

$$C_p = 2p' - n + \frac{RSS/p'}{\hat{\sigma}^2_{\text{full model}}}$$

1. Dec

3. (15 marks) An experiment was conducted to model Y with five explanatory variables X_1, X_2, X_3, X_4 and X_5 . We desire an equation of relating Y to the other variables. The goal is to find variables that should be further studied with the eventual goal of developing a prediction equation. The following table gives RSS for all possible regressions. Total sum of squares is equal to 5.0634 and the number of observations is equal to 20.

No. of parameters in the model	RSS	Model
2	2.0338	X_1
2	5.0219	X_2
2	1.5370	X_3
2	2.5044	X_4
2	1.5563	X_5
3	1.5921	X_1, X_2
3	1.4397	X_1, X_3
3	1.7462	X_1, X_4
3	1.4963	X_1, X_5
3	1.4707	X_2, X_3
3	2.4381	X_2, X_4
3	1.4388	X_2, X_5
3	1.4590	X_3, X_4
3	1.0850	X_3, X_5
3	1.3287	X_4, X_5
4	1.2582	X_1, X_2, X_3
4	1.4257	X_1, X_2, X_4
4	1.2764	X_1, X_2, X_5
4	1.3894	X_1, X_3, X_4
4	1.0644	X_1, X_3, X_5
4	1.3204	X_1, X_4, X_5
4	1.3900	X_2, X_3, X_4
4	0.9871	X_2, X_3, X_5
4	1.2178	X_2, X_4, X_5
4	1.0634	X_3, X_4, X_5
5	1.2199	X_1, X_2, X_3, X_4
5	0.9871	X_1, X_2, X_3, X_5
5	1.1565	X_1, X_2, X_4, X_5
5	1.0388	X_1, X_3, X_4, X_5
5	0.9653	X_2, X_3, X_4, X_5
6	0.9652	X_1, X_2, X_3, X_4, X_5

$$\Rightarrow C_p = 2 \times 2 - 20 + \frac{1.5370}{0.9652/14} = 6.294$$

$$\Rightarrow C_p = 2 \times 3 - 20 + \frac{1.085}{0.9652/14} = 1.738$$

Best model = X_3, X_5

$$\Rightarrow C_p = 2 \times 4 - 20 + \frac{0.9871}{0.9652/14} = 2.318$$

$$\Rightarrow C_p = 2 \times 5 - 20 + \frac{0.9653}{0.9652/14} = 4.001$$

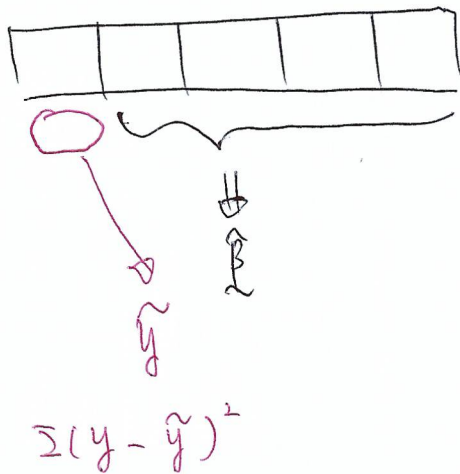
$$\Rightarrow C_p = 2p' - n + \frac{0.9652}{0.9652/(n-p)} = p' = 6$$

Find the best model by C_p , forward selection, backward selection and stepwise selection. Write down how to get the best model on details. Choose critical values for both ENTRY and STAY to be 2. Comment the results.

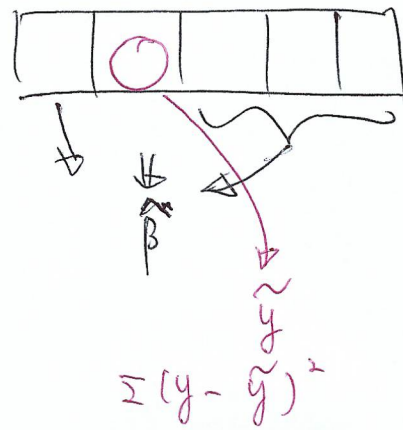
$$\hat{\sigma}^2_{\text{full model}} = \frac{0.9652}{20 - 6} = \frac{0.9652}{14} = 0.06894$$

(6) Cross-validation

①



②



Calculate $\sum \sum (y - \tilde{y})^2$ all obs. ~~without~~ without i th obs.
CV PRESS

