Chapter 6: Diagnostics

Diagnostics

- Checking error assumptions
 - Linearity
 - Normality
 - Constant variance
 - Independent predictors
- Finding unusual points (outlier, leverage)

Checking Error Assumptions

Assumption made so far: $\epsilon \sim N(0, \sigma^2 I)$

This includes

- $\mathbb{E}(\epsilon) = 0$
- $Var(\epsilon) = \sigma^2 I$
- ullet ϵ 's are independent, identically distributed, normal

Graphical and numerical diagnostic methods

Graphical methods

- Scatter Plot
- Residual vs. Fitted plot
- Normal QQ plot
- Cook's Distance plot
- Standardized Residual vs. Fitted plot

Residual vs. Fitted Plot

Plot $\hat{\epsilon}$ against \hat{y} . Can show

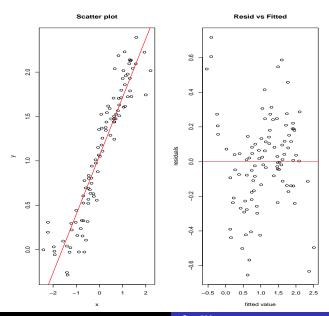
- Homoscedasticity (constant variance)
- Heteroscedasticity (non-constant variance)
- Non-linearity

Residual vs. Fitted Plot

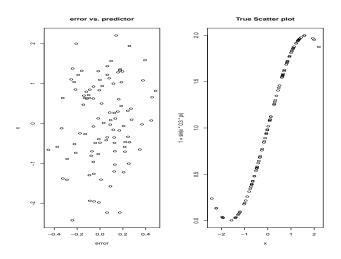
Limitations

- The Residual vs. Fitted Plot is very useful in general.
- It is sometimes NOT enough.
 - Big errors
 - Combination of assumption violations
 - No threshold

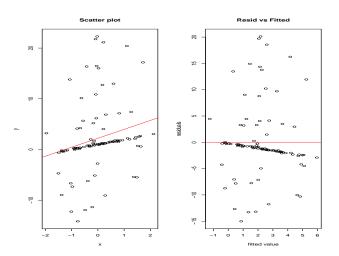
Residual vs. Fitted Plot:



Residual vs. Fitted Plot: Non-linearity

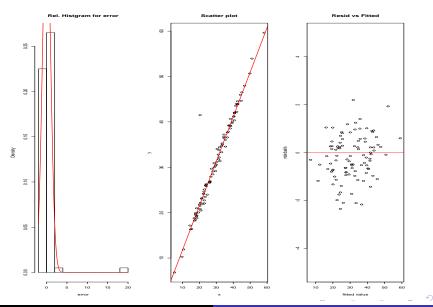


Residual vs. Fitted Plot:

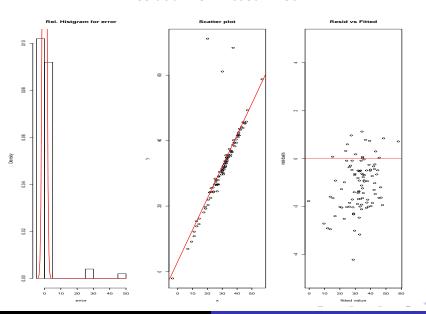


- What is the problem?

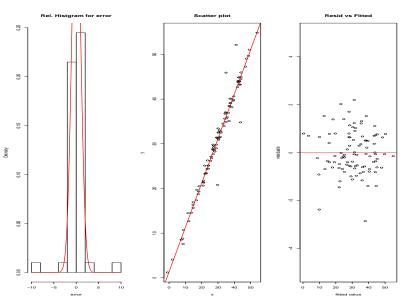
Residual vs. Fitted Plot: Unusual point, Outlier



Residual vs. Fitted Plot



Residual vs. Fitted Plot



Remaining Question

- How to determine if there are outliers
 - Studentized (Standardized) Residual
 - Cook's Distance
- How to fix the assumptions

What to Do

- Non-constant variance
 - Nothing
 - Weighted least squares (Ch 8.2)
 - Transformation of the response (Ch 9.1, 9.2)
- Nonlinearity: change the model (e.g., polynomial model (Ch 9.4))
- Unusual point: either remove it or do nothing

