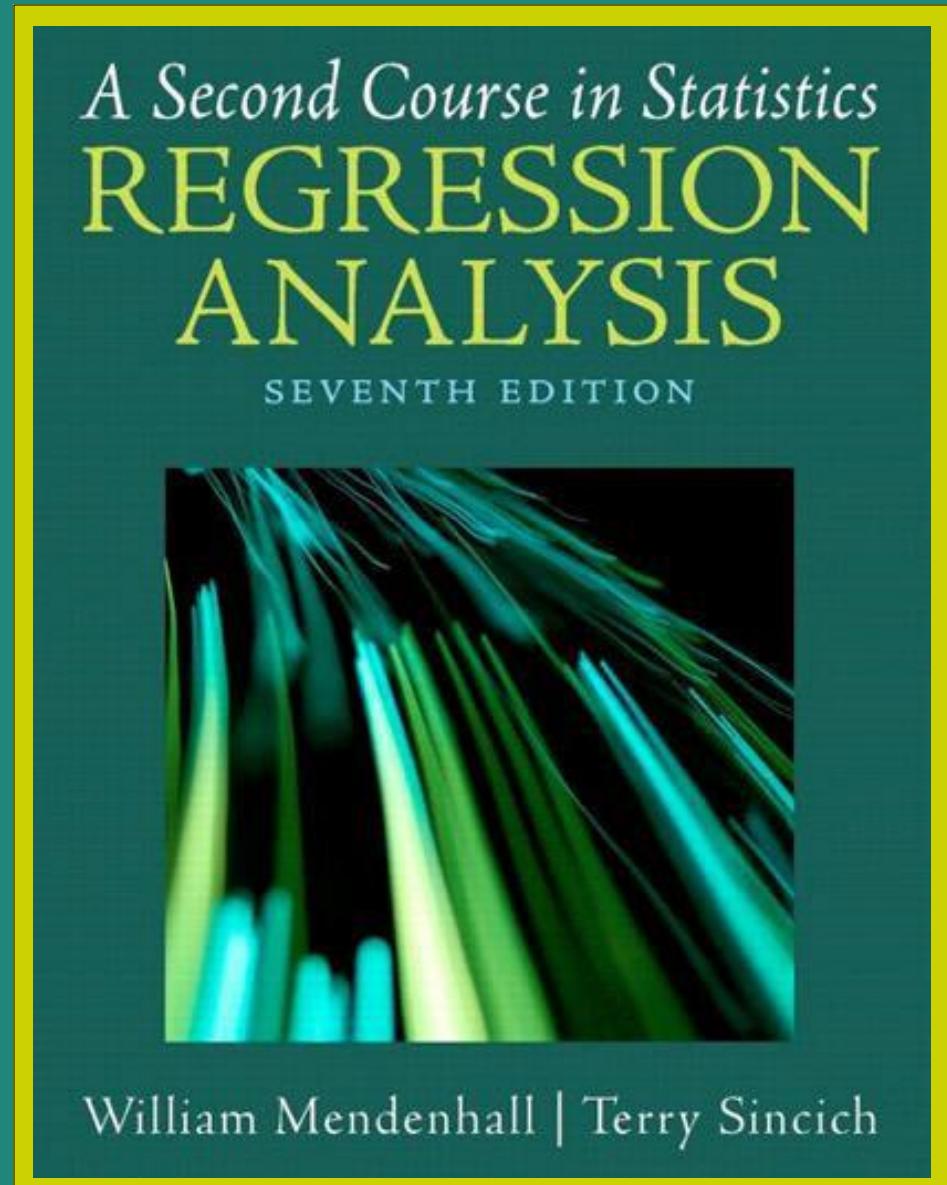


Chapter 8

Residual Analysis

Lecture 1

Dr Brenda Vo



STAT210/410 Study Plan



Topic	Weeks covered	Readings	Assessment
Topic 1: Simple Linear regression (SLR)	Wk 1	Chapter 3	Online Quiz due 9 th March
Topic 2: Multiple Linear Regression (MLR)	Wk 2 & 3	Chapter 4	Written Assessment A2 due 23 rd March
Topic 3: Model building	Wk 4	Chapter 5	
Topic 4: Variable Screening and regression pitfalls	Wk 5	Chapters 6, 7	
Topic 5: Residual Analysis	Wk 6	Chapter 8	Written Assessment A3 due 13 th April
Topic 6 Generalised Linear Models (GLMs)	Wk 9 & 10	Chapter 9	
Topic 7: Principles of Experimental Design	Wk 11	Chapter 11	Written Assessment A4 due 11 th May
Topic 8: ANOVA, contrasts	Wk 12 & 13	Chapter 12	
STAT410 ONLY			
ART: Nonparametric Regression		Section 9.9	Written Assessment ART due 18 th May



Chapter 8 outline

Lecture 1:

- ❖ Review assumptions of linear model
- ❖ Detect lack of fit
- ❖ Power transformations

Lecture 2:

- ❖ Detect outliers and influential points

Assumptions of the linear model



$$\varepsilon \sim N(0, \sigma^2)$$

The residuals

- are normally distributed,
 - have a mean of 0
 - have constant variance
 - are independent
-
- Also check for *outliers* and *influential* points



Violated Assumptions

Issues....

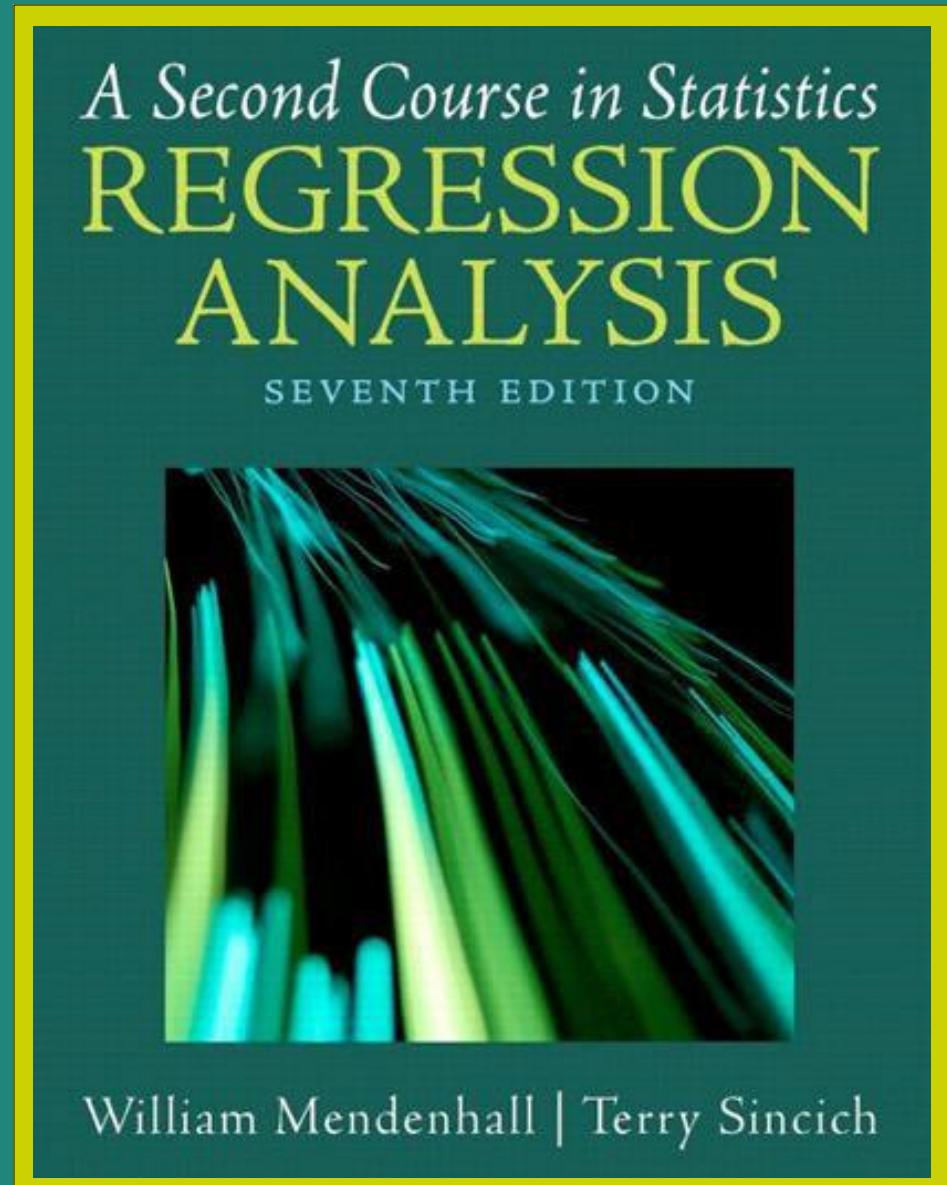
- Using model for estimation or prediction may be invalid
- Assumptions are reasonably “robust”

Solutions....

- Transform response and/or predictor variables
- Weighted regression (constant variance)
- Generalized Linear Models - assume a non-normal error distribution

Section 8.3

Detecting Lack of Fit



Detecting Lack of Fit



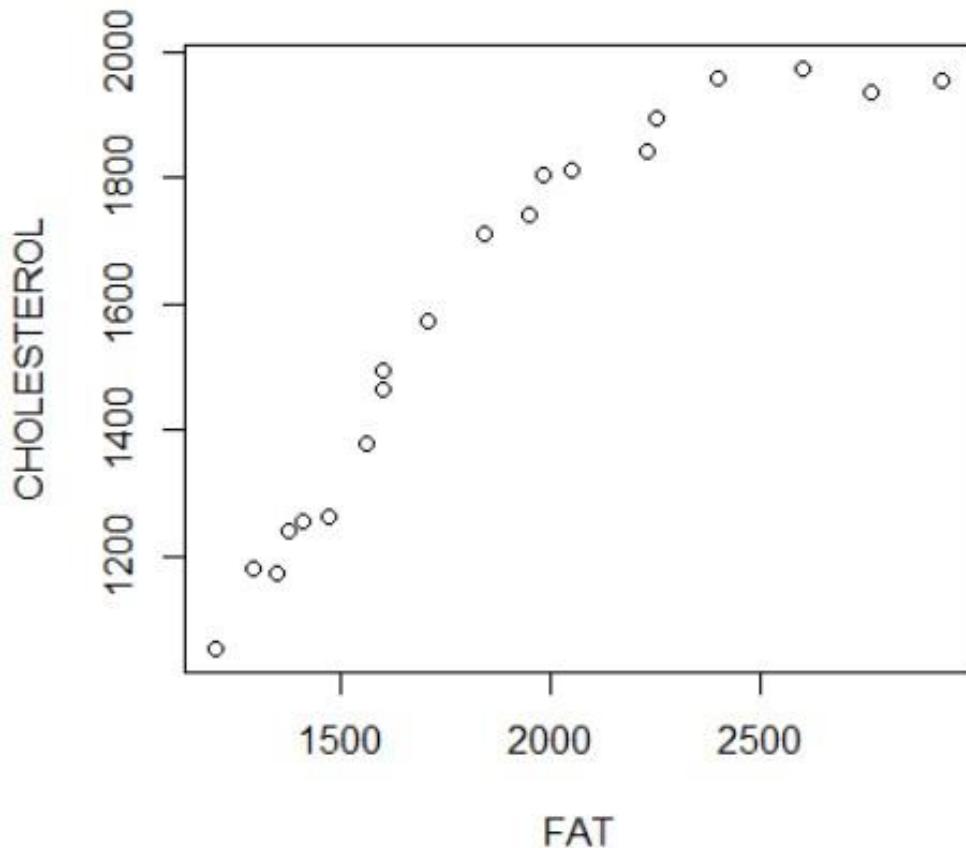
- Plot the residuals versus each of the independent variables $x_1, x_2 \dots x_k$
- Plot the residuals against the fitted value
- In each plot, look for trends, dramatic changes in variability.