PRESS statistic
↑
Predicted

$n_1 = n - 1 \rightarrow$ fit a model
 $\Rightarrow \hat{\beta}$

$n_2 = 1 \rightarrow \tilde{y}_{i(-i)} \quad i = 1, \dots, n$
↑
 i th obs

$(y_i - \tilde{y}_{i(-i)})$
PRESS residual

$$\text{PRESS} = \sum_{i=1}^n (y_i - \tilde{y}_{i(-i)})^2$$

$$= \sum_{i=1}^n \frac{\hat{e}_i^2}{(1 - h_{ii})^2}$$

$\hat{e}_i = y_i - \hat{y}_i$ — residual

$h_{ii} = (i, i)^{\text{th}} \text{ element in } H$

where $H = X(X^T X)^{-1} X^T$

leverage $h_{ii} = \underline{x}_i^T (X^T X)^{-1} \underline{x}_i$
 \underline{x}_i^T — i th row in X

Simple linear regression

$$y_i = \beta_0 + \beta_1 x_i + e_i \quad i=1, \dots, n$$

Centred model

$$\Rightarrow \tilde{X}^T \tilde{X} = \begin{pmatrix} n & 0 \\ 0 & S_{xx} \end{pmatrix} \quad (\tilde{X}^T \tilde{X})^{-1} = \begin{pmatrix} \frac{1}{n} & 0 \\ 0 & \frac{1}{S_{xx}} \end{pmatrix}$$

$$h_{ii} = \begin{pmatrix} 1 & x_i - \bar{x} \end{pmatrix} \begin{pmatrix} \frac{1}{n} & 0 \\ 0 & \frac{1}{S_{xx}} \end{pmatrix} \begin{pmatrix} 1 \\ x_i - \bar{x} \end{pmatrix}$$

$$= \frac{1}{n} + \frac{(x_i - \bar{x})^2}{S_{xx}} \quad \leftarrow \text{diff. between } x_i \text{ \& } \bar{x}$$

$$\boxed{1} \geq h_{ii} \geq \boxed{\frac{1}{n}} \quad \leftarrow \text{semi } I - \frac{1}{n} J \text{ is positive definite}$$

$$\uparrow \quad I - H \text{ is positive semi-definite (Chapt 1)}$$

\Rightarrow all ~~diagonal~~ diagonal elements are non-negative

$$\Rightarrow 1 - h_{ii} \geq 0$$

$$\Rightarrow 1 \geq h_{ii}$$

Define $H_c = \tilde{X}_c (\tilde{X}_c^T \tilde{X}_c)^{-1} \tilde{X}_c^T$

$$\text{Model} = \underline{y} = \hat{\alpha} \underline{1} + \tilde{X}_c \hat{\beta} + \underline{e}$$

$$\hat{\underline{y}} = \hat{\alpha} \underline{1} + \tilde{X}_c \hat{\beta}$$

$$= \hat{\alpha} \underline{1} + \tilde{X}_c (\tilde{X}_c^T \tilde{X}_c)^{-1} \tilde{X}_c^T \underline{y}$$

$$= \left[\frac{1}{n} J + H_c \right] \underline{y}$$

\uparrow matrix with ~~eq~~ all elements equal to 1

$$= H \underline{y}$$

$$\Rightarrow \underline{H} = \frac{1}{n} \underline{J} + \underline{H}_c$$

$$\Rightarrow \underline{H} - \frac{1}{n} \underline{J} = \underline{H}_c$$

\nwarrow ^{semi} positive definite

\Rightarrow all diagonal elements of $\underline{H} - \frac{1}{n} \underline{J}$ are non-negative

$$\Rightarrow h_{ii} - \frac{1}{n} \geq 0$$

$$\Rightarrow h_{ii} \geq \frac{1}{n}$$

$$\underline{PRESS} = \sum_{i=1}^n \frac{\hat{e}_i^2}{(1-h_{ii})^2} \quad - \text{smallest } \underline{PRESS}$$

c) largest $R^2 = 1 - \frac{\text{Res S.S.}}{\text{total S.S.}}$

\Leftrightarrow smallest Res S.S.

