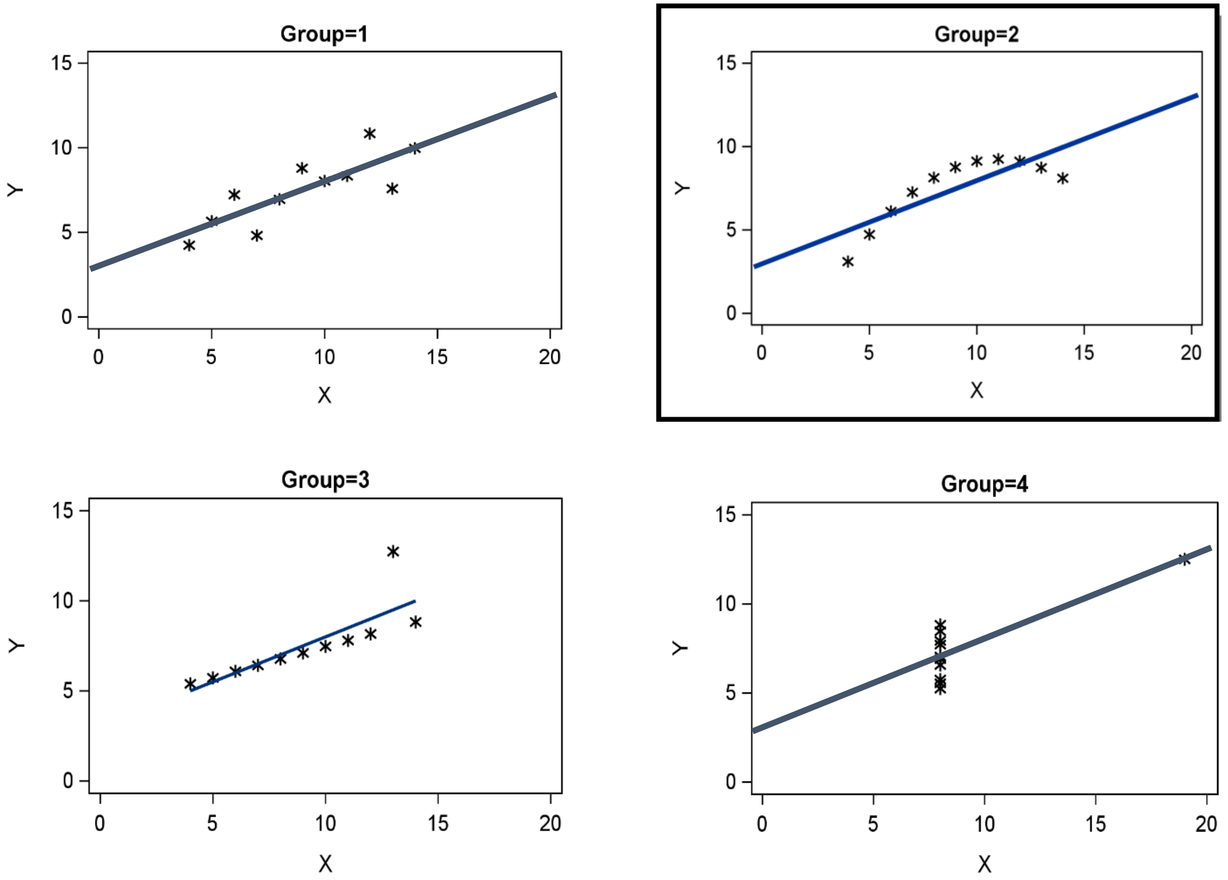
"The most wasted of all days is one without laughter." – E. E. Cummings

Diagnostics

Class of 2025

Before we start discussing diagnostics, it is ESSENTIAL that you visualize your data!!

Y-hat=3+0.5X
R^2 = 0.67



Diagnostics

- Examining Residuals
- Misspecified Model
- Lack of Constant Variance
- Lack of Normality
- Correlated error terms
- Influential points and outliers
- Multicollinearity

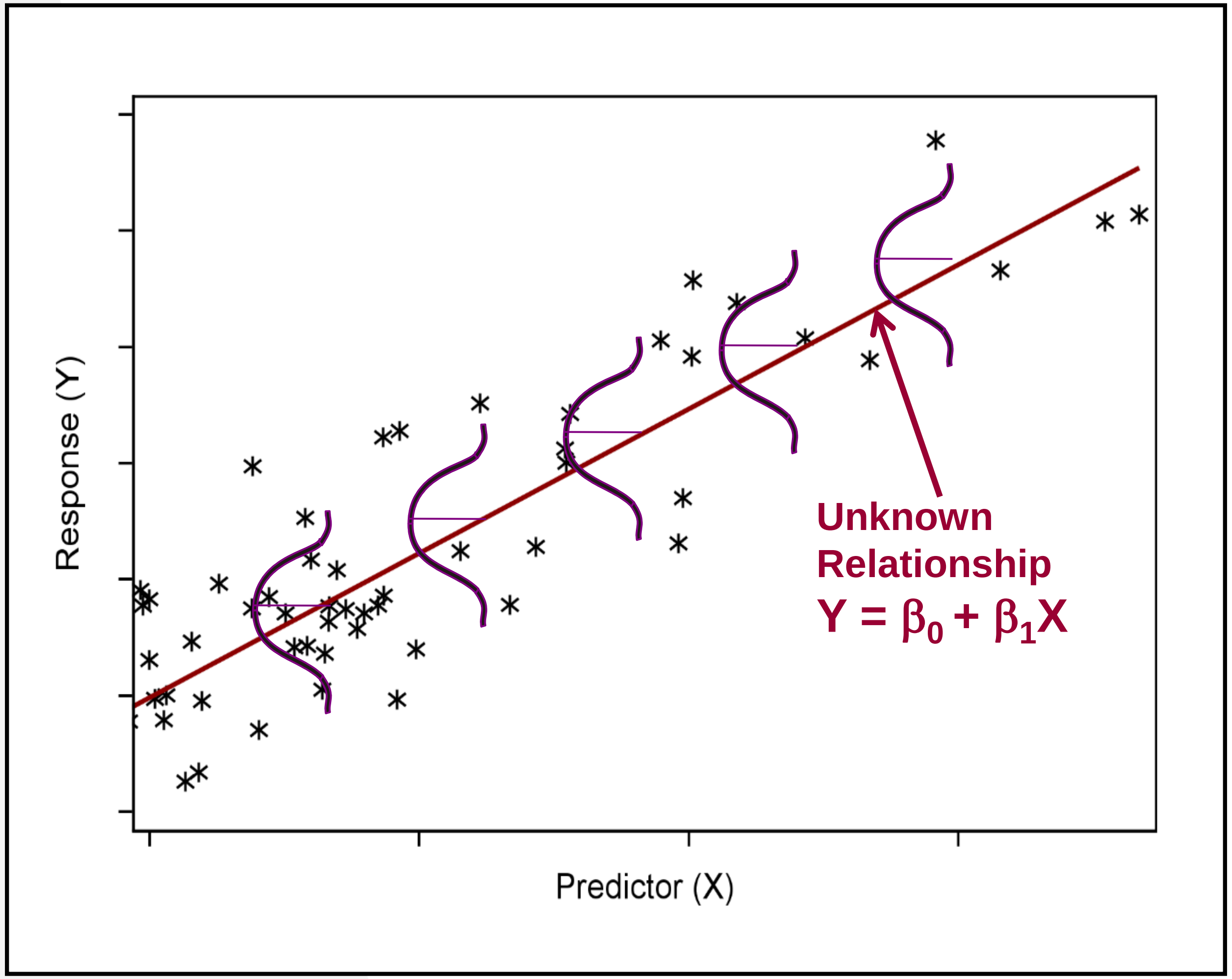
- Complete example

Examining Residuals

Linear Regression Assumptions

- The mean of the Ys is accurately modeled by a **linear** function of the Xs.
- The random error term, ε, is assumed to have a **normal** distribution with a mean of zero.
- The random error term, ε, is assumed to have a **constant variance**, σ^2.
- The errors are **independent**.
- **No perfect collinearity**

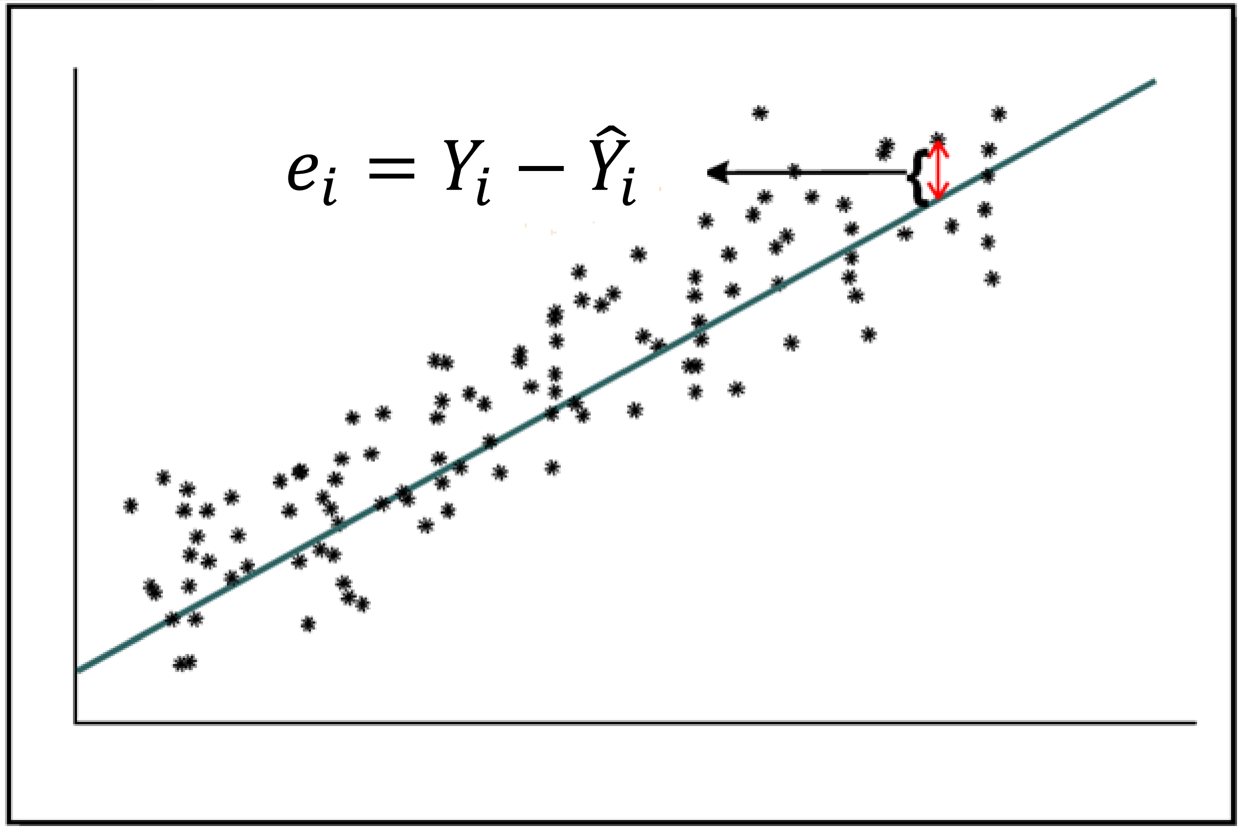
Linear Regression Assumptions



Violation of Model Assumptions

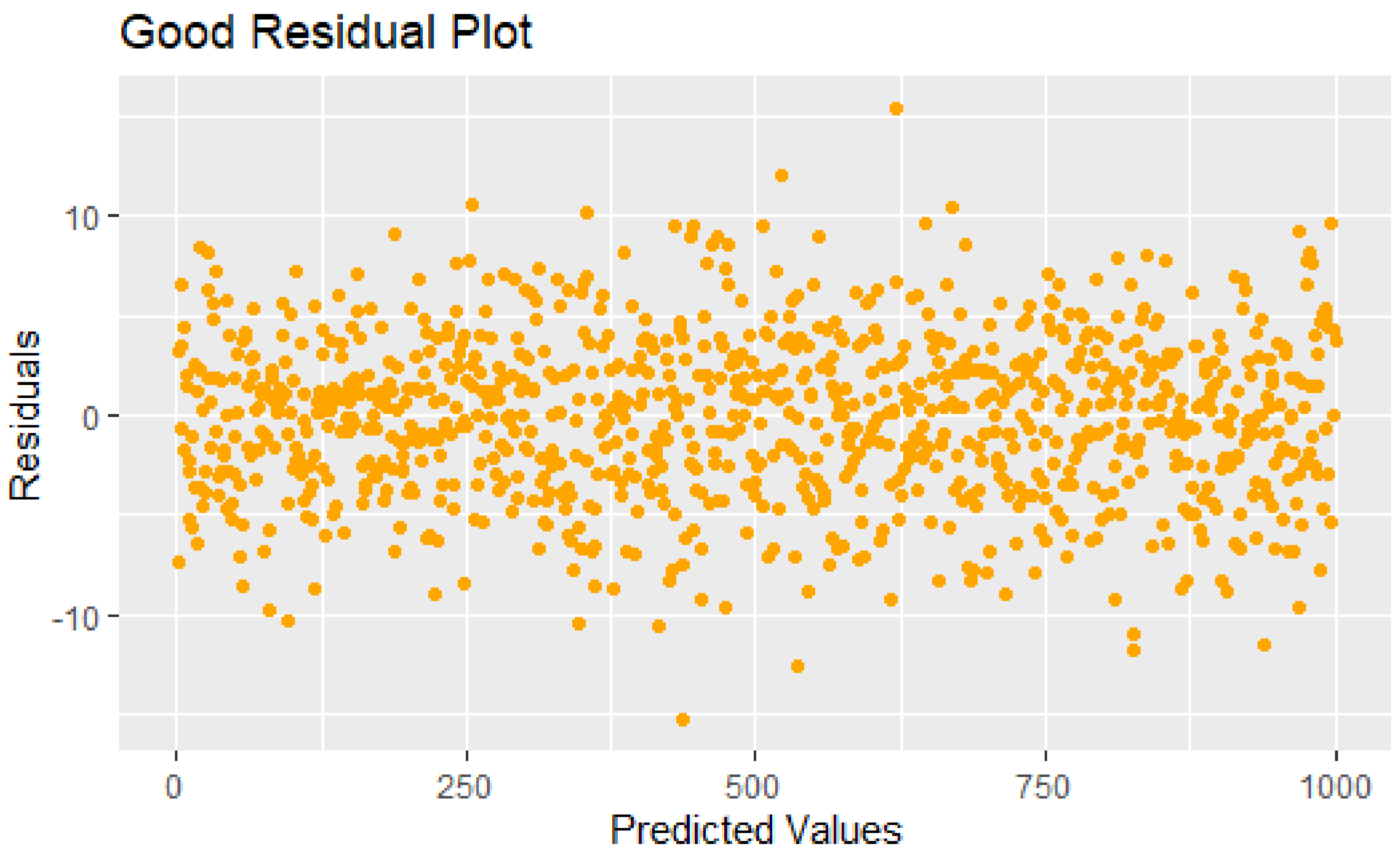
- **Linearity in the parameters** –a ***misspecified model***, and therefore the results are not meaningful.
- **Constant Variance** – does not affect the parameter estimates, but the standard errors are compromised.
- **Normality** – does not affect the parameter estimates, but it affects the test results.
- **Independent observations** – does not affect the parameter estimates, but the standard errors are compromised.

Many assumptions are investigated using residuals



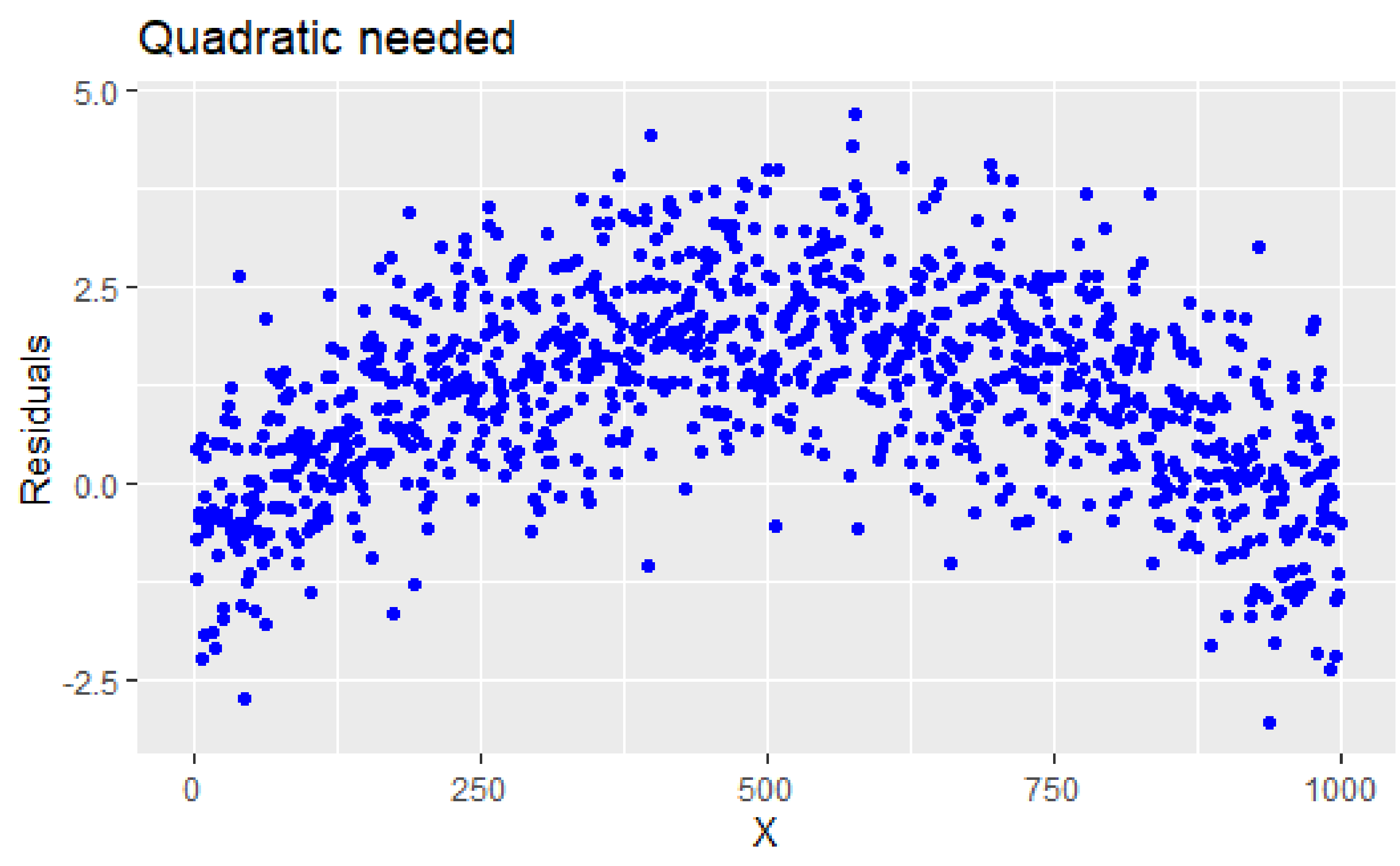
Examining Residual Plots (good residual plot)

- Plot residuals(y-axis) versus each x(x-axis) (or residuals(y-axis) versus predicted value(x-axis))
  - Residuals are randomly scattered about zero reference line.
  - No patterns found.
  - Model form appears to be adequate.