Table 8.1 Data for 20 Olympic athletes

Athlete	Fat intake x , milligrams	Cholesterol y , milligrams/liter
1	1,290	1,182
2	1,350	1,172
3	1,470	1,264
4	1,600	1,493
5	1,710	1,571
6	1,840	1,711
7	1,980	1,804
8	2,230	1,840
9	2,400	1,956
10	2,930	1,954
11	1,200	1,055
12	1,375	1,241
13	1,410	1,254
14	1,560	1,377
15	1,600	1,465
16	1,950	1,741
17	2,050	1,810
18	2,250	1,893
19	2,600	1,972
20	2,760	1,935

Scatterplot



```
oly<-read.table("OLYMPIC.txt", header=T)
plot(CHOLESTEROL~FAT, data=oly)
```

R printout for first-order model



```
mod<-lm(CHOLESTEROL~FAT)
anova(mod)
summary(mod)
#####
Analysis of Variance Table
```

Response: CHOLESTEROL

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FAT	1	1617913	1617913	122	1.8e-09
Residuals	18	237980	13221		

Coefficients:

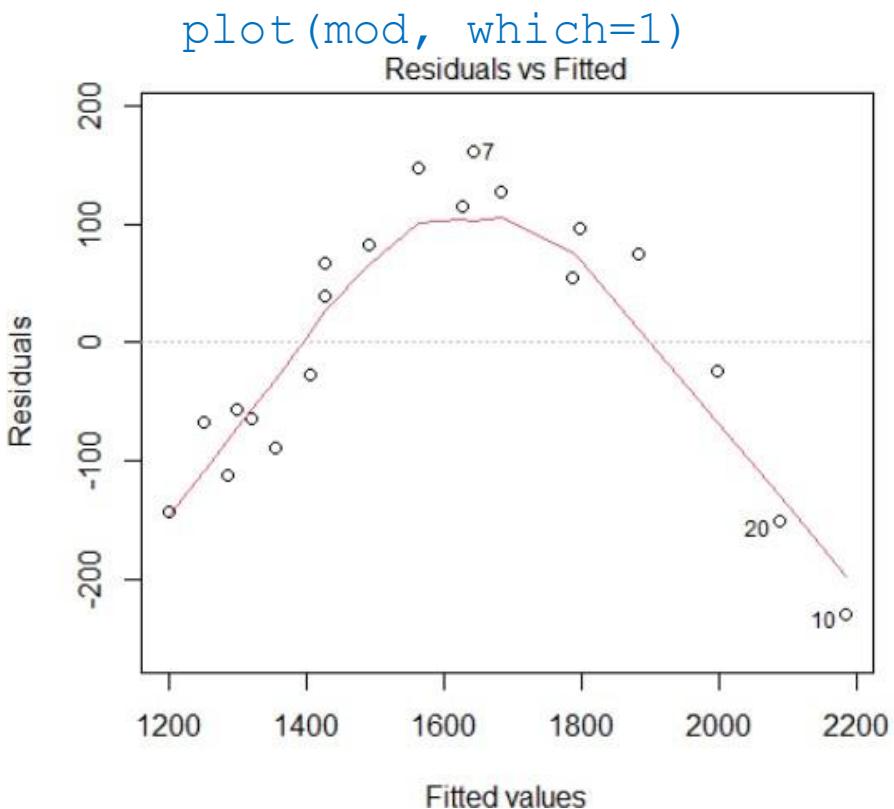
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	515.7050	99.9789	5.16	6.6e-05
FAT	0.5692	0.0515	11.06	1.8e-09

Residual standard error: 115 on 18 degrees of freedom

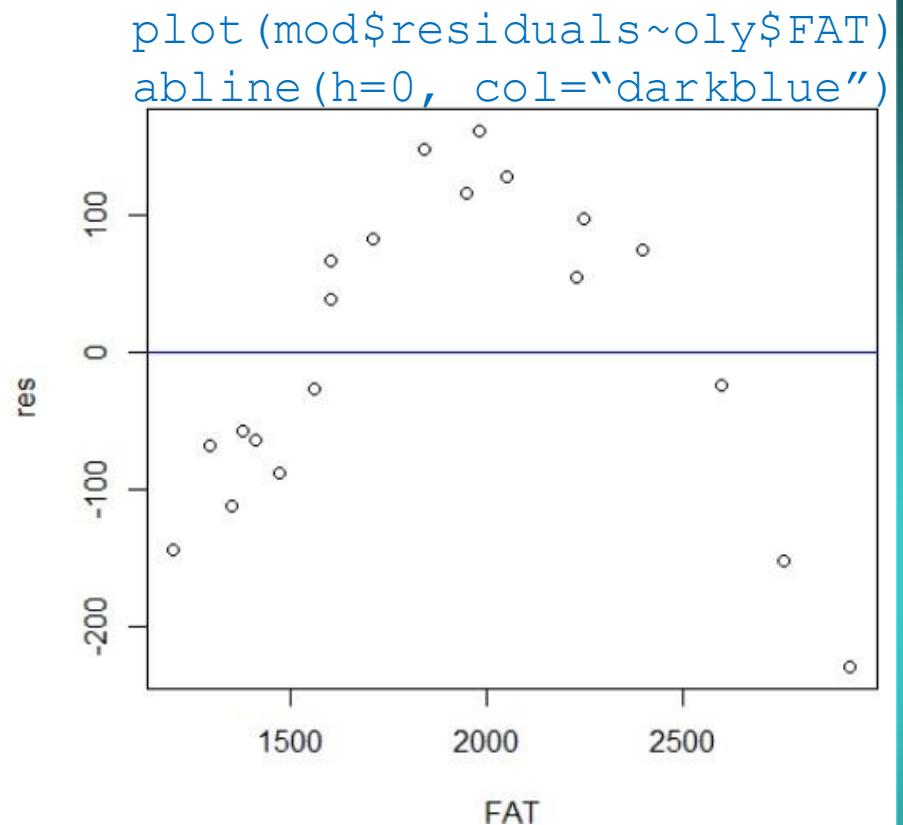
Multiple R-squared: 0.872, Adjusted R-squared: 0.865

F-statistic: 122 on 1 and 18 DF, p-value: 1.85e-09

Plots of residuals



Residuals vs fitted value of y



Residuals vs x values

Observed, predicted and residuals

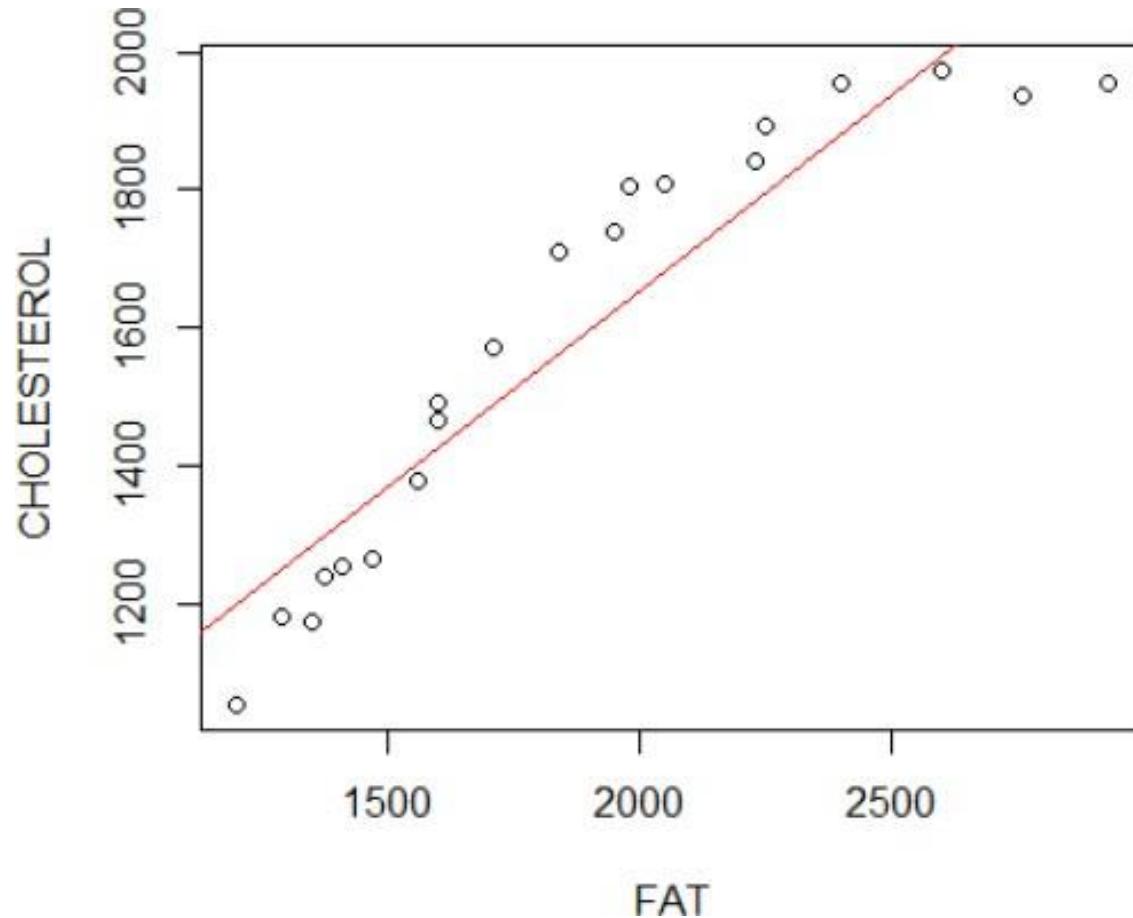


```
res<-mod$residuals  
preds<-predict(mod)  
cbind(FAT, CHOLESTEROL, preds, res)  
#####  


|    | FAT  | CHOLESTEROL | preds | res     |
|----|------|-------------|-------|---------|
| 1  | 1290 | 1182        | 1250  | -67.96  |
| 2  | 1350 | 1172        | 1284  | -112.11 |
| 3  | 1470 | 1264        | 1352  | -88.41  |
| 4  | 1600 | 1493        | 1426  | 66.59   |
| 5  | 1710 | 1571        | 1489  | 81.98   |
| .  | ..   | ..          | ..    | ..      |
| 17 | 2050 | 1810        | 1683  | 127.46  |
| 18 | 2250 | 1893        | 1796  | 96.62   |
| 19 | 2600 | 1972        | 1996  | -23.60  |
| 20 | 2760 | 1935        | 2087  | -151.67 |


```

Scatterplot with SLR line



Quadratic Model

```
mod2<-lm(CHOLESTEROL~FAT + I(FAT^2), data = oly)
anova(mod2)
summary(mod2)
```

Analysis of Variance Table

Response: CHOLESTEROL

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FAT	1	1617913	1617913	1300	< 2e-16
I(FAT^2)	1	216817	216817	174	2.3e-10
Residuals	17	21163	1245		

Coefficients:

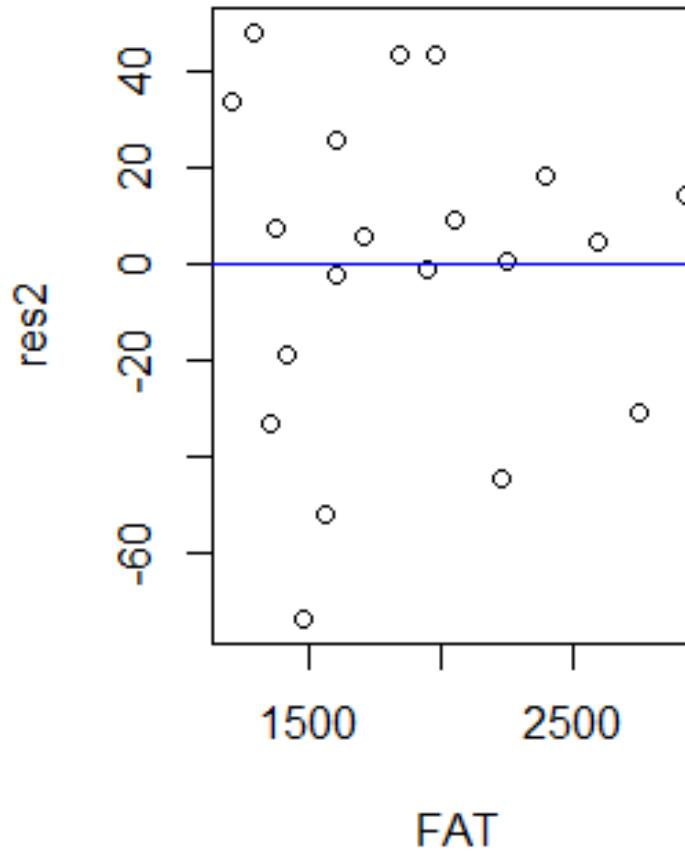
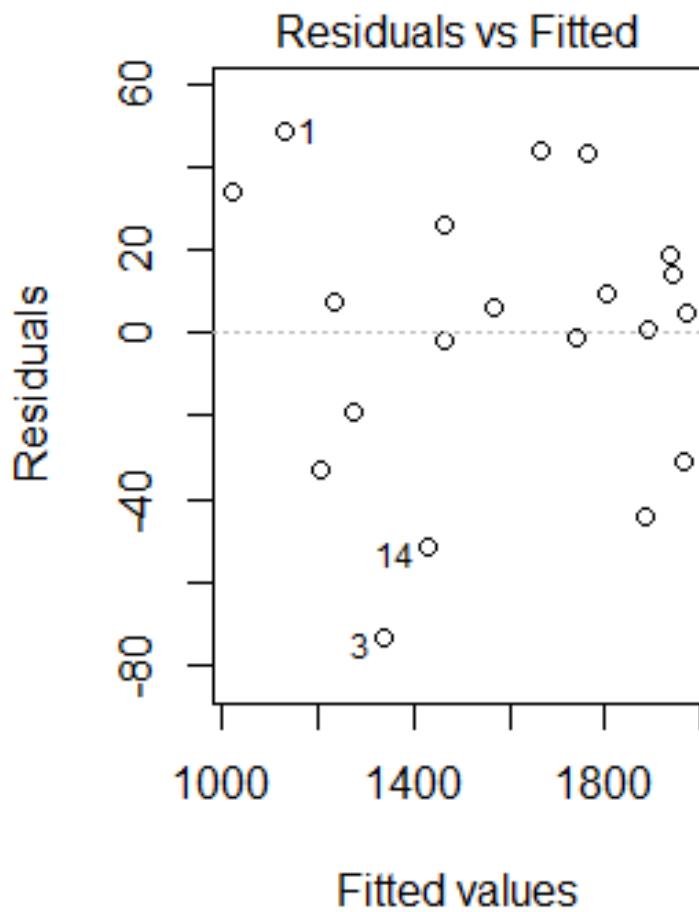
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-1.16e+03	1.31e+02	-8.88	8.6e-08
FAT	2.34e+00	1.35e-01	17.31	3.1e-12
I(FAT^2)	-4.39e-04	3.33e-05	-13.20	2.3e-10