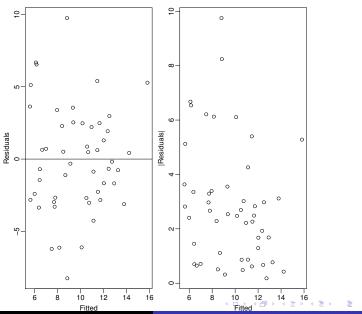
Checking Constant Variance: Savings Example

- 50 different countries, 1960 − 1970
- Response: aggregate personal saving divided by disposable income (sr)
- Predictors: per capital disposable income (dpi), percentage rate of change in per capita disposable income (ddpi), percentage of population under 15 (pop15), percentage of population over 75 (pop75)
- > data(savings)

Savings Example Ctd

```
> plot(result, which = 1)
> plot(result$fitted.values, abs(result$residuals),
xlab = "Fitted", ylab = "|residuals|")
```

Savings Example Ctd



Checking Normality

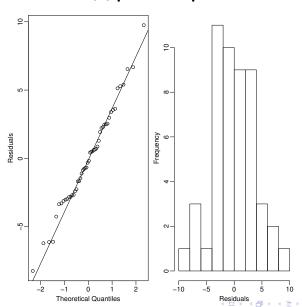
QQ-plot

- ① Sort the residuals $\hat{\epsilon}_{[1]} \leq \hat{\epsilon}_{[2]} \cdots \leq \hat{\epsilon}_{[n]}$
- **2** Compute $u_i = \Phi^{-1}\left(\frac{i}{n+1}\right)$
- **3** Plot $\hat{\epsilon}_{[i]}$ against u_i .

```
## QQ-plot
```

- > qqnorm(result\$residual, ylab="Residuals")
- > qqline(result\$residual)
- ## Histogram
- > hist(result\$residual, xlab="Residuals")

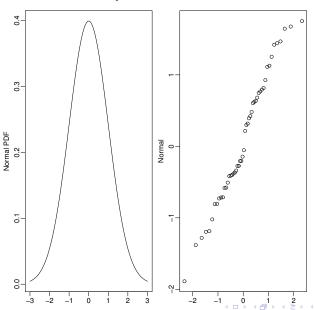
QQ-plot Example



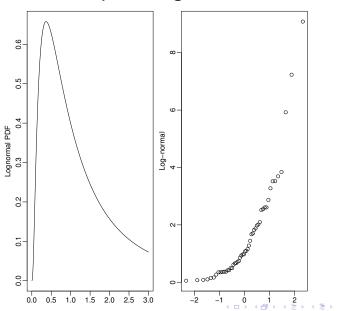
Non-Normality

- Skewed distribution (e.g., log-normal)
- Long-tailed distribution (e.g., Cauchy)
- Short-tailed distribution (e.g., uniform)

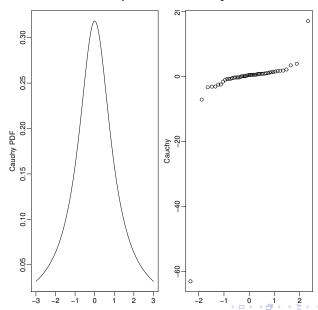
QQ-plot of Normal



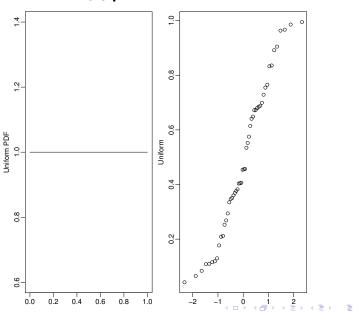
QQ-plot of Log-normal



QQ-plot of Cauchy



QQ-plot of Uniform



Shapiro-Wilk test for normality

 H_0 : samples are normally distributed $H_A: H_0$ is not true.

Shapiro-Wilk test for normality

Not very helpful (QQ plots are better).

- Small n little power
- Large n non-normality is less important

What to do about non-normal errors

- Transformation of the response (Ch 9)
- Robust methods (long-tailed distribution (difficult))
- Nothing

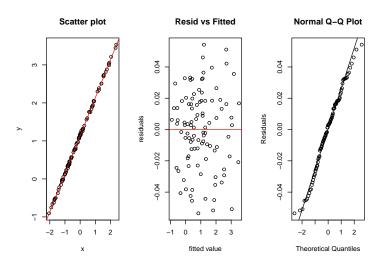
Correlated Errors

Temporally related data

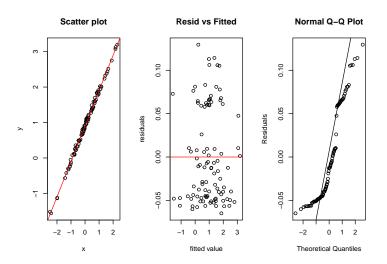
- ullet Plot $\hat{\epsilon}$ against time
- Plot $\hat{\epsilon}_i$ against $\hat{\epsilon}_{i-1}$
- Time series analysis may be more appropriate

No temporal relationship or other ordering in the variables \Rightarrow checking independence is very hard.

