

Linear Regression ¹

Shaobo Li

University of Kansas

¹Partially based on Hastie, et al. (2009) ESL, and James, et al. (2013) ISLR

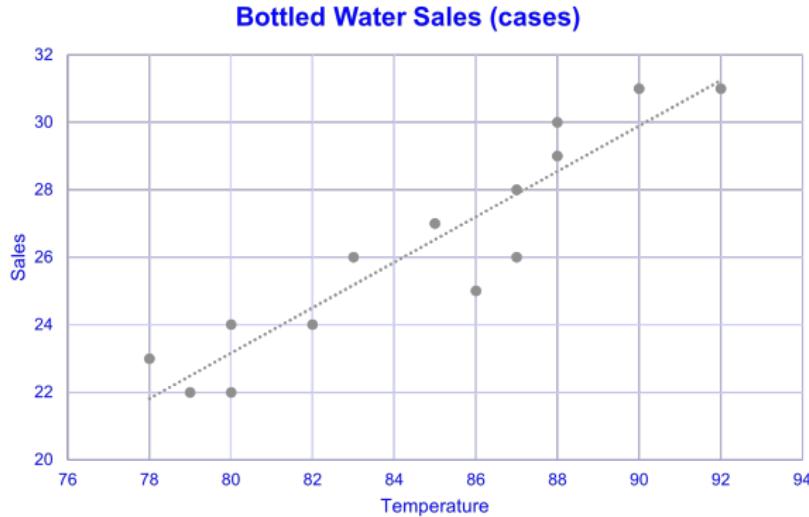
Linear regression – a fundamental learning algorithm

- Supervised learning method
- It assumes the dependence of Y on X is linear
- Largely used in many disciplines
- Simple and interpretable
- Fundamental in data science

What can linear regression do?

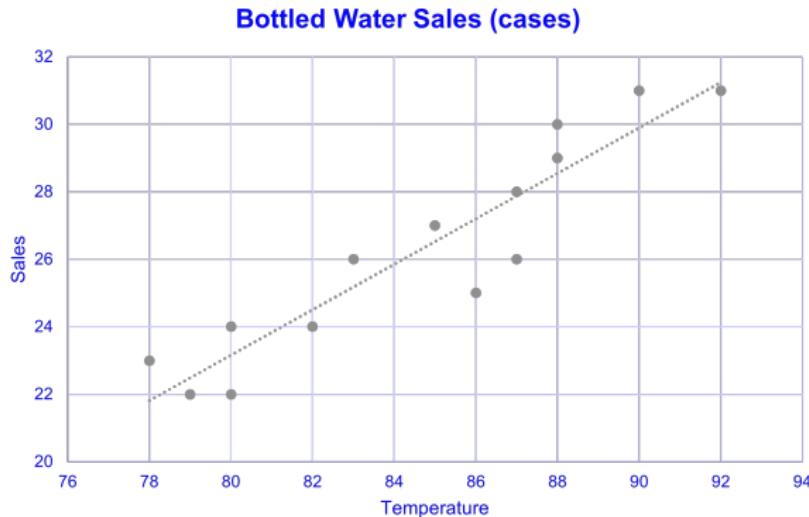
- Is there an association between X and Y ?
- If yes, how strong is this association?
- Is this association linear?
- If there are multiple X 's (X_1 , X_2 and X_3), which of them are related to Y and which are not?
- Can we predict the value of Y for any given X ?
- How accurate is such prediction?

An example – bottled water sales



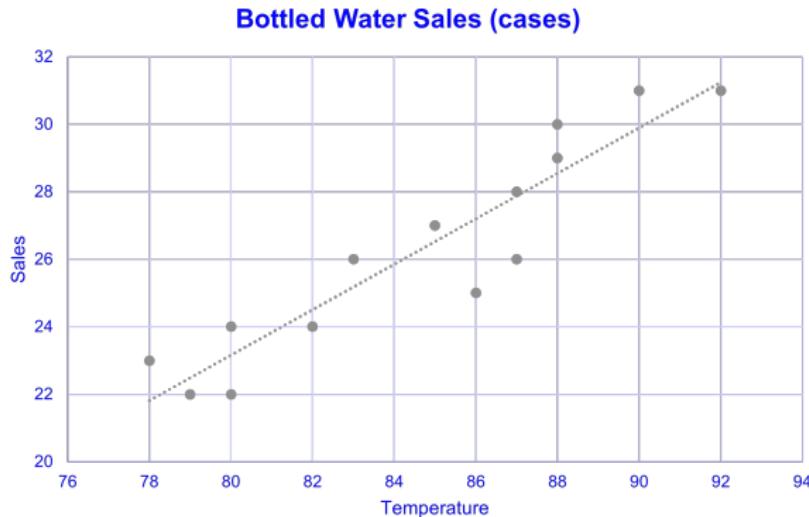
- Is there an association between *Temperature* and *Sales*?