Residual standard error: 35.3 on 17 degrees of freedom

Multiple R-squared: 0.989, Adjusted R-squared: 0.987

F-statistic: 737 on 2 and 17 DF, p-value: <2e-16

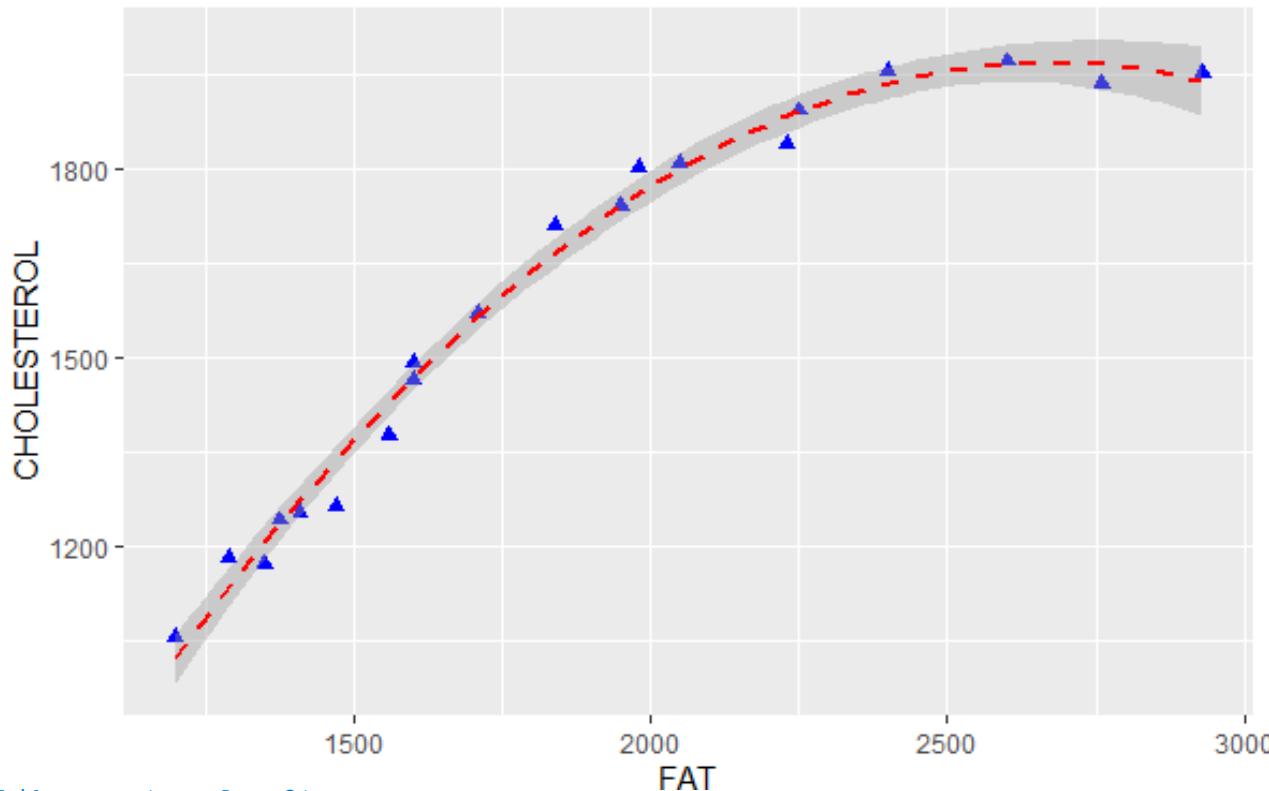
Plots of residuals: Quadratic model



Quadratic model



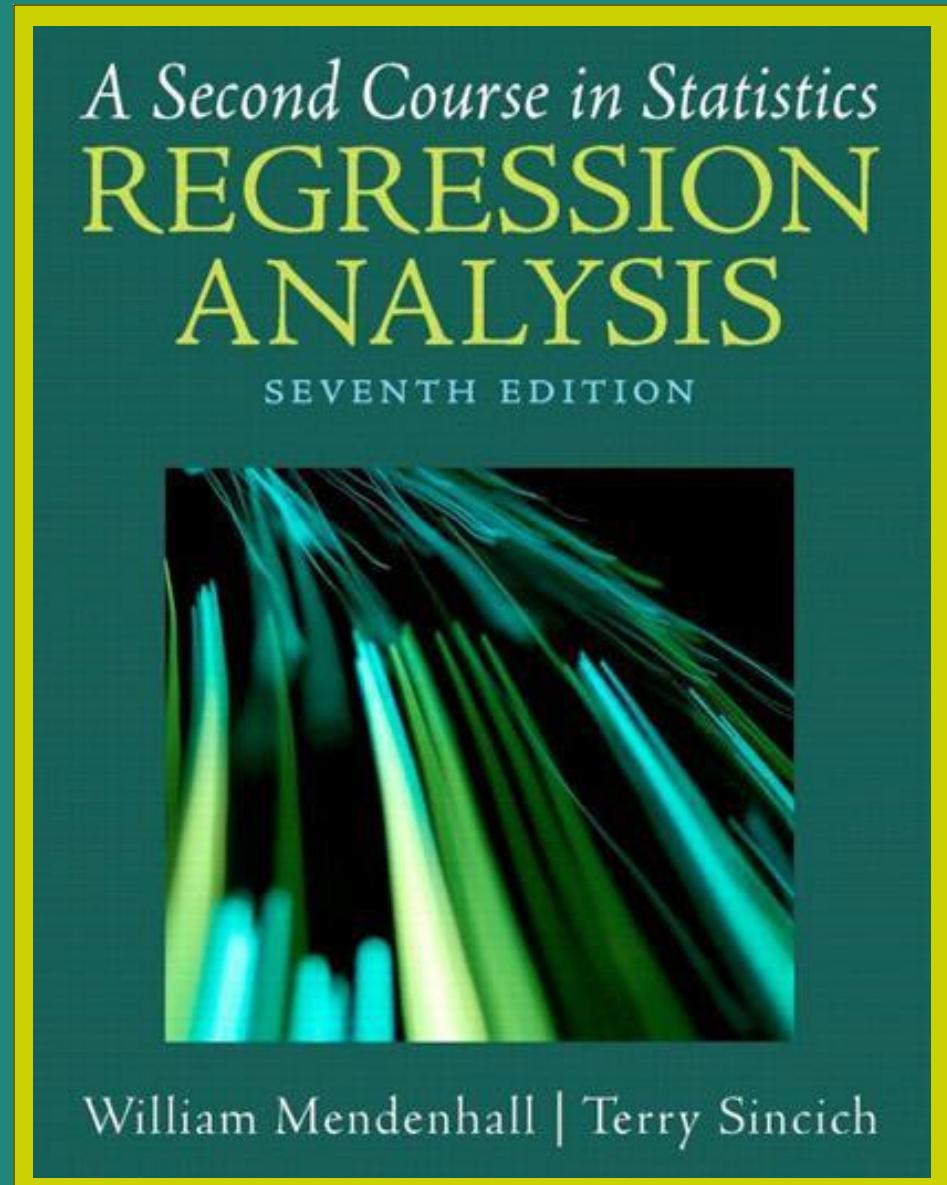
2th degree polynomial with 95% confidence bands



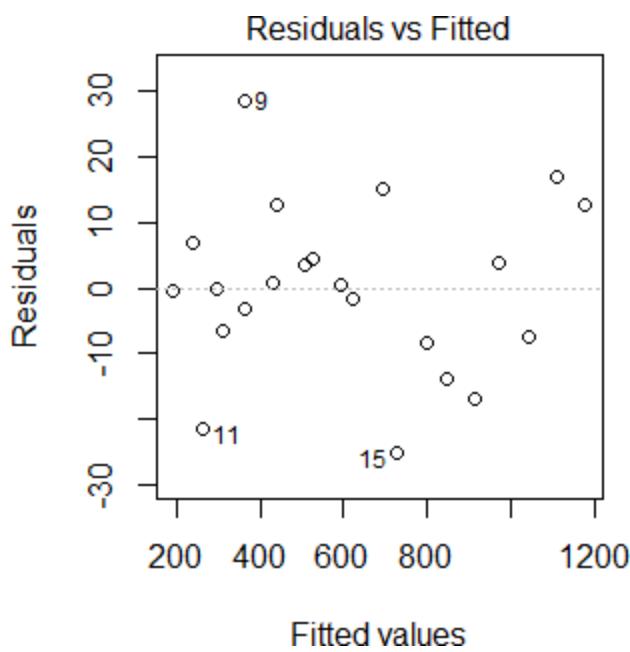
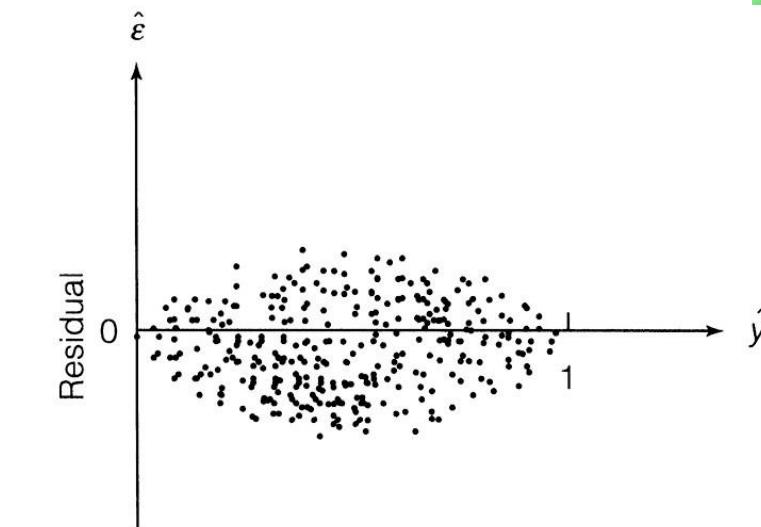
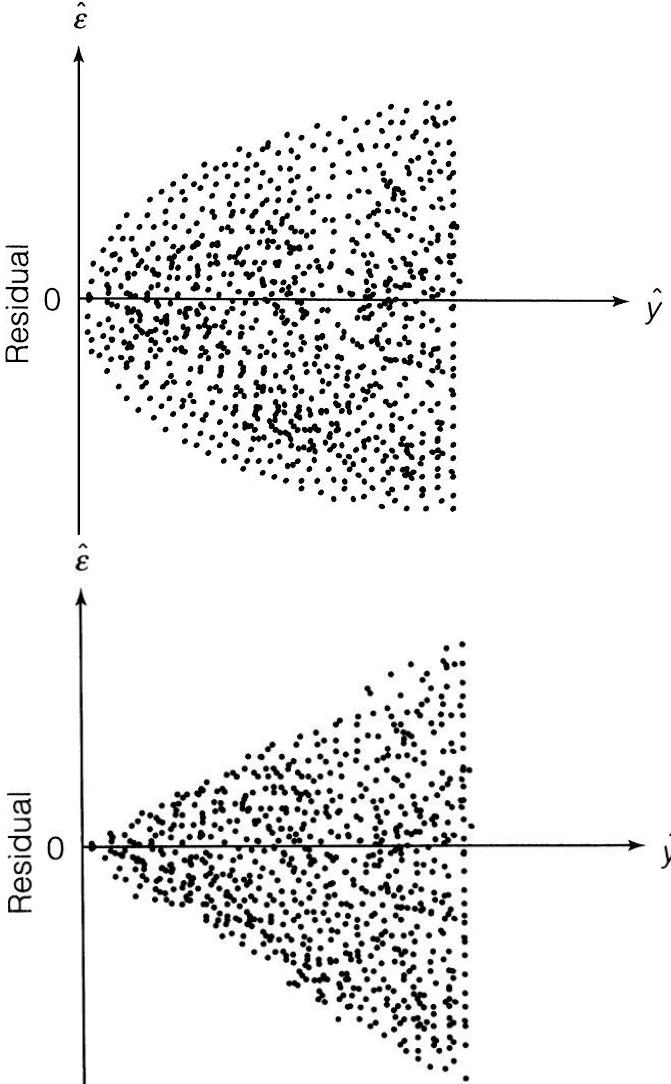
```
library(ggplot2)
par(mfrow =c(1,1))
ggplot(data=oly, aes(x=FAT, y=CHOLESTEROL)) +
  geom_point(pch=17, color="blue", size=2) +
  geom_smooth( method = "lm", formula = y ~ poly(x, 2), color="red",
  linetype=2) +
  labs(title="2th degree polynomial with 95% confidence bands",
  x="FAT", y="CHOLESTEROL")
```

