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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
$$E(Y_i) = \beta_0 + \beta_1 x_i \tag{2}$$

$$Var(Y_i) = \sigma^2 \tag{3}$$
- Mean:  $\beta_0 + \beta_1 x_i$
- Variance:  $\sigma^2$

Assumptions

- $\epsilon_1 \dots \epsilon_n$
- $E(\epsilon_i) = 0, var(\epsilon_i) = \sigma^2$ , 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

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

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x} \tag{6}$$

- $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$  (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

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

Properties of Residuals

- $\sum_{i=1}^n \hat{\epsilon}_i = 0$
- 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  $Y_i$ )

$$s^2 = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 \tag{7}$$

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

Notes

- $\hat{Y}_i$  is an estimator of  $E(Y_i) = \beta_0 + \beta_1 x_i$  in which two parameters are estimated ( $\beta_0$  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.

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

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

$$s.e.(\hat{\beta}_1) = \sqrt{\frac{MSE}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (10)$$

$$MSE = s^2 \quad (11)$$

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

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

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

**Decision Rules**

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

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

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

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

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

$$k = 0, 1 \quad (14)$$

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 $\beta_0$

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

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

### 2.3 Inference about $\hat{Y}$

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

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

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

### 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:

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

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

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

$$SSTO = SSR + SSE \quad (20)$$

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

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

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

$$(24)$$

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.

$$MSR = \frac{SSR}{1} \quad (25)$$

$$MSE = \frac{SSE}{n - 2} \quad (26)$$

$$(27)$$

**F-Statistic**

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

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   | df  | MS  | 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  $x$ ).

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO} \quad (29)$$

Coefficient of correlation:

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

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

Properties of  $R^2$  and  $r$

- $0 \leq R^2 \leq 1$      $-1 \leq r \leq 1$
- $R^2 \approx 1$  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

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

$$= E(XY) - E(X)E(Y) \quad (33)$$

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

where  $\mu_X = E(X)$ ,  $sd(X) = \sqrt{\text{var}(X)}$ , 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  $\rho < 0$ )

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

## 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 distributed.
- Check **constant variance** - residuals are random and don't 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.
- QQ plot is nonlinear  $\implies$  non normal residuals.

## 3.2 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

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

where  $z(p)$  is the  $p$ th 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  $\hat{\epsilon}_{i2}, i = 1, \dots, n_2$  be the residuals for the second part, where  $n_1 + n_2 = n$ .

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

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

3. Compute t score.

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

$$s^2 = \frac{\sum_{i=1}^{n_1} (d_{i1} - \bar{d}_1)^2 + \sum_{i=1}^{n_2} (d_{i2} - \bar{d}_2)^2}{n - 2} \quad (38)$$

4. Test  $H_0 : \sigma_1^2 = \sigma_2^2$  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:  $Y_{ij} = \beta_0 + \beta_1 x_j + \epsilon_{ij}, j = 1 \dots c, i = 1 \dots n_j$  where  $x_j$  is the  $j$ th value of  $x$ ,  $c$  is the number of

different  $x$  values, and  $Y_{ij}, i = 1 \dots n_j$  are the  $Y$  values corresponding to the same  $x_j$ .

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

F-statistic:

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

where

$$SSE(R) = \sum_j \sum_i (Y_{ij} - \hat{Y}_{ij})^2 \quad (40)$$

$$SSE(F) = \sum_j \sum_i (Y_{ij} - \hat{\mu}_j)^2 \quad (41)$$

with  $\hat{Y}_{ij} = \hat{\beta}_0 + \hat{\beta}_1 x_j$  and  $\hat{\mu}_j = \bar{Y}_j - n_j^{-1} \sum_{i=1}^{n_j} Y_{ij}, df_R = n - 2$  with  $n = \sum_{j=1}^c n_j$  and  $df_F = n - c$ .

Under  $H_0$  : The assumed model is correct,  $F \sim F_{c-2, n-c}$ .

