PSTAT 126

Regression Analysis

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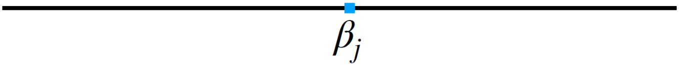
Lecture 8 & 9
Confidence intervals and Diagnostics

Confidence intervals (CIs) for β

We consider the MLR model: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} \sim N_n(\mathbf{0}, \sigma^2 \boldsymbol{I}_n)$

Confidence intervals (CIs) provide an alternative way of expressing the uncertainty in the estimates of $\boldsymbol{\beta}$. We construct confidence intervals based on a confidence level $(1-\alpha) * 100\%$, which represents the proportion of intervals among all possible intervals that contain the true value of the unknown parameter.



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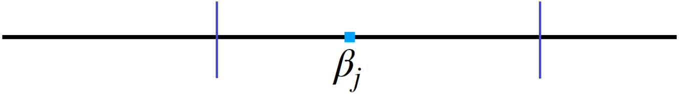

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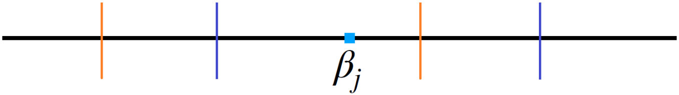

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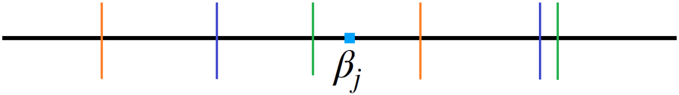

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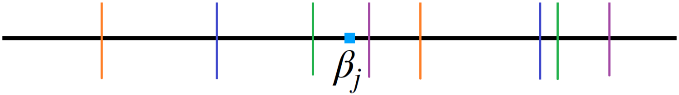

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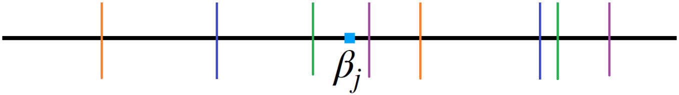


Each data set will produce a different confidence interval. If we construct an infinite number of intervals based on an infinite number of data sets, approximately 95% of them will contain the true value of β_j.

CIs for individual parameters

For individual parameter β_j, the CI takes the form:

$$\hat{\beta}_j \pm t_{(1-\alpha/2;n-p^*)} SE(\hat{\beta}_j)$$

Where $SE = \hat{\sigma}\sqrt{(\boldsymbol{X}^T\boldsymbol{X})^{-1}_{jj}}$, is the standard error of $\hat{\beta}_j$.

Duality between CIs and hypothesis tests: For a significance level α, we can test the hypothesis: $H_0 : \beta_j = 0 \quad vs \quad H_1 : \beta_j \neq 0$, by using the CI with confidence level $(1-\alpha)$:

If the CI contains zero, we fail to reject $\boldsymbol{H}_0$

CIs for Predictions

There are two kind of predictions made from regression models:

1. Prediction of response mean: We want to predict $\mu_0 = E(y_0|x_0) = x_0^T\boldsymbol{\beta}$, which represents the "average" response for a subject with characteristics x_0.
2. Prediction of a future observation: We seek to predict $y_0 = \mu_0 + \epsilon_0 = x_0^T\boldsymbol{\beta} + \epsilon_0$, which represents the response of a new observation with characteristics x_0.

Point-wise Prediction: For a new set of predictors x_0, the predicted response is $\hat{y}_0 = x_0^T\hat{\boldsymbol{\beta}}$ for both cases 1 and 2.

CIs for Predictions

Interval Prediction: We need to assess the uncertainty of this prediction as decision makers need more than just a point estimate to make rational choices.

