Multiple Regression and ANOVA (Ch. 9.2)

Yifan Zhu

Iowa State University

Outline

Multiple Regression and ANOVA

- **Analysis of variance (ANOVA)**: the use of sums of squares to construct a test statistic for comparing nested models.
- **Nested models**: a pair of models such that one contains all the parameters of the other.
    - Examples:
        - Full model: $Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i$ with the reduced model: $Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$.
        - Full model: $Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \varepsilon_i$ with the reduced model: $Y_i = \beta_0 + \varepsilon_i$

Sums of Squares

- **Total sum of squares (SST)**: the total amount of variation in the response.

$$SST = \sum_i (y_i - \overline{y})^2$$

- **Regression sum of squares (SSR)**: the amount of variation in response explained by the model.

$$SSR = \sum_i (\widehat{y}_i - \overline{y})^2$$

- **Error sum of squares (SSE)**: the amount of variation in the response *not* explained by the model.

$$SSE = \sum_i (y_i - \widehat{y}_i)^2$$

Properties of Sums of Squares

- They add up:

$$SST = SSR + SSE$$

- We can use them to calculate R^2:

$$R^2 = \frac{SST - SSE}{SST} = \frac{SSR}{SST}$$

- We can calculate the **mean squared error (MSE)**:

$$MSE = \frac{1}{n-p} SSE$$

which satisfies:

$$E(MSE) = \boxed{\sigma^2}$$

$MSE = \boxed{s_{LF}^2}$ for simple linear regression and $\boxed{s_{SF}^2}$ for multiple regression.

- The **regression mean square (MSR)** is:

$$MSR = \frac{1}{p-1} SSR$$

→ # of predictors.

Inference: deciding between nested models

- Suppose I have the full model:

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \cdots + \beta_{p-1} x_{p-1,i} + \varepsilon_i$$

p parameters. (p−1) predictors.

- And an intercept-only reduced model:

$$Y_i = \beta_0 + \varepsilon_i$$

1 parameter.

- I want to do a hypothesis test to decide if the full model works better than the reduced model.
  - Does the full model explain significantly more variation in the response than the reduced model?
  - This is a job for the sums of squares.

The hypothesis test: intercept-only model vs. full model

the reduced model is true.

1.
   - $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$
   - H_a : not all of the β_i's $= 0$ $(i = 1, 2, \ldots, p-1)$
2. α is some sensible value (< 0.1).
3. The test statistic is:

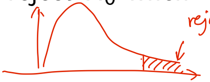
in SLR: $p = 2$, $H_0: \beta_1 = 0$, $H_a: \beta_1 \neq 0$. $F = \frac{SSR/1}{SSE/(n-2)}$

$$F = \frac{SSR/(p-1)}{SSE/(n-p)} = \frac{MSR}{MSE} \sim F_{p-1,\ n-p}$$

Assume:

   - H_0 is true.
   - The full model is valid with the ε_i's iid N$(0,\sigma^2)$

4. Reject H_0 if observed F $> F_{p-1,n-p,1-\alpha}$. Or use the p-value: $P(F_{p-1,n-p} > observedF)$; reject H_0 when p-value is small.



rejection region.

Example: stack loss

1. Consider a chemical plant that makes nitric acid from ammonia.
2. We want to predict stack loss (y, 10 times the % ammonia that escapes from the absorption column) using:
   - x_1: air flow, the rate of operation of the plant
   - x_2, inlet temperature of the cooling water
   - x_3: (% circulating acid - 50%)$\times$10

Example: stack loss

i, Observation Number	x_{1i}, Air Flow	x_{2i}, Cooling Water Inlet Temperature	x_{3i}, Acid Concentration	y_i, Stack Loss
1	80	27	88	37
2	62	22	87	18
3	62	23	87	18
4	62	24	93	19
5	62	24	93	20
6	58	23	87	15
7	58	18	80	14
8	58	18	89	14
9	58	17	88	13
10	58	18	82	11
11	58	19	93	12
12	50	18	89	8
13	50	18	86	7
14	50	19	72	8
15	50	19	79	8
16	50	20	80	9
17	56	20	82	15

Example: stack loss

- Given:
  - $n = 17$
  - y: stack loss of nitrogen from the chemical plant.
  - x_1: air flow, the rate of operation of the plant
  - x_2, inlet temperature of the cooling water
  - x_3: (% circulating acid - 50%)×10
- We'll test the full model:

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

against the reduced model:

$$Y_i = \beta_0 + \varepsilon_i$$

at $\alpha = 0.05$.

