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1 Simple Linear Regression

1.1 Least Squares Estimate

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# 1 Simple Linear Regression

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad i = 1 \dots n \tag{1}$$

If assumptions hold true,

•  $Y_i$  is normally distributed

$$E(Y_i) = \beta_0 + \beta_1 x_i \tag{}$$

$$Var(Y_i) = \sigma^2 \tag{3}$$

- Mean:  $\beta_0 + \beta_1 x_i$
- Variance:  $\sigma^2$

# Assumptions

- $\epsilon_1 \dots \epsilon_n$
- $E(\epsilon_i) = 0, var(\epsilon_i) = 0$ , where  $\sigma^2$  is an unknown constant.
- $\epsilon_i$  is normal. (normality assumption)

# 1.1 Least Squares Estimate

$$\sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 x_i)^2 \tag{4}$$

Take the first order derivative with respect to  $\beta_0, \beta_1$  to minimize equation (4) to find optimal  $\beta_0, \beta_1$ .

#### LS estimators

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(Y_i - \bar{Y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
 (5)

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x} \tag{0}$$

- $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$  (sample mean of the  $x_i$ 's)
- $\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$  (sample mean of the  $Y_i$ 's)
- Regression Line:  $y = \hat{\beta}_0 + \hat{\beta}_1 x$

#### Properties of LS Estimators

•  $E(\hat{\beta}_0) = \beta_0$ ,  $E(\hat{\beta}_1) = \beta_1$ . The average of many sample beta values will approach the true beta values.

Fitted (or predicted) values are estimates. The fitted value for  $Y_i$  is  $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ 

 $\hat{Y}$  is an unbiased estimator of  $E(Y) = \beta_0 + \beta_1 x$  so  $E(\hat{Y}) = E(Y)$ 

# 1.2 Residuals

Residuals :  $\hat{\epsilon}_i = Y_i - \hat{Y}_i, i = 1 \dots n$ Properties of Residuals

- $\bullet \ \Sigma_{i-1}^n \hat{\epsilon}_i = 0$
- The residuals are not independent.
- If one residual is positive, another residual has to compensate.

#### 1.3 Variance

Estimation of  $\sigma^2$ , the variance of the errors (which is the same as the variance of  $Y_i$ )

$$s^{2} = \frac{1}{n-2} \sum_{i=1}^{n} (Y_{i} - \hat{Y}_{i})^{2}$$
 (7)

where  $\hat{Y}_i$  is the estimate of  $E(Y_i)$ .

# (4) Notes

- $\hat{Y}_i$  is an estimator of  $E(Y_i) = \beta_0 + \beta_1 x_i$  in which two parameters are estimated  $(\beta_0 \text{ and } \beta_1) \implies 2$  degrees of freedoms are subtracted.
- $E(s^2) = \sigma^2$

When errors are normally distributed, the LS estimators of  $\beta_0$ ,  $\beta_1$  is equal to the MLEs (Maximum Likelihood Estimators) of  $\beta_0$ ,  $\beta_1$ , but the MLE of  $\sigma^2$ ,  $\hat{\sigma}^2$ , is different from  $s^2$   $s^2$  is just (7)

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \hat{\epsilon}_i^2 \tag{8}$$

# 2 Inference in regression and correlation analysis

# 2.1 Inference about $\beta_1$

For testing  $\beta_1$ 

 $H_0: \beta_1 = \beta_{10}, \beta_{10}$  is a given value such as 0.

 $H_a: \beta_1 \neq \beta_{10}, \beta_1 > \beta_{10}, \text{ or } \beta_1 < \beta_{10}$ 

Test statistic: A statistic whose distribution is known under the null hypothesis.

$$t = \frac{\hat{\beta}_1 - \beta_{10}}{s.e.(\hat{\beta}_1)} \tag{9}$$

where  $\hat{\beta}_1$  is the LS estimate of  $\beta_1$ , and

$$s.e.(\hat{\beta}_1) = \sqrt{\frac{MSE}{\sum_i (x_i - \bar{x})^2}}$$
 (10)

$$MSE = s^2 \tag{11}$$

If normal,  $T \sim t_{n-1}$ 

$$T = \frac{\hat{\beta}_1 - \beta_1}{s.e.(\hat{\beta}_1)} \tag{12}$$

Therefore under the  $H_0$ :  $\beta_1 = \beta_{10}, t \sim t_{n-2}$ Decision Rules

