adjusted R-squared: 0.422
F-statistic: 29.79 on 2 and 77 df, p-value: 2.6e-10
```



- **Q:** What's the big deal? All we did was get rid of the third order term, pH_i^3 .
- **A:** Suppose we are interested in a 95% CI for β_1 :

Model	b_1	s.e.	$CI(eta_1)$
3rd order	7.08	3.60	(-0.12, 14.28)
2nd order	2.82	0.53	(+1.75, 3.89)

We can do all of this stuff with more than 1 predictor. Suppose we have (X_{i1}, X_{i2}, Y_i) , i = 1, ..., n.

2nd order model:

$$\mathsf{E}(Y_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i1}^2 + \beta_4 X_{i2}^2 + \beta_5 X_{i1} X_{i2}$$

We could test $H_0: \beta_3 = \beta_4 = \beta_5 = 0$. That is: "Is a 1st order model sufficient?" Test statistic:

$$F^* = \frac{\mathsf{SSR}(X_1^2, X_2^2, X_1X_2 | X_1, X_2)/3}{\mathsf{MSE}(X_1, X_2, X_1^2, X_2^2, X_1X_2)}$$

Rejection rule: Reject H_0 if $F^* > F(0.95; 3, n-6)$.