Example: stack loss

full model.

$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1} + \varepsilon$ ← p parameters

reduced model → 1 parameters.

$Y = \beta_0 + \varepsilon$. ⇒ $\hat{y}_i = \bar{y}$

$k = p - 1$

$SSR_f = SSR$. $SSR_r = \Sigma(\hat{y}_i - \bar{y})^2 = \Sigma(\bar{y} - \bar{y})^2 = 0$

$(SSR_f - SSR_r)/k = SSR/(p-1)$.

1. ▶ $H_0 : \beta_1 = \beta_2 = \beta_3 = 0$
   ▶ Not all of the β_i's are 0, $i = 1, 2, 3$.
2. $\alpha = 0.05$
3. The test statistic is: are for the full model. → SSR_f SSE_f

$$F = \frac{SSR/\underbrace{(p-1)}_{=k}}{SSE/(n-p)} = \frac{MSR}{MSE} \sim F_{p-1,\ n-p}$$

Assume:

▶ H_0 is true.
▶ The full model is valid with the ε_i's iid N(0,σ^2)

Reject H_0 if $F > F_{p-1,\ n-p,\ 1-\alpha} = F_{4-1,\ 17-4,\ 1-0.05} = F_{3,13,0.95} = 3.41$.

Table B.6.

Example: stack loss

4. In JMP, fit the full model and look at the **ANOVA table**:

Analysis of Variance

\# of predictors = p-1 SSR MSR obs. F.

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	3	795.83449	265.278	169.0432
Error	13	20.40080	1.569	**Prob > F**
C. Total	16	816.23529		<.0001*

n-p SSE MSE p-value.

by reading directly from the table, we can see:

- $p-1=3$, $n-p=13$, $n-1=16$
- $SSR = 795.83, SSE = 20.4, SST = 816.24$
- $MSR = SSR/(p-1) = 795.83/3 = 265.28$
- $MSE = SSE/(n-p) = 20.4/13 = 1.57$
- $observedF = MSR/MSE = 265.78/1.57 = 169.04$
- Prob>F gives the p-value,
  $P(F_{3,13} > observedF) < 0.0001$.

5. With $F = 169.04 > 3.41$, we reject H_0 and conclude H_a.
6. There is overwhelming evidence that at least one of air flow, inlet temperature, and % circulating acid is important in explaining the variation in stack loss.

What if I want to compare different nested models?

if $x_{l_1}, x_{l_2}, x_{l_3}, \dots, x_{l_k}$ are not used in the reduced model.
$\Rightarrow \beta_{l_1} = \beta_{l_2} = \cdots = \beta_{l_k} = 0$.

1.
   - $H_0 : \beta_{l_1} = \beta_{l_2} = \cdots = \beta_{l_k} = 0$
   - H_a : not all of $\beta_{l_1}, \beta_{l_2}, \cdots, \beta_{l_k}$ are 0.
   - (For example, $H_0 : \beta_2 = \beta_3 = 0$ vs H_a : either β_2 or $\beta_3 \neq 0$ or both. The model is $Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \beta_3 x_{i,3} + \beta_4 x_{i,4} + \varepsilon_i$, and $k = 2$)

     $Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_4 x_{i,4}$ ← reduced model.

     difference in the # of parameters in the reduced and full models.
2. α is some sensible value.
3. The test statistic is:

   extra variation explained by the full model over the reduced model.

   extra # of parameters.

$$F = \frac{(SSR_f - SSR_r)/k}{SSE_f/(n-p)} \sim F_{k,\ n-p}$$

- SSR_r is for the reduced model and SSR_f is for the full model.
- Of course, we assume H_0 is true and the full model is valid with the ε_i's iid $N(0, \sigma^2)$.

What if I want to compare different nested models?