 $H_1: \beta_1 \neq \beta_{10}, reject \ H_0 \ if \ |t| > t_{n-2,\alpha/2}$ 

 $H_1: \beta_1 > \beta_{10}, reject \ H_0 \ if \ |t| > t_{n-2;\alpha}$  $H_1: \beta_1 < \beta_{10}, reject \ H_0 \ if \ |t| < -t_{n-2;\alpha}$ 

Alternatively, Reject  $H_0$  if the p-value of t is  $\leq \alpha$  **Error** 

- Type I : Reject  $H_0$  when it is true.
- Type II: Fail to reject  $H_0$  when it is false.

# Level of Significance $\alpha$

 $\alpha$  is the upper bound for the probability of Type I error. **P-value** 

p-value is the observed level of significance: the actual probability that the test statistic is as extreme as observed given  $H_0$  is true.

#### Power

Power is the probability of rejecting  $H_0$  when the alternative holds at a given value.

If  $\beta_{10} = 0, \beta_1 = 1, s.d.(\hat{\beta}_1) = 0.5$ , we have  $\delta = \frac{1}{0.5} = 2$  Let  $\alpha = 0.05$ . From table B.5 we find the power is 0.48.

#### Confidence interval for $\beta_k$

Assuming normality, a  $100(1-\alpha)\%$  c.i. for  $\beta_k$  is

$$\hat{\beta}_k \pm t_{n-2} (1 - \frac{alpha}{2} * s.e.(\hat{\beta}_j))$$
 (13)

$$k = 0, 1 \tag{14}$$

where  $s.e.(\hat{\beta}_1)$  can be found with eq(10) and  $s.e.(\hat{\beta}_0)$  can be found with eq(15).

# 2.2 Inference about $\beta_0$

$$s.e.(\beta_0) = \sqrt{mse(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2})}$$
 (15)

Confidence intervals for  $\beta_0$  can be found with (13)

# 2.3 Inference about $\hat{Y}$

Confidence Interval for  $E(Y) = \beta_0 + \beta_1 x$ 

$$\hat{Y} \pm t_{n-2}(1 - \frac{alpha}{2}) * s.e.(\hat{Y})$$
 (16)

$$s.e.(\hat{Y}) = \sqrt{MSE(\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2})}$$
 (17)

# 2.4 Prediction interval for $\hat{Y}$

A  $100(1-\alpha)\%$  prediction interval for  $Y = E(Y) + \epsilon = \beta_0 + \beta_1 x + \epsilon$ , where Y is the future observation and  $\epsilon$  is the new error:

$$\hat{Y} \pm t_{n-2}(1 - \frac{\alpha}{2}) * p.s.e.(\hat{Y})$$
 (18)

$$p.s.e.(\hat{Y}) = \sqrt{MSE(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2})}$$
(19)

Where p.s.e. is the percent standard error.

The 1 in the p.s.e is because the variance of  $\epsilon = \sigma^2$ . If  $var(\epsilon) = \frac{\sigma^2}{2}$  change the 1 to  $\frac{1}{2}$ .

# 2.5 ANOVA and F-test

$$SSTO = SSR + SSE \tag{20}$$

$$= \sum_{i=1}^{n} (Y_i - \bar{Y})^2 \tag{21}$$

$$SSR = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 \tag{22}$$

$$SSE = \sum_{i=1}^{n} (Y_i - \hat{Y})^2$$
 (23)

(24)

Sum of Squares of Regression (SSR) explains the variability in Y due to the regression model compared to the baseline model. Sum of Squares of Errors (SSE) is the remaining unexplained variability of Y found from SSTO - SSR.