Correlated Errors (1)



Correlated Errors (2)

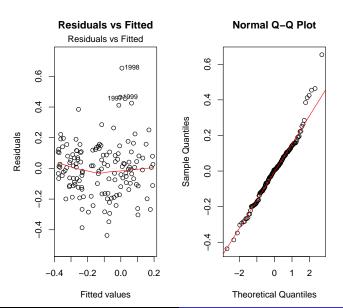


- 145 samples , 1856 2000
- Response: temperature (nhtemp)
- Predictors: wusa, jasper, westgreen, chesapeake, tornetrask, urals, mongolia, tasman,
- 'Year' is not considered as a predictor
- > data(globwarm)
- > head(globwarm)

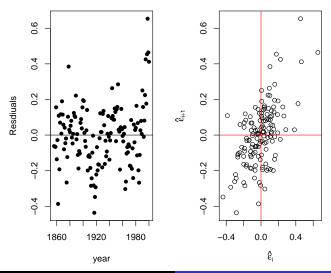
	${\tt nhtemp}$	wusa	jasper	westgreen	chesapeake	tornetrask	urals	mongolia	tasman	year
1000	NA	-0.66	-0.03	0.03	-0.66	0.33	-1.49	0.83	-0.12	1000
1001	NA	-0.63	-0.07	0.09	-0.67	0.21	-1.44	0.96	-0.17	1001
1002	NA	-0.60	-0.11	0.18	-0.67	0.13	-1.39	0.99	-0.22	1002
1003	NA	-0.55	-0.14	0.30	-0.68	0.08	-1.34	0.95	-0.26	1003
1004	NA	-0.51	-0.15	0.41	-0.68	0.06	-1.30	0.87	-0.31	1004
1005	NA	-0.47	-0.15	0.52	-0.68	0.07	-1.25	0.77	-0.37	1005

```
## fitting model
> result = lm( nhtemp ~ wusa+ jasper+ westgreen+ chesapeake
   + tornetrask+ urals+ mongolia+ tasman, data = globwarm)
## fitted model
> summarv(result)
Coefficients:
      Estimate Std. Error t value Pr(>|t|)
0.077384 0.042927 1.803 0.073647 .
wiisa
jasper -0.228795 0.078107 -2.929 0.003986 **
westgreen 0.009584 0.041840 0.229 0.819168
chesapeake -0.032112
                    0.034052 -0.943 0.347346
tornetrask 0.092668
                   0.045053 2.057 0.041611 *
          0.185369 0.091428 2.027 0.044567 *
urals
mongolia
          0.041973 0.045794 0.917 0.360996
tasman
           0.115453 0.030111 3.834 0.000192 ***
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
```

```
## Diagnotic Plots
> par(mfrow = c(1,2))
> plot(result, which = 1, main = "Residuals vs Fitted")
> qqnorm(residuals(result))
> qqline(residuals(result), col = "red")
```



```
## Scatter Plots: Residual vs Year and i th Residual vs i+1 th R
> n = length(residuals(result))
> plot(residuals(result) ~year, na.omit(globwarm), ylab ="Resdiu"> abline(h= 0)
> plot(tail(residuals(result), n-1) ~head(residuals(result), n-1)
> abline(h=0, v=0, col = "red")
```



Durbin-Watson test for Correlated Errors

 H_0 : the errors are uncorrelated vs. H_A : H_0 is not true.

```
## load library
> require(lmtest)
## Durbin-Watson test
> dwtest( nhtemp ~ wusa+ jasper+ westgreen+ chesapeake
   + tornetrask+ urals+ mongolia+ tasman, data = globwarm)
Durbin-Watson test
DW = 0.81661, p-value = 1.402e-15
alternative hypothesis: true autocorrelation is greater than 0
```

Suppose that there is quadratic relationship between a predictor and the response.