1. $100 * (1-\alpha)\%$ CI for the response mean:

$$\hat{y}_0 \pm t_{(1-\alpha/2;n-p^*)}\hat{\sigma}\sqrt{x_0^T(\boldsymbol{X}^T\boldsymbol{X})^{-1}x_0}$$

2. $100 * (1-\alpha)\%$ CI for a single future observation:

$$\hat{y}_0 \pm t_{(1-\alpha/2;n-p^*)}\hat{\sigma}\sqrt{1 + x_0^T(\boldsymbol{X}^T\boldsymbol{X})^{-1}x_0}$$

Regression Diagnostics

Consider the MLR model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} \sim N_n(\mathbf{0}, \sigma^2 \boldsymbol{I}_n)$$

Inference from this model depends on several assumptions, that should be checked by using *regression diagnostics* before using the model. Potential problems can be divided into three categories:

1. **Error**: We have assumed $\boldsymbol{\epsilon} \sim N_n(\mathbf{0}, \sigma^2 \boldsymbol{I}_n)$, which involves three assumptions on the errors: 1) Independence, 2) Constant variance and 3) Normality.
2. **Unusual observations** There might be a few observations that do not fit the model.
3. **Model structure**: We have assumed linearity of the response: $E(\boldsymbol{y}) = \boldsymbol{X}\beta$.

Checking Error Assumptions

Note that errors $\boldsymbol{\epsilon}$ are not observable, however we can examine the residuals $\hat{\boldsymbol{\epsilon}}$ as proxies. Recall that:

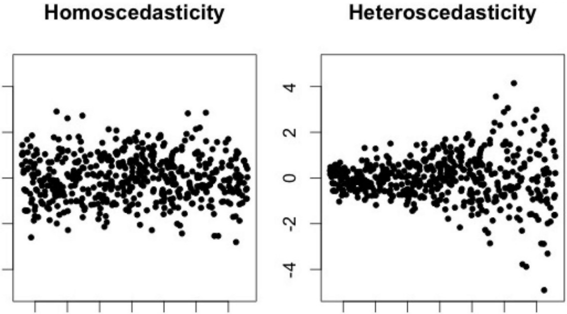
$$\hat{\boldsymbol{\epsilon}} = \boldsymbol{y} - \hat{\boldsymbol{y}} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}$$

with $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T$. Although the errors and the residuals are not interchangeable in general (residuals have no constant variance, neither are they independent, since $Var(\hat{\boldsymbol{\epsilon}}) = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$), diagnostics can reasonably be applied to the residuals in order to check assumptions on the error.

Checking Error Assumptions

1. **Constant Variance**: The most useful diagnostic is the plot of the residuals $\hat{\epsilon}$ (vertical axis) against the fitted values $\hat{y}$ (horizontal axis).

If $Var(\epsilon) = \sigma^2, \quad i = 1, \ldots, n$, we should observe constant symetrical variation (*Homoscedasticity*) in the vertical direction.



Checking Error Assumptions

- We mentioned that even when $Var(\epsilon) = \sigma^2 I$, the residuals do not have constant variance: $Var(\hat{\boldsymbol{\epsilon}}) = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$.
- But it is easy to fix it! Just divide each $\hat{\epsilon}_i$ by its variance (using an estimator for σ^2):

$$r_i = \frac{\hat{\epsilon}_i}{\sqrt{\hat{\sigma}(1 - h_i i)}},$$

  where $h_i i$ is the element in the i-th row, i-th column of $\boldsymbol{H}$.
- These are called the **standardized residuals** or "internally studentized residuals"
- See the function `rstudent` in `R`.
- Faraway's opinion: *Some authors recommend using [internally] studentized rather than raw residuals in all diagnostic plots. However, in many cases, the [internally] studentized residuals are not effectively very different from the raw residuals. Only when there is unusually large leverage will the differences be noticeable.*

Checking Error Assumptions

2. **Normality:** Recall all inference (hypotheses tests/CIs) is based on the assumption of normal errors.

   - The most commonly used diagnostic is the **Q-Q plot** , which compares the residuals to ideal normal distributions based on the quantiles. We plot the sorted residuals against $\phi^{-1}\left(\frac{i}{n+1}\right), \quad i = 1, \ldots, n.$

   - A more formal way to test normality is by using the **Shapiro-Wilk** test, whose null hypothesis is H_0 : Residuals are normal.