4. We can construct a combined ANOVA table:

Source	SS	df	MS	F
Reg (full)	SSR_f	$p-1$		
Reg (reduced)	SSR_r	$p-k-1$		
Reg (full | red)	$SSR_f - SSR_r$	k	$\frac{SSR_f - SSR_r}{k}$	$\frac{MSR_{f\|r}}{MSE_f}$
Error	SSE_f	$n-p$	$\frac{SSE_f}{n-p}$	
Total	SST	$n-1$		

5. Reject H_0 if observed F $> F_{\overset{k}{\cancel{p-1}},n-p,1-\alpha}$. Or use the p-value: $P(F_{\underset{k}{\cancel{p-1}},n-p} > observedF)$; reject H_0 when p-value is small.

Example: stack loss

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

$Y_i = \beta_0 + \beta_1 x_{i,1}.$

1.
   - $H_0 : \beta_2 = \beta_3 = 0$
   - H_a : either $\beta_2 \neq 0$ or $\beta_3 \neq 0$
2. $\boxed{\alpha = 0.05}$
3. The test statistic is:

$$F = \frac{(SSR_f - SSR_r)/k}{SSE_f/(n-p)} = \frac{(SSR_f - SSR_r)/2}{SSE_f/(17-4)}$$
$$= \frac{(SSR_f - SSR_r)/2}{SSE_f/13}$$

- Assume H_0 is true and the full model is valid with the ε_i's iid $N(0, \sigma^2)$.
- Then, $F \sim F_{k,\ n-p} = F_{2,13}$.
- I will reject H_0 if $F > F_{2,13,0.95} = 3.81$.

Example: stack loss

4. Look at the ANOVA tables in JMP for both the full model $(Y_i = \beta_0 + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \beta_3 x_{3,i} + \varepsilon_i)$:

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	3	795.83449	265.278	169.0432
Error	13	20.40080	1.569	**Prob > F**
C. Total	16	816.23529		<.0001*

and the reduced model $(Y_i = \beta_0 + \beta_1 x_{1,i} + \varepsilon_i)$:

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	775.48219	775.482	285.4318
Error	15	40.75311	2.717	**Prob > F**
C. Total	16	816.23529		<.0001*

Example: stack loss

I construct a different ANOVA table for this test:

Source	SS	df	MS	F
Reg (full)	795.83	4		
Reg (reduced)	775.48	2		
Reg (full | red)	20.35	2	10.18	6.48
Error	20.4	13	1.57	
Total	SST	16		

5. With $observedF = 6.48 > 3.81$, I reject H_0 and conclude H_a.
6. There is enough evidence to conclude that at least one of inlet temperature and % circulating acid is associated with stack loss.

Example: stack loss

reduced model
$Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_3 x_{i,3} + \varepsilon_i$.

- Attempt to eliminate inlet temperature (x_2) from the model at $\alpha = 0.05$. Here is the ANOVA table for the full model:

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	3	795.83449	265.278	169.0432
Error	13	20.40080	1.569	**Prob > F**
C. Total	16	816.23529		<.0001*

and for the reduced model:

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	2	776.84496	388.422	138.0520
Error	14	39.39033	2.814	**Prob > F**
C. Total	16	816.23529		<.0001*

Example: stack loss

1. $H_0 : \beta_2 = 0,\ H_a : \beta_2 \neq 0$
2. $\alpha = 0.05$
3. The test statistic is:

$$F = \frac{(SSR_f - SSR_r)/k}{SSE_f/(n-p)} = \frac{SSR_f - SSR_r}{SSE_f/(17-4)}$$
$$= \frac{SSR_f - SSR_r}{SSE_f/13}$$

- Assume H_0 is true and the full model is valid with the ε_i's iid $N(0, \sigma^2)$.
- Then, $F \sim F_{k,\ n-p} = F_{1,13}$.
- I will reject H_0 if $F > F_{1,13,0.95} = 4.67$.

Example: stack loss

4. I construct a different ANOVA table for this test:

Source	SS	df	MS	F
Reg (full)	795.83	4		
Reg (reduced)	776.84	3		
Reg (full | red)	18.99	1	18.99	12.10
Error	20.4	13	1.57	
Total	SST	16		

5. With $observedF = 12.10 > 4.67$, we reject H_0.
6. There is enough evidence to conclude that stack loss varies with inlet temperature.

Example: stack loss

- The F test for eliminating one parameter is analogous to the t test from before:

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-37.65246	4.732051	-7.96	<.0001*
x1	0.7976856	0.067439	11.83	<.0001*
$\beta_2 \rightarrow$ x2	0.5773405	0.165969	3.48	0.0041*
x3	-0.06706	0.061603	-1.09	0.2961

- The t statistic for $H_0 : \beta_2 = 0$ vs. $H_a : \beta_2 \neq 0$ is 3.48.
- But $3.48^2 = 12.1$, which is our F statistic from the ANVOA test!