$R^2 \uparrow$ when # of indep. variables \uparrow

\Rightarrow Best model = full model

d) largest $R^2_{adj} = 1 - \frac{\text{MSE} \leftarrow \text{Res S.S.}/(n-p')}{\text{total M.S.} \leftarrow \text{total S.S.}/(n-1)}$

$$= 1 - \frac{\text{Res S.S.}}{\text{total S.S.}} * \frac{n-1}{n-p'}$$

R^2_{adj} may be negative

f) AIC = Akaike Information Criteria — smallest

$$= -2 \log L + 2 \underbrace{p'}_{\text{penalty}}$$

g) BIC = Bayesian Information Criteria — smallest

$$= -2 \log L + \underbrace{\ln n * p'}_{\text{penalty}}$$

~~$\ln n > 2$~~
 $\log_e(n) > 2$

Linear Regression

$$L(\beta, \sigma^2) = \frac{1}{(2\pi)^{n/2} (\hat{\sigma}^2)^{n/2}} \exp \left\{ - \frac{\sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2}{2 \hat{\sigma}^2} \right\}$$

$$\Rightarrow \log L = - \frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\hat{\sigma}^2) - \frac{n}{2}$$

$$\begin{aligned} \Rightarrow -2 \log L &= n \ln(2\pi) + n \ln(\hat{\sigma}^2) + n \\ &= n \ln \left(\frac{\text{ResSS}}{n} \right) + \text{constant} \end{aligned}$$

$$\Rightarrow \text{AIC} = n \ln \left(\frac{\text{ResSS}}{n} \right) + 2p'$$

$$\text{BIC} = n \ln \left(\frac{\text{ResSS}}{n} \right) + \ln(n) * p'$$

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2}{n} \quad \text{m.l.e.}$$

$\hat{\sigma}^2 = \frac{\text{ResSS}}{n - p'}$ to est.
 $\hat{\sigma}^2$ (unbiased est.)

Chapter 5 Residual Analysis

Assume - $e_i \sim N(0, \sigma^2)$

- y & x are linear related

$$\left. \begin{aligned} \text{Residual } \hat{e}_i &= y_i - \hat{y}_i & E(\hat{e}_i) &= 0 \\ & & \text{Var}(\hat{e}_i) &= \sigma^2(1 - h_{ii}) \\ & & & \neq \text{constant} \end{aligned} \right\} \leftarrow \text{Chapter 1}$$

Standardized residual

① $r_i = \frac{\hat{e}_i}{\sqrt{\hat{\sigma}^2(1 - h_{ii})}}$ — (internally studentized residual)

② $t_i = \frac{\hat{e}_i}{\boxed{\hat{\sigma}_{(-i)}} \sqrt{1 - h_{ii}}}$ — (externally studentized residual)

$x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n$
 $y_1, \dots, y_{i-1}, y_i, y_{i+1}, \dots, y_n$

ignore the i th obs

$\Rightarrow (n-1)$ obs \Rightarrow Fit a model of y on x

$\hat{\beta}_0(-i), \hat{\beta}_1(-i), \dots, \hat{\beta}_p(-i), \hat{\sigma}_{(-i)}^2$

Put x_i into the fitted model

$\Rightarrow \hat{y}_{i(-i)}$

$$\frac{\text{Res S.S.}(-i)}{(n-1) - p'}$$

$\underbrace{\hspace{1cm}}$ $\underbrace{\hspace{1cm}}$
 $\# \text{ of obs.}$ $\# \text{ of unknown}$
 para. in
 the model

$t_i \sim t(n-1-p')$?

Use t_i to detect outlier ①

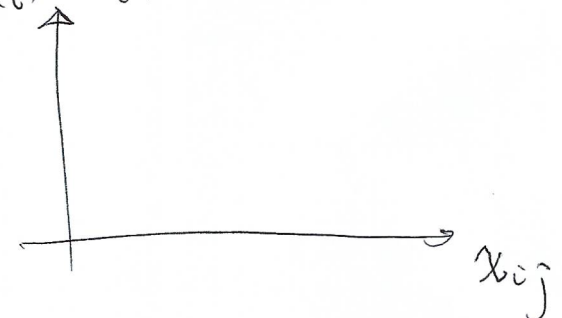
Residual Plot

check: linearity

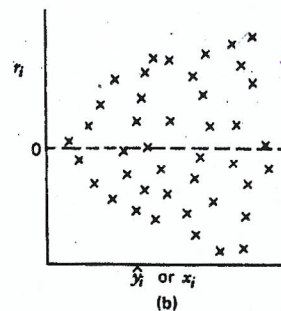
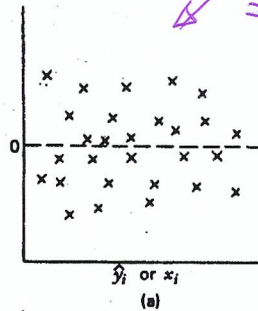
constant variance