Checking Error Assumptions

3. **Uncorrelated errors**: Difficult to check since there are too many possible patterns of correlation that may occur. Examples of correlated data: Temporal & Spatial: Variations are explained by structural dependencies in time and space.

- In temporal data it would be useful to plot *time* against *residuals*. If the errors were uncorrelated, we would expect a random scatter of points above and bellow $\hat{\epsilon} = 0$.

- Alternative plot: Plot successive pair of residuals $(\hat{\epsilon}_i, \hat{\epsilon}_{i+1})$. Any trend will mean correlation.

- *Durbin-Watson Test*: The null hypothesis: H_0: Uncorrelated errors. This test uses the statistic:

$$DW = \frac{\sum_{i=2}^{n} (\hat{\epsilon}_i - \hat{\epsilon}_{i-1})^2}{\sum_{i=1}^{n} \hat{\epsilon}_i^2}$$

Species Example: 95% Confidence Intervals

```
summary(fit1)$coefficients
```

```
##                 Estimate  Std. Error      t value     Pr(>|t|)
## (Intercept)  7.068220709 19.15419782  0.369016796 7.153508e-01
## Area        -0.023938338  0.02242235 -1.067610554 2.963180e-01
## Elevation    0.319464761  0.05366280  5.953187968 3.823409e-06
## Nearest      0.009143961  1.05413595  0.008674366 9.931506e-01
## Scruz       -0.240524230  0.21540225 -1.116628222 2.752082e-01
## Adjacent    -0.074804832  0.01770019 -4.226216850 2.970655e-04
```

```
CIs<- cbind(summary(fit1)$coefficients[, 1]-qt(0.975, fit1$df.residual)*summary(fit1)$coefficients[, 2] ,
            summary(fit1)$coefficients[, 1]+qt(0.975,fit1$df.residual)*summary(fit1)$coefficients[, 2])
CIs ## Using Formula
```

```
##                   [,1]        [,2]
## (Intercept) -32.4641006 46.60054205
## Area         -0.0702158  0.02233912
## Elevation     0.2087102  0.43021935
## Nearest      -2.1664857  2.18477363
## Scruz        -0.6850926  0.20404416
## Adjacent     -0.1113362 -0.03827344
```

```
confint(fit1) #Using Built in Function
```

```
##                   2.5 %      97.5 %
## (Intercept) -32.4641006 46.60054205
## Area         -0.0702158  0.02233912
## Elevation     0.2087102  0.43021935
## Nearest      -2.1664857  2.18477363
## Scruz        -0.6850926  0.20404416
## Adjacent     -0.1113362 -0.03827344
```

Species Example: Prediction Interval

```
x0<- data.frame(Area=20.6, Elevation= 46, Nearest=1.9, Scruz=8.0, Adjacent=0.78  )
pred.y0<-t(x0.vector)%*%fit1$coefficients ; pred.y0
```

```
##         [,1]
## [1,] 19.3053
```

```
se2.betas<- t(x0.vector)%*%(solve(t(X)%*%X))%*%x0.vector
sigma<- sigma(fit1)
predmean.CI<- c(pred.y0 - sigma*qt(0.975,fit1$df.residual)*sqrt(se2.betas),
            pred.y0 + sigma* qt(0.975,fit1$df.residual)*sqrt(se2.betas)); predmean.CI #Using Formula
```

```
## [1] -16.42255  55.03315
```

```
predict(fit1, newdata = x0, interval = "confidence")  #Using Built-in function
```

```
##       fit       lwr      upr
## 1 19.3053 -16.42255 55.03315
```

```
pred.CI<- c(pred.y0 - sigma*qt(0.975,fit1$df.residual)*sqrt(1+se2.betas),
            pred.y0 + sigma* qt(0.975,fit1$df.residual)*sqrt(1+se2.betas)); pred.CI #Using Formula
```