# Degrees of Freedom

$$SSRdf = 1$$
  

$$SSEdf = n - 2$$
  

$$SSTOdf = n - 2 + 1 = n - 1$$

# Mean Squares

Mean squares is SS divided by its degrees of freedom.

$$MSR = \frac{SSR}{1} \tag{25}$$

$$MSE = \frac{SSE}{n-2} \tag{26}$$

(27)

# F-Statistic

$$F = \frac{MSR}{MSE} = \frac{SSR * (n-2)}{SSE}$$
 (28)

ANOVA table: Analysis of variance.

The distribution of F under the null hypothesis  $H_0: \beta_1 = 0$  is  $F_{1,n-2}$ .

Source	SS	$\mathrm{d}\mathrm{f}$	MS	$\mathbf{F}$
Regression	SSR	1	MSR	F
Error	SSE	n-2	MSE	
Total	SSTO	n-1		

# 2.6 Inference about $\rho$

 $R^2$ : a measure of goodness of fit, which is the proportion of variation in Y explained by the regression (i.e. by x).

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO} \tag{29}$$

Coefficient of correlation:

$$r = \pm \sqrt{R^2} = \begin{cases} +\sqrt{R^2} & \text{if } \hat{\beta}_1 > 0\\ -\sqrt{R^2} & \text{if } \hat{\beta}_1 < 0 \end{cases}$$
 (30)

$$r = \frac{\sum_{i} (Y_i - \bar{Y})(x_i - \bar{x})}{\sqrt{\sum_{i} (Y_i - \bar{Y})^2 \sum_{i} (x_i - \bar{x})^2}}$$
(31)

# Properties of $R^2$ and r

- $0 < R^2 < 1 1 < r < 1$
- $R^2 \approx 1$  or  $r \approx \pm 1$ , if there is a strong linear association between x and Y.
- $R^2 \approx 0$ , or  $r \approx 0$ , if there is a weak or no linear association between x and Y.
- Both  $R^2$  and r are measures of linear association only.

# Covariance and correlation between two random variables

$$cov(X, Y) = E\{(X - \mu_X)(Y - \mu_Y)\}$$
 (32)

$$= E(XY) - E(X)E(Y) \tag{33}$$

$$cor(X,Y) = \frac{cov(X,Y)}{sd(X)sd(Y)}$$
(34)

where  $\mu_X = E(X), sd(X) = \sqrt{var(X)}$ , etc.

Special case: (X,Y) has a bivariate normal distribution.

# Testing for $\rho$

Assume that the bivariate normal distribution holds for (X,Y).

$$H_0: \rho = 0$$

 $H_a: \rho \neq 0 ( or \rho > 0 or \rho < 0 )$ 

$$t^* = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} \sim t_{n-2} \text{ under } H_0$$
 (35)

# 3 Diagnostics

The goal of diagnostics is to examine the departures from the simple linear regression model with normal errors. Typical departures and corresponding diagnostic plots/tests are:

- The regression is not linear residual plots(residual against the predictor variable, or against the fitted values), lack of fit test.
- The error terms are not normally distributed histogram, boxplot/dot plot of residuals, normal probability plot (aka QQ plot), Shapiro-Wilk's test, correlation test for normality.
- The error terms do not have constant variance residual plots, Brown Forsythe (BF) test.
- The error terms are not independent residual against time.
- The model fits all but one or a few outlier observations (semistudentized) residual plots, box plots, dot plots, stem and leaf plots.
- Some important predictors are missing residual plots (residual against other possibly important predictors).

# 3.1 Residual Plots

Residuals can be used to check whether

- The regression function is not linear.
- The variance of the errors is not constant.
- The errors are not independent.
- Outliers
- The errors are not normal.
- Some important predictors are missing.

#### **Scatter Plot**

- Check linearity residuals normally disributed.
- Check constant variance residuals are random and dont follow a cone pattern.

#### Box Plot and Dot Plot

• Normality - residuals should be centered and symmetric about 0.

# Normality probability plot - QQ Plot

- QQ plot is linear  $\implies$  normal residuals.
- ullet QQ plot is nonlinear  $\Longrightarrow$  non normal residuals.