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon.$$

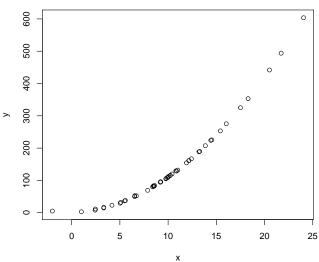
However we consider the simple linear model (missing predictor).

$$Y = \beta_0 + \beta_1 X + \epsilon.$$

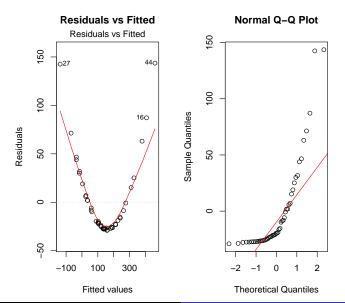
```
## Sample Size
n = 50
## Predictor
x = rnorm(n, 10, 5)
z = x^2
## Reponse Variable
y = 1 + x + z + rnorm(n, 0, 1)
## Fitting Model (Missing z variable)
result= lm(y ~ x)
summary(result)
```

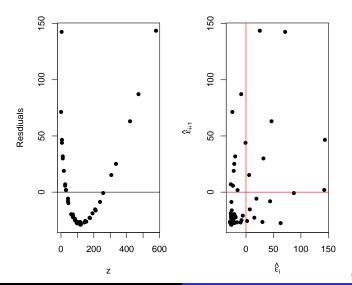
Residual standard error: 41.49 on 48 degrees of freedom Multiple R-squared: 0.8948, Adjusted R-squared: 0.8926 F-statistic: 408.4 on 1 and 48 DF, p-value: < 2.2e-16





```
> par(mfrow = c(1,2))
> plot(result, which = 1, main = "Residuals vs Fitted")
> qqnorm(residuals(result))
> qqline(residuals(result), col = "red")
```





Durbin-Watson test for Correlated Errors

 H_0 : the errors are uncorrelated vs. H_A : H_0 is not true. ## Durbin-Watson test > dwtest(y ~ x) Durbin-Watson test data: y ~ x DW = 1.2681, p-value = 0.003285 alternative hypothesis: true autocorrelation is greater than 0

Studentized Residuals

Since $Var(\hat{\epsilon}_i) = \sigma^2(1 - h_i)$ where $h_i = H_{ii}$, let

$$r_i = \frac{\hat{\epsilon}_i}{\hat{\sigma}\sqrt{1 - h_i}}$$

These are called (internally) studentized residuals

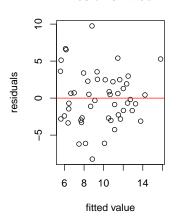
- It is better to use studentized residuals for diagnostic plots (QQ-plot and testing constant variance)
- In practice, usually little difference

Savings Example

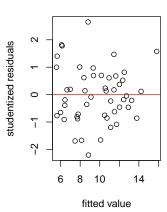
```
## Compute studentized residuals
> result.s <- summary(result)</pre>
> sigma.s <- result.s$sig</pre>
> hat.s <- lm.influence(result)$hat</pre>
> stud.res <- result$residuals/(sigma.s * sqrt(1-hat.s))
> par(mfrow = c(1,2))
> plot(result$fitted.values, result$residuals, xlab = "fitted va
ylab = "residuals", main = "Resid vs Fitted")
> abline(h = 0, col = "red")
> plot(result$fitted.values, stud.res, xlab = "fitted value",
ylab = "studentized residuals", main = "Studentized Resid vs Fit
>abline(h = 0, col = "red")
```

Studentized Residual vs. Fitted Plot

Resid vs Fitted



Studentized Resid vs Fitted



Studentized Residuals

If absolute values of studentized residuals are greater than 2.5, they are more likely to be unusal points.