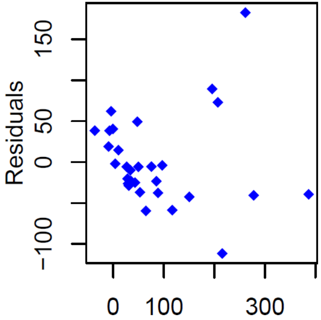
```
## [1] -111.5146  150.1252
```

```
predict(fit1, newdata = x0, interval = "prediction")  #Using Built-in function
```

```
##       fit       lwr      upr
## 1 19.3053 -111.5146 150.1252
```

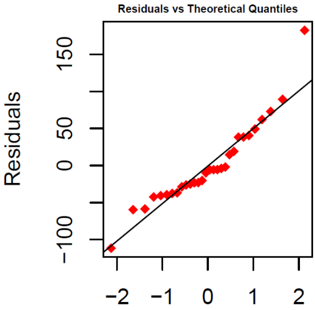
Species Example: Checking Homoscedasticity

```r
par(mar = c(5, 5, 1, 2))
plot(fitted(fit1), residuals(fit1), xlab="",
     ylab="", col="blue", pch=18);mtext(side=2, text="Residuals", line=2)
```



Species Example: Checking Normality

```r
par(mar = c(5, 5, 1, 2))
qqnorm(residuals(fit1), ylab="Residuals",
       main="", pch=18, col="red")
qqline(residuals(fit1));title("Residuals vs Theoretical Quantiles", cex.main=0.5)
```



Species Example: Checking Normality

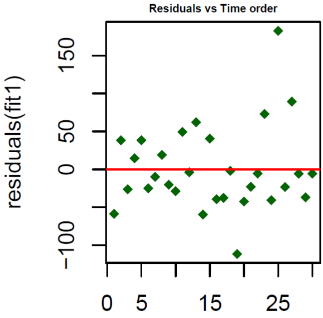
```
shapiro.test(residuals(fit1))
```

```
##
##  Shapiro-Wilk normality test
##
## data:  residuals(fit1)
## W = 0.91351, p-value = 0.01826
```

- H_0 : population is normally distributed.
- p value less than chosen $\alpha \Rightarrow$ reject H_0 (data is not Gaussian)
- If the sample size is sufficiently large this test may detect even trivial departures from the null hypothesis

Species Example: Checking Correlation

```
par(mar = c(5, 5, 1, 2))
plot(1:length(gala$Species), residuals(fit1), col="darkgreen", pch=18)
abline(h=0. ,col="red")
title("Residuals vs Time order", cex.main=0.5)
```



Species Example: Checking Correlation

```
dwtest( Species ~ Area+Elevation+Nearest+ Scruz+ Adjacent, data=gala)
```

```
##
##  Durbin-Watson test
##
## data:  Species ~ Area + Elevation + Nearest + Scruz + Adjacent
## DW = 2.4759, p-value = 0.9017
## alternative hypothesis: true autocorrelation is greater than 0
```

- Null hypothesis: H_0: Uncorrelated errors

Finding Unusual Observations

Consider the MLR model:

$$\mathbf{y} = \mathbf{X}\beta + \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} \sim N_n(\mathbf{0}, \sigma^2 \boldsymbol{I}_n)$$

Which fits observations $(y_1, \boldsymbol{X}_1), (y_2, \boldsymbol{X}_2) \ldots, (y_n, \boldsymbol{X}_n)$. However there may be three kind of observations that don't "agree" with this model.

- ***High Leverage Points:*** Data points that are extreme in the predictor space. (Extreme values $\boldsymbol{X}_i$).
- ***Outliers:*** Extreme observations in the response given the predictors. (Unusual values y_i given $\boldsymbol{X}_i$).
- ***Influential Observations:*** Data points that change the fit of the model substantially.

Leverage

Recall the hat matrix: $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T$. The ***leverage score*** for the i^{th} independent observation $\boldsymbol{X}_i$ are given by the diagonal elements of $\boldsymbol{H}$: $h_i = [\boldsymbol{H}]_{ii}$.

Interpretation: The leverage score can be seen as the “weighted” distance between X_i and the average point of the X_i's. It can also be interpreted as the degree by which y_i influences $\hat{y}_i$.