Section 8.4

Detecting Unequal Variances

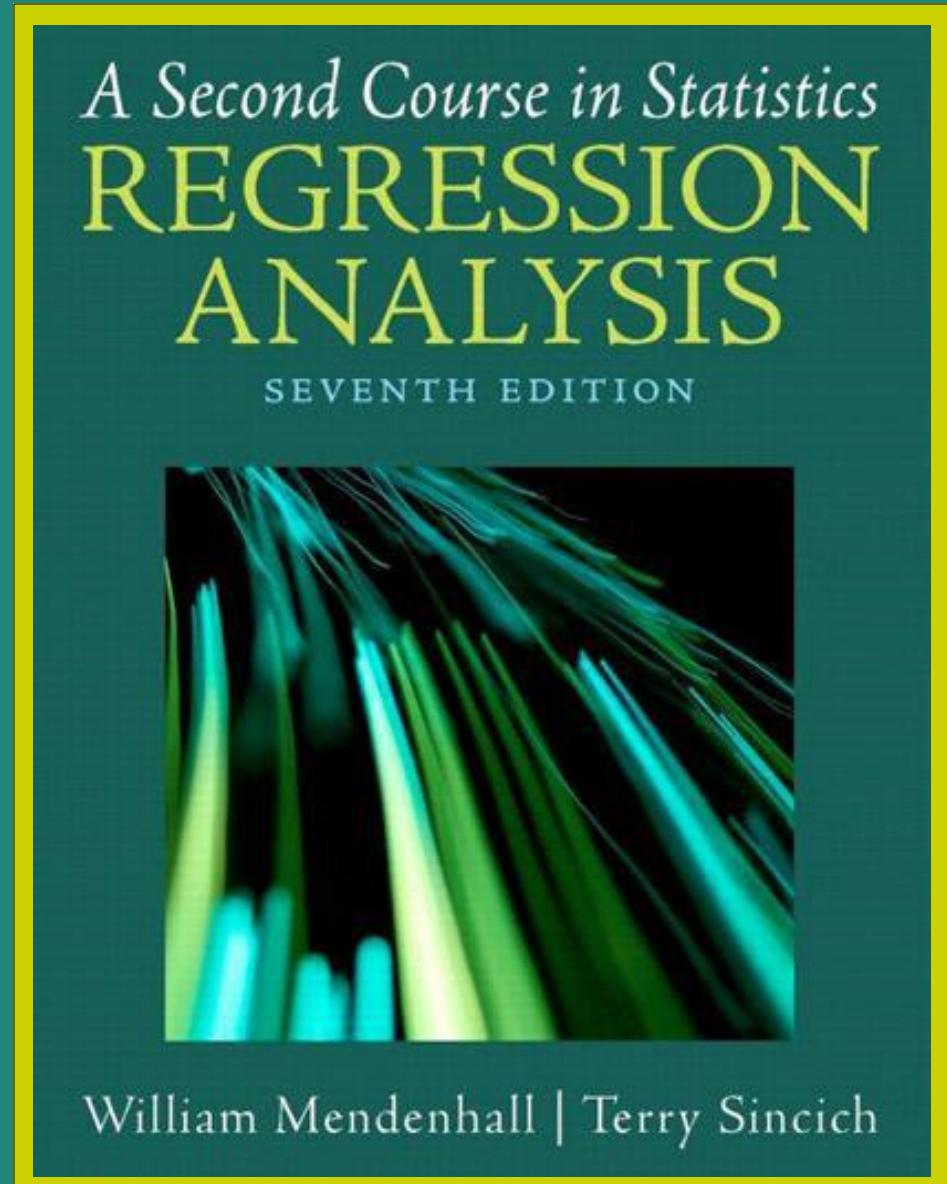


plot of residuals vs fitted values



Section 8.5

Checking the Normality Assumption



Assumption of normally distributed residuals



- This is the least restrictive of the assumptions.
- Regression is robust to departures from normality
- Inferences derived from the analysis remain valid even if the assumption is not exactly satisfied
- Moderate departures have little impact on CIs for the model parameters



Formal test

```
shapiro.test(model$residuals)
```

Limitations:

- Formal tests only useful for relatively small samples.
- Tests have low ***power*** i.e. the probability of detecting a non-normal error distribution when it exists is low



Power Transformations

How can we address the problem of violated model assumptions?

One approach is to transform the response variable.



Example

The following table gives the counts of numbers of poppies grown under six different treatment regimes. We will analyse the data and check the assumptions.

	1	2	3	4	mean	sd
A	538	422	377	315	413	94
B	438	442	319	380	395	58
C	77	61	157	52	87	48
D	115	57	100	45	79	34
E	17	31	87	16	38	34
F	18	26	77	20	35	28

Example



```
## Create data frame

poppies <- expand.grid(Block = 1:4,
                        Treatment = LETTERS[1:6])
poppies$Block <- factor(poppies$Block)
poppies$count <- c(538, 422, 377, 315,
                  438, 442, 319, 380,
                  77, 61, 157, 52,
                  115, 57, 100, 45,
                  17, 31, 87, 16,
                  18, 26, 77, 20)

## Fit a MLR model
mod1 <- lm(count ~ Block + Treatment, data = poppies)
summary(mod1)
```

Example



Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	439.04	31.54	13.919	5.55e-10	***
Block2	-27.33	29.74	-0.919	0.3726	
Block3	-14.33	29.74	-0.482	0.6368	
Block4	-62.50	29.74	-2.102	0.0529	.
TreatmentB	-18.25	36.42	-0.501	0.6236	
TreatmentC	-326.25	36.42	-8.957	2.08e-07	***
TreatmentD	-333.75	36.42	-9.163	1.56e-07	***
TreatmentE	-375.25	36.42	-10.303	3.37e-08	***
TreatmentF	-377.75	36.42	-10.371	3.09e-08	***

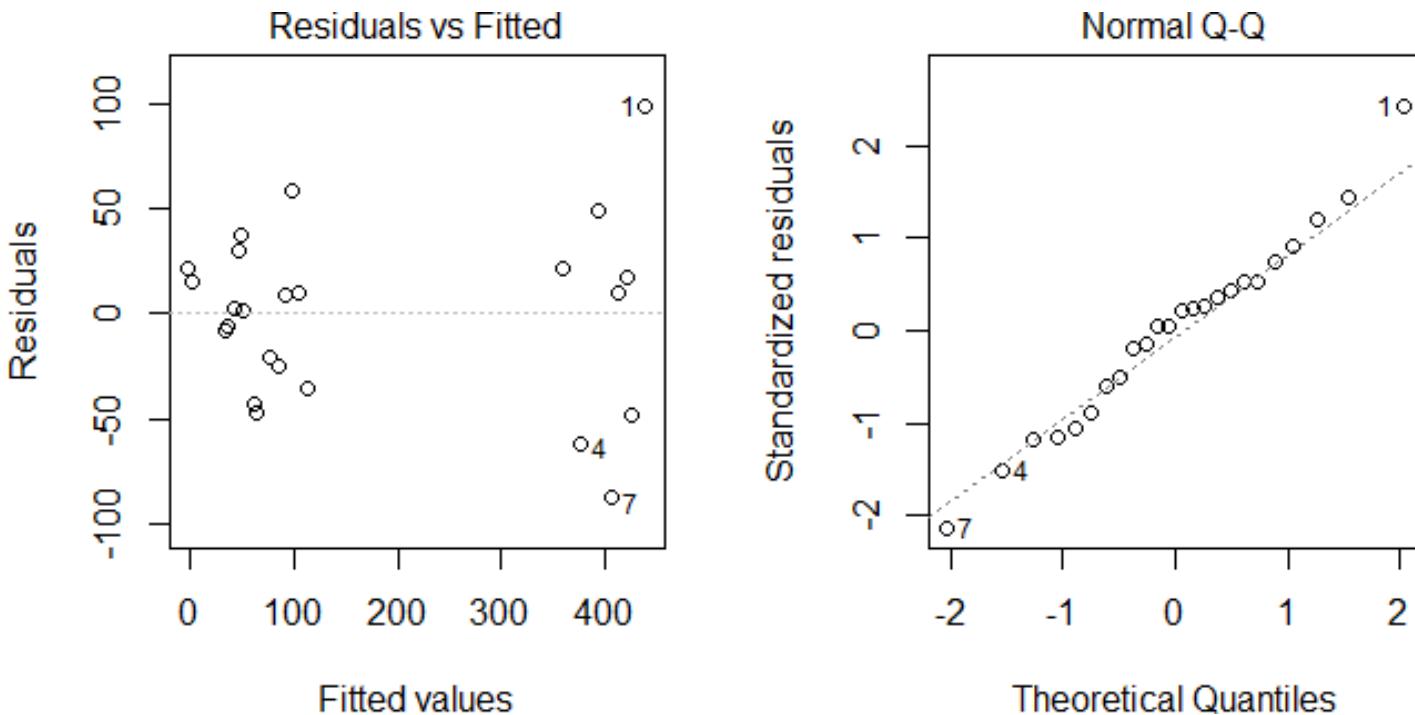
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1					

Residual standard error: 51.51 on 15 degrees of freedom

Multiple R-squared: 0.9426, Adjusted R-squared: 0.912

F-statistic: 30.81 on 8 and 15 DF, p-value: 5.927e-08

Example



```
par(mfrow =c(1,2))
plot(mod1,which=1:2,add.smooth = F)
```



Transformations

- Transform the data to a different scale and carry out the analysis in the new scale.
- Transformations often can be used to solve problems of non-homogeneity of variance and non-normal error distribution.
- Power transformations can make a skewed distribution more symmetric and stabilize the spread of the data.

Power Transformations



The most commonly used power transformations ($Y' = Y^\lambda$) in *order of increasing strength* are:

Transformation	Y'	λ	Back Transform
No transform	Y	1	
Square root	\sqrt{Y}	0.5	Y^2
Log Natural log	$\log_e Y$	0 (by definition)	e^Y
Reciprocal	$1/Y$	-1	$1/Y$

Choosing a transformation



The most appropriate transformation is that for which the data

- Shows no sign of a variance-mean relationship
- Shows least difference between the group variances as expressed by

$$F_{max} = \frac{\text{largest group variance}}{\text{smallest group variance}}$$

Comparing transforms



Treat	Y	var	$Y^{1/2}$	var	$\log_e(Y)$	var
A	413.00	8869	20.23	5.24	6.00	0.05
B	394.75	3353	19.83	2.21	5.97	0.02
C	86.75	2300	9.08	5.70	4.37	0.24
D	79.25	1126	8.75	3.69	4.30	0.20
E	37.75	1125	5.75	6.18	3.38	0.62
F	35.25	786	5.65	4.48	3.37	0.44
F_{max}		11.31		2.81		31.00

Q What does this table suggest?