Misspecified Model

Examining Residual Plots-Misspecified Model



- Residuals: $y_i - \hat{y}_i$
- Pattern is detected (for example, curvilinear) in residuals.
- Model form is incorrect.
- Possible remedies, depending on pattern, include polynomial terms, interactions, splines, and so on.

Polynomial Regression Models

- Quadratic Polynomial Model

$$Y_j = \beta_0 + \beta_1 X_j + \beta_2 X_j^2 + \varepsilon_j$$

- Cubic Polynomial Model

$$Y_j = \beta_0 + \beta_1 X_j + \beta_2 X_j^2 + \beta_3 X_j^3 + \varepsilon_j$$

- Polynomial Model with a Cross-Product Term

$$Y_j = \beta_0 + \beta_1 X_{1j} + \beta_2 X_{2j} + \beta_3 X_{1j} X_{2j} + \varepsilon_j$$

Model Hierarchy

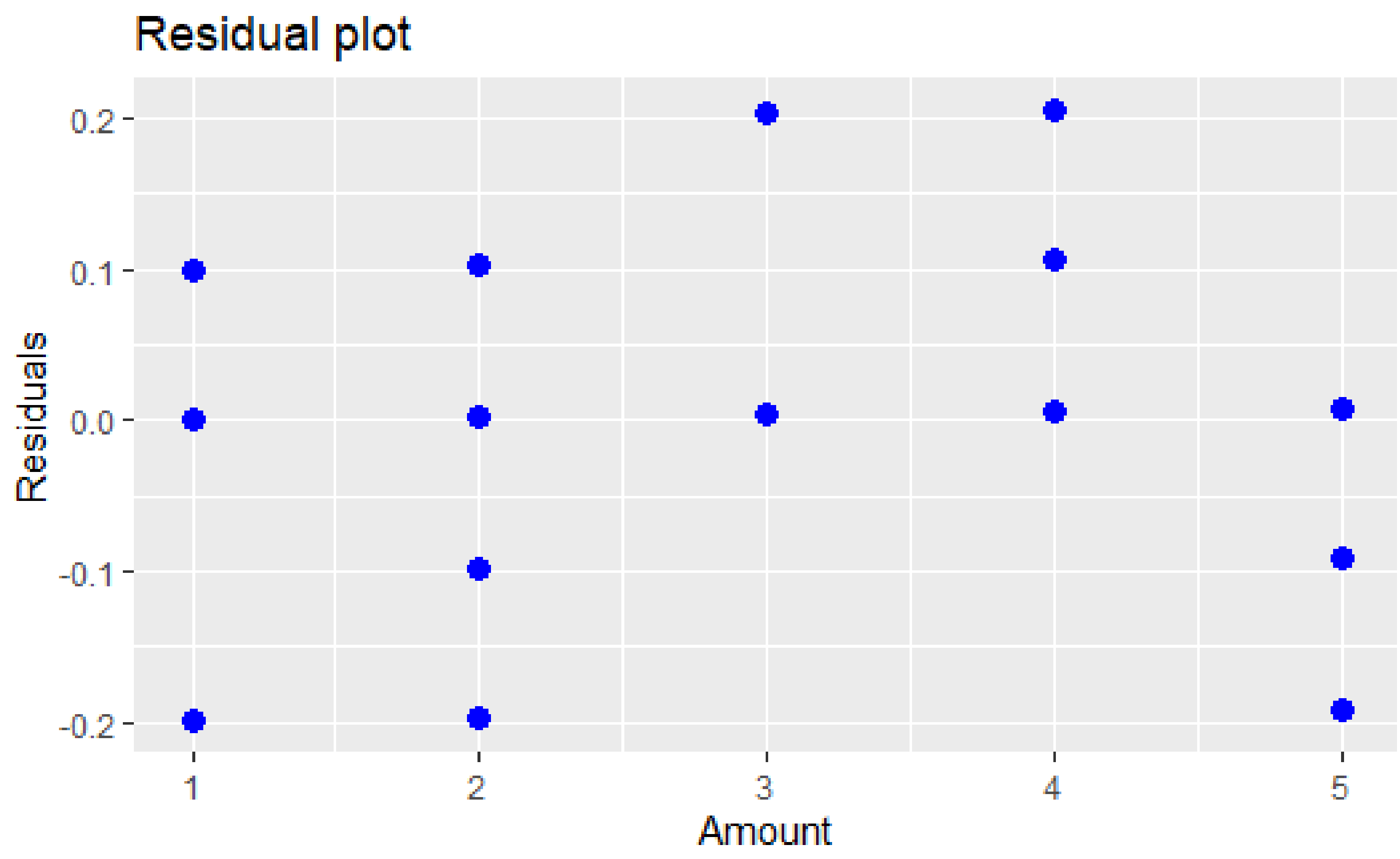
- When adding higher order terms (power terms and/or interactions), you should have ALL lower terms included in the model.
- For example, if x^3 is in the model, you should have x and x^2 also in the model
- If you include an interaction between x_3 and x_4 (x_3x_4) in the model, then x_3 AND x_4 should also be included in the model
- This is referred to as model hierarchy
- If you do have higher order terms in the model, you should center the variable (i.e. take each value and subtract the mean)

Example of polynomial regression

A researcher is interested in studying the effect of a chemical additive on paper strength. The response variable is the amount of force required to break the paper (strength) and the explanatory variable is the amount of chemical additive (amount).

Example

```
lm.quad=lm(strength~amount)
 summary(lm.quad)

ggplot(lm.quad,aes(x=amount,y=resid(lm.quad)))+geom_point(
color="blue",size=3)+labs(title="Residual plot", x="Amount",
y="Residuals")
```



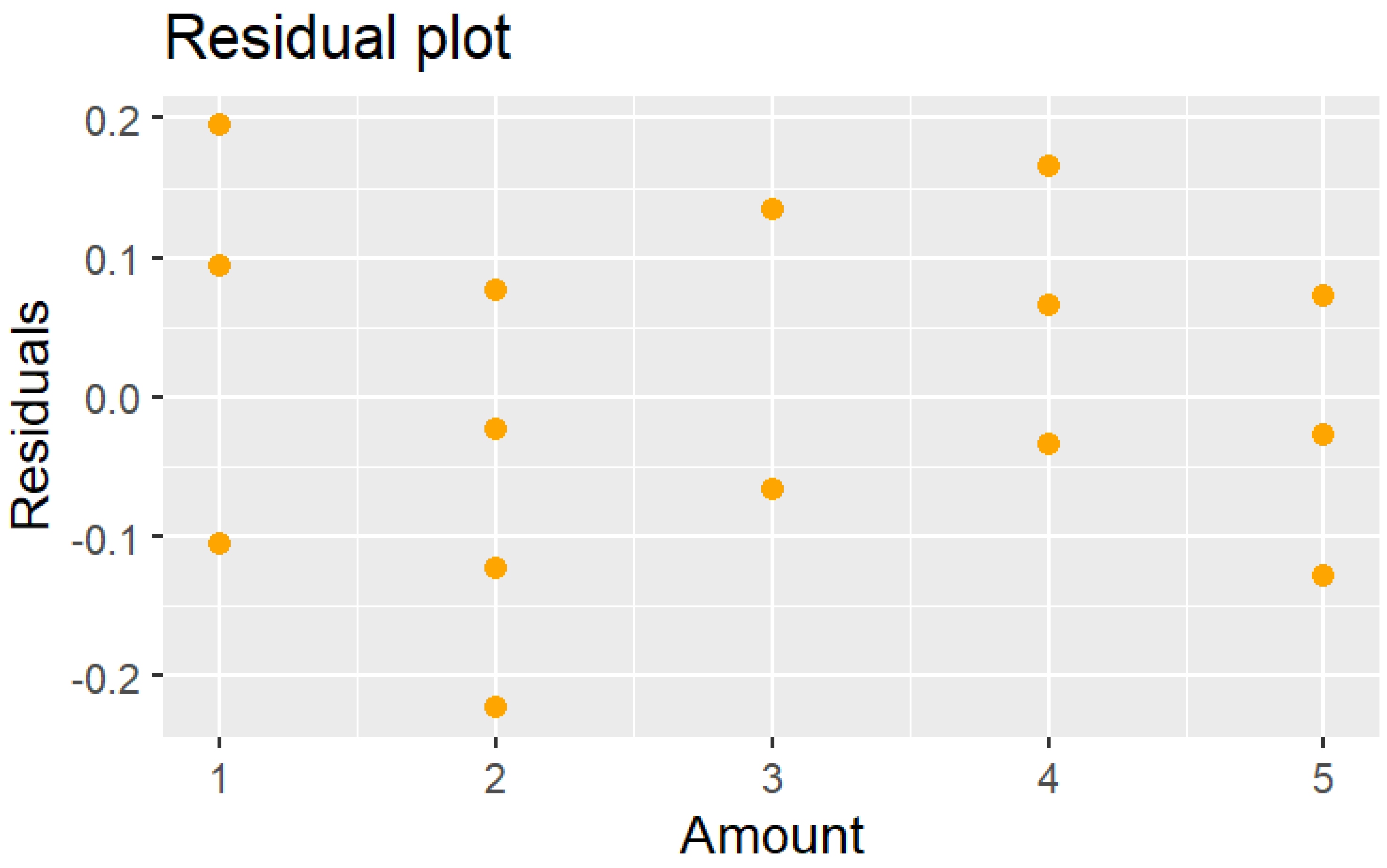
Fitting a Quadratic

```
amount.c<-scale(amount,scale=F)
lm.quad=lm(strength~amount.c + I(amount.c^2))
summary(lm.quad)
```

$$\hat{Y}_i = 2.88 + 0.09(x_i - \bar{x}) - 0.04(x_i - \bar{x})^2$$

```
Call:
lm(formula = strength ~ amount.c + I(amount.c^2))


Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    2.88358    0.03783  76.228  < 2e-16 ***
amount.c       0.09202    0.01807   5.091 6.49e-05 ***
I(amount.c^2) -0.03728    0.01535  -2.428   0.0253 *
```

Residual Plot



Third degree polynomial

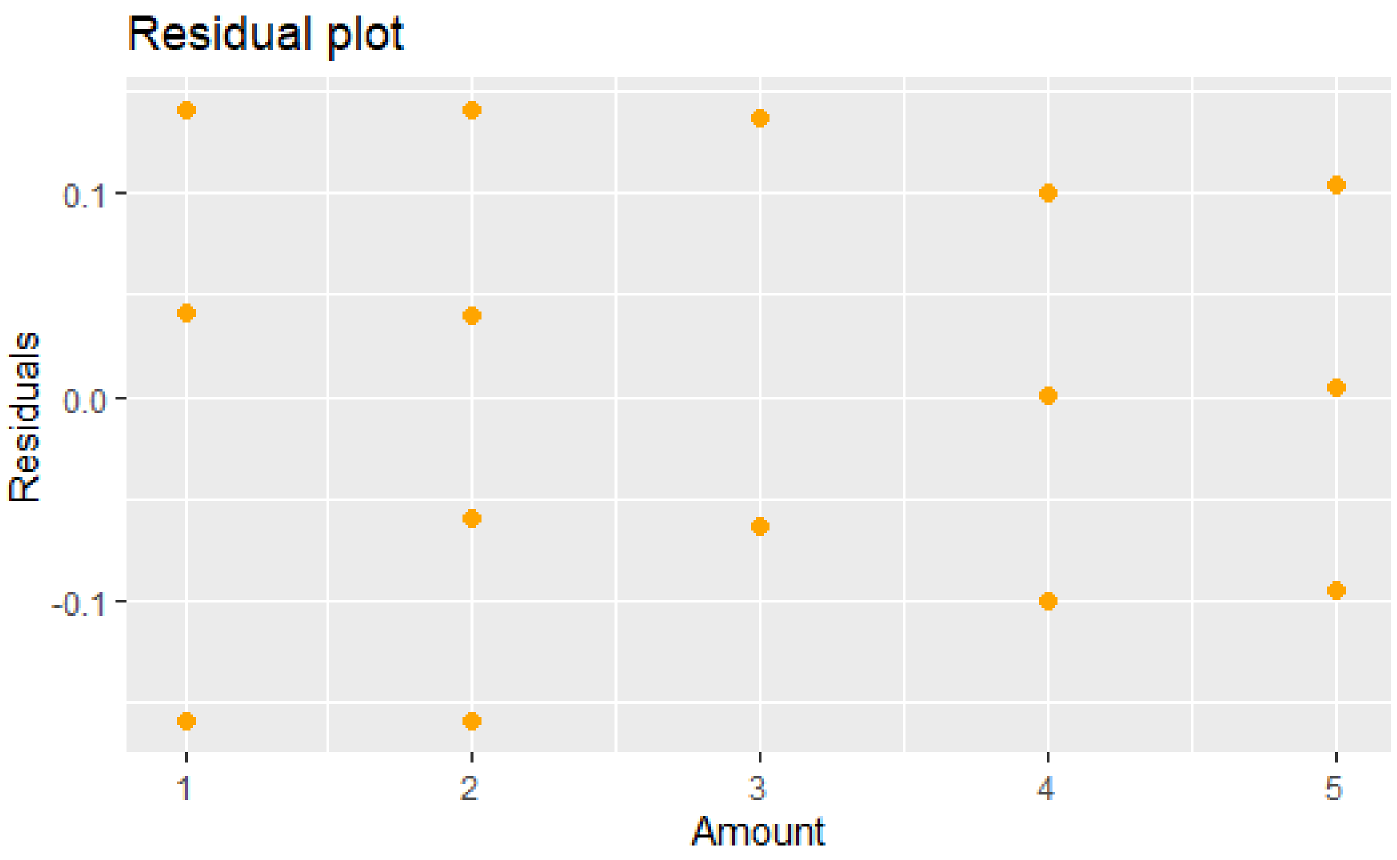
```
lm.quad=lm(strength ~ amount.c + I(amount.c^2) + I(amount.c^3))

summary(lm.quad)
ggplot(lm.quad,aes(x=amount,y=resid(lm.quad)))+geom_point(color="orange",size=2)+labs(title="Residual plot", x="Amount", y="Residuals")
```

Model:

```
Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)     2.89841    0.03495  82.934  < 2e-16 ***
amount.c        0.18335    0.04372   4.194 0.000546 ***
I(amount.c^2) -0.04979    0.01500  -3.320 0.003805 **
I(amount.c^3) -0.02862    0.01270  -2.254 0.036927 *
```

$$\hat{Y}_i = 2.90 + 0.18(x_i - \bar{x}) - 0.05(x_i - \bar{x})^2 - 0.03(x_i - \bar{x})^3$$

Residual Plot



When a straight line is inappropriate

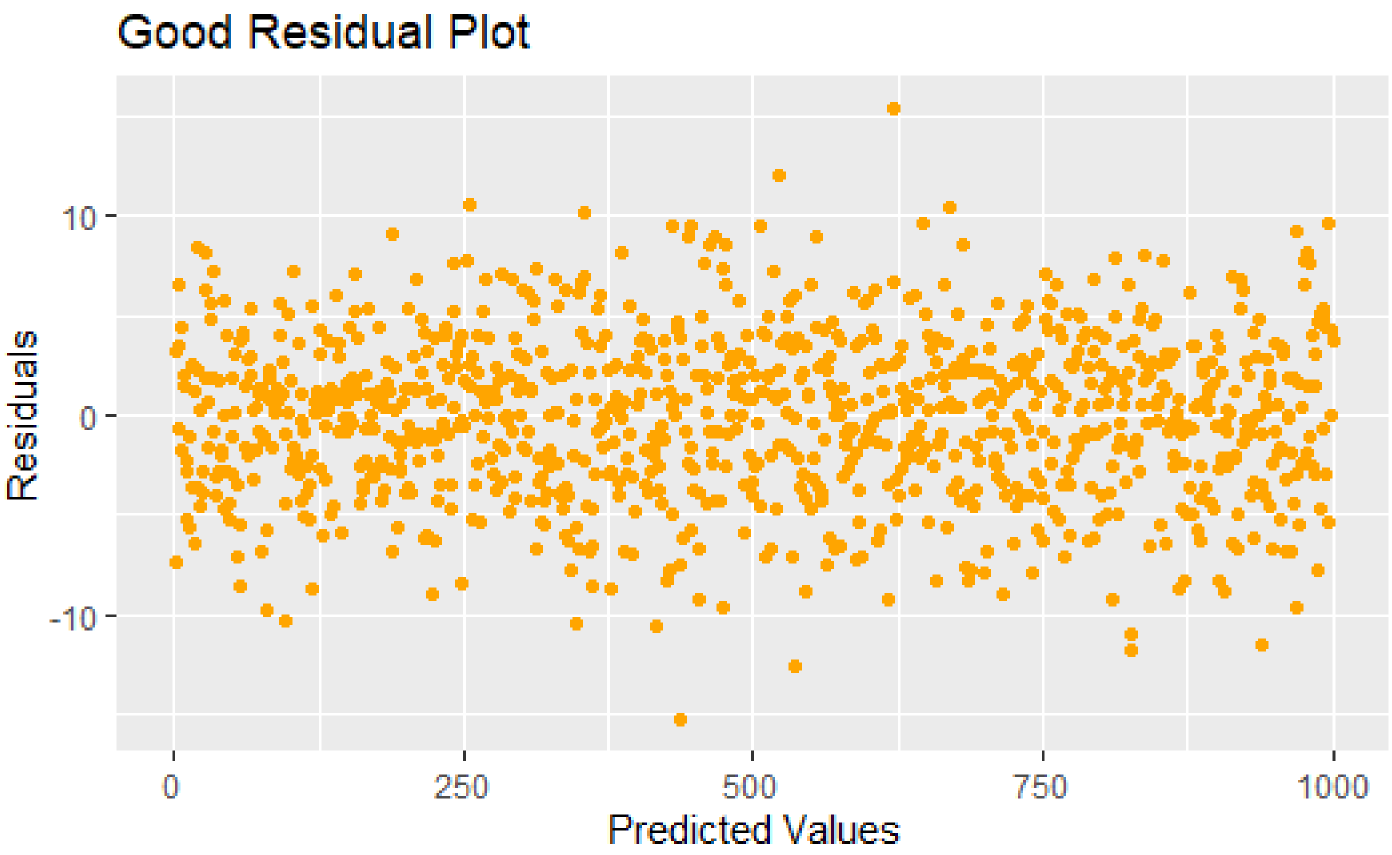
Consider the following options:

- Fit a polynomial/more complex regression model.
- Transform the dependent and/or independent variables to obtain linearity.
- Fit a nonlinear regression model, if appropriate.
- Fit a nonparametric regression model (for example, LOESS or Splines)