Properties:

1. $0 \leq h_{ii} \leq 1 \qquad \forall i = 1, \ldots, n.$
2. $\sum_{i=1}^{n} h_{ii} = p^* = p + 1$

Reminder: The trace of a square matrix is the sum of its diagonal elements

Leverage properties:

1. ***Proof:*** We use that the hat matrix is symmetric and idempotent:

$$\begin{aligned} \boldsymbol{H}^2 = \boldsymbol{H} &\Rightarrow [\boldsymbol{H}]^2_{ii} = [\boldsymbol{H}]_{ii} \\ &\Rightarrow h_{ii} = h_{ii}^2 + \sum_{j \neq i} h_{ij} h_{ji} = h_{ii}^2 + \sum_{j \neq i} h_{ij}^2 \geq 0 \\ \sum_{j \neq i} h_{ij}^2 \geq 0 &\Rightarrow h_{ii} \geq h_{ii}^2 \Rightarrow h_{ii} \leq 1 \\ &\Rightarrow 0 \leq h_{ii} \leq 1 \end{aligned}$$

2. ***Proof:*** We use $Tr(\boldsymbol{A}^T\boldsymbol{B}) = Tr(\boldsymbol{A}\boldsymbol{B}^T)$

$$\begin{aligned} \sum_{i=1}^{n} h_{ii} &= Tr(\boldsymbol{H}) = Tr(\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T) \\ &= Tr(\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}) = Tr(\boldsymbol{I}_{p^*}) = p^* = p + 1 \end{aligned}$$

Effect on Residual Variance

Recall that $\hat{\boldsymbol{\epsilon}} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y} \Rightarrow Var(\hat{\boldsymbol{\epsilon}}) = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$. This implies:

$$Var(\hat{\epsilon}_i) = \sigma^2(1 - h_i)$$

This means that large leverage score h_i will make $Var(\hat{\epsilon}_i) = Var(y_i - \hat{y}_i)$ small, so that the regression line will be attracted toward y_i.

Extreme $\boldsymbol{X}_i$'s $\Rightarrow$ Large values of h_i $\Rightarrow$ Large influence of $\hat{y}_i$ on y_i

Since $\sum_{i=1}^{n} h_{ii} = p^* \Rightarrow \bar{h} = \frac{p^*}{n}$. We should look at observations that greatly exceed $\bar{h}$. **The Rule of thumb:** We consider large leverage score $h^* > 2\bar{h}$.

High Leverage points - Savings data

Savings data: - sr: savings rate - pop15: % population under age 15 - pop75: % population under age 75 - dpi: per-capita disposable income - ddpi: percent growth rate of dpi

```
library(faraway);data(savings)
```

```
## Warning: package 'faraway' was built under R version 4.1.3
```

```
lmod<- lm(sr ~ pop15 + pop75+ dpi+ ddpi, savings)
X<- model.matrix(lmod)
hatv <- diag(X%*%(solve(t(X)%*%X))%*%t(X)) #Using formula
hatv2<- hatvalues(lmod)  #Using built in formula
all.equal(hatv, hatv2)
```

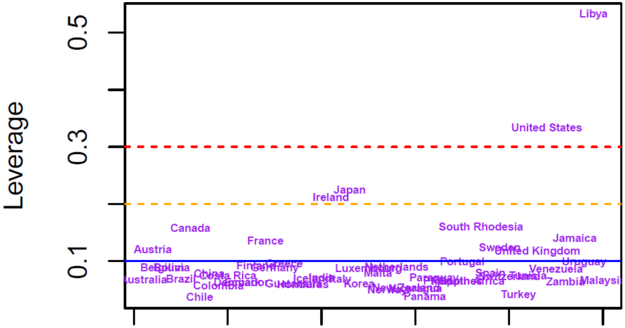
```
## [1] TRUE
```

```
sum(hatv2)  # sum h_i = p+1
```

```
## [1] 5
```