Square root transform



```
mod2<-lm(sqrt(count) ~ Block + Treatment, data = poppies)
```

```
anova(mod2)
```

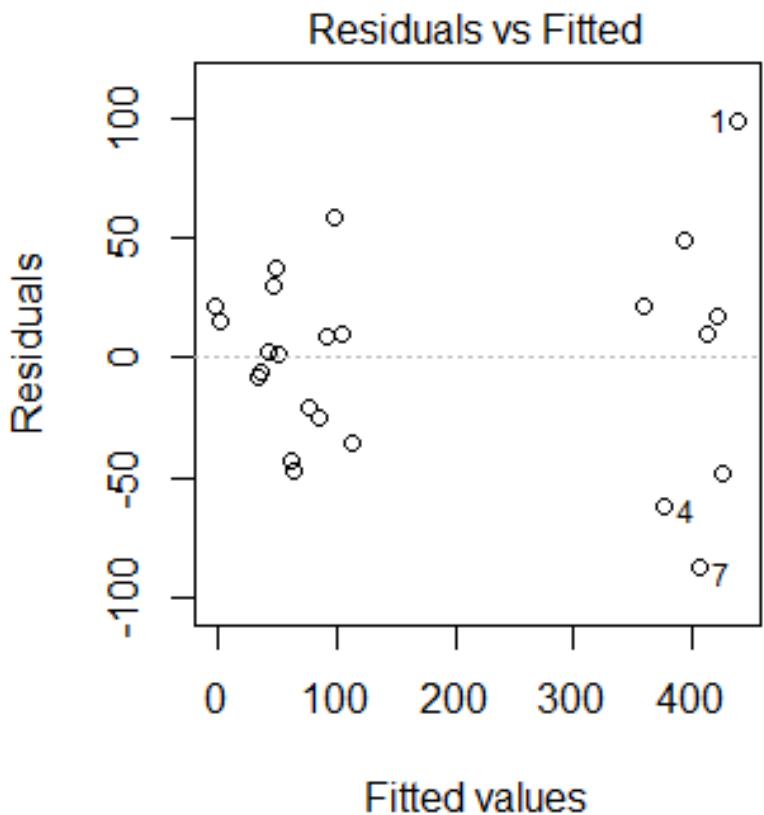
```
#####
```

Analysis of Variance Table

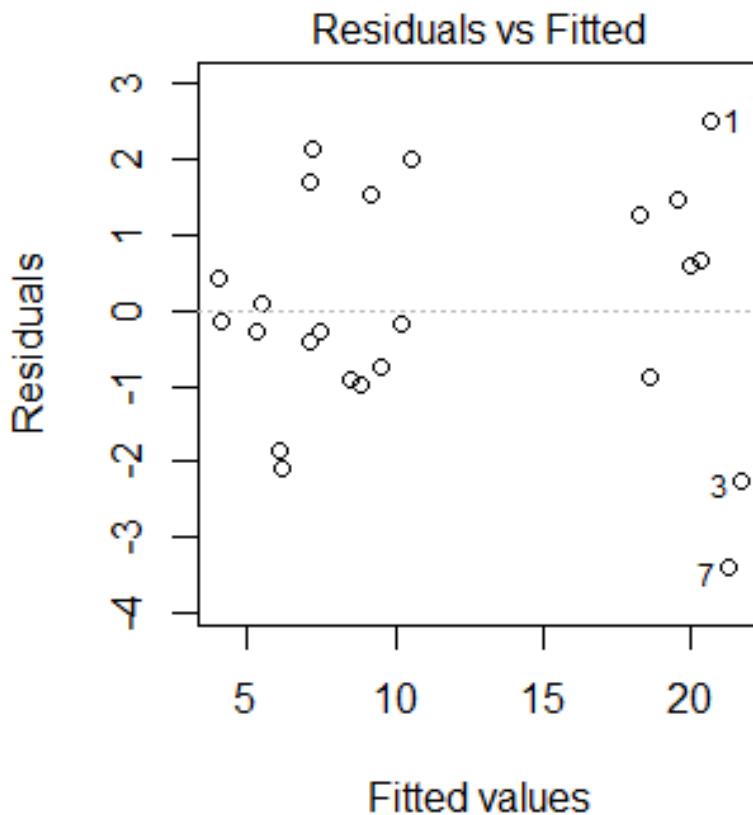
Response: sqrt(count)

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
Block	3	29.62	9.872	2.8014	0.07578	.
Treatment	5	904.62	180.925	51.3405	6.628e-09	***
Residuals	15	52.86	3.524			

Compare diagnostics



count ~ Block + Treatment



$\text{sqrt(count)} \sim \text{Block} + \text{Treatment}$

Square root transform: Block 1 means



`sqrt(count) ~Treatment + Block`

```
mod2a<-lm(sqrt(count) ~Treatment+Block-1, data=poppies)  
confint(mod2a)
```

	Estimate	Std. Error	2.5 %	97.5 %
TreatmentA	20.677	1.15	18.23	23.127
TreatmentB	20.278	1.15	17.83	22.728
TreatmentC	9.533	1.15	7.08	11.983
TreatmentD	9.197	1.15	6.75	11.647
TreatmentE	6.206	1.15	3.76	8.656
TreatmentF	6.098	1.15	3.65	8.549

Back transformations



- Tests, inference and CIs are made in the transformed scale.
- To express the results in the original scale of measurement make a second transformation
 - ➔ transforming the results back to the original scale.
- This process is known as back transformation

Back transformations



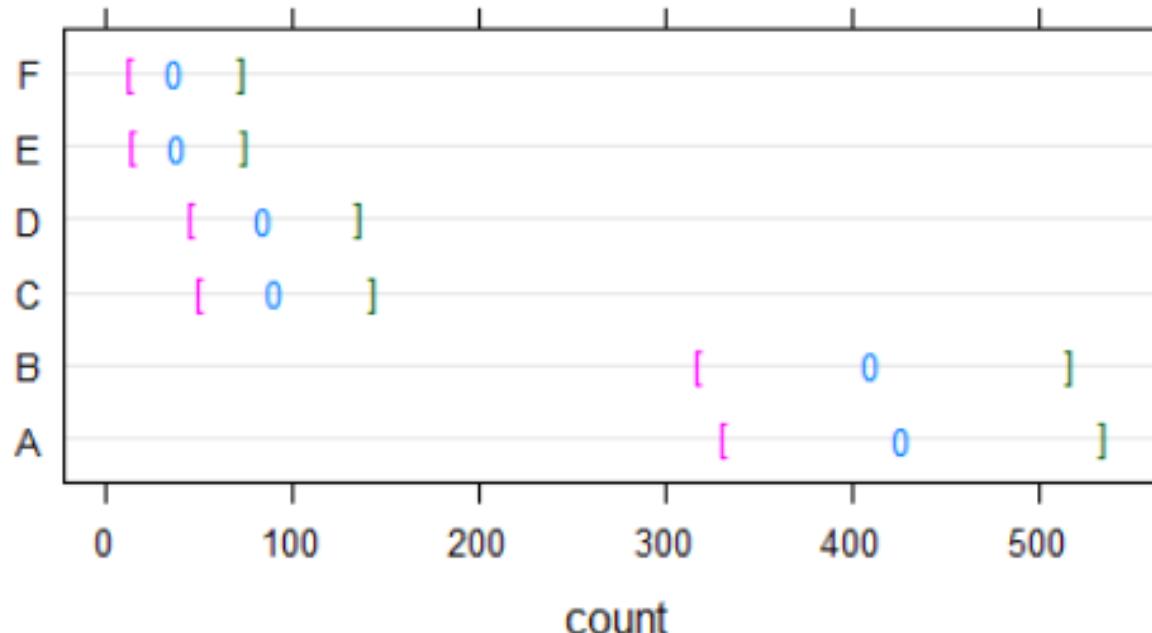
```
## back transforming  
pred.df <- data.frame(Block=1,Treatment=LETTERS[1:6])  
pred.df$Block <- factor(pred.df$Block)  
preds <- predict(mod2,newdata=pred.df,interval="confidence")  
pred.df <- cbind(pred.df,preds)  
  
#square results (Backtransform of sqrt)  
pred.df$backT_fit <- pred.df$fit^2  
pred.df$backT_lwr <- pred.df$lwr^2  
pred.df$backT_upr <- pred.df$upr^2
```

Backtransformations



```
> pred.df
```

	Block	Treatment	fit	lwr	upr	backT_fit	backT_lwr	backT_upr
1	1	A	20.68	18.23	23.13	427.5	332.2	534.9
2	1	B	20.28	17.83	22.73	411.2	317.8	516.6
3	1	C	9.53	7.08	11.98	90.9	50.2	143.6
4	1	D	9.20	6.75	11.65	84.6	45.5	135.6
5	1	E	6.21	3.76	8.66	38.5	14.1	74.9
6	1	F	6.10	3.65	8.55	37.2	13.3	73.1



The Box – Cox procedure

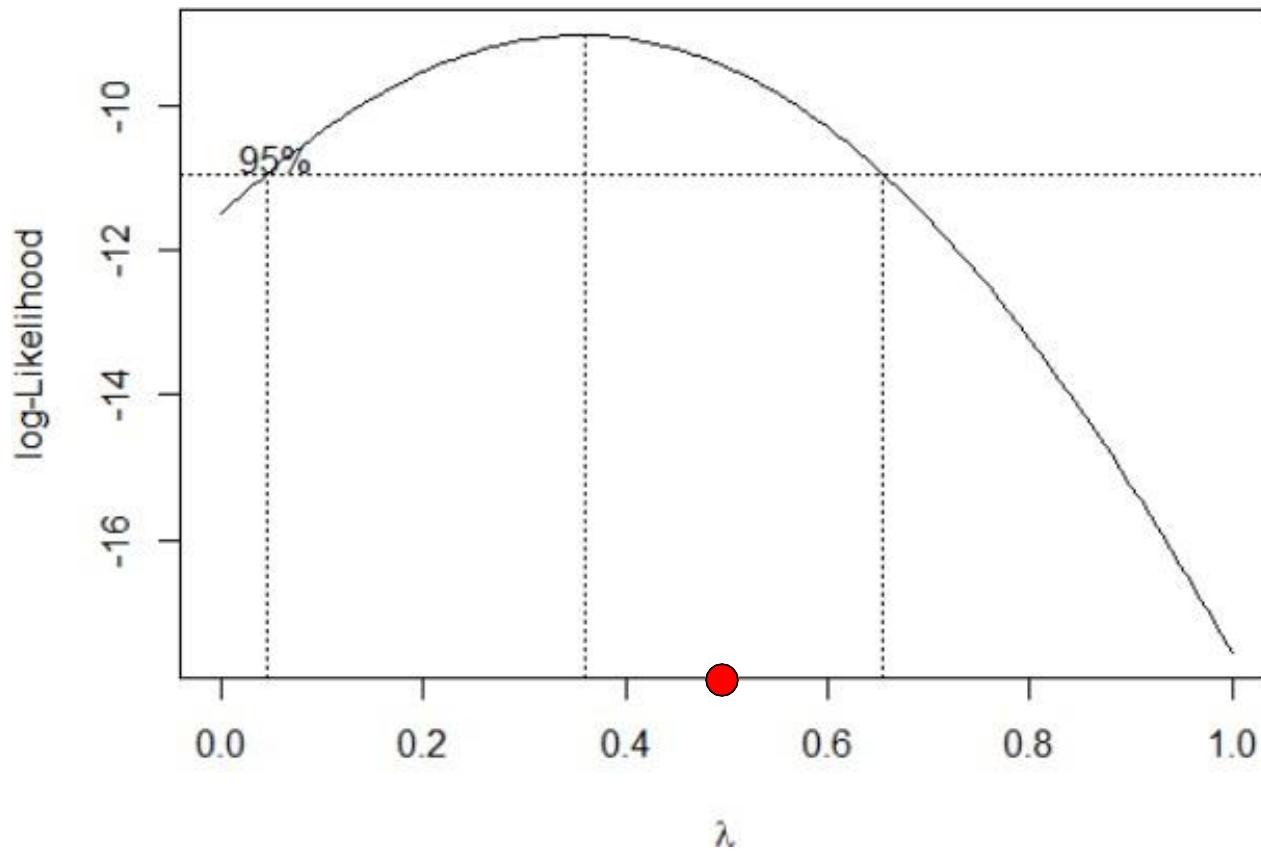


The Box-Cox procedure offers a method of finding a suitable value of λ for a power transformation of the type Y^λ .