pattern \Rightarrow transformation of y
 $\& x$

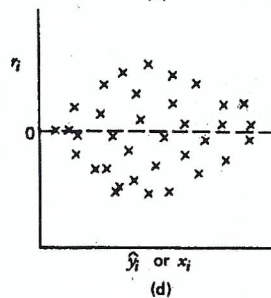
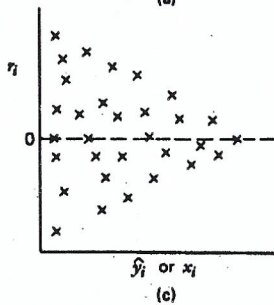
$\#$ If there is pattern
 \hat{e}_i, r_i, t_i



$\hat{\epsilon}_i, r_i, t_i$ no pattern
⇒ Assumptions are valid



variance (variation of residuals) increases as \hat{y}_i or x_i increases



non-linear →

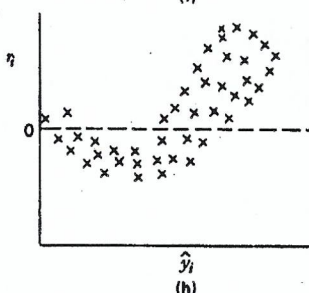
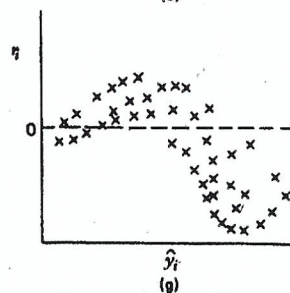
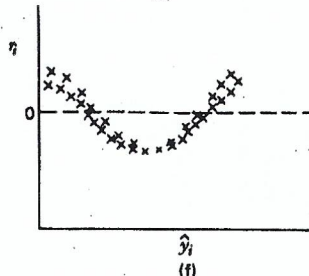
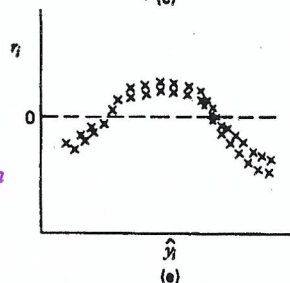


Figure 6.3 Residual plots: (a) null plot; (b) right-opening megaphone; (c) left-opening megaphone; (d) double outward bow; (e) nonlinearity; (f) nonlinearity; (g) nonlinearity and nonconstant variance; (h) nonlinearity and nonconstant variance.

⇒ transformation of y and/or x

e.g. count data $\Rightarrow \sim \text{Poisson}(\mu)$ $E(y) = \mu$

$-\sqrt{y}, \log(y)$

y - area m^2

x - perimeter m

\sqrt{y}	$\log(y)$	y
x	$\log(x)$	x^2

$\text{Var}(y) = \mu$
 smallest $-2\log L$
 largest likelihood

Smallest Res.S.S.