F-test and t-test are equivalent for testing $H_0: \beta_2 = 0$ vs $H_a: \beta_2 \neq 0$.

a two-sided test for one parameter.

- Fun fact:

$$F_{1,\ \nu} = t_\nu^2$$

Note: the ANOVA F-test is always a two-sided test.

The F test statistic and R^2

- If F is the test statistic from a test of $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$ vs. H_a : not all of $\beta_1, \beta_2, \ldots, \beta_{p-1}$ are 0, then F can be expressed in terms of the coefficient of determination of the full model:

$$F = \frac{R^2/(p-1)}{(1-R^2)/(n-p)}$$

- For the stack loss example, the full model's $R^2 = 0.975$, and so:

$$F = \frac{0.975/(4-1)}{(1-0.975)/(17-4)} = 169$$

The F test statistic and R^2

Summary of Fit

RSquare	0.975006
RSquare Adj	0.969238
Root Mean Square Error	1.252714
Mean of Response	14.47059
Observations (or Sum Wgts)	17

Analysis of Variance

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C. Total	16	816.23529		<.0001*

The F test statistic and R^2

- For $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$ vs. H_a : not all of $\beta_1, \beta_2, \ldots, \beta_{p-1}$,

$$F = \frac{SSR \frac{1}{p-1}}{SSE \frac{1}{n-p}} = \frac{\frac{SSR}{SST} \frac{1}{p-1}}{\frac{SSE}{SST} \frac{1}{n-p}} = \frac{\frac{SSR}{SST} \frac{1}{p-1}}{\frac{SST-SSR}{SST} \frac{1}{n-p}} = \frac{\frac{SSR}{SST} \frac{1}{p-1}}{\left(1 - \frac{SSR}{SST}\right) \frac{1}{n-p}}$$

$$= \frac{R^2 \frac{1}{p-1}}{(1 - R^2) \frac{1}{n-p}}$$

The F test statistic and R^2

- If F is the test statistic from a test of $H_0 : \beta_{l_1} = \beta_{l_2} = \cdots = \beta_{l_k} = 0$ vs. H_a : not all of $\beta_{l_1}, \beta_{l_2}, \ldots, \beta_{l_k}$ are 0, then F can be expressed in terms of the coefficient of determination of the full model (R_f^2) and that of the reduced model (R_r^2):

$$F = \frac{(R_f^2 - R_r^2)/k}{(1 - R_f^2)/(n-p)}$$

- For the stack loss example when we tested $H_0 : \beta_2 = \beta_3 = 0$, $R_f^2 = 0.975$ and $R_r^2 = 0.95$.

$$F = \frac{(0.975 - 0.95)/2}{(1 - 0.975)/(17 - 4)} = 6.50$$

which is close to the test statistic of 6.48 that we calculated before.

The F test statistic and R^2

- When we tested $H_0 : \beta_2 = 0$, R_r^2 was 0.9517, so:

$$F = \frac{(0.975 - 0.9517)/1}{(1 - 0.975)/(17 - 4)} = 12.117$$

which is close to the test statistic of 12.10 that was calculated directly from the ANOVA table.

The F test statistic and R^2

$$F = \frac{(SSR_f - SSR_r)\frac{1}{k}}{SSE_f \frac{1}{n-p}} = \frac{\frac{SSR_f - SSR_r}{SST}\frac{1}{k}}{\frac{SSE_f}{SST}\frac{1}{n-p}} = \frac{\left(\overset{R_f^2}{\frac{SSR_f}{SST}} - \overset{R_r^2}{\frac{SSR_r}{SST}}\right)\frac{1}{k}}{\frac{SST - SSR_f}{SST}\frac{1}{n-p}}$$

$$= \frac{\left(\frac{SSR_f}{SST} - \frac{SSR_r}{SST}\right)\frac{1}{k}}{\left(1 - \frac{SSR_f}{SST}\right)\frac{1}{n-p}} = \boxed{\frac{\left(R_f^2 - R_r^2\right)\frac{1}{k}}{\left(1 - R_f^2\right)\frac{1}{n-p}}}$$

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