Lack of Constant Variance

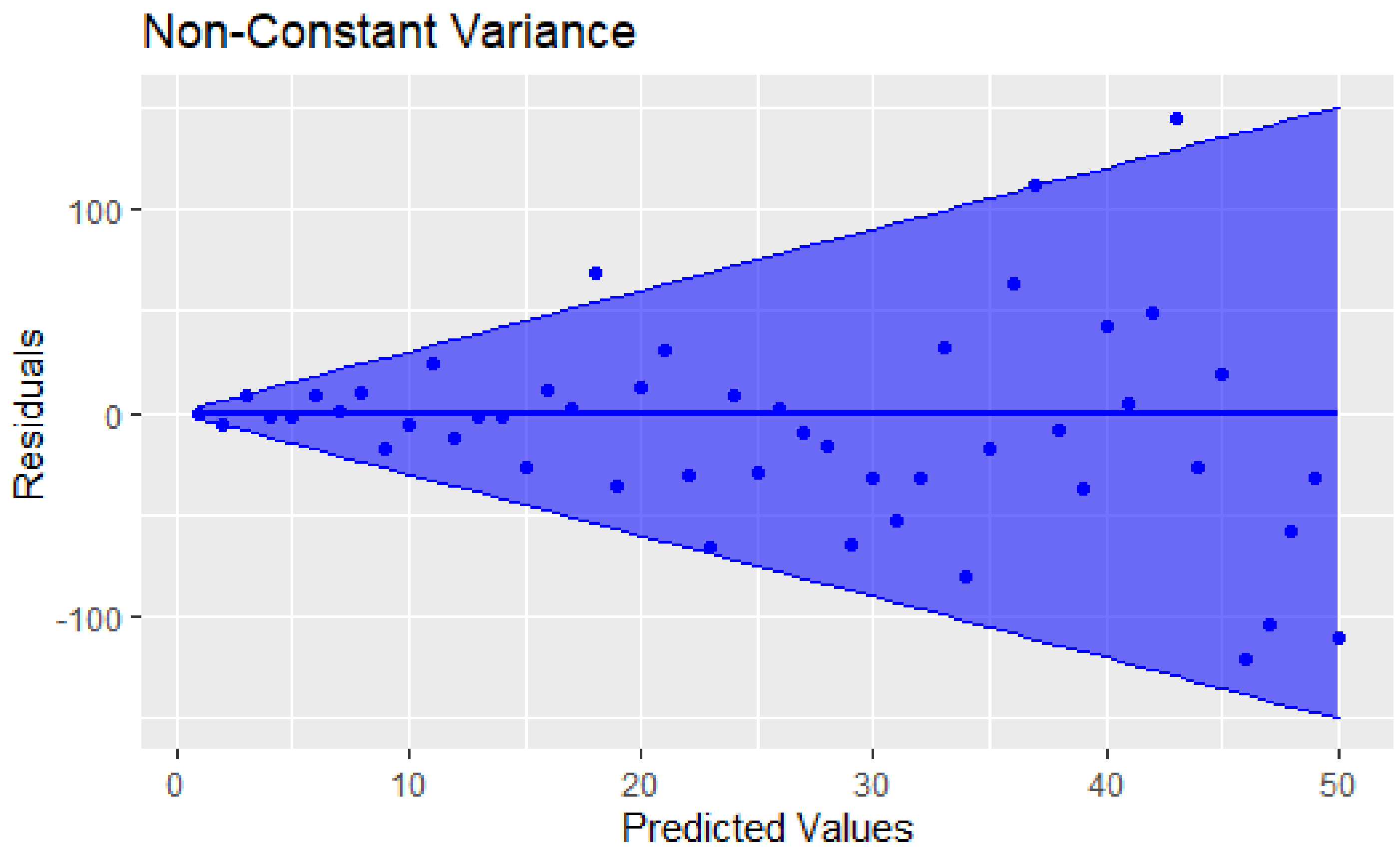
Homoscedasticity

- The random error term, ε, is assumed to have a constant variance, σ^2 (**homoscedasticity**).



Homoscedasticity

- The random error term, ε, is assumed to have a constant variance, σ^2 (**homoscedasticity**).
- This is an example of **heteroscedasticity**.
  - Does ***not*** affect the calculation of the parameter estimates.
  - Does affect the standard errors of the parameter estimates.



Heteroscedasticity

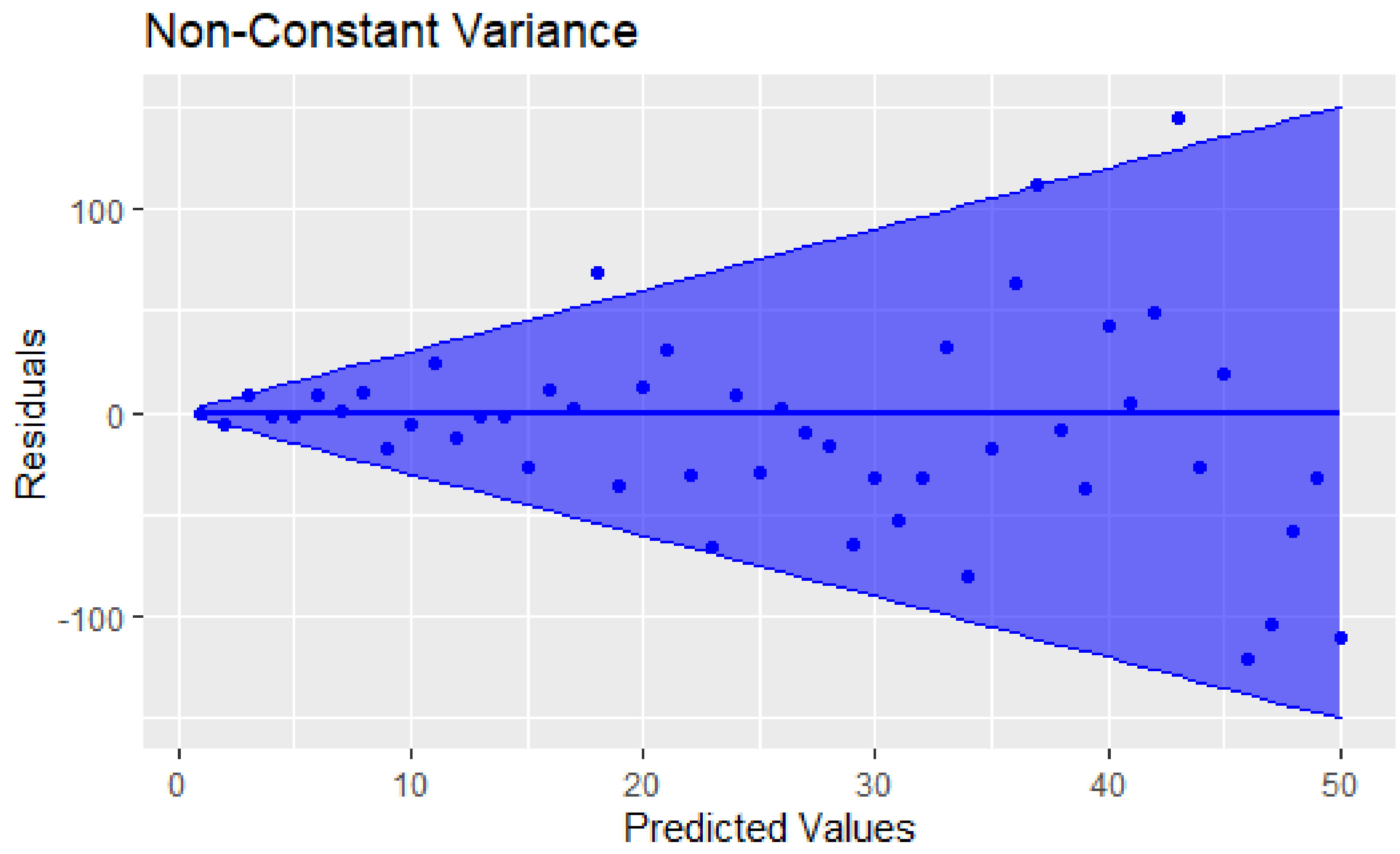
- Any inferences under the traditional assumptions will be incorrect.
- Hypothesis tests and confidence intervals based on the t, F, χ^2 distributions will not be valid.

Detecting Heteroscedasticity

- There are a couple of approaches to detecting heteroscedasticity in a data set.
  1. Plotting residuals and looking for patterns.
  2. Spearman Rank Correlation

The Spearman correlation uses ranks of the data (still between -1 and 1)

Detecting Heteroscedasticity



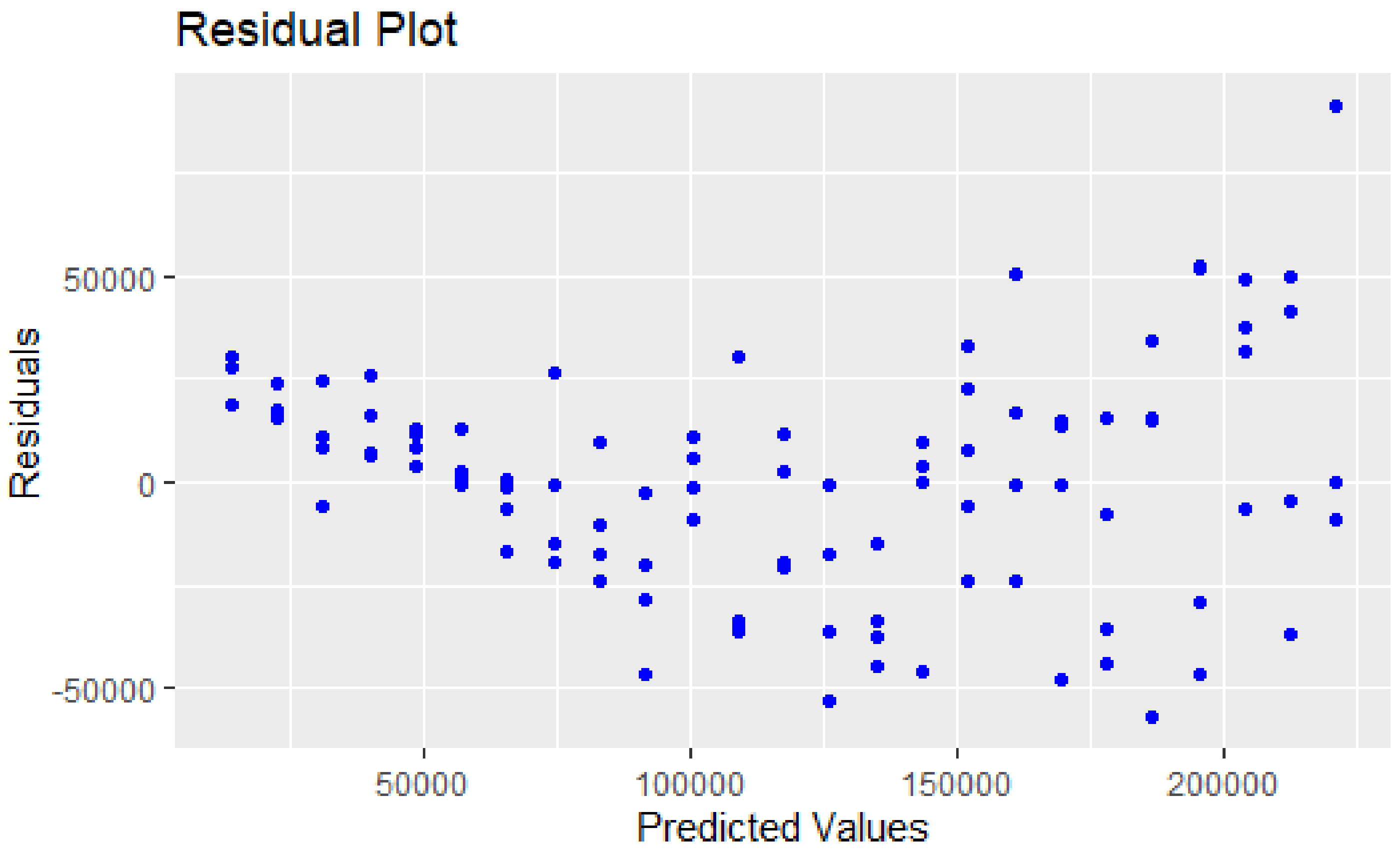
Plotting residuals and looking for patterns.

Spearman Rank Correlation

- If the Spearman rank correlation coefficient between the ***absolute value of the residuals*** and the ***predicted values*** is
  - close to zero, then the variance is potentially homoscedastic
  - positive, then the variance increases as the mean increases
  - negative, then the variance decreases as the mean increases
  - Can perform a test: H_0: variance is homoscedastic
    H_A: variance is heterscedastic
  - If there is a relationship between the absolute value of residuals and predicted value but it is not linear, this test will NOT discover it

Transformations

Salary data set



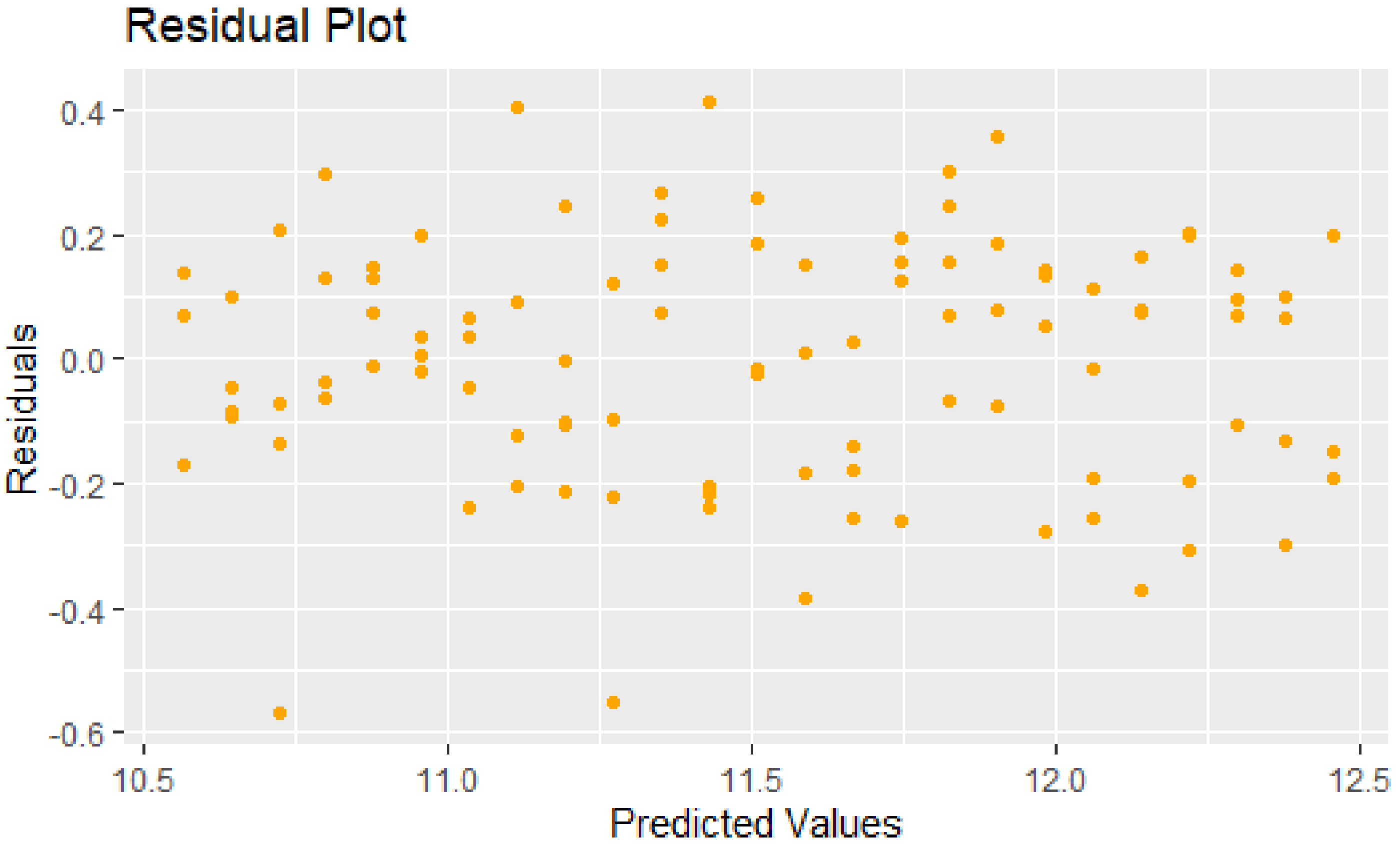

```
lm.var=lm(salary~years)

ggplot(lm.var,aes(x=fitted(lm.var),y=resid(lm.var)))+geom_point(color=
"blue")+labs(title="Residual Plot", x="Predicted Values",y="Residuals")
```

Spearman rank correlation test

```
cor.test(abs(resid(lm.var)),fitted.values(lm.var),method="spear
man",exact=T)

        Spearman's rank correlation rho

data:  x and y
S = 115122, p-value = 0.001747
alternative hypothesis: true rho is not equal to 0
sample estimates:
      rho
0.3091986
```

Use variance-stabilizing transformation

```
lm.var=lm(log(salary)~years)

ggplot(lm.var,aes(x=fitted(lm.var),y=resid(lm.var)))+geom_point(color=
"orange")+labs(title="Residual Plot", x="Predicted
Values",y="Residuals")
```



Weighted Least Squares

Weighted Least Squares (WLS)

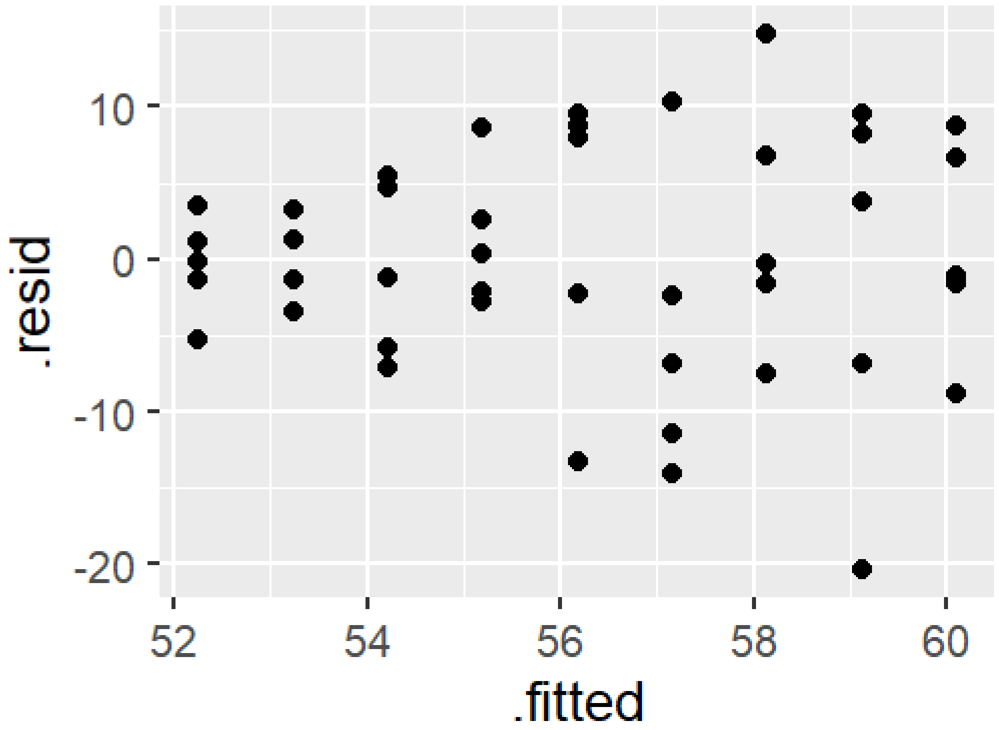
- The idea is that we are placing a “weight” on each observation
- This weight is used to calculate the standard error (adjusts for the varying variances across the fitted values
- The hardest part is deciding what the weights should be?
- Some possible ideas: 1/fitted values^2 OR if you have several observations at each x, you can estimate the standard deviation of the observations within each x-value and use the weights: 1/(standard deviation)^2

Example:

Create data and run model

```
x<-c(rep(2:10,each=5))
set.seed(26785)
error<-rnorm(length(x),0,x)
y<-50 + 1.2*x + error
model1<-lm(y~x)
ggplot(model1, aes(x = .fitted, y =
.resid)) +  geom_point()
```