An example – bottled water sales



- Is there an association between *Temperature* and *Sales*?
- If yes, how strong is this association?

An example – bottled water sales



- Is there an association between *Temperature* and *Sales*?
- If yes, how strong is this association?
- Is this association linear?

An example – bottled water sales

- We can write this relationship as

$$Sales \approx \beta_0 + \beta_1 \times Temperature$$

- We use “ \approx ” because the model always approximates the “truth”.
- This is a *simple linear regression*.
- β_0 is called intercept and β_1 is slope.
- Given the data points we observed, the model is estimated to be

$$Sales \approx -30.70 + 0.67 \times Temperature$$

- This is the straight line we saw before.
- How do we interpret this model?

Linear regression models

- More generally, a simple linear regression model is

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

and a multiple linear regression model is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon,$$

where ϵ catches the error of the “model” from the “truth”.

- Y is called dependent variable (or response, outcome).
- X is called independent variable (or covariates, explanatory variable).

Linear regression model in matrix form

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \\ 1 & X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

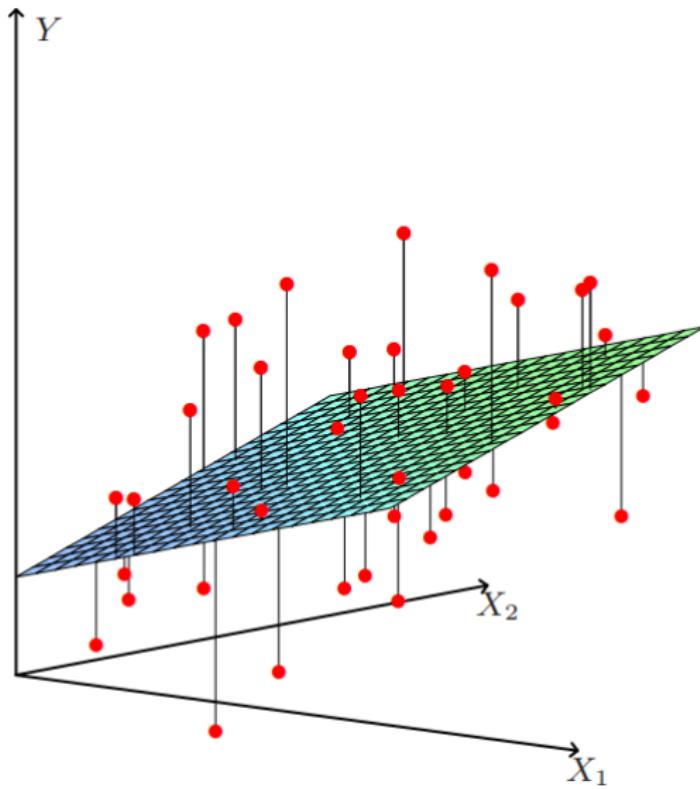
- \mathbf{X} is called design matrix

- The *estimated linear regression model* is

$$\hat{\mathbf{y}} = \mathbb{E}(\mathbf{y}|\mathbf{X}) = \mathbf{X}\hat{\boldsymbol{\beta}}$$

- We need to figure out $\hat{\boldsymbol{\beta}}$, the estimates of $\boldsymbol{\beta}$
- Method to use: *ordinary least square (OLS)*

Least square solution



Least square solution

- We want to minimize residual sum squares (RSS)

$$\begin{aligned} RSS(\beta) &= \sum_{i=1}^n (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \end{aligned}$$

- Take first-order derivative with respect to $\boldsymbol{\beta}$ and set to 0

$$\begin{aligned} 0 &= \frac{\partial RSS(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ \mathbf{X}^T\mathbf{y} &= \mathbf{X}^T\mathbf{X}\boldsymbol{\beta} \end{aligned}$$

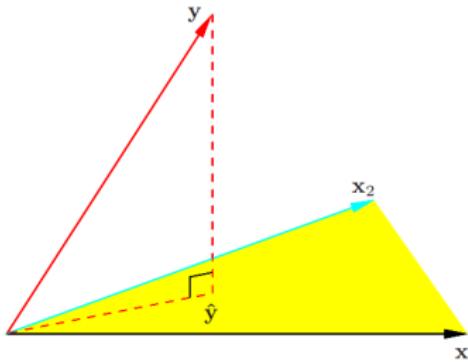
- This is called *normal equation*.