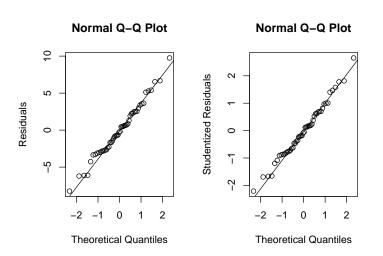
```
> which.max( abs(stud.res) )
Zambia
46
> stud.res[46]
Zambia
2.650915
```

Savings Example

```
> qqnorm(result$residual, ylab="Residuals")
```

- > qqline(result\$residual)
- > qqnorm(stud.res, ylab="Studentized Residuals")
- > qqline(stud.res)

Studentized Residual QQ Plot



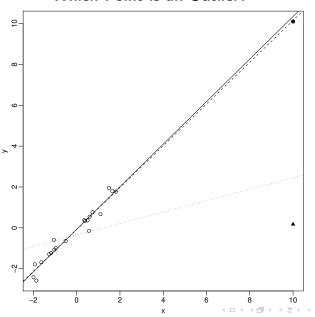
Finding Unusual Points

- 1 Outliers do not fit the model well
- 2 Leverage extreme in the predictor space, but not necessarily influence the fit

A point can be none, one, or both of these.

Influential points – affect the fit of the model substantially

Which Point is an Outlier?



Leverage

Recall the hat matrix $H = X(X^TX)^{-1}X^T$.

Leverage of point i: $h_i = H_{ii}$.

- h_i depends only on X
- $var(\hat{\epsilon}_i) = \sigma^2(1 h_i)$
- $\sum_{i} h_{i} = p + 1$
- Average of h_i is $\frac{p+1}{n}$

Rule of thumb: Leverages greater than $2 \times \frac{p+1}{n}$ are considered high.

Savings Example

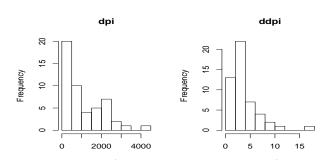
Libya

49

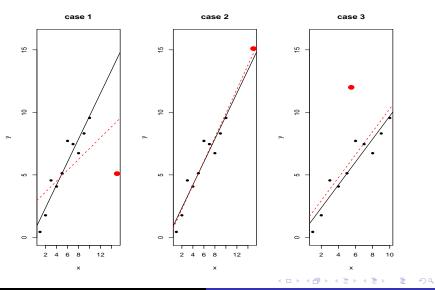
Savings Example

```
> savings$dpi[c(44)]
[1] 4001.89
> savings$ddpi[c(23, 49)]
[1] 8.21 16.71
```

- > par(mfrow= c(1,2))
- > hist(savings\$dpi, main ="dpi")
- > hist(savings\$ddpi, main ="ddpi")



Examples: Outliers



Outliers

How do we distinguish between truly unusual points and large residuals?

Compare two models:

Model 1:
$$Y = X\beta + \epsilon$$
, vs. Model 2: $Y_{-i} = X_{-i}\beta + \epsilon'$,

 \iff

Compare residuals for i^{th} observation.

Outliers

How do we distinguish between truly unusual points and large residuals?

- Exclude point *i*, recompute $\hat{\beta}_{(i)}$ and $\hat{y}_{(i)} = x_i^T \hat{\beta}_{(i)}$.
- If $|y_i \hat{y}_{(i)}|$ is large, then observation i is an outlier; but how large is large?

Outliers

Note that

•

$$\widehat{\text{var}}(\hat{y}_{(\text{pred})}) = \hat{\sigma}\sqrt{1 + x_{new}^T (X^T X)^{-1} x_{new}}$$

•

$$\widehat{\text{var}}(y_i - \hat{y}_{(i)}) = \hat{\sigma}_{(i)} \sqrt{1 + x_i^T \left(X_{(i)}^T X_{(i)} \right)^{-1} x_i}$$

•

$$\frac{\hat{\cdot} - \cdot}{\hat{\mathsf{se}}(\cdot)} \sim t_{n-(p+1)}.$$

Externally Studentized Residuals

It turns out

$$t_{i} = \frac{y_{i} - \hat{y}_{(i)}}{\hat{\sigma}_{(i)} \sqrt{1 + x_{i}^{T} \left(X_{(i)}^{T} X_{(i)}\right)^{-1} x_{i}}}$$

$$\sim t_{(n-1)-(p+1)}$$

The book also calls these jackknife or cross-validated residuals.

Multiple Hypothesis Tests

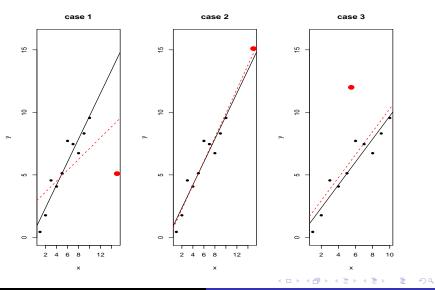
- If $|t_i|$ is too large, reject and conclude observation i is an outlier (because p-value is $P(|t_{(n-1)-(p+1)}| > |t_i|)$.
- For each observation *i*, compare $|t_i|$ with $t_{n-(p+1)-1}^{\alpha/2}$.
- Will fail to reject too many points. Why?