## 3.3 Remedial Measures

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

**Transformation of Y:** for nonnormality/unequal variance.

### Box Cox transformation

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

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

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

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

$$K_1 = \frac{1}{\lambda K_2^{\lambda-1}} \quad (44)$$

## 4 Simultaneous Inference

### 4.1 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.

SCI's for  $E(Y_h) = \beta_0 + \beta_1 x_h, h \in G, g = |G|$

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

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

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

Where,

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

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

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

## 4.2 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.

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

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

where  $B = (49)$

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

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

$$(54)$$

## 5 Multiple Linear Regression

Matrix expression for multiple linear regression,

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

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

$$Y = X\beta + \epsilon \quad (56)$$

Given

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

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

### LS Estimate

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

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \cdots \\ \hat{\beta}_{p-1} \end{bmatrix} = (X'X)^{-1}X'Y \quad (59)$$

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

#### 1. Manual

- `$\hat{\beta} = \text{solve}(t(X) \%*\% X) \%*\% (t(X) \%*\% Y)$`
- `$\%*\%$`  denotes the matrix product.

#### 2. Using built in functions

- `$\text{result} = \text{lsfit}(X, Y, \text{intercept} = F)$`
- `$\text{bhat} = \text{result}\$coef$`

## 5.1 ANOVA Table

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

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

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

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

$$MSE = \frac{SSE}{(n-p)} \quad (64)$$

$$F = \frac{MSR}{MSE} \quad (65)$$

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

| Source     | SS   | df    | MS    | F   |
|------------|------|-------|-------|-----|
| Regression | SSR  | $p-1$ | $MSR$ | $F$ |
| Error      | SSE  | $n-p$ | $MSE$ |     |
| Total      | SSTO | $n-1$ |       |     |

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

## 5.2 Inference about Regression Parameters

### Step 1

$H_0 : \beta_k = \beta_{k0}$

$H_1 : \beta_k \neq \beta_{k0} (> \beta_{k0}, < \beta_{k0})$  where  $\beta_{k0}$  is a specified value (e.g. 0).

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

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

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

Under  $H_0$ ,  $t \sim t_{n-p}$

### Step 2

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

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

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

## 5.3 Estimation of Mean Responses

$$E(Y_h) = x'_h \beta = \beta_0 + \beta_1 x_{h,1} + \cdots + \beta_{p-1} x_{h,p-1} \quad (70)$$

First compute  $\hat{Y}_h = x'_h \hat{\beta}$  and

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

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

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

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

## 5.4 Prediction Interval

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

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

$$Scheffe : \hat{Y}_h \pm S * pse(\hat{Y}_h), S = \sqrt{g * F_{g, n-p}(1 - \alpha)} \quad (75)$$

$$Bonfer : \hat{Y}_h \pm B * pse(\hat{Y}_h), B = t_{n-p} \left( 1 - \frac{\alpha}{2g} \right) \quad (76)$$

## 5.5 Multiple Predictor SS

$$SSR(x_2|x_1) = SSR(x_1, x_2) - SSR(x_1) \\ = SSE(x_1) - SSE(x_1, x_2)$$

$$SSR(x_3|x_1, x_2) = SSR(x_1, x_2, x_3) - SSR(x_1, x_2) \\ = SSE(x_1, x_2) - SSE(x_1, x_2, x_3)$$

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

## 5.6 ANOVA with extra SS

| Source         | SS                   | df      |
|----------------|----------------------|---------|
| 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

$$H_0 : \beta_3 = 0$$

$$H_1 : \beta_3 \neq 0$$

$$SSE(Full) = SSE(x_1, x_2, x_3)$$

$$SSE(Reduced) = SSE(x_2, x_2)$$

$$F = \frac{SSR(R) - SSR(F)/(df_R - df_F)}{SSR(F)/df_F} \quad (77)$$

$$F = \frac{MSR(x_3|x_1, x_2)}{MSE(x_1, x_2, x_3)} \quad (78)$$

$$df_R = n - 3, df_F = n - 4$$

$$\text{Under } H_0, F \sim F_{1, n-4}$$

## 5.8 Coefficient of Partial Determination

$$R_{Y, x_2|x_1}^2 = R_{Y, 2|1}^2 = \frac{SSR(x_2|x_1)}{SSE(x_1)} = 1 - \frac{SSE(x_1, x_2)}{SSE(x_1)} \quad (79)$$