Least square solution

- By assuming $p < n$, the OLS solution is

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

- The predicted value is $\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$
- $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ is called hat matrix or projection matrix
- That is, $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$. In other words, $\hat{\mathbf{y}}$ is a linear projection of \mathbf{y}



Some important questions after fitting the model

- How to interpret the model?
- Is at least one of the predictors useful to predict and explain the response?
- Do all predictors help to explain response, or just a subset?
- How well does the model fit the data?
- Given a set of predictor values, what response value does the model predict? How accurate is the prediction?

Hypothesis testing – test multiple coefficients

Is at least one X useful?

- F -test for overall significance

- $H_0: \beta_1 = \dots = \beta_p = 0; H_1: \text{at least one } \beta \neq 0$
- F statistics

$$F^* = \frac{(TSS - RSS)/p}{RSS/(n - p - 1)} \sim F_{p, n-p-1}$$

where $TSS = \sum_{i=1}^n (y_i - \bar{y})^2$, is total sum squares

Hypothesis testing – test individual coefficients

Is a specific X relevant?

- Testing for individual β
 - $H_0: \beta_j = 0; H_1: \beta_j \neq 0$
 - Using T-test since the true variance is unknown

$$T = \frac{\hat{\beta}_j}{se(\hat{\beta}_j)} = \frac{\hat{\beta}_j}{\hat{\sigma} \sqrt{v_j}} \sim t_{n-p-1}$$

where v_j is the j th diagonal element of $(\mathbf{X}^T \mathbf{X})^{-1}$

- Reject H_0 if p-value $< \alpha$ or $|T| > T_{1-\alpha}^{(n-p-1)}$
- Confidence interval: $\hat{\beta} \pm se(\hat{\beta}) \times T_{1-\alpha}^{(n-p-1)}$

R output for bottle water example

```
> model1<- lm(Sales~Temperature, data = sales)
> summary(model1)
```

Call:

```
lm(formula = Sales ~ Temperature, data = sales)
```

Residuals:

Min	1Q	Median	3Q	Max
-2.1994	-0.5016	0.2908	0.8350	1.4542

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-30.69720	6.38033	-4.811	0.000425 ***
Temperature	0.67322	0.07529	8.942	1.18e-06 ***

Signif. codes: 0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.184 on 12 degrees of freedom

Multiple R-squared: 0.8695, Adjusted R-squared: 0.8586

F-statistic: 79.96 on 1 and 12 DF, p-value: 1.182e-06

Model Assessment – R Square and MSE

- It is proportion of variation in Y explained by the model

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

R^2 increases monotonically as number of X 's increasing.

- Adjusted R^2

$$R_{adj}^2 = 1 - \frac{n - 1}{n - p - 1} \frac{RSS}{TSS}$$

- Mean Squared Error (MSE)

$$MSE = \frac{1}{n - p - 1} \times RSS$$

It is an unbiased estimate of σ^2 , variance of ϵ . (Can you show this?)

Categorical covariate

Suppose we want to know how blood pressure (Y) is associated with Weight (X_1) and Gender (X_2) using linear regression model.

- X_1 is continuous; X_2 is categorical

$$X_2 = \begin{cases} 1 & \text{Female} \\ 0 & \text{Male} \end{cases}$$

- How does the linear model look like?

Categorical covariate

Suppose we want to know how blood pressure (Y) is associated with Weight (X_1) and Gender (X_2) using linear regression model.

- X_1 is continuous; X_2 is categorical

$$X_2 = \begin{cases} 1 & \text{Female} \\ 0 & \text{Male} \end{cases}$$

- How does the linear model look like?

$$\begin{aligned} E(Y|X_1, X_2) &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 \\ &= \begin{cases} \beta_0 + \beta_1 X_1 + \beta_2 & \text{for female} \\ \beta_0 + \beta_1 X_1 & \text{for male} \end{cases} \end{aligned}$$

- How do we interpret this model?
- Can you draw a graph to illustrate this model?

More than two categories

- Consider another covariate – $Race (X_3)$, which has 5 categories: White, Black, Asian, Hispanic, and Others.
- How can we write the model?