Example: Estimate the value of λ needed to transform the poppy count data

```
### Box-Cox procedure  
  
install.packages("MASS")  
library(MASS)  
  
par(mfrow =c(1,1))  
boxcox(count~Block+Treatment, data = poppies,  
       lambda=seq(from=0,to=1, by=0.01))
```

The Box – Cox procedure



$\lambda = 0.5$ lies inside the 95% CI



Lecture 1 recap:

- ❖ Review assumptions of linear model
- ❖ Detect lack of fit using residual plots
- ❖ Power transformations – box-cox procedure

Lecture 2:

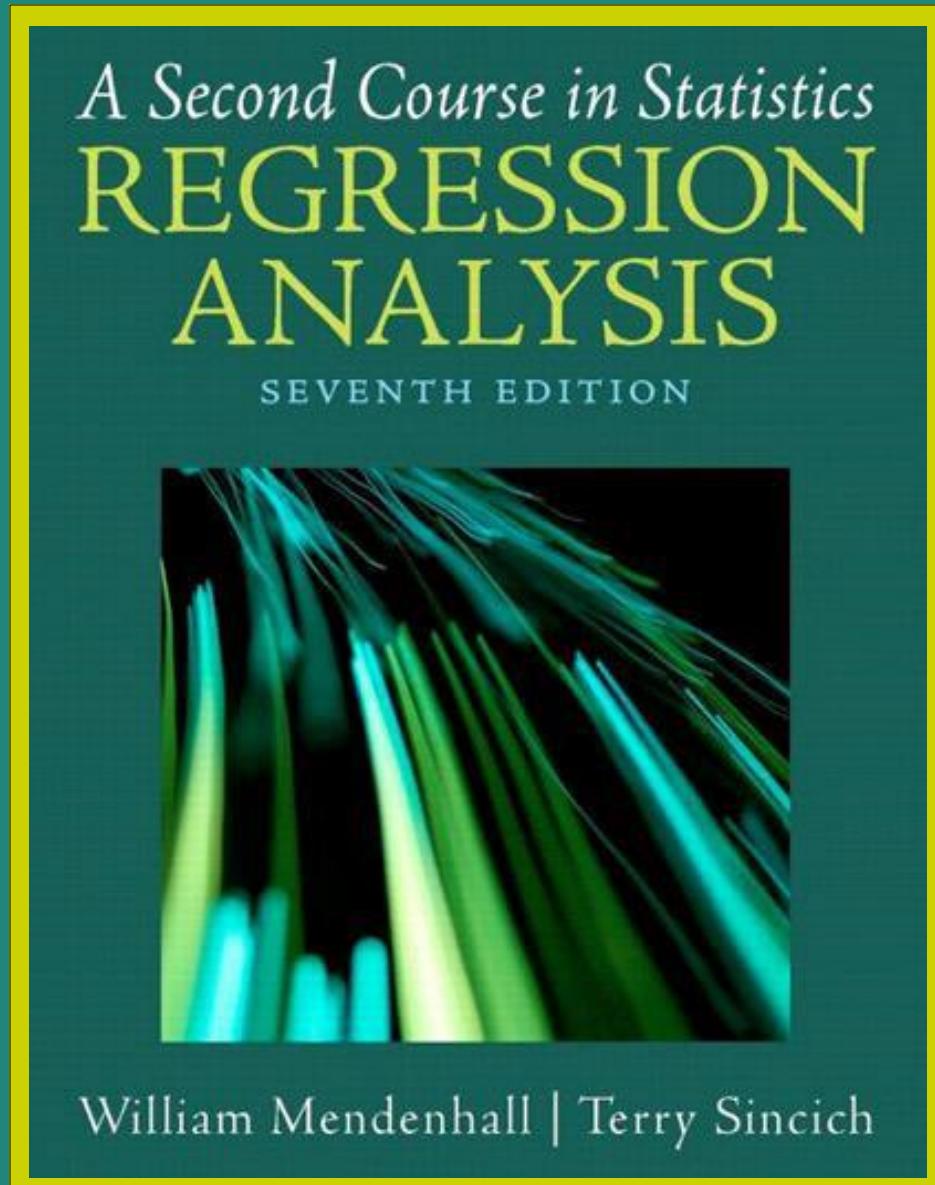
- ❖ Detect outliers and influential points

Chapter 8

Residual Analysis

(Lecture 2)

Dr Brenda Vo





Chapter 8 outline

Lecture 1:

- ❖ Review assumptions of linear model
- ❖ Detect lack of fit
- ❖ Power transformations

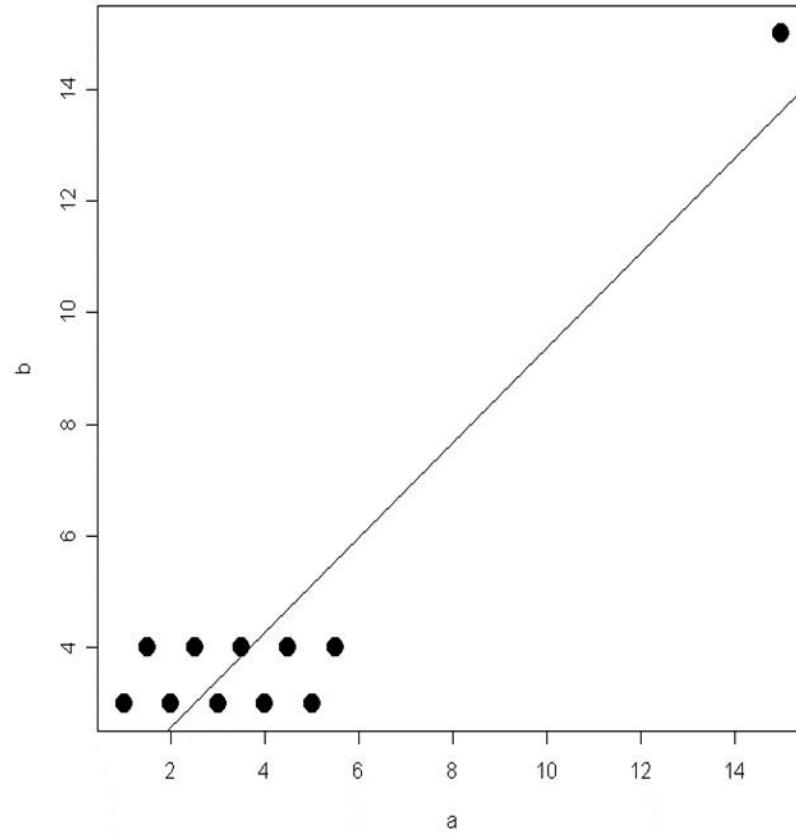
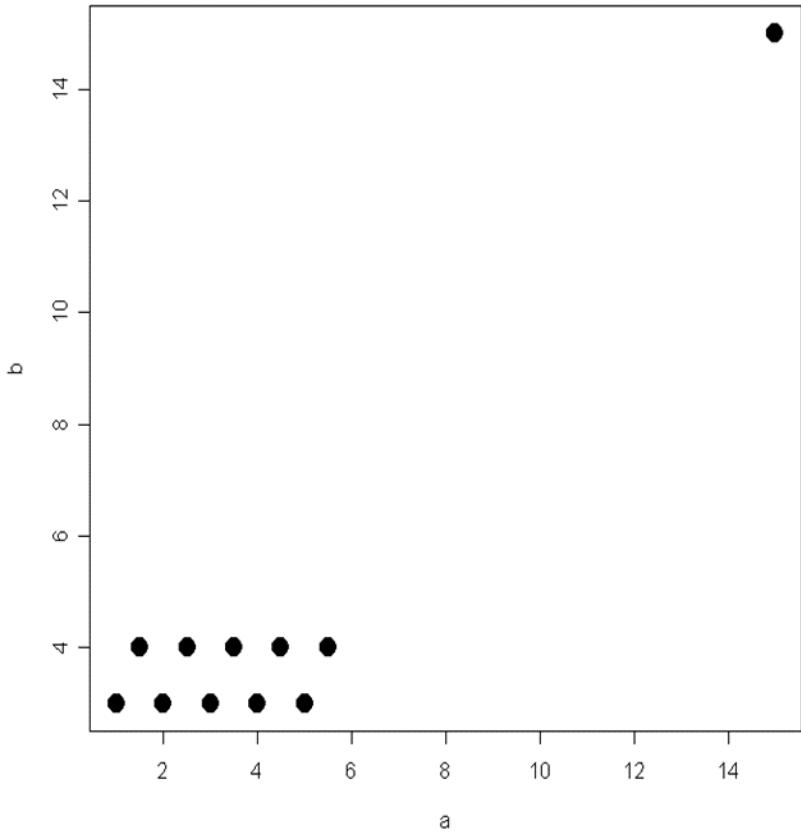
Lecture 2:

- ❖ Detect outliers and influential points (section 8.6)



Q: How would you describe the relationship between a and b ?

Q: What would the line of best fit look like?





Standardised Residuals

The standardised residual for the i^{th} observation

$$z_i = \frac{\hat{\epsilon}_i}{s} = \frac{y_i - \hat{y}_i}{s}$$

Note that this is
simply the z-score
for the residual.
 $Z \sim N(0,1)$

An observation whose absolute value of the standardised residual is

- greater than 2 is a potential outlier.
- greater than 3 is an outlier

Influential points, leverage and Cook's distance



Influential points

- have a large influence on the regression analysis
- their inclusion or exclusion changes the model, the values of the regression parameters, the predictions etc.

Identify influential points using

- Leverage
- Cook's distance

Life Cycle Savings



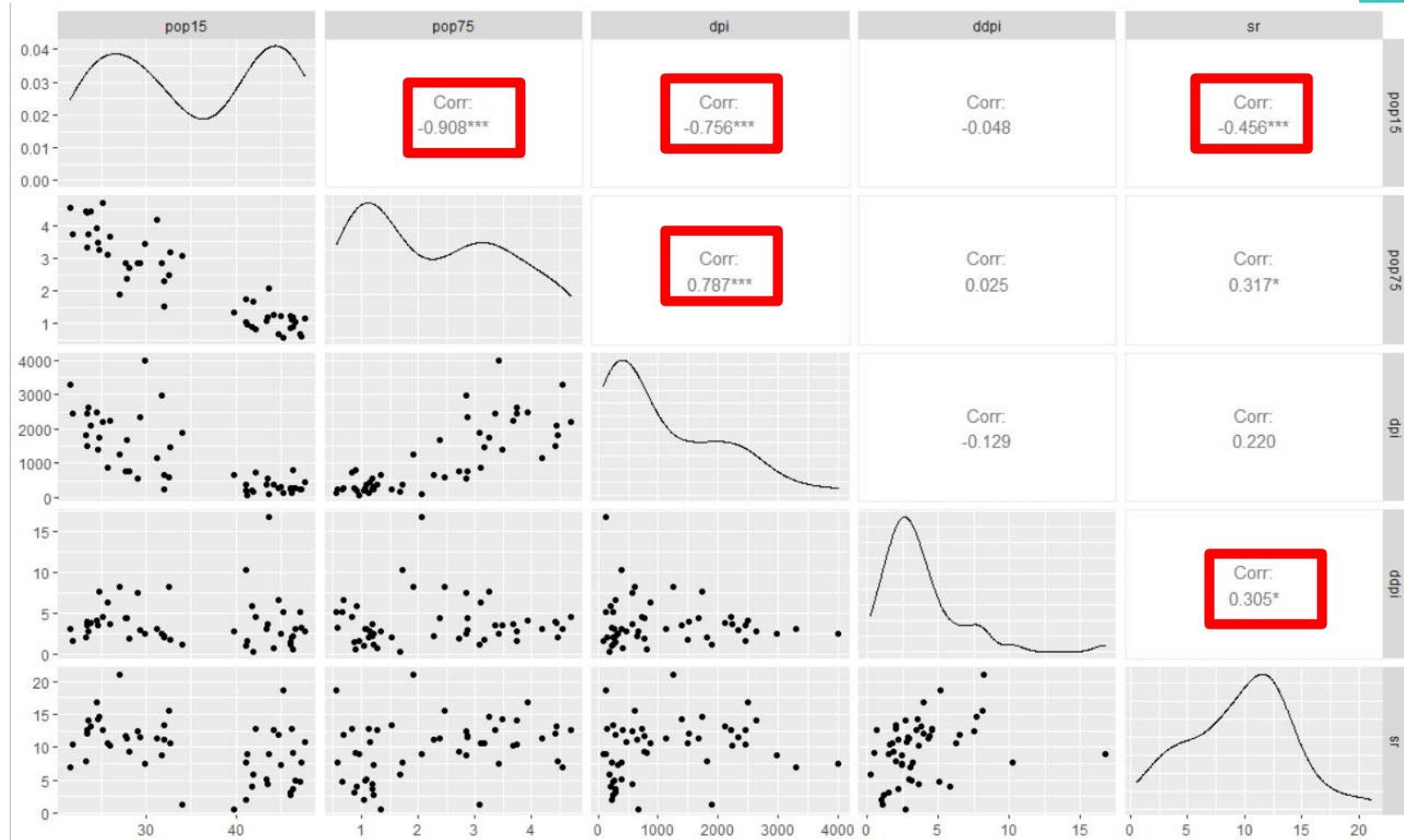
Data on the savings ratio 1960–1970:
50 observations (countries) on 5 variables.