# Diagnostic Tests

# Shapiro Wilk's test

 $H_0 \ data \ \sim N()$ 

 $H_a$ : data not normal.

 $p-val \leq \alpha$  reject normality assumption.

# Correlation test for normality

Step 1. Compute the coefficient of correlation between the ordered residuals and their expected values. The latter are given by

$$\sqrt{MSE}z(\frac{k-0.375}{n+0.25}), \quad k=1,\dots,n$$
 (36)

where z(p) is the pth quantile of the standard normal distribution, that is,  $P[Z \leq z(p)] = p$ , where Z has the standard normal distribution.

Step 2. Compare the coefficient of correlation on I with the critical value from Table B.6, if the coefficient of correlation exceeds the critical value, accept the normality assumption.

#### BF test for constant variance

1. Divide the residuals into two parts according to residual pattern (or no pattern)

Let  $\hat{\epsilon}_{i1} = 1, \dots, n_1$  be the residuals for the first part, and  $\hat{\epsilon}_{i2}$ ,  $i = 1, ..., n_2$  be the residuals for the second part, where  $n_1 + n_2 = n$ .

Compute  $m(\hat{\epsilon}_1) = median \ of \ \hat{\epsilon}_{i1}, i = 1, \dots, n_1 \ and$  $m(\hat{\epsilon}_2)$ .

2. Compute  $d_{i1} = |\hat{\epsilon}_{i1} - m(\hat{\epsilon}_1)|, i = 1 \dots n_1$  and  $d_{i2} = 1 \dots n_1$  $|\hat{\epsilon}_{i2} - m(\hat{\epsilon}_2)|, i = 1 \dots n_2$ 

3. Compute t score.

$$t_{BF} = \frac{\bar{d}_1 - \bar{d}_2}{s\sqrt{n_1^{-1} + n_2^{-1}}} \tag{37}$$

$$s^{2} = \frac{\sum_{i=1}^{n_{1}} (d_{i1} - \bar{d}_{1})^{2} + \sum_{i=1}^{n_{2}} (d_{i2} - \bar{d}_{2})^{2}}{n - 2}$$
(38)

4. Test  $H_0: \sigma_1^2 = \sigma_2^2 \text{ vs } H_a: \sigma_1^2 \neq \sigma_2^2$ 

 $t_{BF} \sim t_{n-2}$  under  $H_0$ . Given  $\alpha$ , use the critical value (or p-value) to test  $H_0$ .

#### F-test for lack of fit

Regression model:  $Y_{ij} = \beta_0 + \beta_1 x_j + \epsilon_{ij}, j = 1 \dots c, i =$  $1 \dots n_i$  where  $x_i$  is the *ith* value of x, c is the number of different x values, and  $Y_{ij}$ ,  $i = 1 \dots n_i$  are the Y values SCI's for  $E(Y_h) = \beta_0 + \beta_1 x_h$ ,  $h \in G$ , g = |G|corresponding to the same  $x_i$ .

Full model:  $Y_{ij} = \mu_j + \epsilon_{ij}, j = 1 \dots c, i = 1 \dots n_j$ F-statistic:

$$F = \frac{SSE(R) - SSE(F)}{df_R - df_F} \{ \frac{SSE(F)}{df_F} \}^{-1}$$
 (39)

where

$$SSE(R) = \sum_{j} \sum_{i} (Y_{ij} - \hat{Y}_{ij})^{2}$$
(40)

$$SSE(F) = \Sigma_j \Sigma_i (Y_{ij} - \hat{\mu}_j)^2 \tag{41}$$

with  $\hat{Y}_{ij} = \hat{\beta}_0 + \hat{\beta}_1 x_i$  and  $\hat{\mu}_i = \bar{Y}_i - n_i^{-1} \sum_{i=1}^{n_j} Y_{ij}, df_R = n-2$ with  $n = \sum_{i=1}^{c} n_i$  and  $df_F = n - c$ . Under  $H_0$ : The assumed model is correct,  $F \sim F_{c-2,n-c}$ .