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**

$$R_{Y, x_p, \dots, x_{p+q-1}|x_1, \dots, x_{p-1}}^2 = 1 - \frac{SSE(x_1, \dots, x_{p+1-1})}{SSE(x_1, \dots, x_{p-1})} \quad (80)$$

## 5.9 Adjusted R

$$R^2 = 1 - \frac{SSE}{SSTO} \quad (81)$$

$$R_a^2 = 1 - \frac{MSE}{MSTO} = \frac{SSE/(n-p)}{SSTO/(n-1)} \quad (82)$$

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 Mallows's C

$$C_p = C_p(x_{i_1}, \dots, x_{i_{p-1}}) = \frac{SSE(x_{i_1}, \dots, x_{i_{p-1}})}{MSE(x_1, \dots, x_{K-1})} - (n-2p) \quad (83)$$

where  $SSE(x_{i_1}, \dots, x_{i_{p-1}}) = SSE$  of fitting the regression with  $x_{i_1}, \dots, x_{i_{p-1}}$  and  $MSE(x_1, \dots, x_{K-1}) = MSE$  of fitting the regression with all candidate predictors.

The best subset of predictors corresponds to the one such that  $C_p$  is small and close to  $p$ . Note:  $C_p = K$ .

## 5.11 AIC and BIC(SBC) criteria

$$AIC_p = n \log(SSE_p/n) + 2p \quad (84)$$

$$SBC_p = n \log(SSE_p/n) + (\log n)p \quad (85)$$

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,

$$r_i = \frac{\hat{\epsilon}_i}{se(\hat{\epsilon}_i)} = \frac{\hat{\epsilon}_i}{\sqrt{MSE(1 - h_{ii})}} \quad (86)$$

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  $i$ th diagonal element of the hat matrix  $H = X(X'X)^{-1}X'$ , also called the **leverage** for the  $i$ th case.

**deleted (jackknife) residual:** Fit the regression with the  $i$ th 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 towards 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,

$$d_i = Y_i - \hat{Y}_{i(-i)} \quad (87)$$

**studentized deleted (externally studentized) residual .**

$$t_i = \frac{d_i}{se(d_i)} = r_i \left( \frac{n-k-2}{n-k-1-r_i^2} \right)^{1/2} \quad (88)$$

$$se(d_i) = \sqrt{\frac{MSE_i}{1 - h_{ii}}} \quad (89)$$

$$MSE_i = \frac{(1 - h_{ii}SSE - \hat{\epsilon}_i^2)}{(n-p-1)(1 - h_{ii})} \quad (90)$$

$$= \frac{n-p}{n-p-1}MSE - \frac{\hat{\epsilon}_i^2}{(n-p-1)(1 - h_{ii})} \quad (91)$$

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

$$\max_{1 \leq i \leq n} |t_i| > t_{n-p-1} \left(1 - \frac{\alpha}{2n}\right) \quad (92)$$

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

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

3. Get max of absolute value  $\max_{1 \leq i \leq n} |t_i|$  if residuals.

4. If  $\max |t_i| < t^*$ , fail to reject  $H_0$  and conclude no outliers.

### 5.16 Identifying outlier x observations

Recall  $h_{ii}$  is the  $i$ th diagonal element of the hat matrix  $H = Px$ , which is called the leverage for the  $i$ th case.

A property:

$$\sum_{i=1}^n h_{ii} = p \quad (93)$$

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**.

$$D = \frac{\sum_{j=1}^n (\hat{Y}_j - \hat{Y}_{j(-i)})^2}{p * MSE} \quad (94)$$

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  $i$ th case.

Large values of  $D_i$  indicate a potentially influential case. Another more computationally convenient expression is,

$$D_i = \frac{h_{ii} \hat{\epsilon}_i^2}{p(1 - h_{ii})^2 MSE} \quad (95)$$