sr	numeric	aggregate personal savings
pop15	numeric	% of population under 15
pop75	numeric	% of population over 75
dpi	numeric	real per-capita disposable income
ddpi	numeric	% growth rate of dpi

Data set available in R: `data("LifeCycleSavings")`

```
library(Ggally)
ggpairs(LifeCycleSavings[,c(2,3,4,5,1)])
```

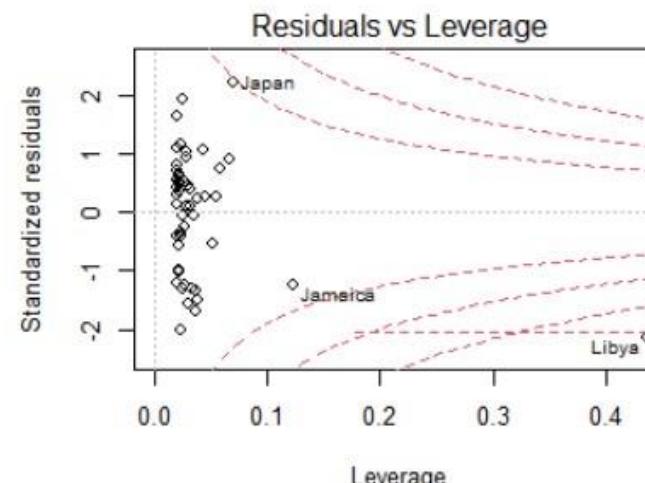
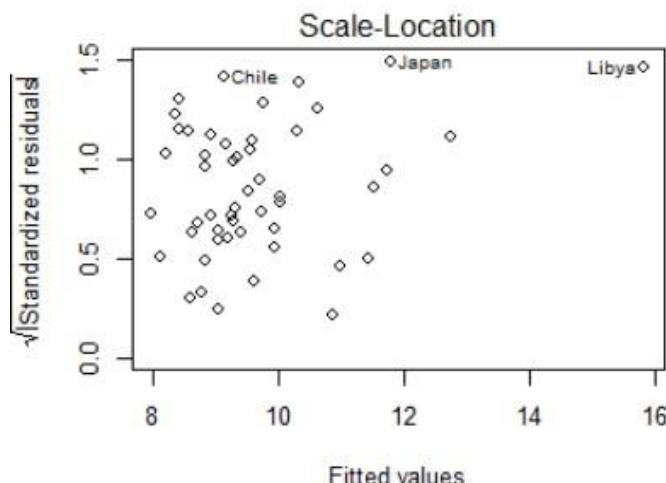
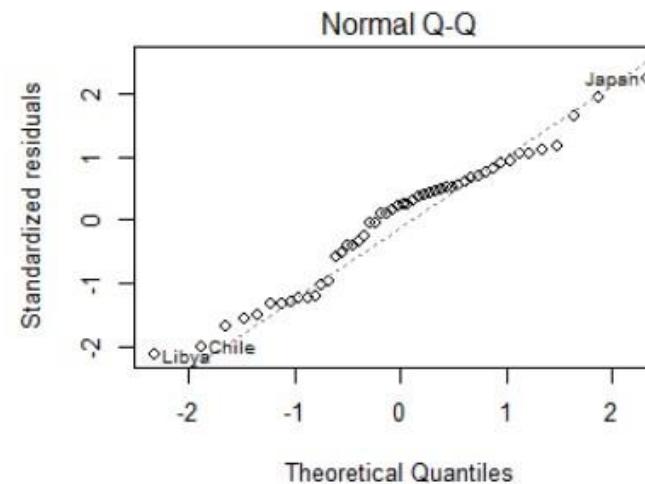
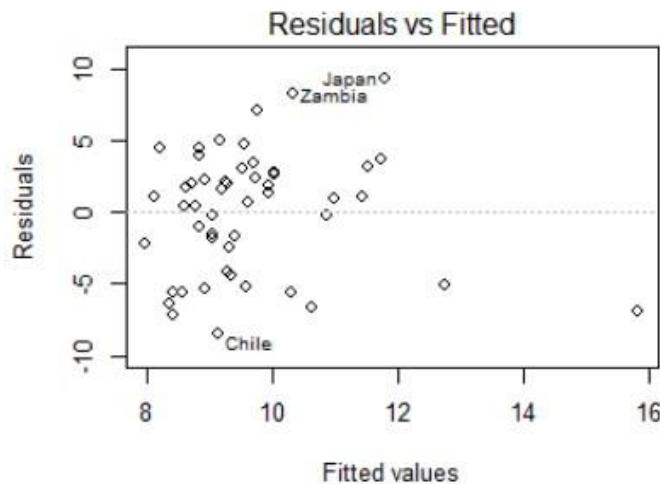
LifeCycleSavings pairs plot



```

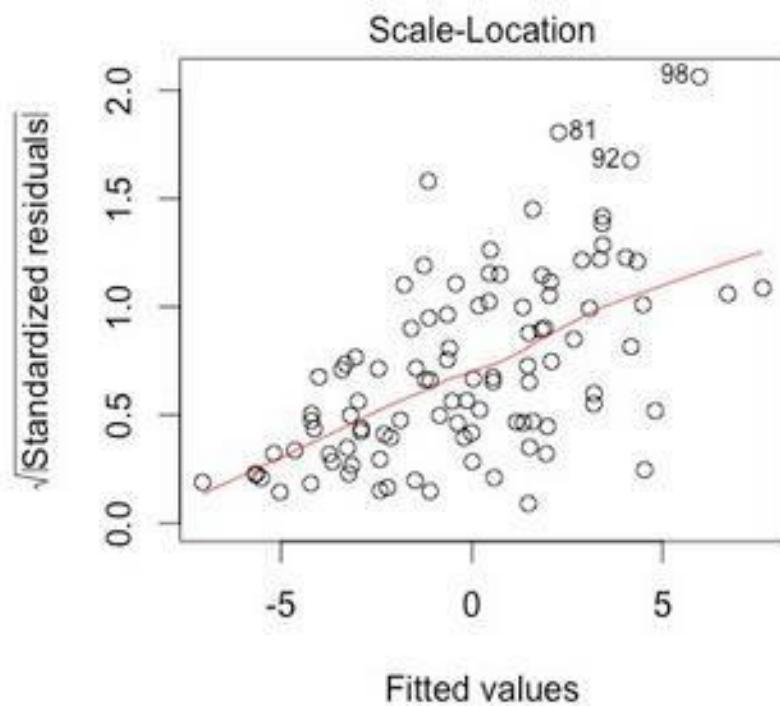
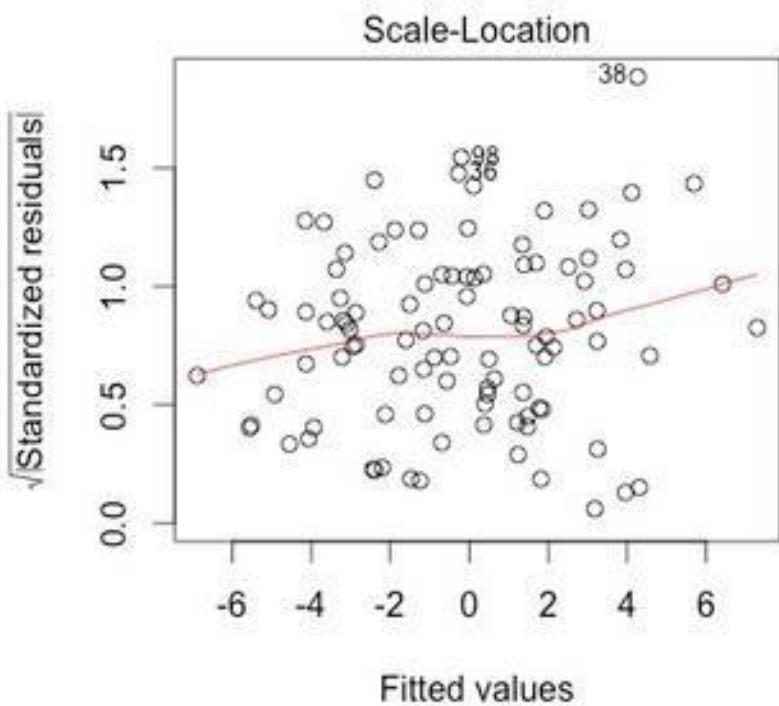
mod1 <- lm(sr ~ ddpi, data = LifeCycleSavings)
summary(mod1)
par(mfrow = c(2, 2))
plot(mod1, add.smooth=F, cook.levels=c(0.2,0.5,1.0))

```



Influential point

Scale-Location plot



- Check the assumption of equal variance (homoscedasticity)
- Check if residuals are spread equally along the x-axis.

Influential Points: Leverage



- The leverage for i^{th} observation is denoted as h_i
- The leverage h_i measures the influence of y_i on its predicted value \hat{y}_i

Rule of Thumb for Detecting Influence with Leverage

The observed value of y_i is influential if

$$h_i > \frac{2(k + 1)}{n}$$

where h_i is the leverage for the i th observation and $k =$ the number of β 's in the model (excluding β_0).

For Life Savings example

$$\frac{2(k + 1)}{n} = \frac{2(1 + 1)}{50} = 0.08$$

Libya has $h_i \approx 0.42 > 0.08 \rightarrow$ Libya is an influential point



Influential Points: Cook's Distance

Cook's distance, D_i , of an observation i is a measure of *the overall influence of that observation on the estimated regression parameters β*

$$D_i = \frac{(y_i - \hat{y})^2}{(k+1)MSE} \left[\frac{h_i}{(1 - h_i)^2} \right] \quad i = 1, \dots, n$$

D_i depends on

- The residual $(y_i - \hat{y})$
- The leverage h_i
- Large value of D_i indicates that the observed value i^{th} has strong influence on the estimated β coefficients.



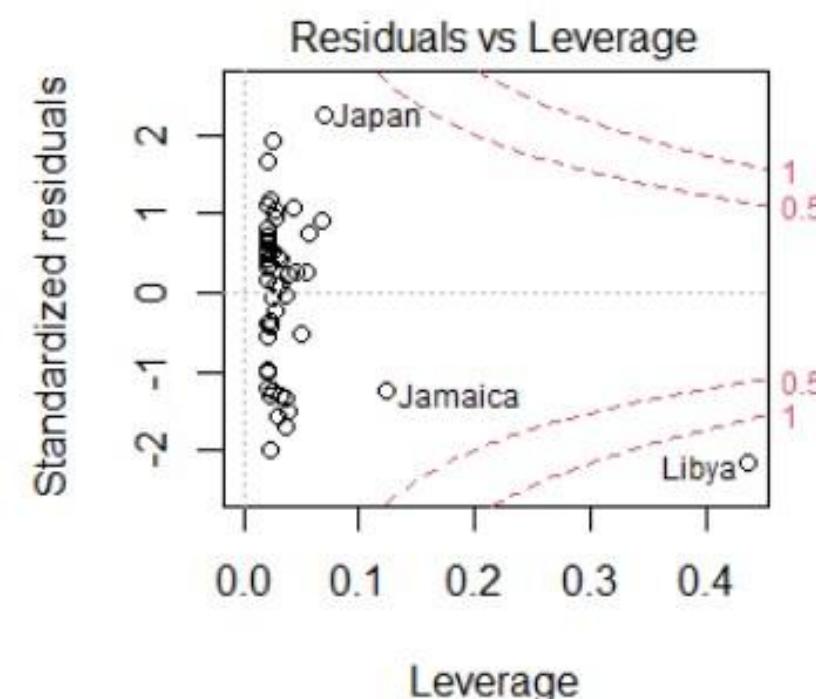
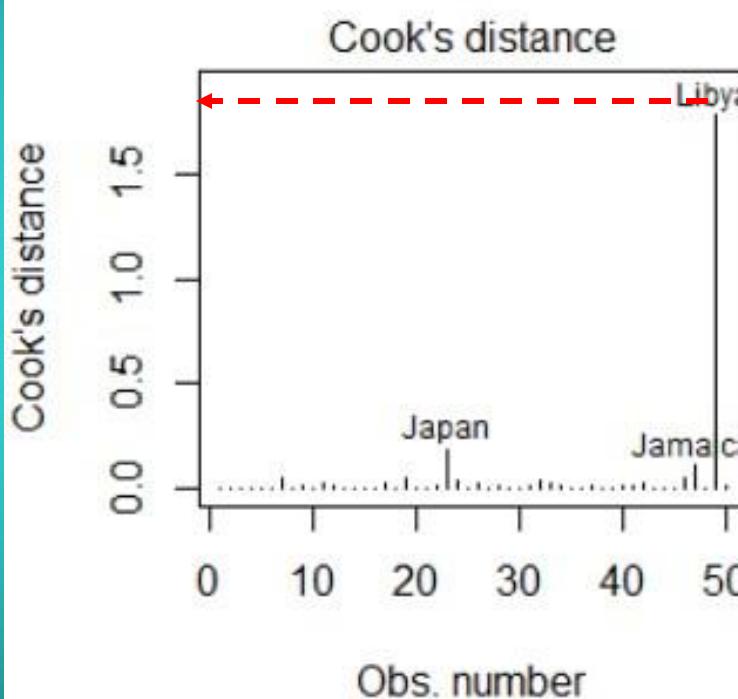
Influential Points: Cook's Distance