Bonferroni Correction

Type I Error =
$$Pr_{H_0}$$
 (reject at least one test)
 $\leq \sum_{i} Pr_{H_0}$ (reject test i)
= $n\alpha$

Bonferroni correction: test each hypothesis at level α/n

Examples: Outliers



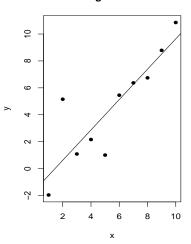
```
## Externally Studentized Residuals
> round( rstudent(res1), 3)
        1        2        3        4        5        6        7        8        9        10        11
-1.066 -0.552        1.732 -0.108 -0.002        2.150        0.437 -1.547 -0.735 -0.422        0.556
## P-values
> round( 2 * ( pt( abs(rstudent(res1)), 11 - 1 - 2, lower.tail = F)), 3)
        1        2        3        4        5        6        7        8        9        10        11
0.318        0.596        0.121        0.917        0.998        0.064        0.674        0.160        0.484        0.684        0.594
```

Examples: Outliers

case 4: multiple outliers 15 10 > 2 0 2 10 6 8

х

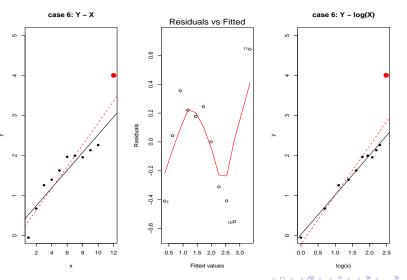
case 5: large error variance



```
## Externally Studentized Residuals
> round( rstudent(res1), 3)
    1     2     3     4     5     6     7     8     9     10     11     12
-0.480 -0.280     0.447 -0.088 -0.036     0.581     0.146 -0.479 -0.234 -0.112     3.550 -2.418

## P-values
> round( 2 * ( pt( abs(rstudent(res1)), 11 - 1 - 2, lower.tail = F)), 3)
    1     2     3     4     5     6     7     8     9     10     11     12
0.644 0.786 0.667 0.932 0.972 0.577 0.887 0.645 0.821 0.914 0.008 0.042
```

Examples: Outliers



Case 6: $Y \sim X$

Externally Studentized Residuals

Case 6: $Y \sim \log(X)$

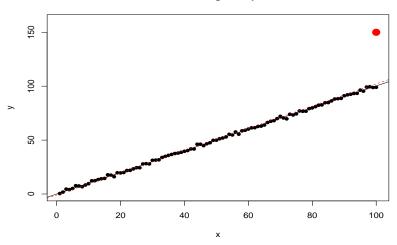
Externally Studentized Residuals

```
> round( rstudent(res1), 3)
1          2     3     4     5     6     7     8     9     10     11
0.501     0.089     0.279 -0.196 -0.293 -0.036 -0.393 -0.886 -0.819 -0.831 13.206
## P-values
> round( 2 * ( pt( abs(rstudent(res1)), 11 - 1 - 2, lower.tail = F)), 3)
1          2     3     4     5     6     7     8     9     10     11
```

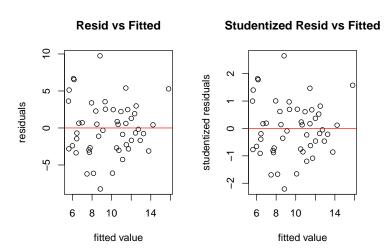
0.630 0.931 0.787 0.850 0.777 0.972 0.704 0.401 0.437 0.430 0.000

Examples: Outliers

case 7: large samples



Savings Example: Studentized Residual vs. Fitted Plot



Savings Example

```
## Compute (externally) studentized residuals
> ti <- rstudent(result)</pre>
> max(abs(ti))
[1] 2.853558
> which(ti == max(abs(ti)))
Zambia
    46
## Compute p-value
> 2*(1-pt(max(abs(ti)), df=50-1-5))
[1] 0.006566663
## compare to alpha/n
> 0.05/50
[1] 0.001
```

Remarks on Outliers

- Two or more outliers can hide each other.
- Examine the context what could it mean?
 - Occasionally data entry errors occur
 - Hidden variables may be part of the explanation
 - Something going wrong: e.g., fraudulent use of credit cards
 - A new unknown effect (you may get a Nobel prize if you can explain it!)
 - Some patterns just have exceptions...