#### Remedial Measures 3.3

**Transformation of x**: for nonlinear association.

Transformation of Y: for nonnormality/unequal vari-

#### Box Cox transformation

This is a collection of transformations depending on a "tuning parameter",  $\lambda$ .

$$Y_i' = \begin{cases} K_1(Y_i^{\lambda} - 1), & \lambda \neq 0 \\ K_2 log(Y_i), & \lambda = 0 \end{cases}$$
 (42)

where  $K_1, K_2$  are two numbers computed from the data.

$$K_2 = (Y_1 Y_2 \dots Y_n)^{\frac{1}{n}} = e^{\overline{\log Y}} \tag{43}$$

$$K_1 = \frac{1}{\lambda K_2^{\lambda - 1}} \tag{44}$$

# Simultaneous Inference

# Simultaneous Confidence Intervals

An SCI represents the percentage likelihood that a group of confidence intervals will all include the true population parameters or true differences between factor levels if the study were repeated multiple times.

A  $100(1-\alpha)\%$  s.c.i has the following form,

Working-Hotelling's 
$$\hat{Y}_h \pm W * se(\hat{Y}_h)$$
 (45)

Bonferroni's 
$$\hat{Y}_h \pm B * se(\hat{Y}_h)$$
 (46)

Where.

$$se(\hat{Y}_h) = \sqrt{MSE\left(\frac{1}{n} + \frac{(x_h - \bar{x})^2}{\Sigma_i(x_i - \bar{x})^2}\right)}$$
(47)

$$W = \sqrt{2 * F_{2,n-2}(1-\alpha)} \tag{48}$$

$$B = t_{n-2} \left( 1 - \frac{\alpha}{2g} \right) \tag{49}$$

# Simultaneous Prediction Intervals

The goal of a prediction band is to cover with a prescribed probability the values of one or more future observations from the same population from which a given data set was sampled. Just as prediction intervals are wider than confidence intervals, prediction bands will be wider than confidence bands.

Bonferroni's 
$$\hat{Y}_h \pm B * pse(\hat{Y}_h)$$
 (50)

Scheffe's 
$$\hat{Y}_h \pm S * pse(\hat{Y}_h)$$
 (51)

where B = (49)

$$pse(\hat{Y}_h) = \sqrt{MSE\left(1 + \frac{1}{n} + \frac{(x_h - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}\right)}$$
 (52)

$$S = \sqrt{gF_{g,n-2}(1-\alpha)} \tag{53}$$

(54)

# Multiple Linear Regression

Matrix expression for multiple linear regression,

$$Y_i = \beta_0 + \beta_1 x_{i,1} + \dots + \beta_p x_{i,p-1} + \epsilon_i, i = 1 \dots n$$
 (55)

 $\epsilon_i$  has the same assumptions as simple linear regression. Multiple linear regression can be expressed as

$$Y = X\beta + \epsilon \tag{56}$$

Given

$$X = \begin{bmatrix} 1 & x_{1,1} & \dots & x_{1,p-1} \\ 1 & x_{2,1} & \dots & x_{2,p-1} \\ \dots & \dots & \dots & \dots \\ 1 & x_{n,1} & \dots & x_{n,p-1} \end{bmatrix}$$
(57)

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_{p-1} \end{bmatrix}, Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \dots \\ Y_n \end{bmatrix}, \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \dots \\ \epsilon_n \end{bmatrix}$$
 (58)

#### LS Estimate

Find  $\beta$  that minimizes  $|Y - X\beta|^2$ , where for a vector 5.2  $v = (v_1 \dots v_n)', |v|^2 = \sum_{i=1}^n v_i^2$ , the solution is given by

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \dots \\ \hat{\beta}_{p-1} \end{bmatrix} = (X'X)^{-1}X'Y$$

$$(59) \begin{array}{c} \textbf{Step 1} \\ H_0: \beta_k = \beta_{k0} \\ H_1: \beta_k \neq \beta_{k0} (> \beta_{k0}, < \beta_{k0}) \text{ where } \beta_{k0} \text{ is a specified value} \\ \text{(e.g. 0)}. \end{array}$$

This can be computed in R. Given an n \* p matrix, X.