Residual Plot



WLS

WLS – compare results

```
summary(model1)
weights1<-1/x^2
model2<-lm(y~x, weights =
weights1)
summary(model2)
weights2<-1/model1$fitted.values^2
model3<-lm(y~x,weights=weights2)
summary(model3)
```

Summaries:

MODEL1:

	Estimate	Std. Error	t value
(Intercept)	50.2878	2.8033	17.939
x	0.9811	0.4292	2.286

MODEL2:

	Estimate	Std. Error	t value
(Intercept)	49.9844	1.4734	33.926
x	1.0408	0.3641	2.858

MODEL3:

	Estimate	Std. Error	t value
(Intercept)	50.2946	2.6490	18.986
x	0.9799	0.4194	2.337

Other methods to adjust standard errors

Robust Standard Errors

- There are several methods developed that create robust standard errors (different algorithms for different “robustness”)
- The package estimatr has several methods for this (“HC0” – “HC3”)
- Recommend either “HC1” or “HC2”
- “HC1” is the Eicker-Huber-White variance, this one performs best for small samples
- “HC2” is more efficient than “HC1”

Robust standard errors

OLS:

	Estimate	Std. Error	t value
(Intercept)	50.2878	2.8033	17.939
x	0.9811	0.4292	2.286

WLS:

	Estimate	Std. Error	t value
(Intercept)	50.2487	2.3435	21.44
x	0.9871	0.3948	2.50

HC1: model3<-lm_robust(y~x,se_type = "HC1")

summary(model3)

	Estimate	Std. Error	t value
(Intercept)	50.2878	1.8577	27.070
x	0.9811	0.3802	2.581

HC2: model4<-lm_robust(y~x)

summary(model4)

	Estimate	Std. Error	t value
(Intercept)	50.2878	1.8672	26.932
x	0.9811	0.3825	2.565

Accounting for Heteroscedasticity

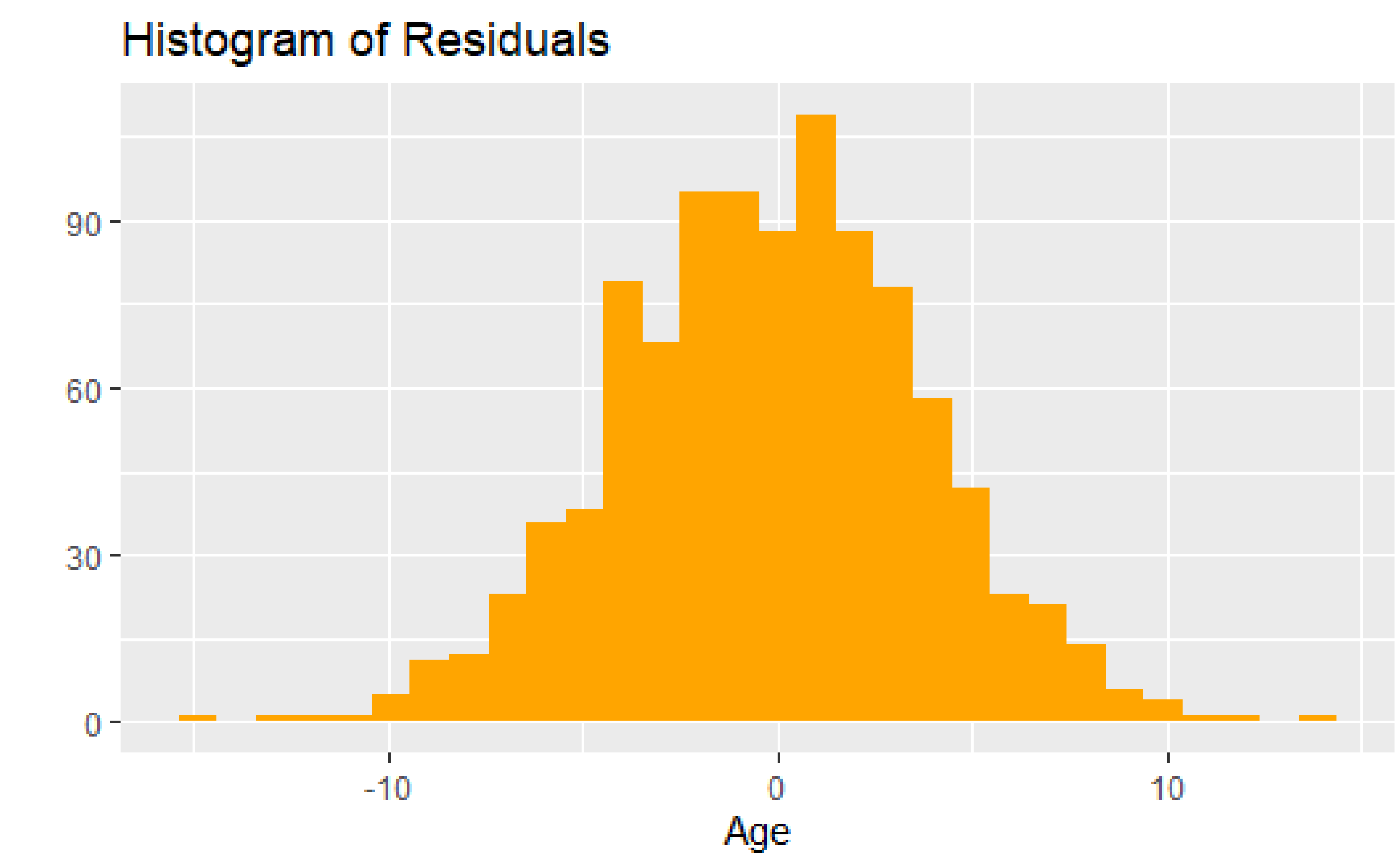
- If heteroscedasticity is evident in your model, you can consider:
  - Transform data.
  - Use Weighted Least Squares (WLS) or iteratively reweighted least squares (IRLS).
  - Use sandwich standard error methods
  - Use a different distribution (for example, if count data, a Poisson distribution is more appropriate….will be discussed later)

Lack of Normality

Detecting Lack of Normality

- Check that the error terms are Normally distributed by examining:
  - Histogram of the residuals
  - Normal probability plot of the residuals (QQ-plot)
  - Formal tests for Normality

Detecting Lack of Normality



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Detecting Lack of Normality

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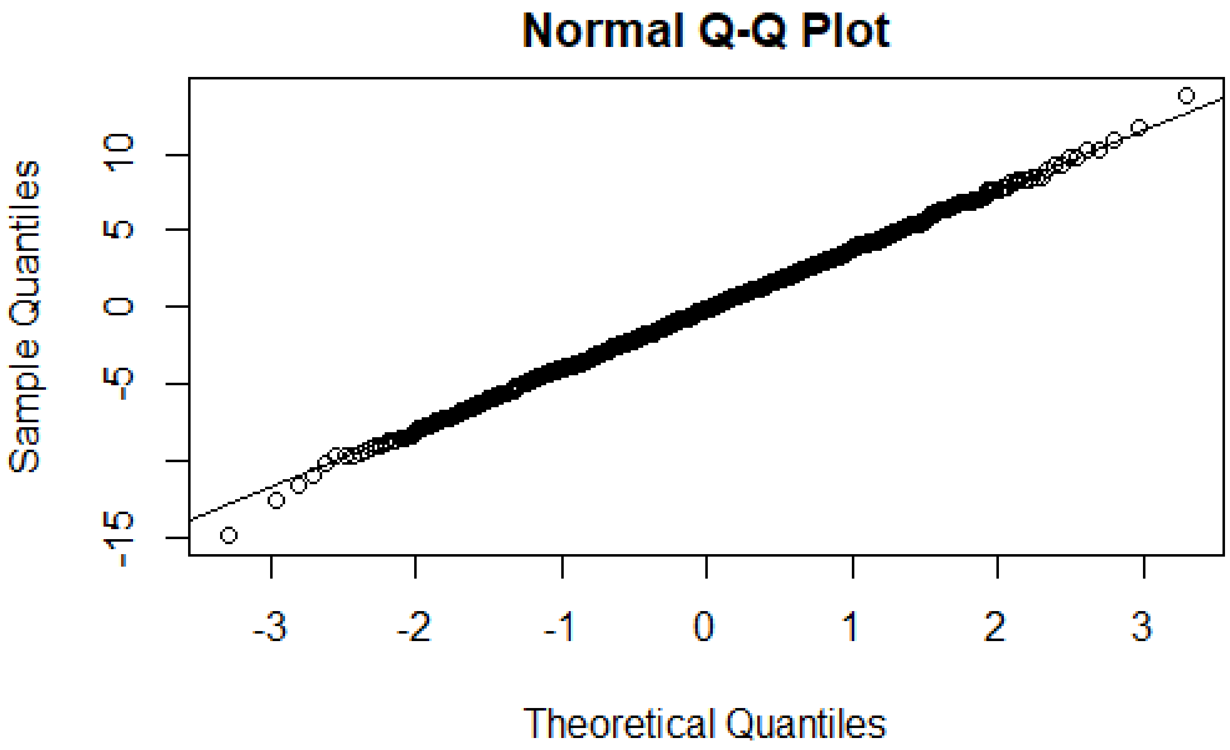
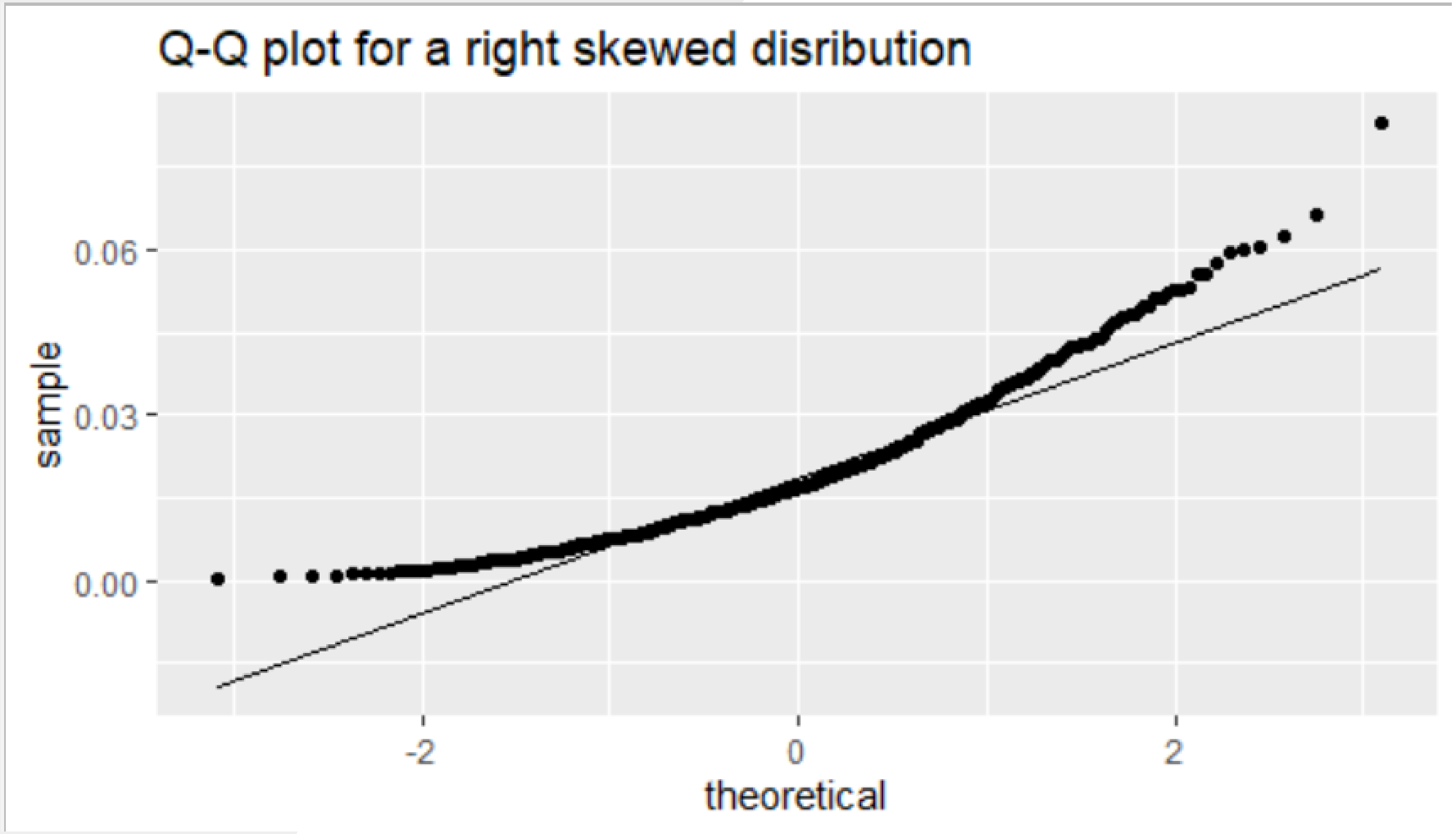
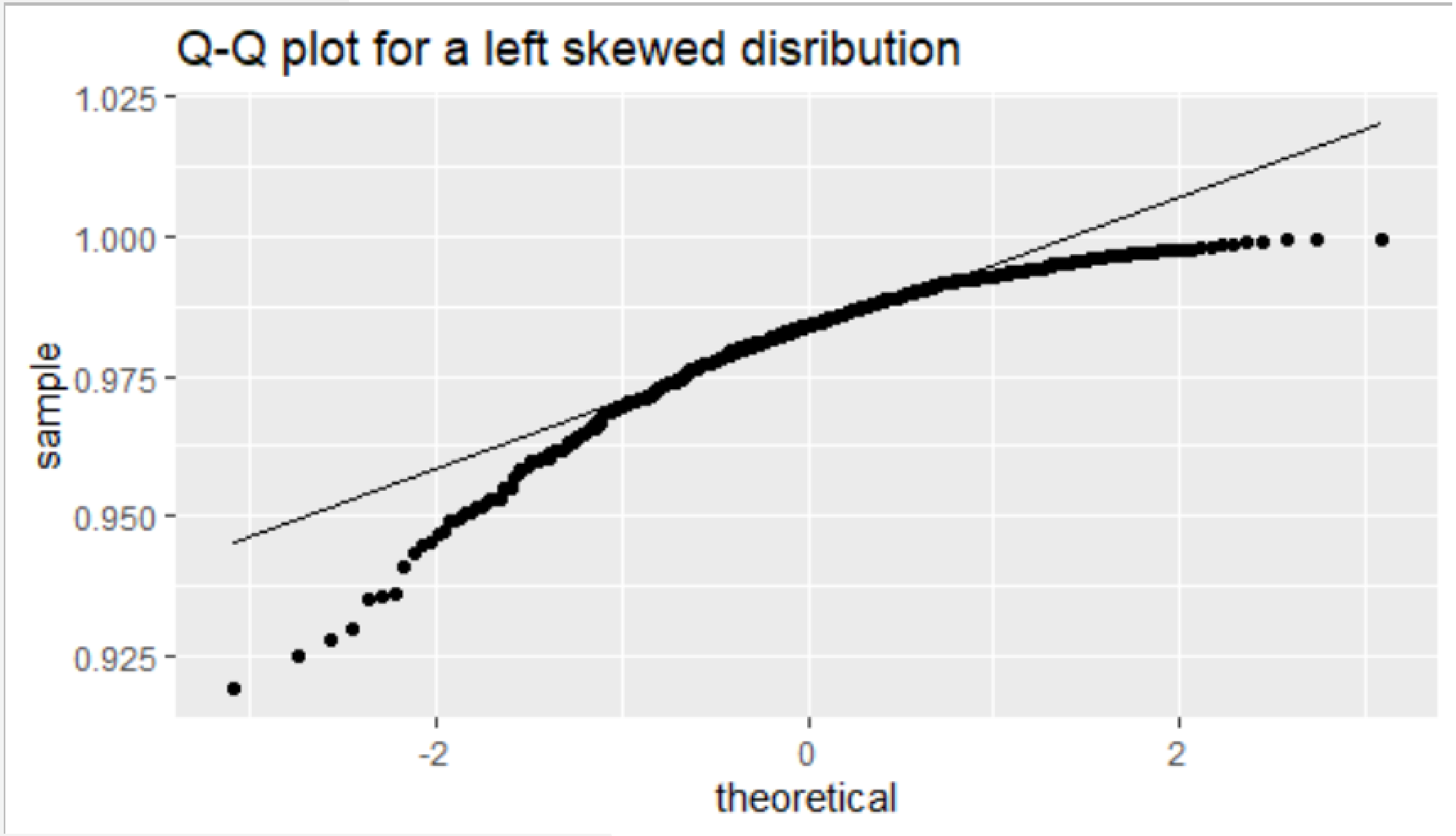
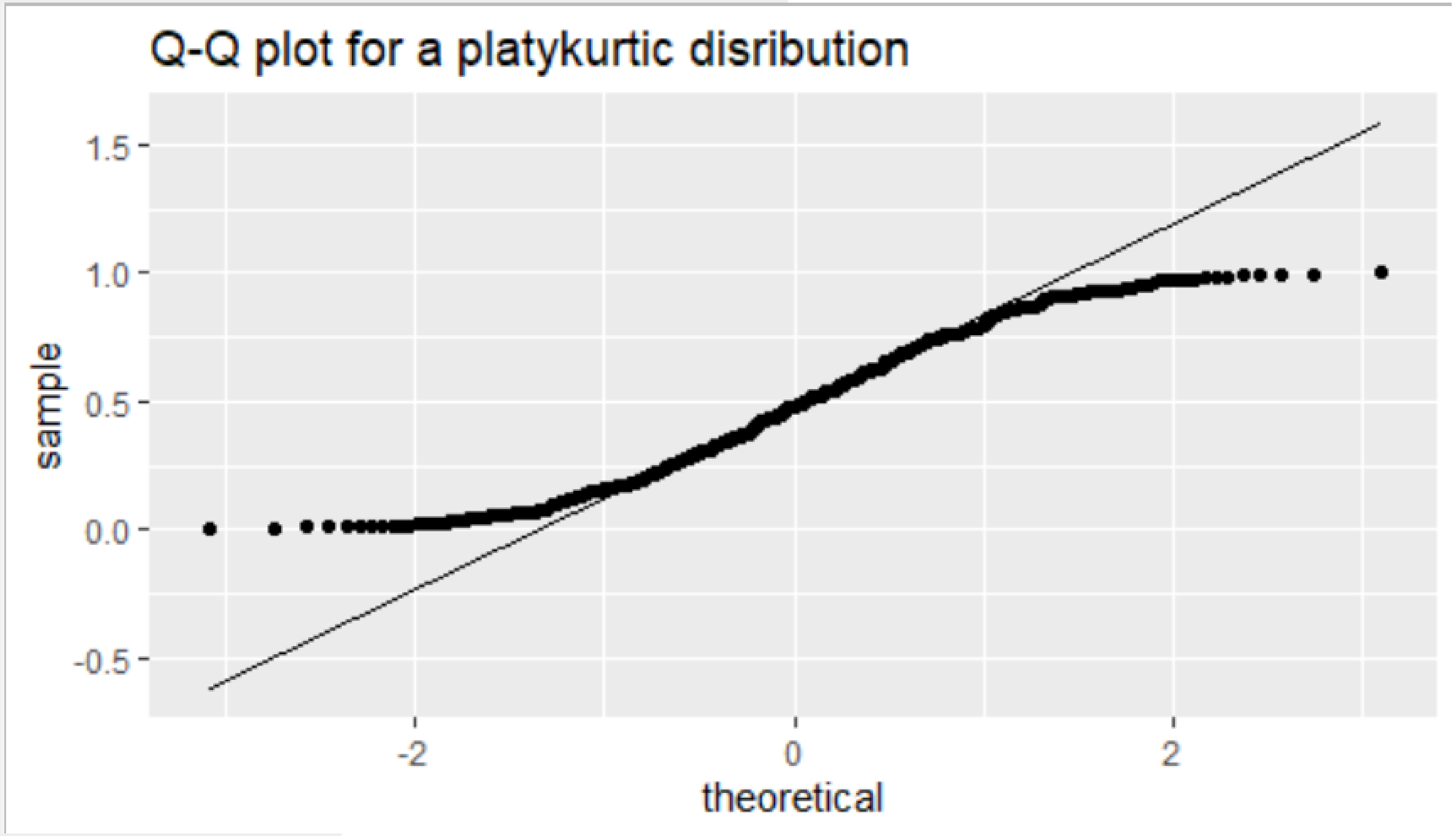
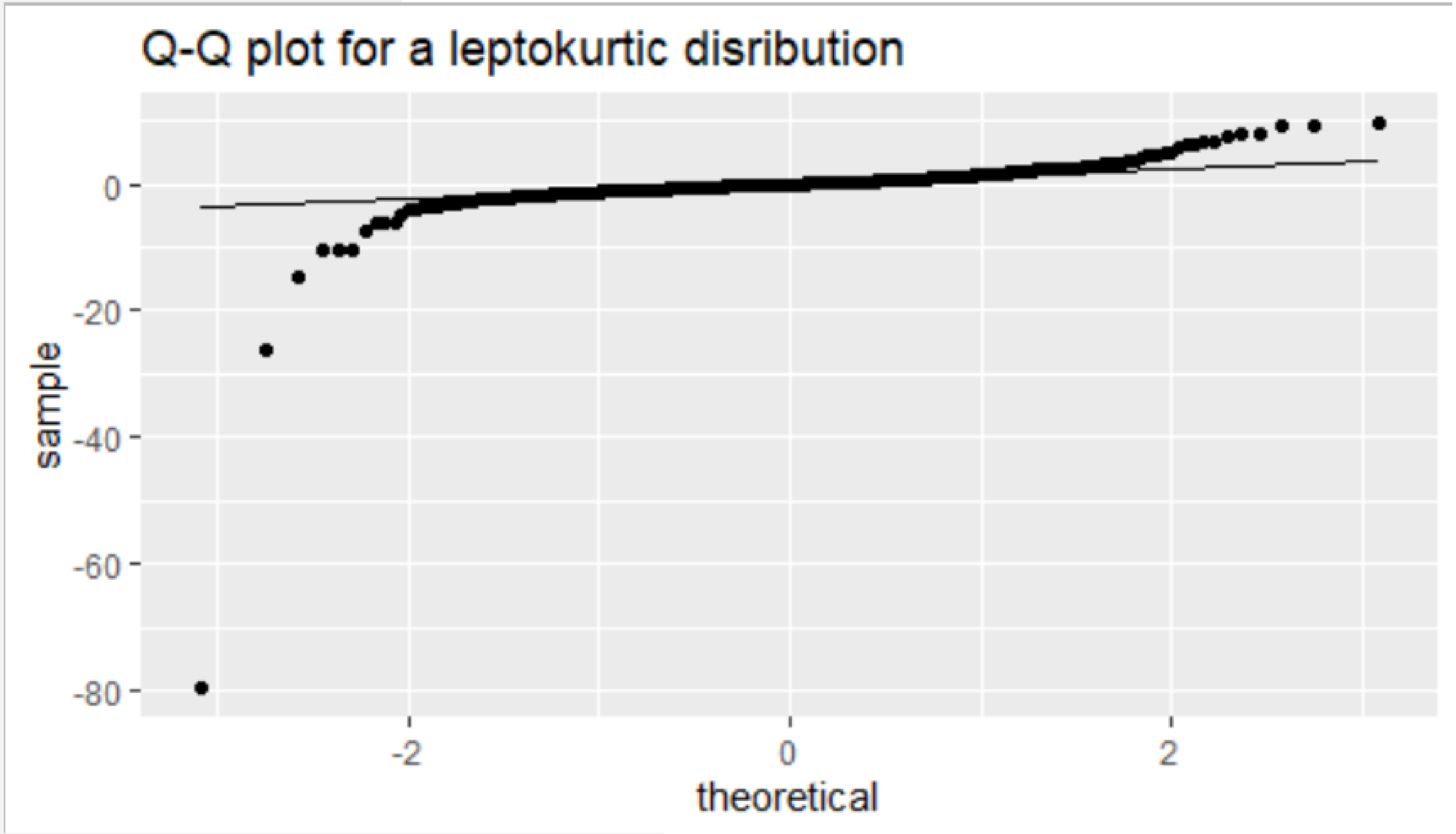