High Leverage points - Savings data

```
data.lev<- data.frame(index=seq(length(hatv)),
                      Leverage=hatv, namesC=rownames(savings))
par(mar = c(4, 4, 0.5, 0.5))
plot(Leverage ~ index, data=data.lev, col="white", pch=NULL)
text(Leverage ~ index, labels=namesC, data=data.lev, cex=0.4, font=2, col="purple")
abline(h = sum(hatv2)/dim(data.lev)[1], col="blue")
abline(h = 2*sum(hatv2)/dim(data.lev)[1], col="orange", lty=2)
abline(h = 3*sum(hatv2)/dim(data.lev)[1], col="red", lty=2)
```



Outliers

We define the **outliers** as points that does not fit the model well, data point for which $y_i - \hat{y}_i$ is large. Outliers may be the result of wrong measurements, or true unusual observations. How do we identify outliers?

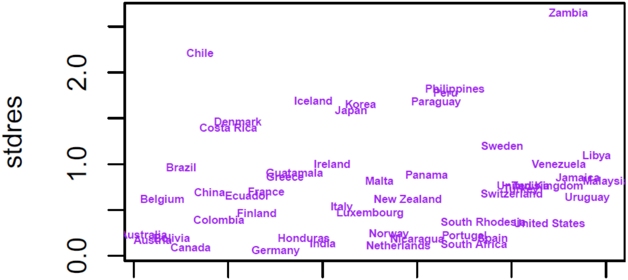
- *Residuals* vs *fitted values* plots
- We consider the **Standardized residuals**: $r_i = \frac{y_i - \hat{y}_i}{\hat{\sigma}\sqrt{1-h_i}}$. We use *the rule of thumb*: Outliers $|r_i| \geq 3$

Outliers - Savings data

```
r1<- residuals(lmod)/(sigma(lmod)*sqrt(1-hatv)) ## Using formula
r2<- rstandard(lmod) ##Built-in function
all.equal(r1,r2)
```

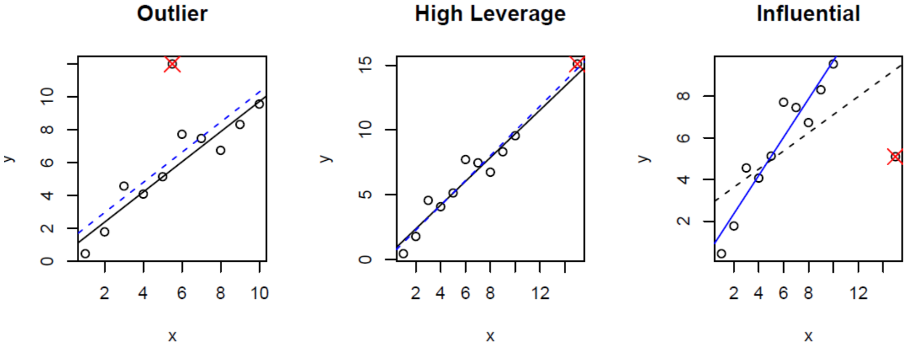
```
## [1] TRUE
```

```
data.sres<- data.frame(index=seq(length(r2)),
                       stdres=abs(r2), namesC=rownames(savings))
par(mar = c(4, 4, 0.5, 0.5))
plot(stdres ~ index, data=data.sres, col="white", pch=NULL)
text(stdres ~ index, labels=namesC, data=data.sres, cex=0.4, font=2, col="purple")
abline(h=3, col="red", lty=2)
```



Influential Observations

An **influential point** is one whose removal from the data set would case a significant change in the model. It may or may not be an outlier and may or may not be a high leverage point. (They tend to have at least one of these two properties)



Cook's Distance

We use Cook Statistics for influence diagnostics, which is defined as:

$$D_i = \frac{(\hat{y} - \hat{y}_{(i)})^T (\hat{y} - \hat{y}_{(i)})}{p^* \hat{\sigma}^2} = \frac{1}{p^*} r_i^2 \frac{h_i}{1 - h_i}$$