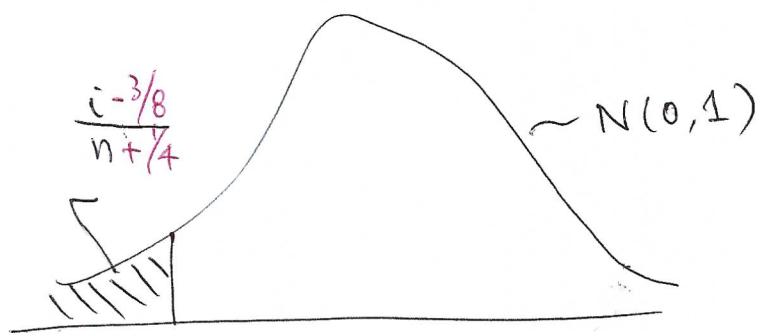
↑
linear regression

Normality assumption

Q-Q plot \Rightarrow ~~normal~~ normality

Arrange t_1, \dots, t_n

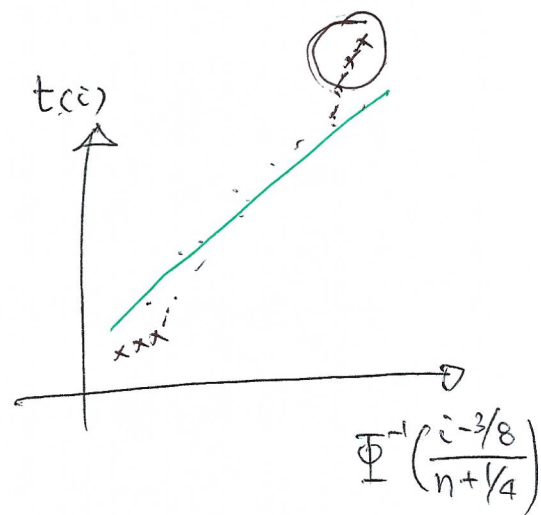
$\Rightarrow t_{(1)}, \dots, t_{(n)}$



$t_{(i)}$
 \uparrow

$$z_{\frac{i}{n}} = \Phi^{-1}\left(\frac{i-3/8}{n+1/4}\right)$$

$\Phi(z) = \text{c.d.f. of } Z = N(0,1)$



Transformation on y Box-Cox transformation (Power \neq transformation)

$$y_i^* = \begin{cases} \frac{y_i^\lambda - 1}{\lambda} & \lambda \neq 0 \\ \log_e(y_i) & \lambda = 0 \end{cases}$$

λ - unknown

\uparrow

Find m.l.e. of λ

Assume $Y^* \sim N(X\beta, \sigma^2 I)$

- Data: Y, X

- dist. of Y is unknown

- dist. of $Y^* \sim N$

\Rightarrow dist. of Y

likelihood $(\beta, \sigma^2, \lambda | Y, X)$

$$= \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left\{-\frac{(Y^* - X\beta)^2}{2\sigma^2}\right\} \times J(\lambda, Y)$$

where $J(\lambda, Y) = \left(\prod_{i=1}^n y_i\right)^{\lambda-1}$

$$= GM(y)^{\lambda-1}$$

\uparrow geometric mean

linear regression

$$\log L = -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\hat{\sigma}^2) - \frac{n}{2}$$

$$= -\frac{n}{2} \log\left(\frac{\text{Res.S.S.}}{n}\right) + \text{constant}$$

log likelihood

$$\text{likelihood}(\lambda) = -\frac{n}{2} \log(\hat{\sigma}^2(\lambda))$$

↑

$$\hat{\sigma}^2(\lambda) = \frac{\mathbf{Y}^{*T} \mathbf{Y}^* - \mathbf{Y}^{*T} \mathbf{X}^* (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}^*}{n}$$

profile likelihood

$$\text{Define } \tilde{\mathbf{Z}}^\lambda = \mathbf{Y}^* / \mathbf{J} \mathbf{Y}_n$$

$$\Rightarrow \log \text{likelihood}(\lambda) = -\frac{n}{2} \log(\text{Res.S.S.}_\lambda(\tilde{\mathbf{Z}}^\lambda))$$

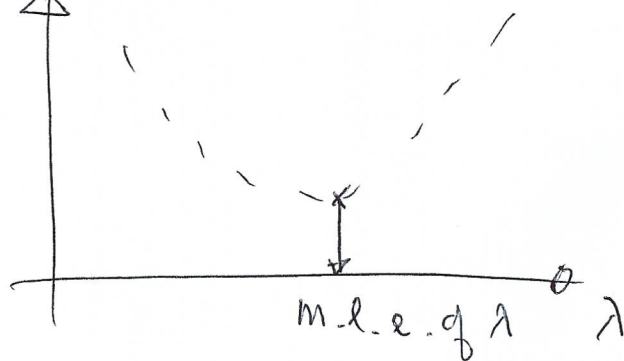
$$\text{where } \tilde{\mathbf{Z}}^\lambda \ni n \times 1 \text{ vector with } Z_i^\lambda = \begin{cases} \frac{y_i^\lambda - 1}{\lambda \text{GM}(y)} \mathbf{J}^{\lambda-1} & \lambda \neq 0 \\ \text{GM}(y) \ln(y_i) & \lambda = 0 \end{cases}$$

For each λ , \Rightarrow calculate Z_i^λ .

fit Z_i^λ on \mathbf{X}

$$\Rightarrow \text{Res.S.S.}_\lambda(\tilde{\mathbf{Z}})$$

$\text{Res.S.S.}_\lambda(\tilde{\mathbf{Z}})$



$$\text{e.g. } \hat{\lambda} = 0.423 \quad \therefore 95\% \text{ of } \hat{\lambda} ?$$

Does it over 0.5 ?