Q-Q plot for a right skewed disribution
sample
0.06
0.03
0.00
-2
0
2
theoretical



Q-Q plot for a left skewed disribution
1.025
1.000
0.975
0.950
0.925
sample
-2
0
2
theoretical


Q-Q plot for a platykurtic disribution
1.5
1.0
0.5
0.0
-0.5
sample
-2
0
2
theoretical



Q-Q plot for a leptokurtic disribution
0
-20
-40
-60
-80
sample
-2
0
2
theoretical

Detecting Lack of Normality

- Check that the error terms are Normally distributed by examining:
  1. Histogram of the residuals
  2. Normal probability plot of the residuals (QQ-plot)
  3. Formal tests for Normality

$$H_0: \text{Normality}$$
$$H_A: \text{Not Normality}$$

Tests for Normality

There are numerous tests for normality. Most have the same null and alternative hypotheses. We will illustrate the following tests:

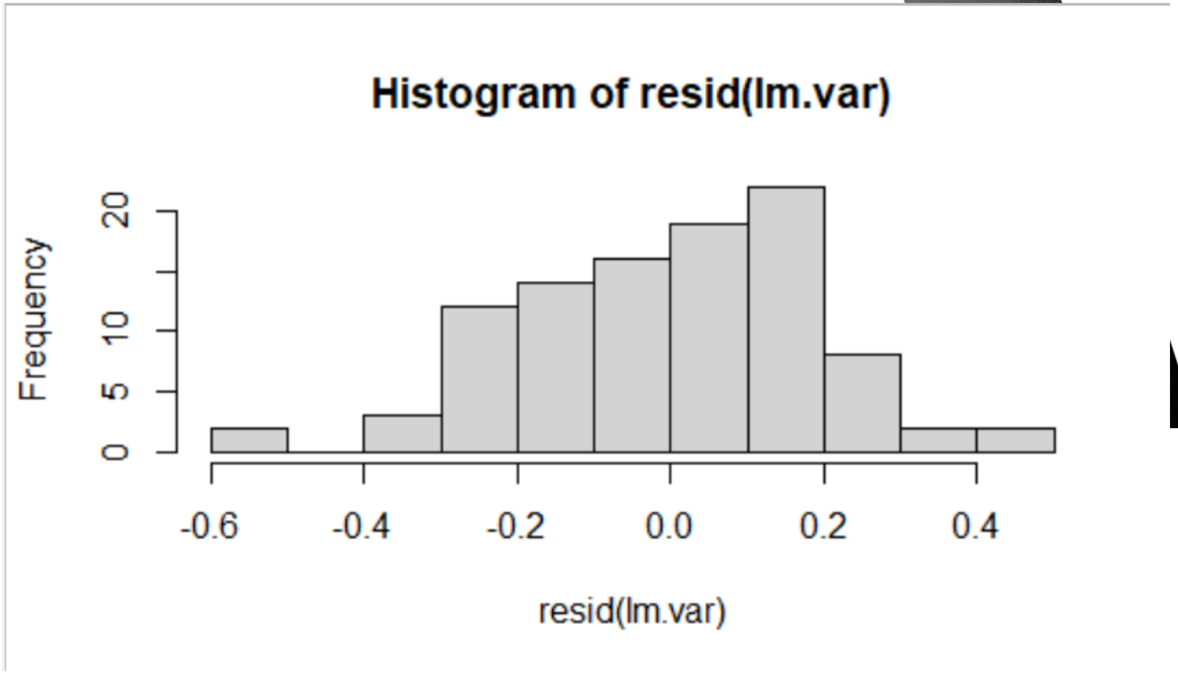
$$H_0\text{: Normally Distributed}$$

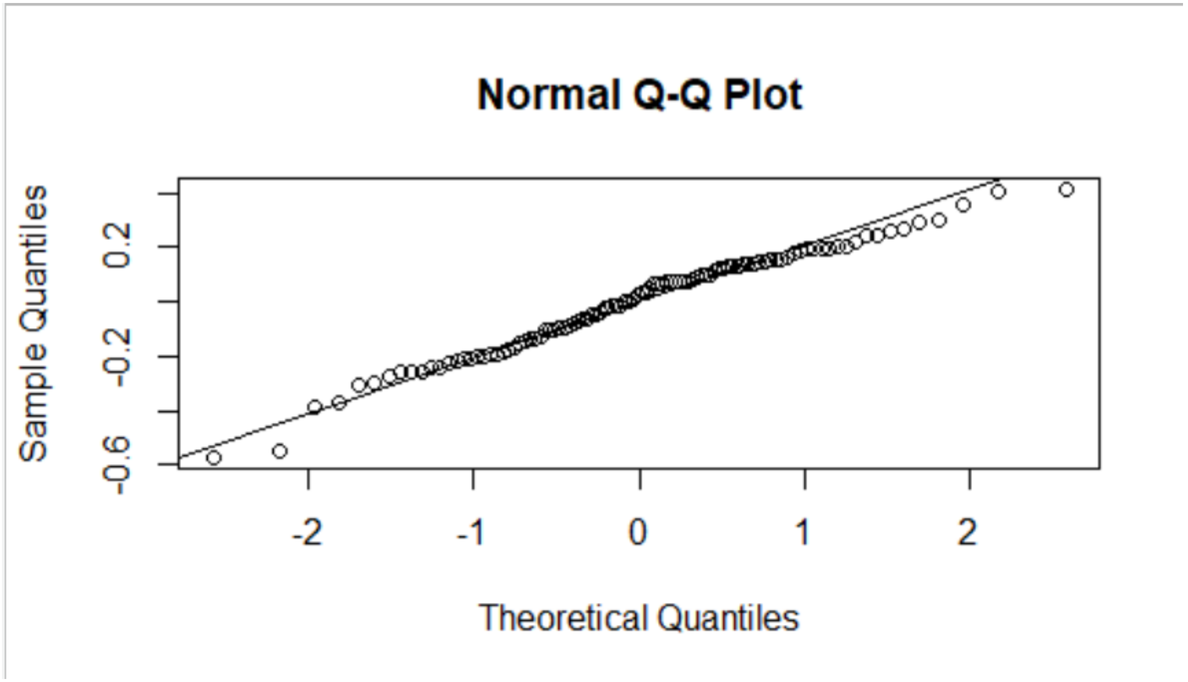
$$H_A\text{: Not Normally Distributed}$$

1. Anderson-Darling is based on the empirical cumulative distribution function of the data and gives more weight to the tails.
2. Shapiro-Wilk test uses the idea of correlation between the sample data and normal scores. The Shapiro-Wilk is better for smaller data sets.

Log(Salary) model (nortest in R)

```
> hist(resid(lm.var))
> qqnorm(resid(lm.var))
> qqline(resid(lm.var))
> ad.test(resid(lm.var))

        Anderson-Darling normality test

data:  resid(lm.var)
A = 0.61387, p-value = 0.1074

> shapiro.test(resid(lm.var))

        Shapiro-Wilk normality test

data:  resid(lm.var)
W = 0.98033, p-value = 0.141
```





Accounting for Lack of Normality

Depends on why the lack of Normality occurred:

- Outliers → Robust Regression (quantile regression or WLS)
- Nonnormal→ Transformation Needed
  - Can try Box-Cox transformation
- Use another distribution (Poisson, Gamma…)

Box-Cox transformation

- Box-Cox (1964) developed a method to determine the best (power) transformation to induce normality.
- The Box-Cox transformation has the following form:

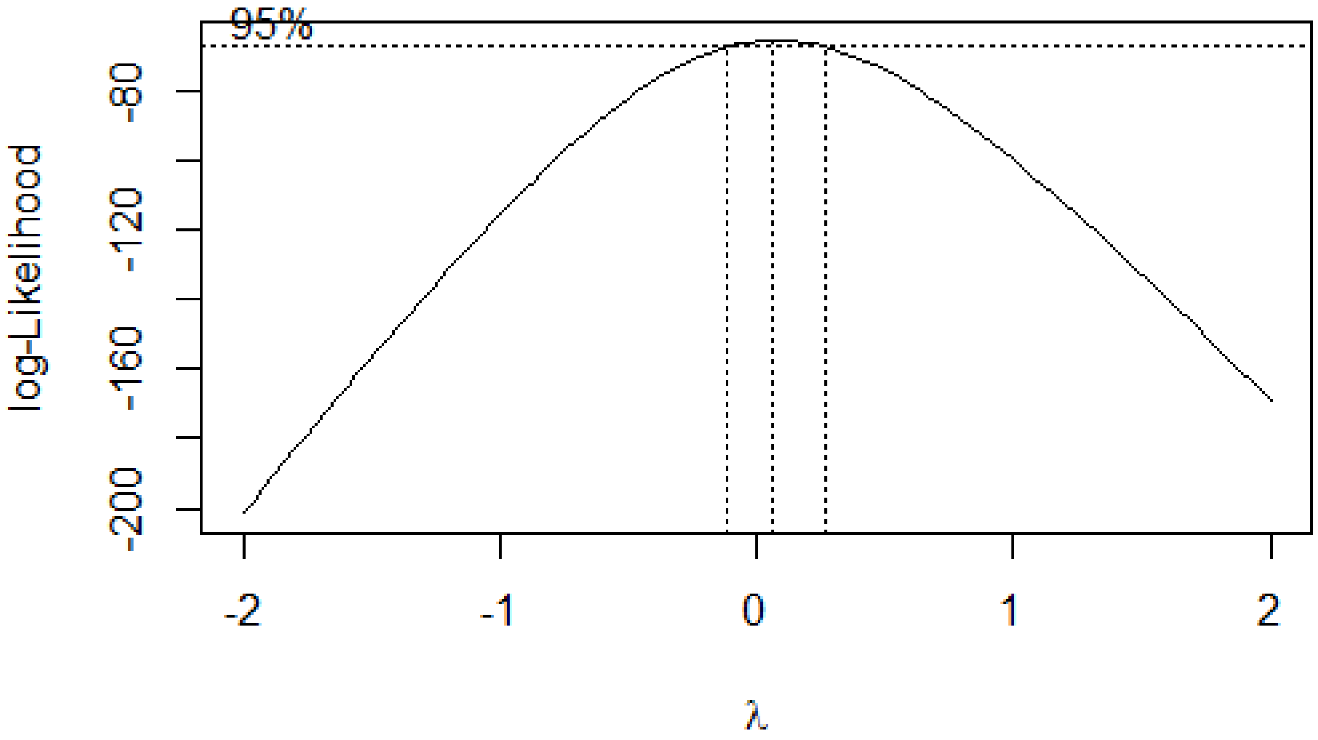
$$\begin{matrix} (y^{\lambda} - 1)/\lambda & \lambda \neq 0 \\ \log(y) & \lambda = 0 \end{matrix}$$

- λ is the power in which the response variable y is raised to (so, if $\lambda = 2$, then we would square y). The exception is when $\lambda=0$ (this the log transformation).

Box-cox on original Salary data set

lm.var=lm(salary~years)

boxcox(lm.var)



Break out and Lab 8

Don’t forget to take the lab check on Moodle!

"Start each day with a positive thought and a grateful heart." – Roy Bennett

Source: Freepik

Correlated Error terms

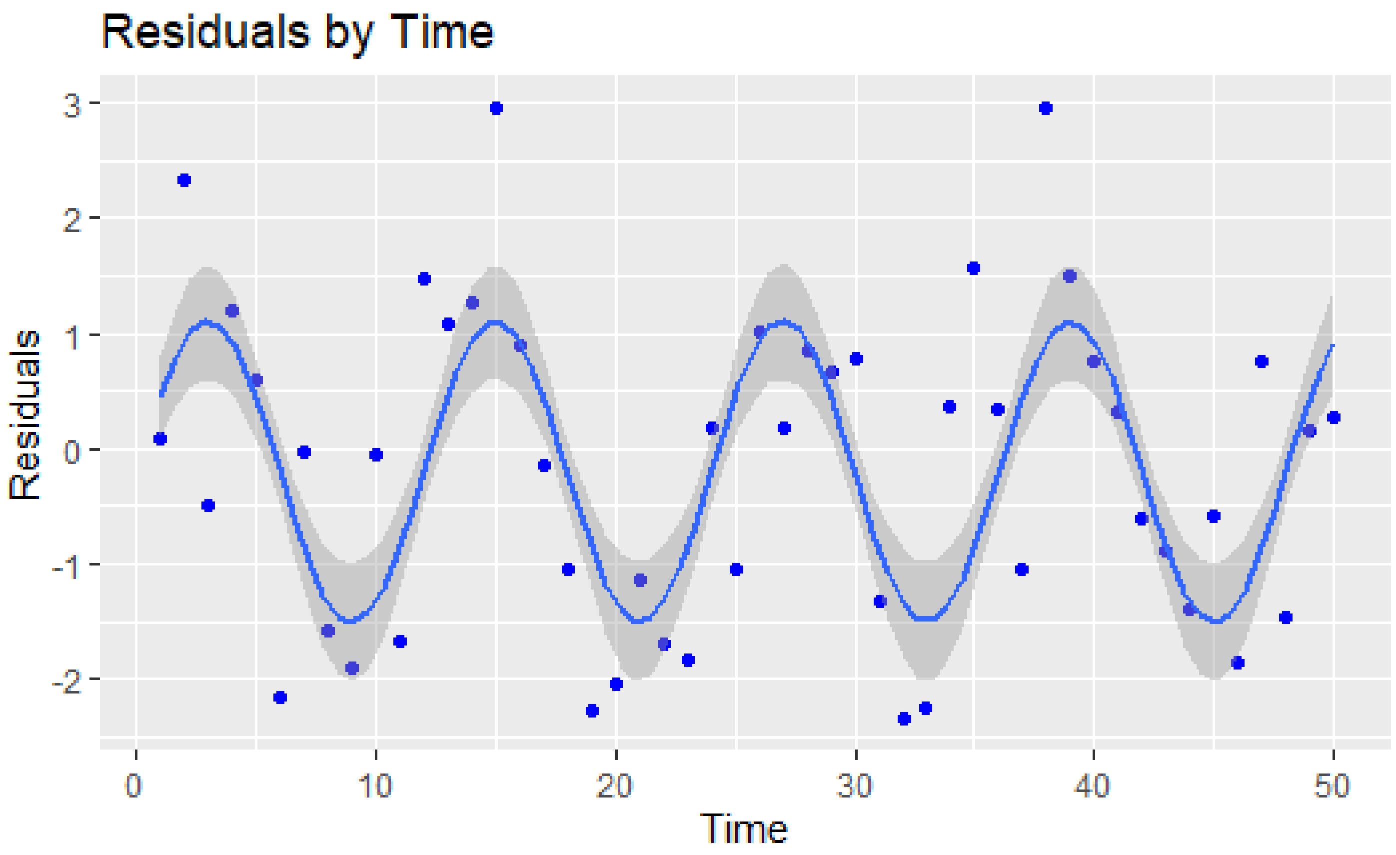
Independence

Know the source of your data:

- Clustered/Grouped data
- Observations connected in some way
- Complex survey designs
- Repeated measures
- Data gathered over time

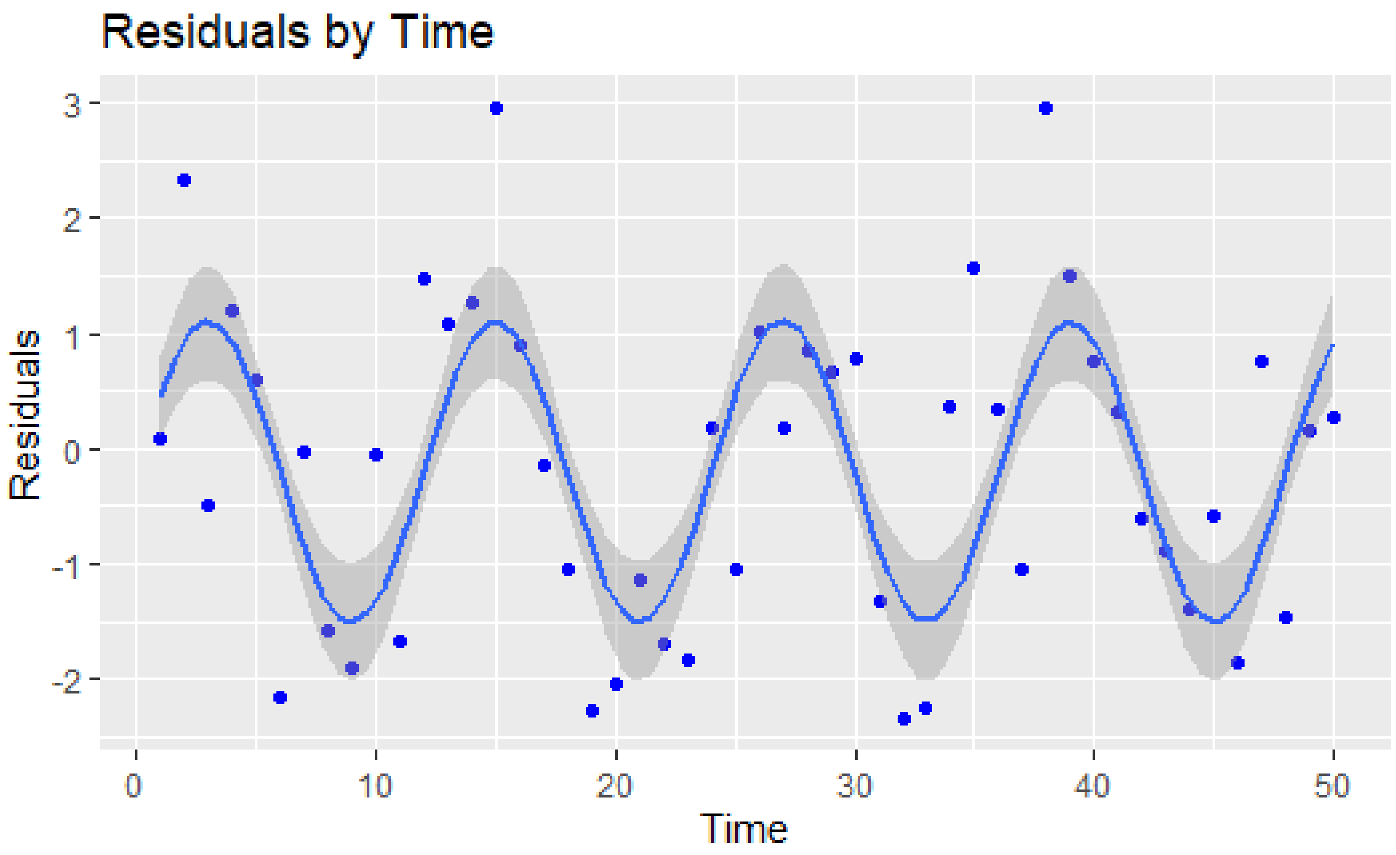
Data dependent on time

- Observations not independent.
- Residuals follow cyclic pattern.
- Collected over time.



Detect non-independence

1. Plots of residuals versus time or other ordering component



Detect non-independence

1. Plots of residuals versus time or other ordering component

2. Durbin-Watson statistic or the first-order autocorrelation statistic for time-series data

H_0: No Residual Correlation
H_A: Residual Correlation

Durbin-Watson test

Statistic:

$$d = \frac{\sum_{t=2}^{T}(e_t - e_{t-1})^2}{\sum_{t=1}^{T} e_t^2}$$

Bounded between 0 and 4. When d=2, we fail to reject H_0 and assume there is not enough evidence supporting autocorrelation. For $d < 2$, possible positive autocorrelation (this is the one usually used). For $d > 2$, there is possible negative autocorrelation.

Google stock data

```
data(google)
x=seq(1,length(google))
lm.model=lm(google~x)
###Testing for POSITIVE AUTOCORRELATION
dwtest(lm.model,alternative="greater")
```

```
        Durbin-Watson test

data:  lm.model
DW = 1.842, p-value = 0.0321
alternative hypothesis: true autocorrelation is greater than 0
```

How to handle correlated error terms

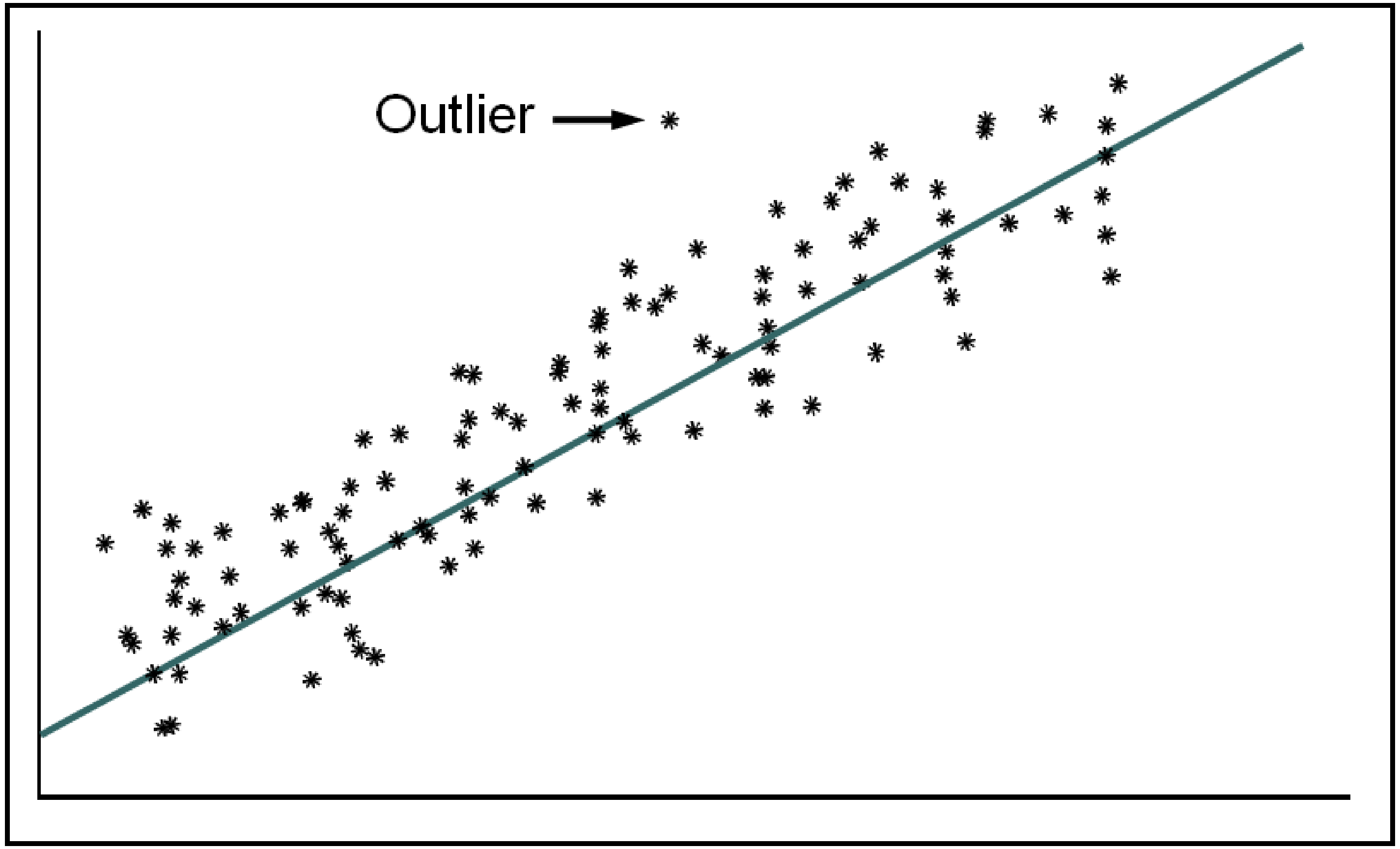
- If correlated due to time, perform time series
- If correlated due to clustered data, perform a hierarchical model
- Longitudinal analysis/panel data

Influential points and outliers

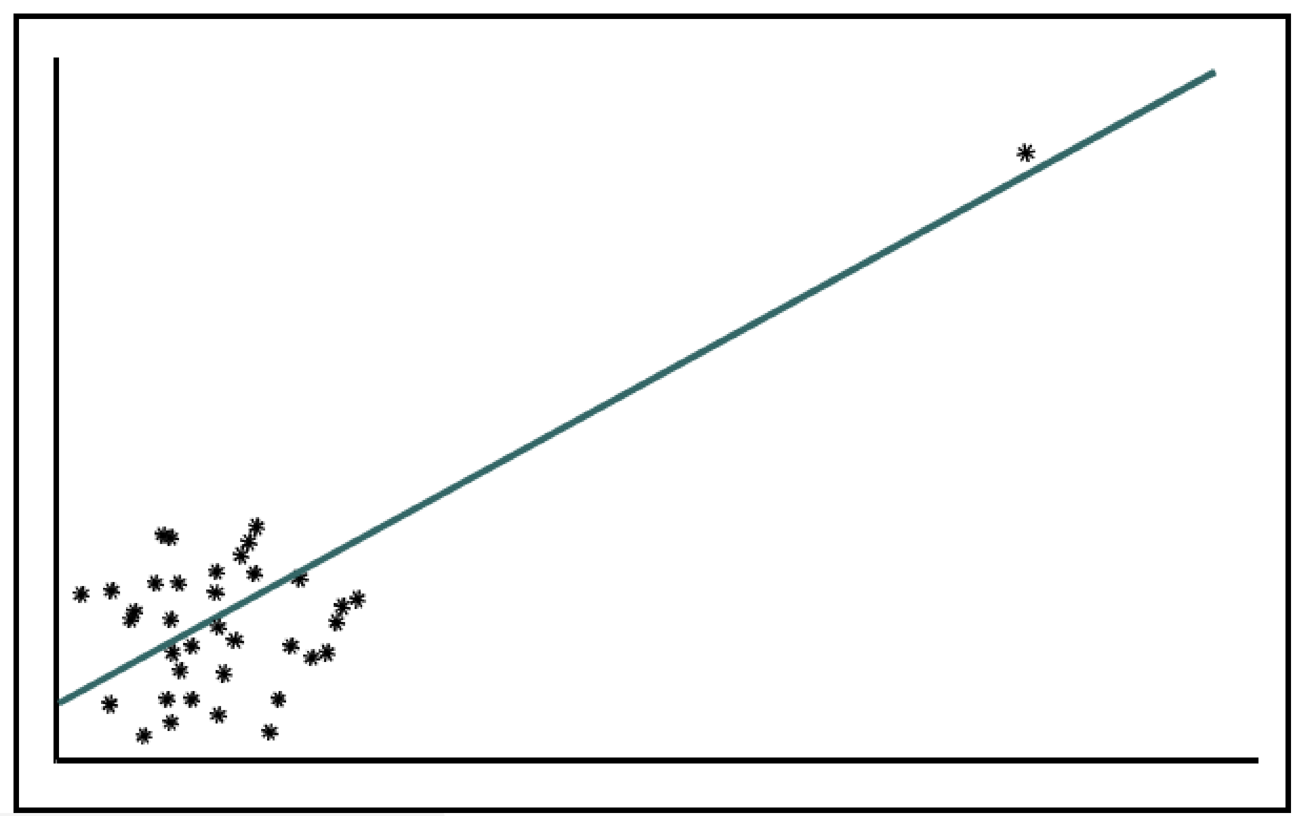
Anomalous observations

- There are two types of anomalous observations that will be discussed:
  1. Outliers – point with a large standardized residual (lie far away from the fitted line in the Y-direction).
  2. Leverage Points – point that falls outside the normal range (far from the mean) in the X-space (possible values of the predictors) and have a large “influence” on the regression line.
- Observations could be one or both of these.

Detecting Outliers

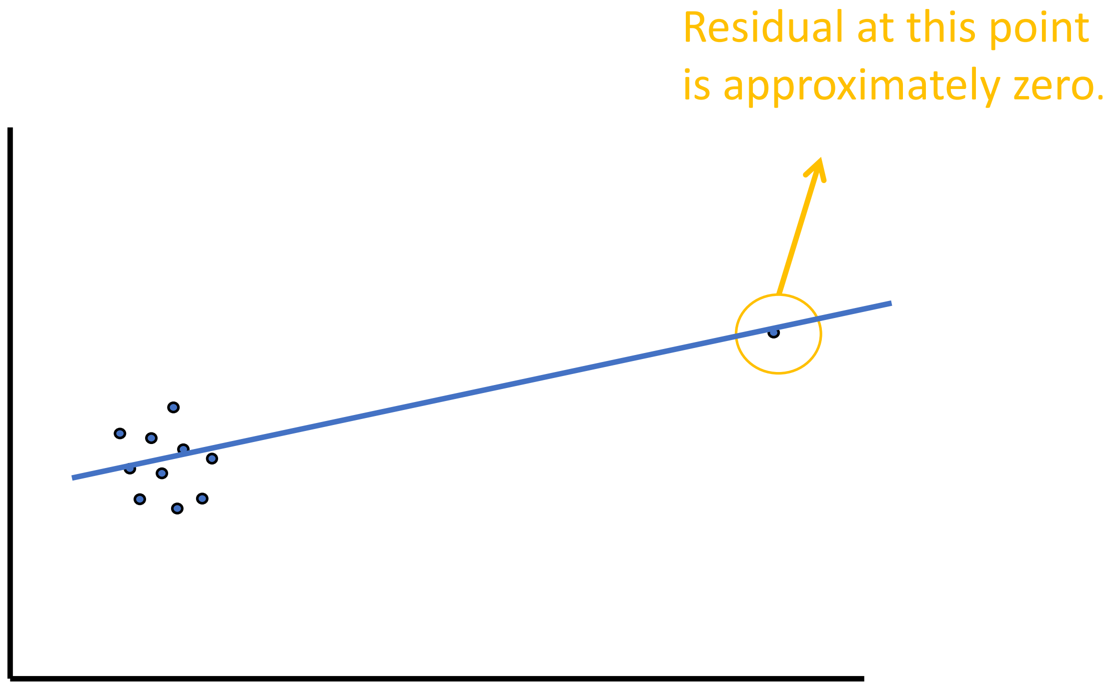


Influential Observations



Residual Analysis

- Don’t only focus efforts on residuals of data.
- Residual analysis only tends to discover outliers instead of leverage points.



Diagnostic Statistics

Statistics that help identify influential observations are the following:

- Standardized residuals (good for detecting outliers)
- Studentized residuals (good for detecting outliers)
- Cook's *D* (good for detecting influential observations)
- DFFITS (good for detecting influential observations)
- DFBETAS (good for detecting influential observations)
- Hat values (good for detecting influential observations)

Studentized Residuals

- Studentized residuals are obtained by dividing the residuals by their standard errors (standard errors are found by deleting that one observation).
- Suggested cutoffs are as follows:
  - $|SR| > 2$ for data sets with a relatively small number of observations
  - $|SR| > 3$ for data sets with a relatively large number of observations

Cook’s D

Cook's distance, also referred to as Cook's D, measures the difference in the regression estimates when the i^{th} observation is left out.
A suggested cutoff is: (other cutoffs suggested: 4/*n*, 0.5, 1)

$$D_i > \frac{4}{n - k - 1}$$

DFFITS

- DFFITS_i measures the impact that the i^{th} observation has on the predicted value.
- A suggested cutoff for influence is shown below:

$$|\,\mathbf{DFFITS_i}\,| > 2\sqrt{\frac{p}{n}}$$

Hat values

- Using matrix notation, the estimate of the parameters is:

$$b = (X'X)^{-1}X'y$$

- Which means the estimated line is:

$$\hat{y} = X(X'X)^{-1}X'y$$

- And the hat values

$$X(X'X)^{-1}X'$$

- A suggested cutoff is:

$$h_{ii} > \frac{2p}{n}$$

DFBETA

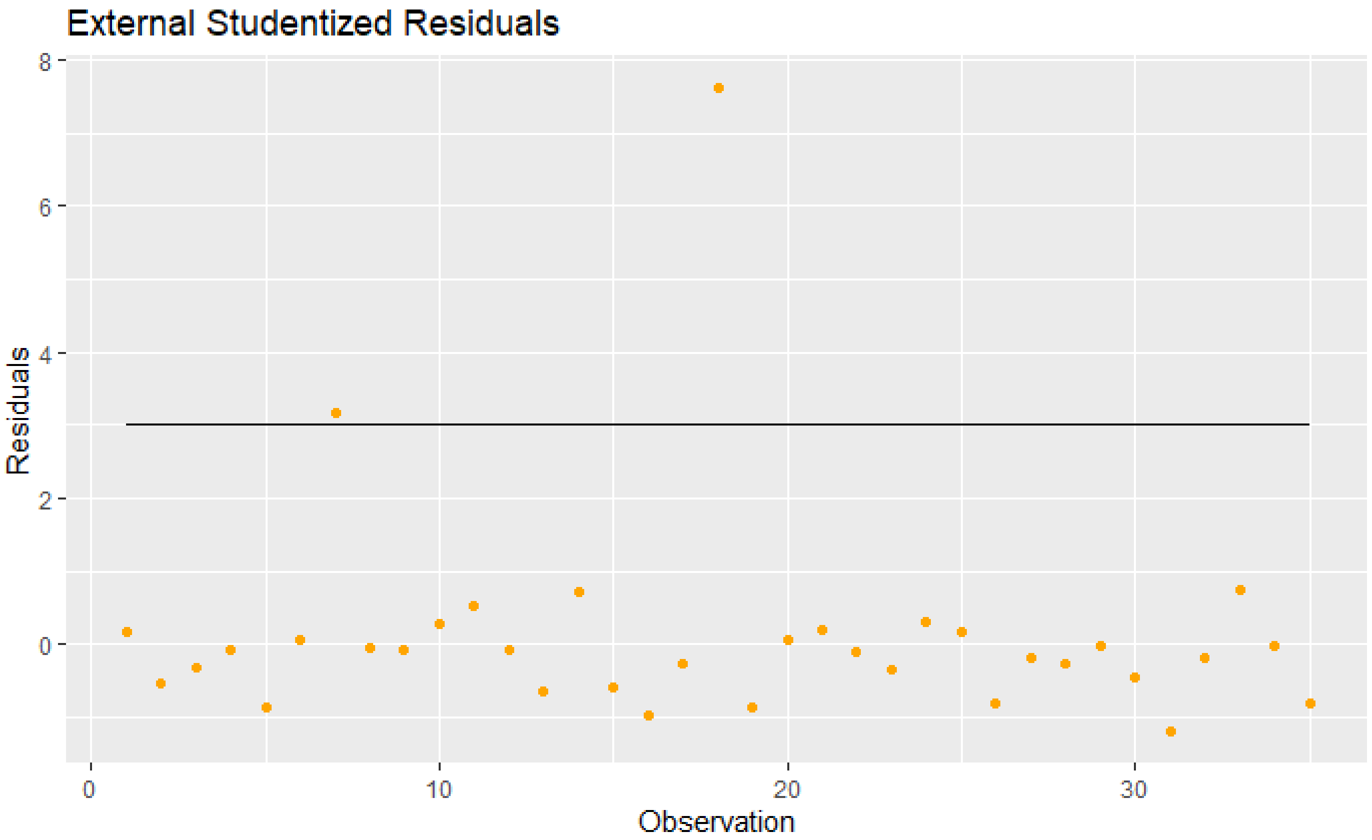
- Measure of change in the j^{th} parameter estimate with deletion of the i^{th} observation
- One DFBETA per parameter per observation
- Helpful in explaining on which parameter coefficient the influence most lies
- A suggested cutoff for influence is shown below:

$$|\mathbf{DFBETA}_{ij}| > 2\sqrt{\frac{1}{n}}$$

Scottish Hill Races

```
url =
'http://www.statsci.org/data/general/hills.txt'
races.table = read.table(url, header=TRUE,
sep='\t')
n.index=seq(1,nrow(races.table))
races.table=cbind(races.table,n.index)
lm.model=lm(Time~Distance+Climb,data=rac
es.table)
```

```
ggplot(lm.model,aes(x=n.index,y=rstudent(lm.mod
el)))+geom_point(color="orange")+geom_line(y=-
3)+geom_line(y=3)+labs(title = "External
Studentized
Residuals",x="Observation",y="Residuals")
```