- $D_i \sim F_{k+1, n-(k+1)}$ where k is the number of estimated parameters
- If D_i lies at or *above the 50th percentile* of the *F distribution*, the ith observation is considered to have a major influence
- if D_i is *below the 20th percentile* then it has little influence

Cook's distance (D_i) and leverage (h_i)



```
par(mfrow = c(1, 2))
plot(mod1, which=4:5, add.smooth = F)
```



Libya has a Cook's distance that lies outside the red lines
→ highly influential

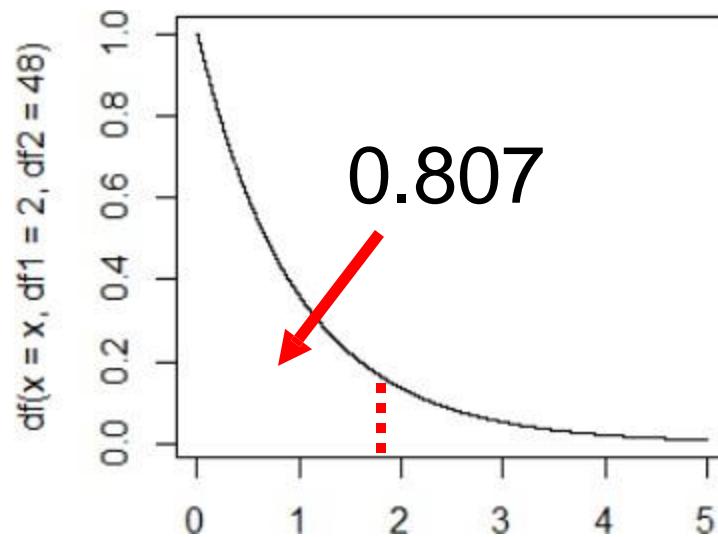
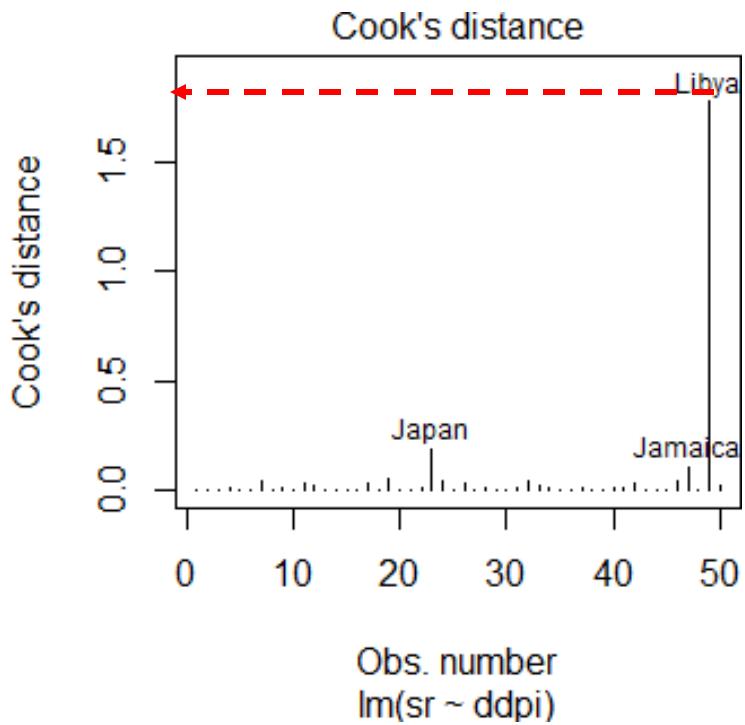
Cook's distance (D_i)



Calculate F percentile

```
> pf(1.7, 2, 48)  
[1] 0.807
```

i.e the Cook's distance of 1.7 lies above the 80th of the F distribution.

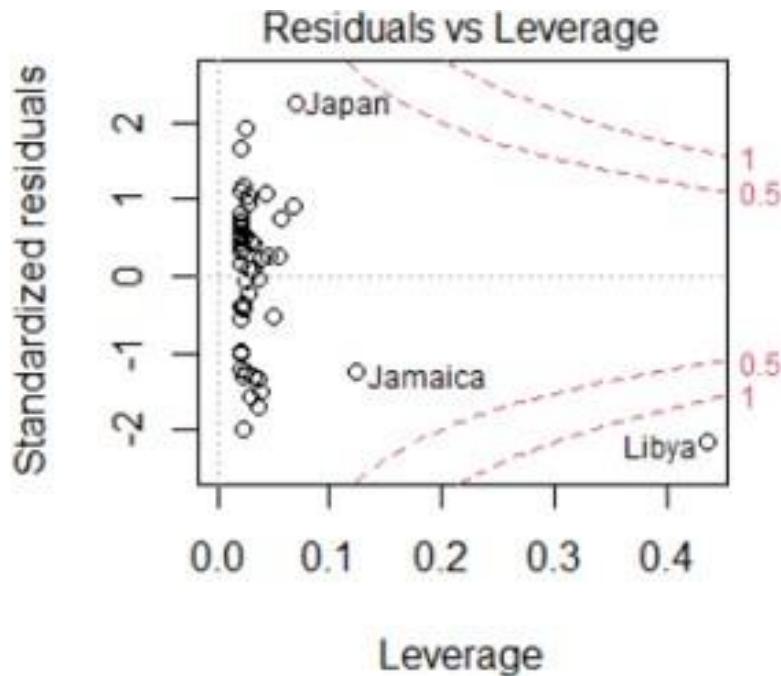


F distribution with 2 and 48 df

Residuals vs leverage plot



- Patterns are not relevant
- Look at observations at the upper right corner and at the lower right corner
- Look for cases outside of the red dashed lines
 - High Cook's distance scores





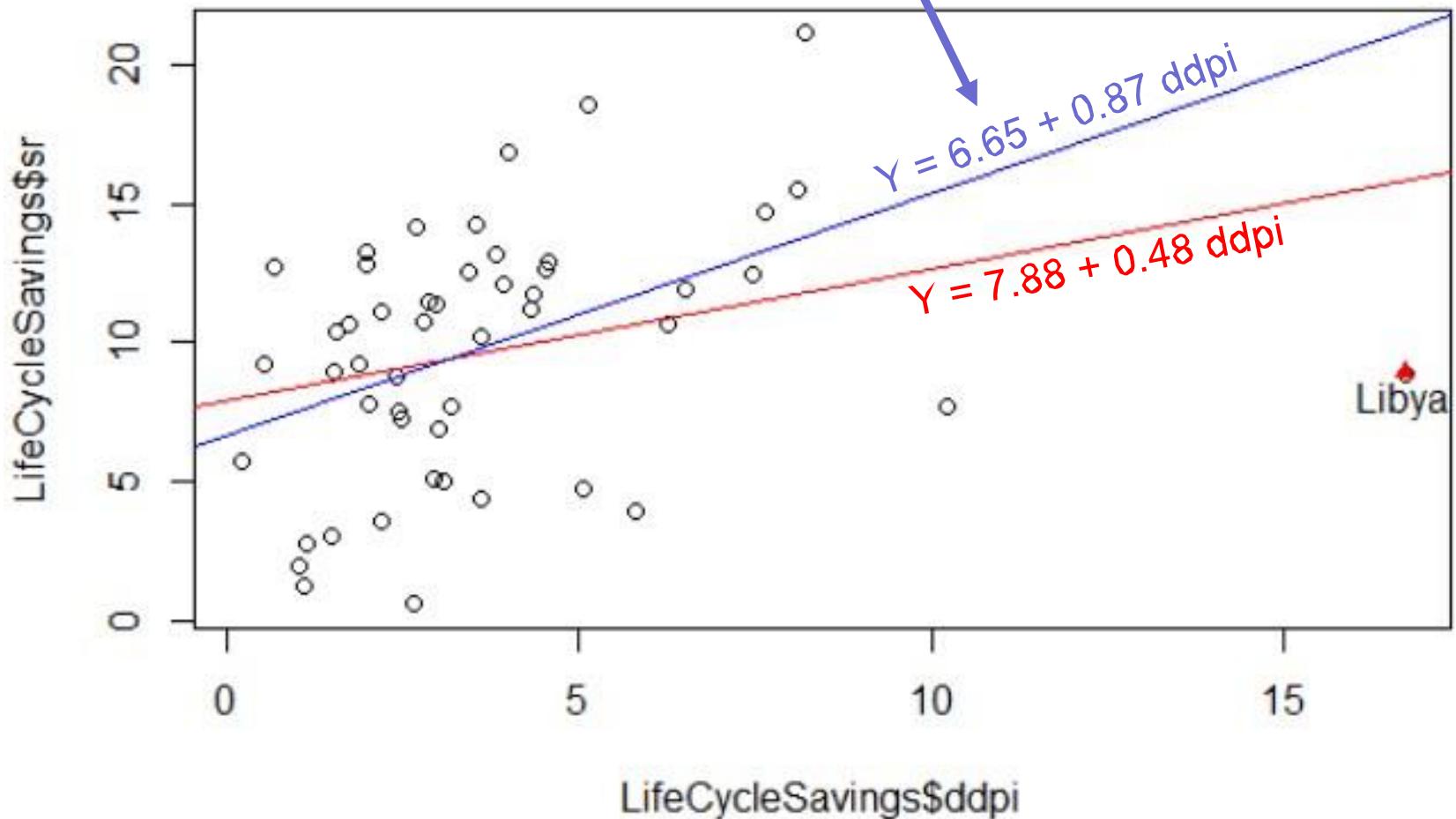
Cook's distance

```
install.packages("car")
library(car)
sort(cooks.distance(mod1))
```

Greece	Canada	India	Uruguay	Norway
4.19e-05	4.28e-05	1.36e-04	1.75e-04	2.33e-04
United Kingdom	China	Finland	United States	Costa Rica
8.31e-04	9.54e-04	9.87e-04	1.52e-03	1.53e-03
Guatemala	Tunisia	Korea	Paraguay	Chile
2.94e-02	3.39e-02	3.87e-02	4.51e-02	4.73e-02
Zambia	Iceland	Jamaica	Japan	Libya
4.74e-02	5.52e-02	1.10e-01	1.86e-01	1.77e+00

LifeCycleSavings

Without Libya



Review



- What are the four indicators of multicollinearity?
- State the assumptions of the linear model.
- List the 5 diagnostic (residuals) plots and explain what information they provide about the model.
- Why would you consider transforming the response variable?
- List the common power transformations discussed in lectures. What value of lambda corresponds to each?



Review

➤ What are the four indicators of multicollinearity?

1. Significant pairwise correlations for the I.V.s
2. Non-significant t-tests for many individual parameters
3. Opposite sign to expected for estimated parameters
4. Variance Inflation Factor, $VIF > 10$

Review



- State the assumptions of the linear model.
Residuals, $\varepsilon \sim N(0, \sigma^2)$, where σ^2 is constant, and residuals are independent.
- List the 5 diagnostic (residuals) plots and explain what information they provide about the model.
 1. Residuals vs fitted: check assumption of constant variance, and residuals are randomly centred around 0
 2. Normal QQ plot: check assumption of normality and also for potential outliers.
 3. Scale location plot: check constant variance assumption when n is small.
 4. Residuals vs leverage plot: check for influential points.
 5. Cook's distance plot: check for influential points.



Review

- Why would you consider transforming the response variable?
 - If the model assumptions have been violated.
- List the common power transformations discussed in lectures. What value of lambda corresponds to each?
 1. Square root transformation, $\lambda = 0.5$
 2. Log transformation, $\lambda = 0$, by definition
 3. Reciprocal, $\lambda = -1$