Influential Points

An influential point is one whose removal from the dataset would cause a large change in the fit. At least one of the following:

- Outlier
- High leverage

How to measure the influence?

- Change in the coefficients $\hat{\beta} \hat{\beta}_{(i)}$
- Change in the fit $X^T(\hat{\beta} \hat{\beta}_{(i)}) = \hat{y} \hat{y}_{(i)}$

Cook's Distance

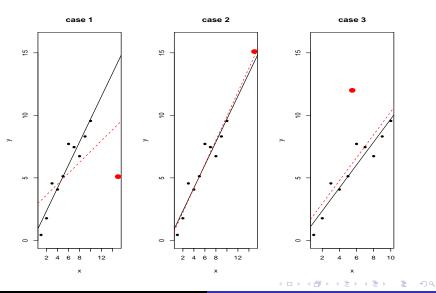
Cook statistic:

$$D_{i} = \frac{(\hat{y} - \hat{y}_{(i)})^{T} (\hat{y} - \hat{y}_{(i)})}{(p+1)\hat{\sigma^{2}}}$$
$$= \frac{1}{p+1} r_{i}^{2} \frac{h_{i}}{1-h_{i}}$$

Combination of residual effect and leverage effect

Rule of thumb: Cook's Distance $D_i > \frac{4}{n-p-1}$ is considered large.

Examples: Influential Points



Case 1

```
## Cook's Distance
> round( cooks.distance(res1), 3)
    1    2    3    4    5    6    7    8    9    10    11
0.365    0.111    0.005    0.003    0.000    0.059    0.030    0.003    0.046    0.145    4.485
## Threshold
> 4 / (11 - 1 - 1)
0.444
```

Case 2

```
## Cook's Distance
> round( cooks.distance(res1), 3)
    1    2    3    4    5    6    7    8    9    10    11
0.202  0.043  0.233  0.001  0.000  0.166  0.011  0.124  0.044  0.020  0.200
## Threshold
> 4 / (11 - 1 - 1)
0.444
```

Case 3

```
## Cook's Distance
> round( cooks.distance(res1), 3)
1     2     3     4     5     6     7     8     9     10     11
0.192     0.057     0.012     0.008     0.004     0.014     0.000     0.071     0.046     0.041     0.374
## Threshold
> 4 / (11 - 1 - 1)
```

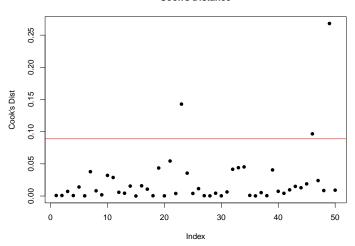
0.444

Savings Example

```
## Compute Cook's distance
> cook <- cooks.distance(result)
> plot( cook, pch = 16 , ylab ="Cook's Dist", main = "Cook's Distance"
> abline(h = 4/ (50 - 4 -1), col="red")
> which(cooks.distance(result) >4/ (50 - 4 -1) )
Japan Zambia Libya
23     46     49
```

Savings Example Continued

Cook's Distance



Savings Example

Recall that Ireland, Japan, United States, and Libya may be leverage points. In addition, there is no outliers from t-tests.

According to the choice of a test or a method, the result may be different.

Checking the Structure of the Model: Linearity

Plot $\hat{\epsilon}$ against \hat{y} and x_j , but other predictors impact the relationship. Consider

- Partial regression plots
- Partial residual plots

Isolate the effect of x_i on y

Partial Regression Plots

- **1** Regress y on all x except x_j , get residuals $\hat{\delta}$
- 2 Regress x_j on all x except x_j , get residuals $\hat{\gamma}$
- ${\color{red} \bullet} \ \, \mathsf{Plot} \,\, \hat{\delta} \,\, \mathsf{against} \,\, \hat{\gamma} \\$

Partial Regression Plots: Intuition

In the summary table below, we have an evidence that X_2 and Y have a significant relationship after removing the effects of other variables.

```
## fitting model
> result = lm( Y ~ X1+ X2+ X3 )
## fitted model
> summary(result)
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.242555
                        0.027011 -8.980 1.97e-15 ***
X 1
            0.077384 0.042927 1.803 0.073647 .
X2
           -0.228795 0.078107 -2.929 0.003986 **
Х3
            0.009584 0.041840
                                  0.229 0.819168
```

Partial Regression Plots: Intuition

Residual is part of Y after removing the effects of predictors.