More than two categories

- Consider another covariate – $Race (X_3)$, which has 5 categories: White, Black, Asian, Hispanic, and Others.
- How can we write the model?
Following the same logic, we can write:

$$E(Y|X_1, X_2, X_3) = \begin{cases} \beta_0 + \beta_1 X_1 + \beta_2 X_2 & \text{for White} \\ \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{3,1} & \text{for Black} \\ \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{3,2} & \text{for Asian} \\ \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{3,3} & \text{for Hispanic} \\ \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{3,4} & \text{for Others} \end{cases}$$

- Can you see how do we handle the categorical variable $Race (X_3)$?
- How do we draw conclusions in testing the significant of X_3 ?

Interaction

- Consider the same example without Race.

$$\begin{aligned}E(Y|X_1, X_2) &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 \\&= \begin{cases} \beta_0 + \beta_1 X_1 + \beta_2 & \text{for female} \\ \beta_0 + \beta_1 X_1 & \text{for male} \end{cases}\end{aligned}$$

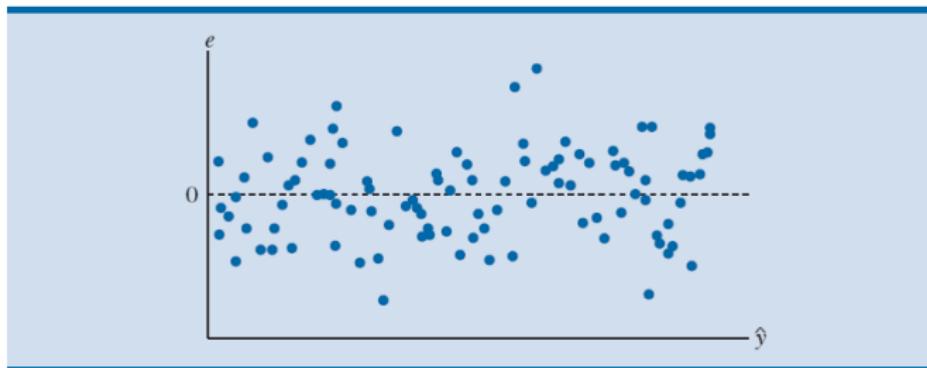
- This model says Weight (X_1) has the same effect regardless the gender. But how do know if this is true or not?
- To answer this question, we need to examine the **interaction effect**

$$E(Y|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3(X_1 * X_2)$$

- Can you break down this model with respect to Gender?
- Can you draw a graph to illustrate this model?

Model Diagnostics

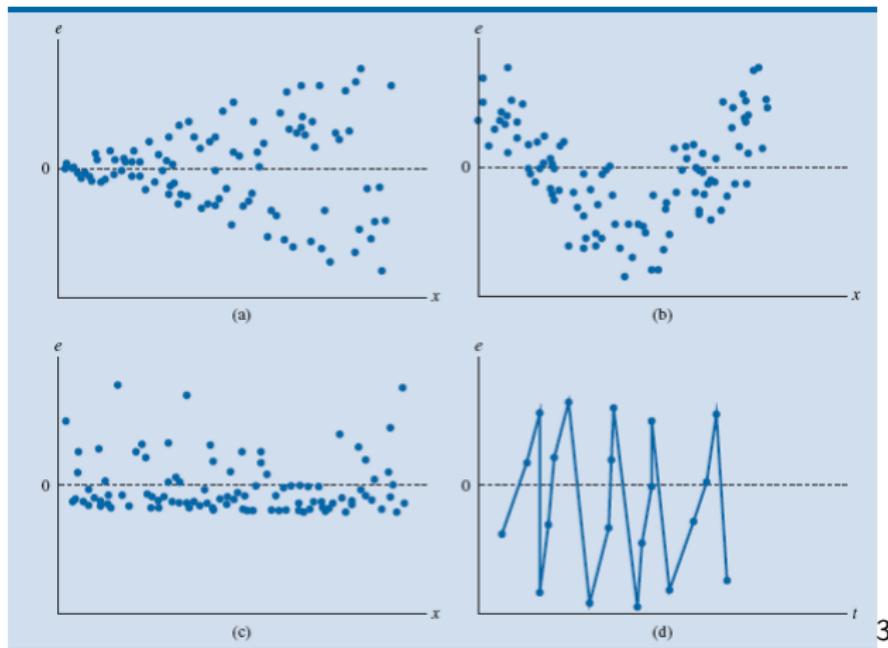
- Model assumptions:
 - Linear relationships between Y and X 's
 - The error term $\{\epsilon_1, \dots, \epsilon_n\} \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$
Independent normal distribution; $\mathbb{E}(\epsilon_i) = 0$; $Var(\epsilon_i) = \text{constant}$.
- Residual plot (an ideal residual plot looks like this)²



²source: Camm, et al., *Essentials of Business Analytics*

Residual plot

Which type of assumption is violated?