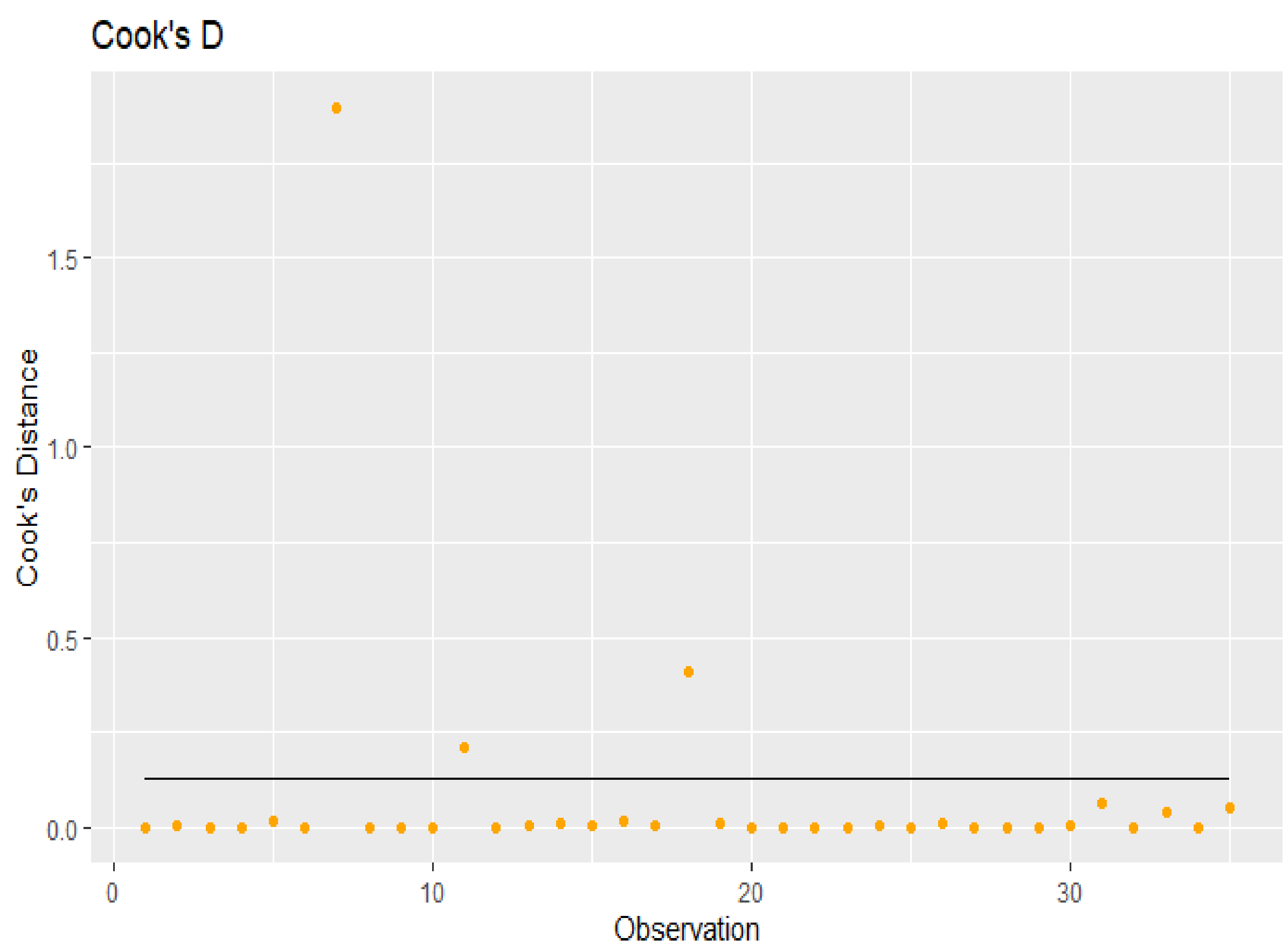
Scottish Hill Races dataset

- This data set is the record-winning times for 35 hill races in Scotland, as reported by Atkinson (1986). The distance travelled and the height climbed in each race is also given.

Variable	Description
Race	Name of race
Distance	Distance covered in miles
Climb	Elevation climbed during race in feet
Time	Record time for race in minutes

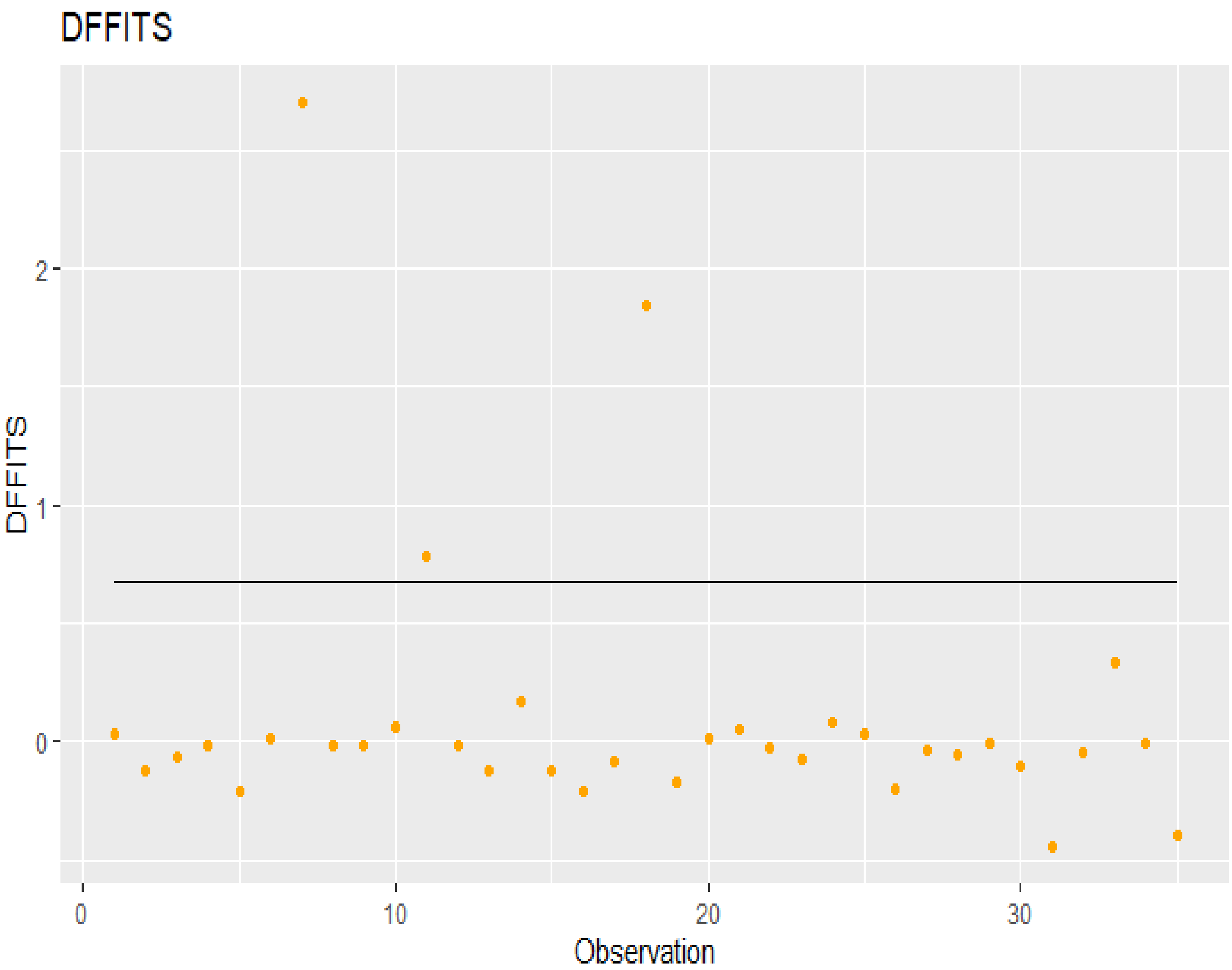
Cook's D

```
##Cook's D
D.cut=4/(nrow(races.table)-3)

ggplot(lm.model,aes(x=n.index,y=cooks.distance(lm.model)))+geom_point(color="orange")+geom_line(y=D.cut)+labs(title = "Cook's D",x="Observation",y="Cook's Distance")
```



DFFITS

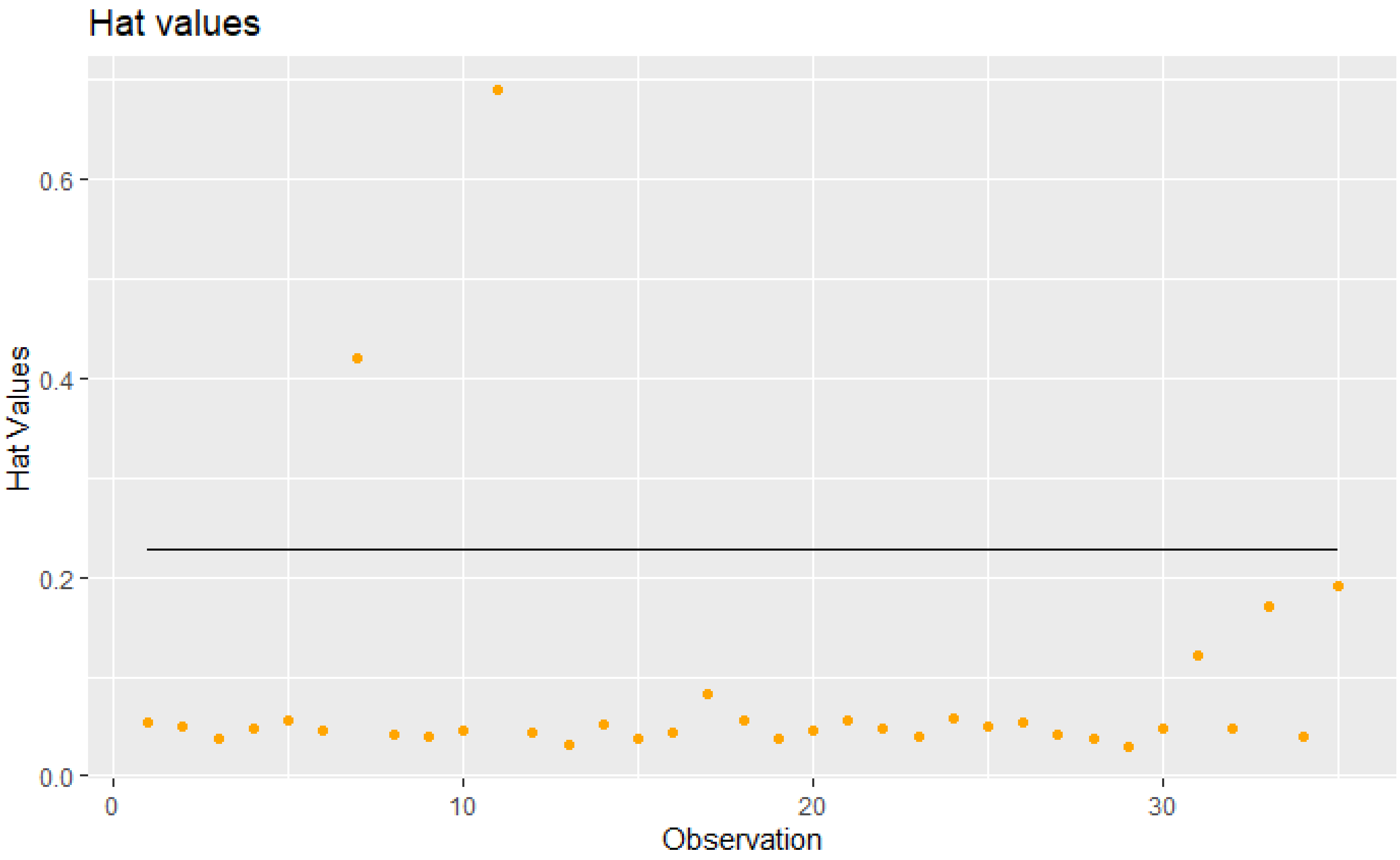
```
df.cut=2*(sqrt((3)/nrow(races.table)))

ggplot(lm.model,aes(x=n.index,y=dffits(lm.model)))+geom_point(color="orange")+geom_line(y=df.cut)+geom_line(y=-df.cut)+labs(title = "DFFITS",x="Observation",y="DFFITS")
```



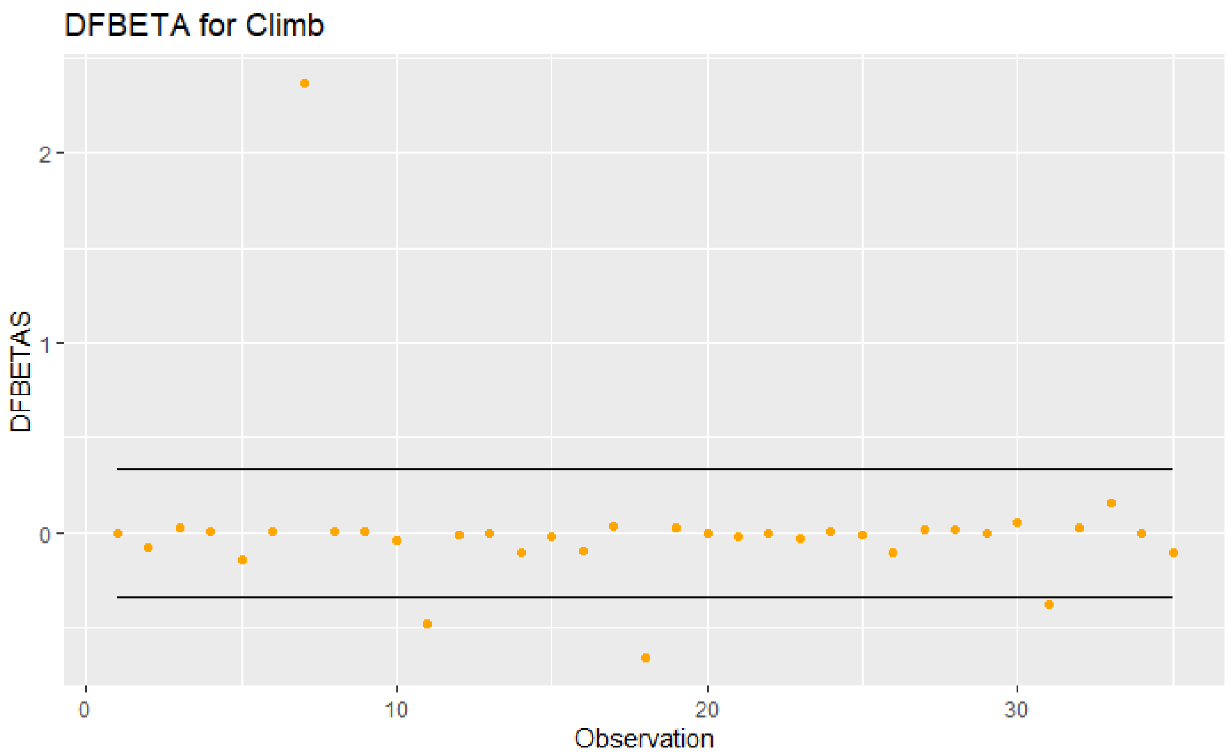
Hat values

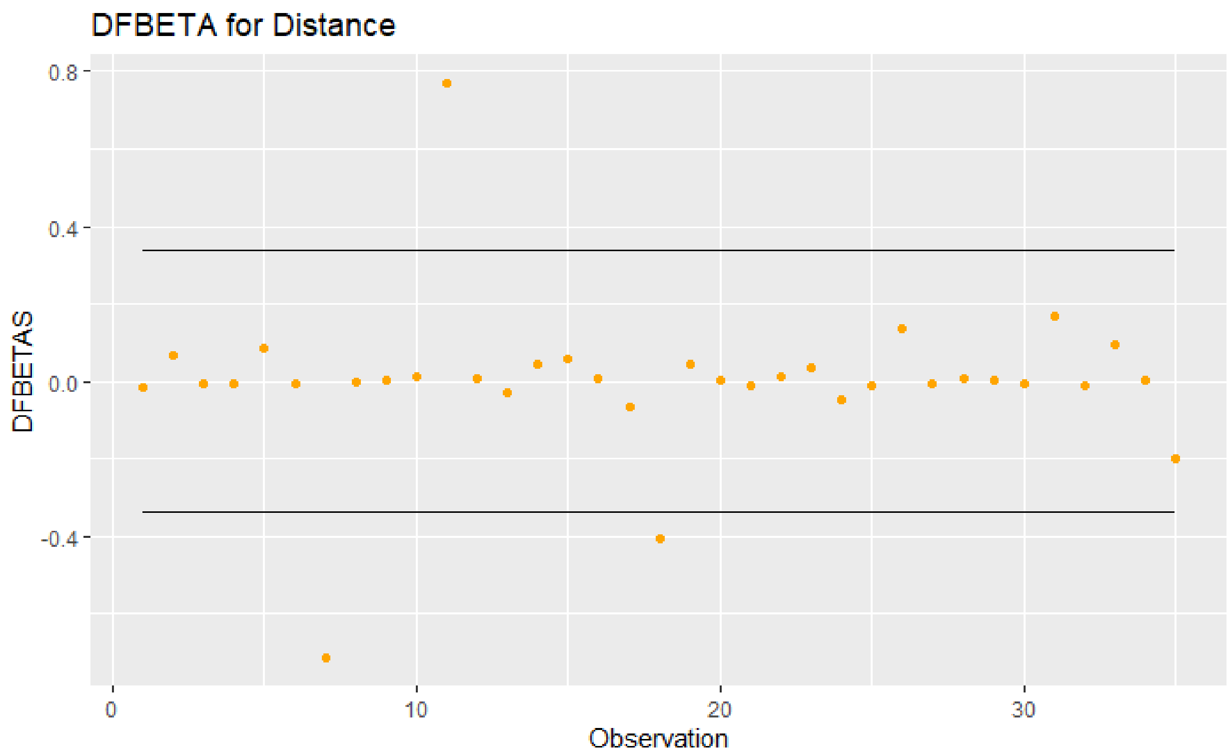
hat.cut=2*(3)/nrow(races.table)

ggplot(lm.model,aes(x=n.index,y=hatvalues(lm.model)))+geom_point(color="orange")+geom_line(y=hat.cut)+labs(title = "Hat values",x="Observation",y="Hat Values")



```
db.cut=2/sqrt(nrow(races.table))

ggplot(lm.model,aes(x=n.index,y=dfbetas(lm.model)[,'Climb']))+geom_point(color="orange")+geom_line(y=db.cut)+geom_line(y=-db.cut)+labs(title = "DFBETA for Climb",x="Observation",y="DFBETAS")

ggplot(lm.model,aes(x=n.index,y=dfbetas(lm.model)[,'Distance']))+geom_point(color="orange")+geom_line(y=db.cut)+geom_line(y=-db.cut)+labs(title = "DFBETA for Distance",x="Observation",y="DFBETAS")
```