- 1. Manual
  - $\hat{\beta} = \text{solve}(\mathsf{t}(\mathsf{X}) \% \% \ \mathsf{X}) \% \% (\mathsf{t}(\mathsf{X}) \% \% \ \mathsf{Y})$
  - %\*% denotes the matrix product.
- 2. Using built in functions
  - result = lsfit(X, Y, intercept = F)
  - bhat = result\$coef

#### ANOVA Table 5.1

$$SSTO = \sum_{i=1}^{n} (Y_i - \bar{Y})^2 \tag{60}$$

$$SSR = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 \tag{61}$$

$$SSE = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$
 (62)

$$MSR = \frac{SSR}{(p-1)} \tag{63}$$

$$MSE = \frac{SSE}{(n-p)} \tag{6}$$

$$F = \frac{MSR}{MSE} \tag{65}$$

Where  $\hat{Y}_i = (56)$ 

Under  $H_0: \beta_1 = \dots = \beta_{p-1} = 0, F \sim F_{p-1, n-p}$  $R^2$  has the same interpretation as in SLR.

# Inference about Regression Parameters

$$t = \frac{\hat{\beta}_k - \beta_{k0}}{se(\hat{\beta}_k)} \tag{66}$$

$$se(\hat{\beta}_k) = \sqrt{MSE * (X'X)_{k,k}^{-1}}$$
 (67)

Where  $(X'X)_{k,k}^{-1}$  is the kth diagonal element of  $(X'X)^{-1}$ . (0 < k < p - 1)

#### Under $H_0, t \sim t_{n-n}$ Step 2

# A $100(1-\alpha)\%$ sci for $\beta_h, h \in G$ with q = |G|

$$\hat{\beta}_h = B * se(\hat{\beta}_h) \tag{68}$$

$$B = t_{n-p} \left( 1 - \frac{\alpha}{2g} \right) \tag{69}$$

# 5.3 Estimation of Mean Responses

$$E(Y_h) = x_h' \beta = \beta_0 + \beta_1 x_{h,1} + \dots + \beta_{p-1} x_{h,p-1}$$
 (70)

(64) First compute  $\hat{Y}_h = x_h' \hat{\beta}$  and

$$se(\hat{Y}_h) = \sqrt{MSE(x'_h(X'X)^{-1}x_h)}$$
 (71)

A  $100(1-\alpha)\%$  sci for  $E(Y_h), h \in G, g = |G|$  is

$$W - H: \hat{Y}_h \pm W * se(\hat{Y}_h), W = \sqrt{p * F_{p,n-p}(1-\alpha)}$$
(72)

Bonf.: 
$$\hat{Y}_h \pm B * se(\hat{Y}_h), B = t_{n-p} \left(1 - \frac{\alpha}{2g}\right)$$
 (73)

# 5.4 Prediction Interval

$$pse(\hat{Y}_h) = \sqrt{MSE(1 + x'_h(X'X)^{-1}x_h)}$$
 (74)

A  $100(1-\alpha)\%$  spi for  $Y_h$ 

Scheffe: 
$$\hat{Y}_h \pm S * pse(\hat{Y}_h), S = \sqrt{g * F_{g,n-p}(1-\alpha)}$$

Bonfer:  $\hat{Y}_h \pm B * pse(\hat{Y}_h), B = t_{n-p} \left(1 - \frac{\alpha}{2a}\right)$ 

# (66) 5.5 Multiple Predictor SS

$$\begin{split} SSR(x_2|x_1) &= SSR(x_1,x_2) - SSR(x_1) \\ &= SSE(x_1) - SSE(x_1,x_2) \\ SSR(x_3|x_1,x_2) &= SSR(x_1,x_2,x_3) - SSR(x_1,x_2) \\ &= SSE(x_1,x_2) - SSE(x_1,x_2,x_3) \end{split}$$

SSR has (number of predictors on the left of the bars) degrees of freedom.