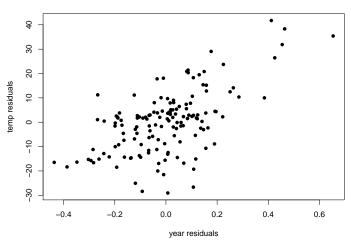
Therefore, partial regression plots show the relationship between a predictor and the response variable after removing the effects of predictors.

Global Warming Example

```
## Load Data
> data(globwarm)
# Remove Missing Values
> id = which( is.na( globwarm$nhtemp ) == FALSE )
> globwarm = globwarm[id,]
## Fitting models
> result.a = lm( nhtemp ~ wusa+ jasper+ westgreen+
   chesapeake+ tornetrask+ urals+ mongolia+ tasman, data = globwarm)
> result.b = lm( year ~ wusa+ jasper+ westgreen+
   chesapeake+ tornetrask+ urals+ mongolia+ tasman, data = globwarm)
## Partial Regression Plot
> plot( residuals(result.a), residuals(result.b), xlab = "year residuals",
   ylab ="temp residuals", main = " Partial Regression", pch = 16 )
```

Global Warming Example





Partial Residual Plots

• Plot $\hat{\epsilon} + \hat{\beta}_j x_j$ against x_j

Where does this come from?

$$y - \sum_{j' \neq j} x_{j'} \hat{\beta}_{j'} = \dots$$

= $x_j \hat{\beta}_j + \hat{\epsilon}$

The slope is $\hat{\beta}_j$. Look for non-linearity and outliers and influential points.

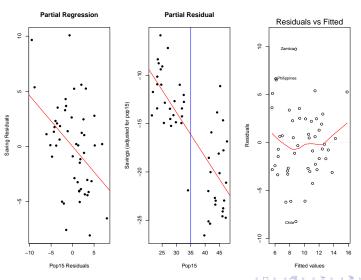
Savings Example

```
## Load Data
> data(savings)

## Partial regression plot
> delta <- residuals(lm(sr ~ pop75 + dpi + ddpi, data=savings))
> gamma <- residuals(lm(pop15 ~ pop75 + dpi + ddpi, data=savings))
> plot(gamma,delta, xlab="Pop15 Residuals", ylab="Saving Residuals", main = "Partial Regression", pch = 16)
> temp <- lm(delta ~ gamma)
> abline(reg=temp, col = "red")
```

> plot(result, which = 1)

Savings Example Continued



Savings Example Continued

- Linearity
- Normality
- Constant Variance
- Independent Errors
- Unusual Points (influential points)
- Leverage Points
- Outliers

- Linearity
- Scatter Plot
- Residual vs Fitted Plot
- Partial Regression Plot
- Partial Residual Plot
- # Prediction (x), Inference (Test, CI) (x)

- Normality
- Normal QQ Plot
- Shapiro-Wilk's Test
- # Prediction (o), Inference (Test, CI) (x)

- Constant Variance
- Residual vs Fitted Plot
- # Prediction (o), Inference (Test, CI) (may be...)

- Independent Errors
- Residual vs Fitted Plot
- ϵ_i vs ϵ_{i+1} Plot
- ϵ vs Time Plot
- Durbin-Watson test
- # Prediction (o), Inference (Test, CI) (x)

- Influential Points
- Histogram, Scatter Plot
- Residual vs Fitted Plot
- Leverage
- Internally and Externally Studentized Residuals
- Cook's Distance
- # Prediction (may be), Inference (Test, CI) (may be)

- Leverage Points
- Histogram, Scatter Plot
- Leverage
- Cook's Distance
- # Prediction (o; however be careful), Inference (Test, CI) (o)

- Outliers
- Histogram, Scatter Plot
- Residual vs Fitted Plot
- Externally Studentized Residuals
- Cook's Distance
- # Prediction (x), Inference (Test, CI) (x)

Summary of Diagnostics

- Just fitting a model is not enough
- Graphical diagnostics are more informative but also more subjective
- Diagnostics often suggest a change in the model and then the whole process is repeated
- Time-consuming... but worth it