Exploring Influential and Outlier Observations

1. Recheck the data to ensure that no transcription or data entry errors occurred.
2. If the data is valid, one possible explanation is that the model is not adequate.
   - A model with higher-order terms, such as polynomials and interactions between the variables, might be necessary to fit the data well.
   - Nonlinear model
3. Determine the robustness of the inference by running the analysis both with and without these observations.
4. Robust Regression (Covered Later in Program)
5. Weighted Least Squares (WLS)

Collinearity

Illustration of Collinearity

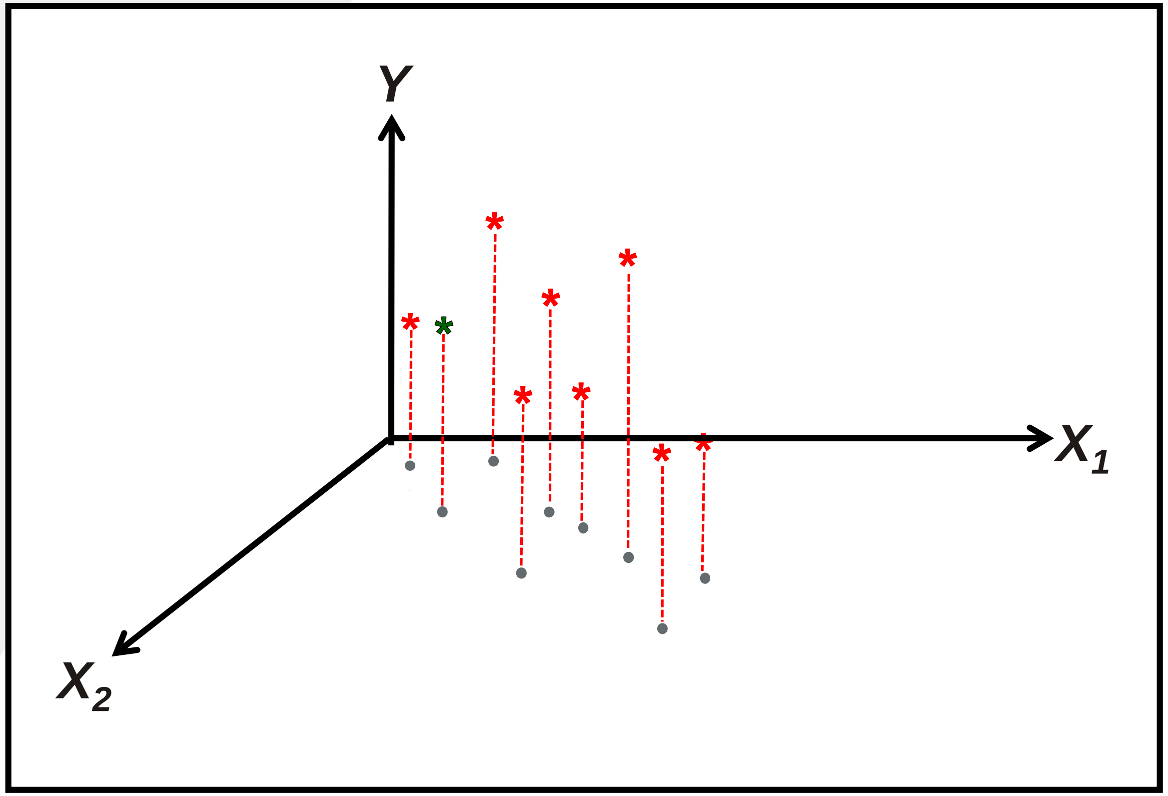


Illustration of Collinearity

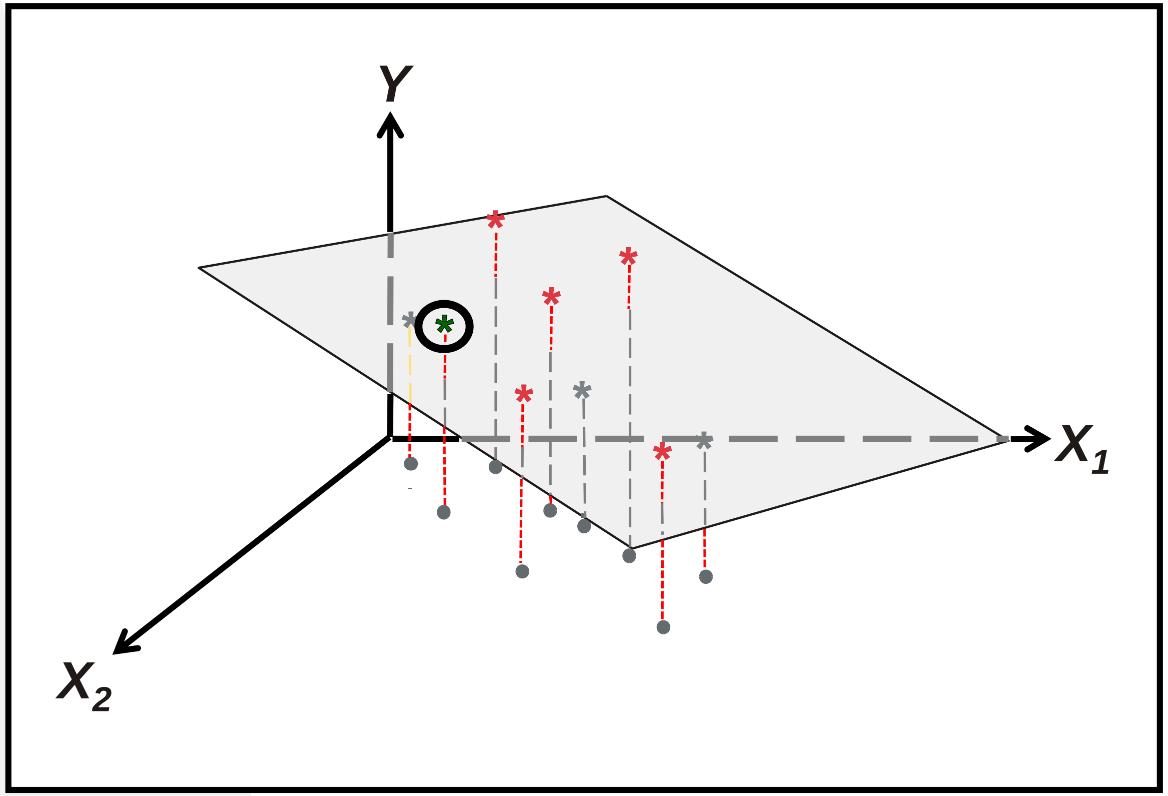
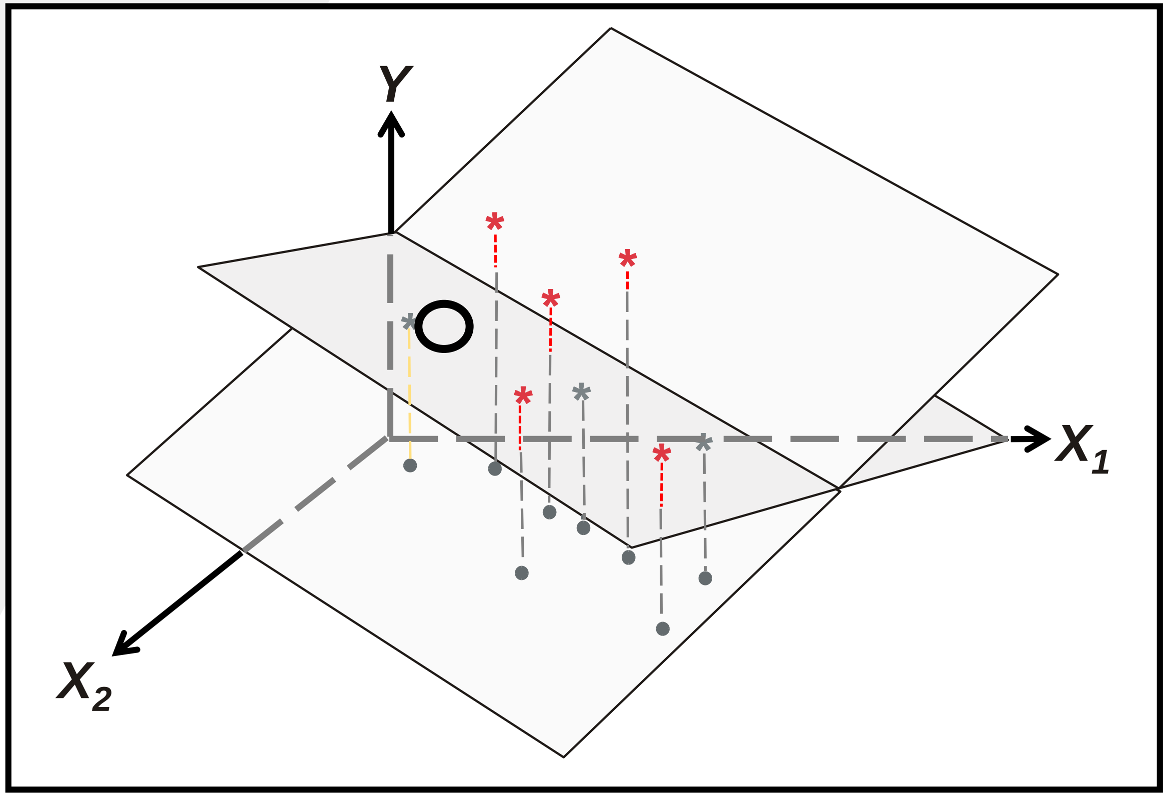


Illustration of Collinearity



Collinearity Diagnostics

- Looking at correlation matrix of predictors
- One of the most commonly used measures is the variance inflation factor (VIF).
- VIF is calculated by

$$VIF_i = \frac{1}{1 - R_i^2}$$

- Values of VIF greater than 10 indicate potential collinearity

MTCARS data set

```
cor(mtcars)
lm.model=lm(mpg~.,data=mtcars)
vif(lm.model)
```

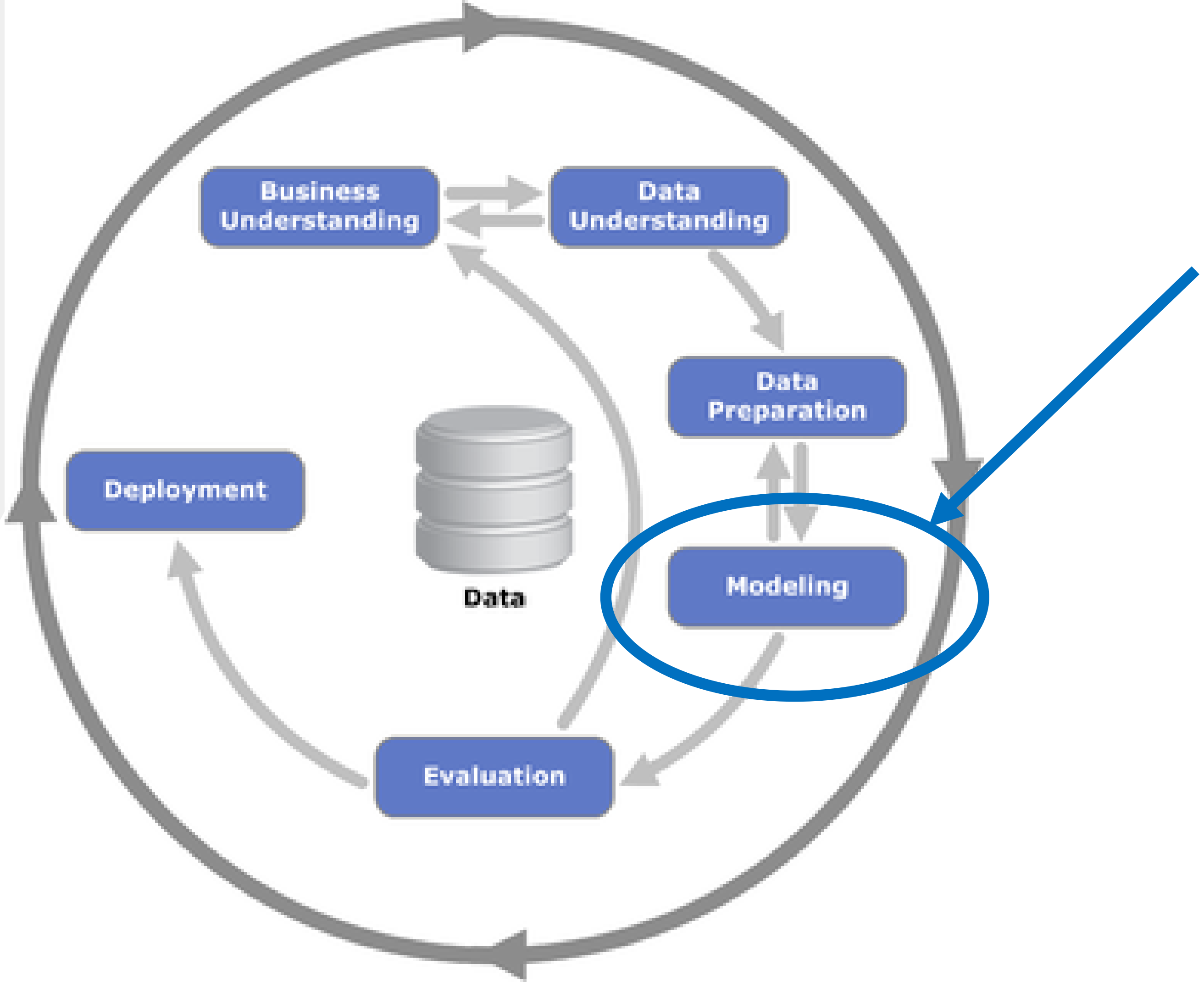
```
      cyl      disp        hp      drat        wt      qsec
15.373833 21.620241  9.832037  3.374620 15.164887  7.527958
       vs        am      gear      carb
 4.965873  4.648487  5.357452  7.908747
```

Dealing with Multicollinearity

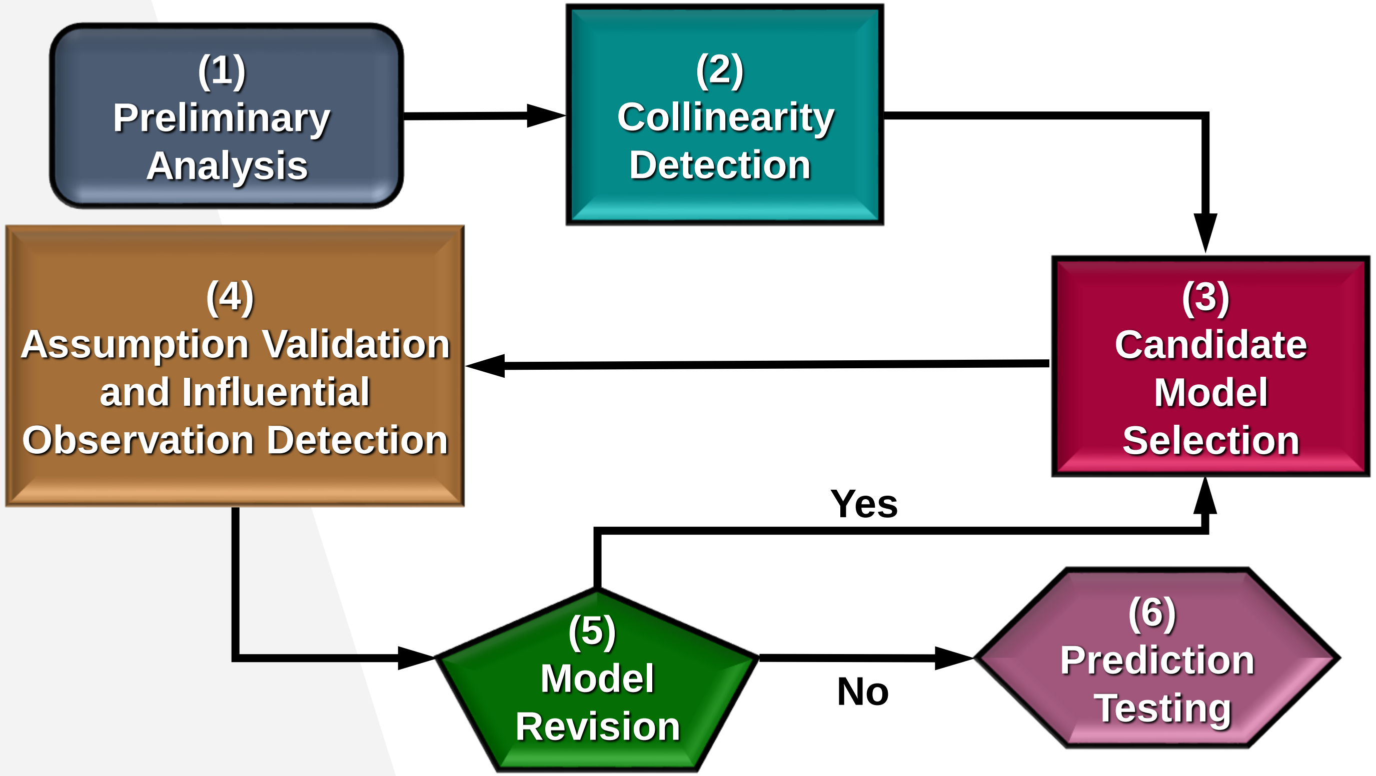
- Exclude redundant independent variables.
- Redefine variables.
- Use biased regression techniques (for example, RIDGE).
- Be sure that you have centered any independent variables in polynomial regression models (or with interactions).

CRISP-DM

Cross-industry standard process for data mining



An Effective Modeling Cycle



Break out and Lab 9

Don’t forget to take the lab check on Moodle!