#### 5.6 ANOVA with extra SS

Source	SS	$\mathrm{d}\mathrm{f}$
Regression	$SSR(x_1, x_2, x_3)$	3
$x_1$	$SSR(x_1)$	1
$x_2 x_1$	$SSR(x_2 x_1)$	1
$x_3 x_1, x_2$	$SSR(x_3 x_1,x_2)$	1
Error	$SSE(x_1, x_2, x_3)$	n-4
Total	SSTO	n-1

Source	MS
Regression	MSR
$x_1$	$MSR(x_1) = SSR(x_1)/1$
$x_{2} x_{1}$	$MSR(x_2 x_1) = SSR(x_2 x_1)/1$
$x_3 x_1, x_2$	$MSR(x_3 x_1,x_2) = SSR(x_3 x_1,x_2)/1$
Error	$MSE(x_1, x_2, x_3) = \frac{SSE(x_1, x_2, x_3)}{(n-4)}$
Total	

# 5.7 F Test for predictors

 $H_0: \beta_3 = 0$   $H_1: \beta_3 \neq 0$   $SSE(Full) = SSE(x_1, x_2, x_3)$  $SSE(Reduced) = SSE(x_2, x_2)$ 

$$F = \frac{MSR(x_3|x_1, x_2)}{MSE(x_1, x_2, x_3)}$$
(77)

 $df_R = n - 3, df_F = n - 4$ Under  $H_0, F \sim F_{1,n-4}$ 

# 5.8 Coefficient of Partial Determination

$$R_{Y,x_2|x_1}^2 = R_{Y,2|1}^2 = \frac{SSR(x_2|x_1)}{SSE(x_1)} = 1 - \frac{SSE(x_1,x_2)}{SSE(x_1)}$$
(78)

It measures the proportionate reduction in the variation of Y due to adding  $x_2$ , given that  $x_1$  is already in the model. More generally

$$R_{Y,x_p,\dots,x_{p+q-1}|x_1,\dots,x_{p-1}}^2 = 1 - \frac{SSE(x_1,\dots,x_{p+1-1})}{SSE(x_1,\dots,x_{p-1})}$$
(79)

# 5.9 Adjusted R

$$R^2 = 1 - \frac{SSE}{SSTO} \tag{80}$$

$$R_a^2 = 1 - \frac{MSE}{MSTO} = \frac{SSE/(n-p)}{SSTO/(n-1)}$$
 (81)

Models with more predictors will always have higher  $R^2$ , but  $R_a^2$  takes into account the number of predictors. Select the model that maximizes  $R_a^2$ .

#### 5.10 Mallow's C

$$C_p = C_p(x_{i_1}, \dots, x_{i_{p-1}}) = \frac{SSE(x_{i_1}, \dots, x_{i_{p-1}})}{MSE(x_{i_1}, \dots, x_{i_{p-1}})} - (n-2p)$$
(82)

where  $SSE(x_{i_1},\ldots,x_{i_{p-1}})=SSE$  of fitting the regression with  $x_{i_1},\ldots,x_{i_{p-1}}$  and  $MSE(x_1,\ldots,x_{K-1})=MSE$  of fitting the regression with all candidate predictors. The best subset of predictors corresponds to the one such

# 5.11 AIC and BIC(SBC) criteria

that  $C_p$  is small and close to p. Note:  $C_p = K$ .

$$AIC_p = n\log(SSE_p \ n) + 2p \tag{83}$$

$$SBC_{p} = n\log(SSE_{p} n) + (\log n)p \tag{84}$$

Choose a subset of predictors (model) that minimizes  $AIC_p(SBC_p)$ .

# 5.12 Forward Stepwise Selection

- 1. Choose the first predictor  $(x_1)$  that has the largest |t| for the slope under a simple linear regression with the predictor.
- 2. Choose the second predictor x(2) that has the largest |t| for the coefficient under a linear regression with  $(x_1)$  and a new predictor.
- 3. Continue until the p-value of the new predictor is greater than 0.10.
- 4. After adding new predictors, check existing predictor p-values. If any are greater than 0.15, remove them from the model.