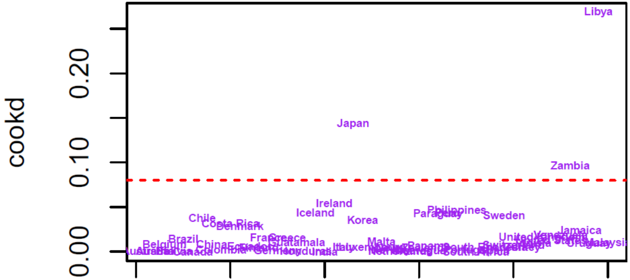
Where $\hat{y}_{(i)}$ indicates the fit without case i, r_i is the standardized residual, h_i is the leverage score. **The rule of thumb**: $D_i > 4/n$

Influential Observations - Savings data

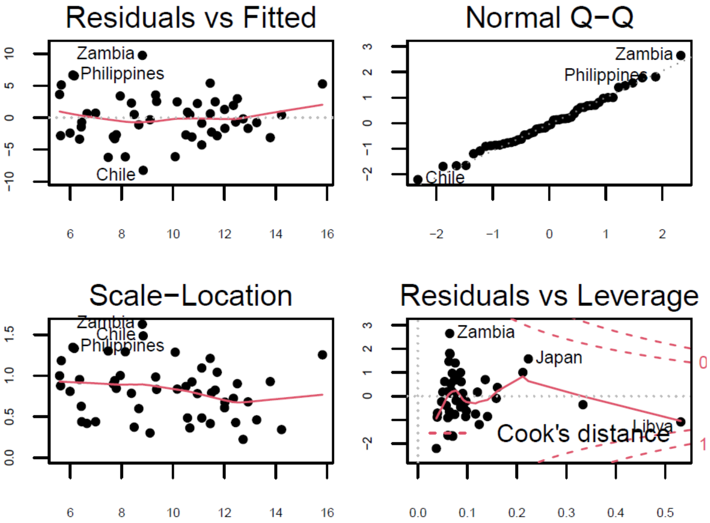
```
cook1<- (r1^2/dim(X)[2])* hatv/(1-hatv) ## Using formula
cook2<- cooks.distance(lmod) ##Built-in function
all.equal(cook1,cook2)
```

```
## [1] TRUE
```

```
data.cook<- data.frame(index=seq(length(r2)),
                      cookd=abs(cook2), namesC=rownames(savings))
par(mar = c(4, 4, 0.5, 0.5))
plot(cookd ~ index, data=data.cook, col="white", pch=NULL)
text(cookd ~ index, labels=namesC, data=data.cook, cex=0.4, font=2, col="purple")
abline(h=4/dim(X)[1], col="red", lty=2)
```



Unusual Observations in a single plot



What to do with Unusual Observations?

What should we do once we find such observations?

1. Check if there is data-entry error
2. Exclude the points
3. Try re-including them later if the model is changed

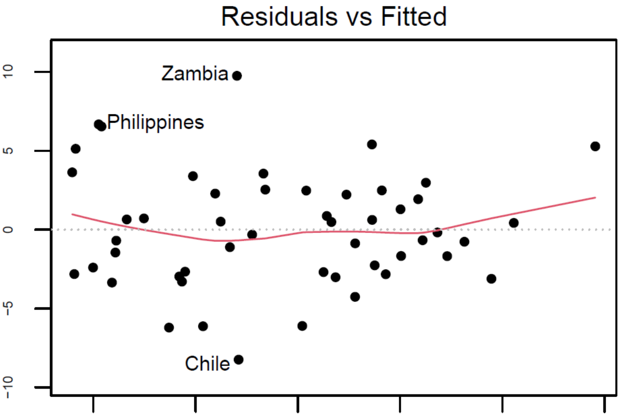
Checking Model Structure

Diagnostics can be used to detect deviations to the linearity assumption $E(\boldsymbol{y}) = \boldsymbol{X}\beta$. ***Residuals*** can show any sign of systematic structure that deviates from the linear assumption.

- Residuals against fitted values
- Residuals against predictors

Model Structure - Savings data

```
par(mar = c(3, 2, 1.5, 0.5))
plot(lmod, cex.main=1, cex.lab=0.5, cex.axis=0.5, pch=20)
```


Residuals vs Fitted
Zambia
Philippines
Chile