# 5.13 Conditional residual plots

 $e(Y|x_2)$  = residual of fitting Y against  $x_2$ .  $e(x_1|x_2)$  = residual of fitting  $x_1$  against  $x_2$ .

A linear pattern in the plot of  $e(Y|x_1)$  against  $e(x_2|x_1)$  suggest that an important predictor,  $x_2$ , is missing in the model.

# 5.14 Identifying outlying Y observations

Internally Studentized (Standardized) residual: Let  $\hat{\epsilon}_i$  denote the residual, the studentized residual is,

$$r_i = \frac{\hat{\epsilon}_i}{se(\hat{\epsilon}_i)} = \frac{\hat{\epsilon}_i}{\sqrt{(MSE(1 - h_{ii}))}}$$
(85)

The motivation for studentizing is that the variance of residuals for different inputs may differ, even if the variances of the errors are equal.

where  $h_{ii}$  is the *ith* diagonal element of the hat matrix  $H = X(X'X)^{-1}X'$ , also called the leverage for the *ith* case.

deleted (jackknife) residual: Fit the regression with the ith case deleted; let  $\hat{Y}_{i(-i)}$  denote the predicted value for  $Y_i$ , under this regression. The idea behind the deleted residual is that an influential data point i, pulls the regression line torwards itself. By removing that data point, the line should bounce back away from the original response, resulting in a large deleted residual.

The deleted residual is,

$$d_i = Y_i - \hat{Y}_{-(-i)} \tag{86}$$

studentized deleted (externally studentized) residual.

$$t_i = \frac{d_i}{se(d_i)} = r_i \left(\frac{n - k - 2}{n - k - 1 - r_i^2}\right)^{1/2}$$
 (87)

$$se(d_i) = \sqrt{\frac{MSE_i}{1 - h_{ii}}} \tag{88}$$

$$MSE_i = \frac{(1 - h_{ii}SSE - \hat{\epsilon}_i^2)}{(n - p - 1)(1 - h_{ii})}$$
(89)

$$= \frac{n-p}{n-p-1}MSE - \frac{\hat{\epsilon}^2}{(n-p-1)(1-h_{ii})}$$
 (90)

Under the null hypothesis  $H_0$ : no outliers,  $t_i \sim t_{n-p-1}$ .

# 5.15 Bonferonni's method for obtaining critical value for studentized deleted residuals

Decision Rule: Reject  $H_0$ : no outliers, if

$$\max_{1 \le i \le n} |t_i| > t_{n-p-1} (1 - \frac{\alpha}{2n})$$

where p is the number of  $\beta$ 's

- 1. Calculate critical value  $t_{n-p-1}(1-\frac{\alpha}{2n})$ .
- 2. Calculate all studentized residuals  $t_i$ .

- 3. Get max of absolute value  $\max_{1 \le i \le n} |t_i|$  if residuals. 5.17
- 4. If  $\max |t_i| < t^*$ , fail to reject  $H_0$  and conclude no outliers.

# 5.16 Identifying outlier x observations

(91) Recall  $h_{ii}$  is the *ith* diagonal element of the hat matrix H = Px, which is called the leverage for the *ith* case. A property:

$$\sum_{i=1}^{n} h_{ii} = p \tag{92}$$

If  $h_{ii} > 2h = \frac{2p}{n}$ , case i is considered outlying in x.

# 5.17 Identifying influential cases

An outlying case isn't necessarily influential, to identify influential cases, consider Cook's Distance .

$$D = \frac{\sum_{j=1}^{n} (\hat{Y}_{j} - \hat{Y}_{j(-i)})^{2}}{p * MSE}$$
(93)

where  $\hat{Y}_j$  is the predicted value of  $Y_j$  via regression with the full data, and  $\hat{Y}_{j(-i)}$  is the predicted value of  $Y_j$  via regression with the data without the *ith* case. Large values of  $D_i$  indicate a potentially influential case. Another more computationally convenient expression is,

$$D_i = \frac{h_{ii}\hat{\epsilon}_i^2}{p(1 - h_{ii})^2 MSE} \tag{94}$$