Other Diagnostic Plots

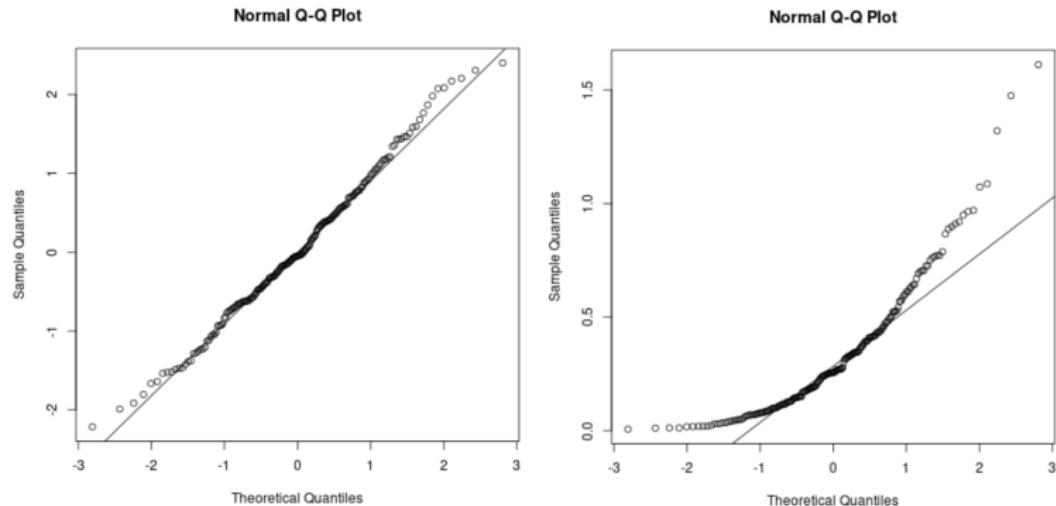
■ Normal Quantile-Quantile Plot

- It plots the standardized residual vs. theoretical quantiles
- An easy way to visually test the normality assumption
- If residual follows normal distribution, you should expect all dots lie on the diagonal straight line.

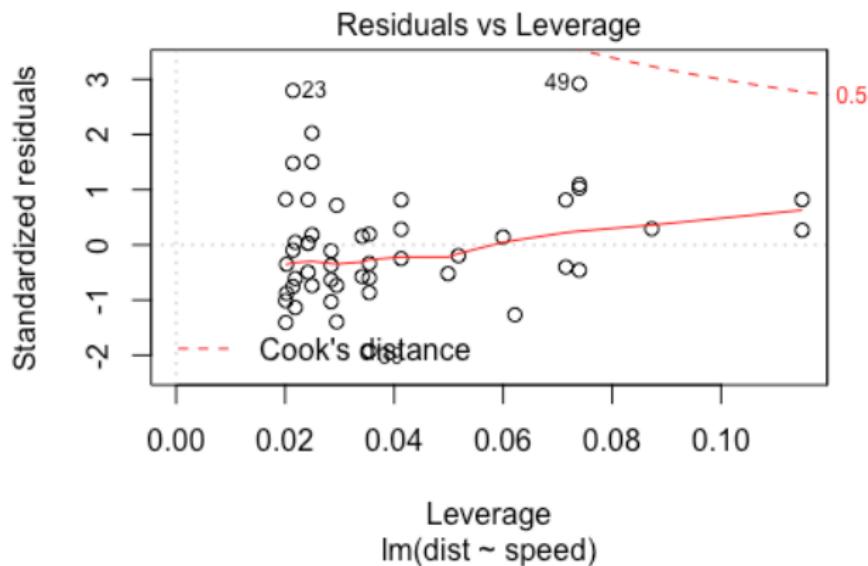
■ Residual-Leverage Plot

- This plot checks if there are any influential points, which could alter your analysis by excluding them
- The points that lie outside the dashed line, Cook's distance, are considered as influential points

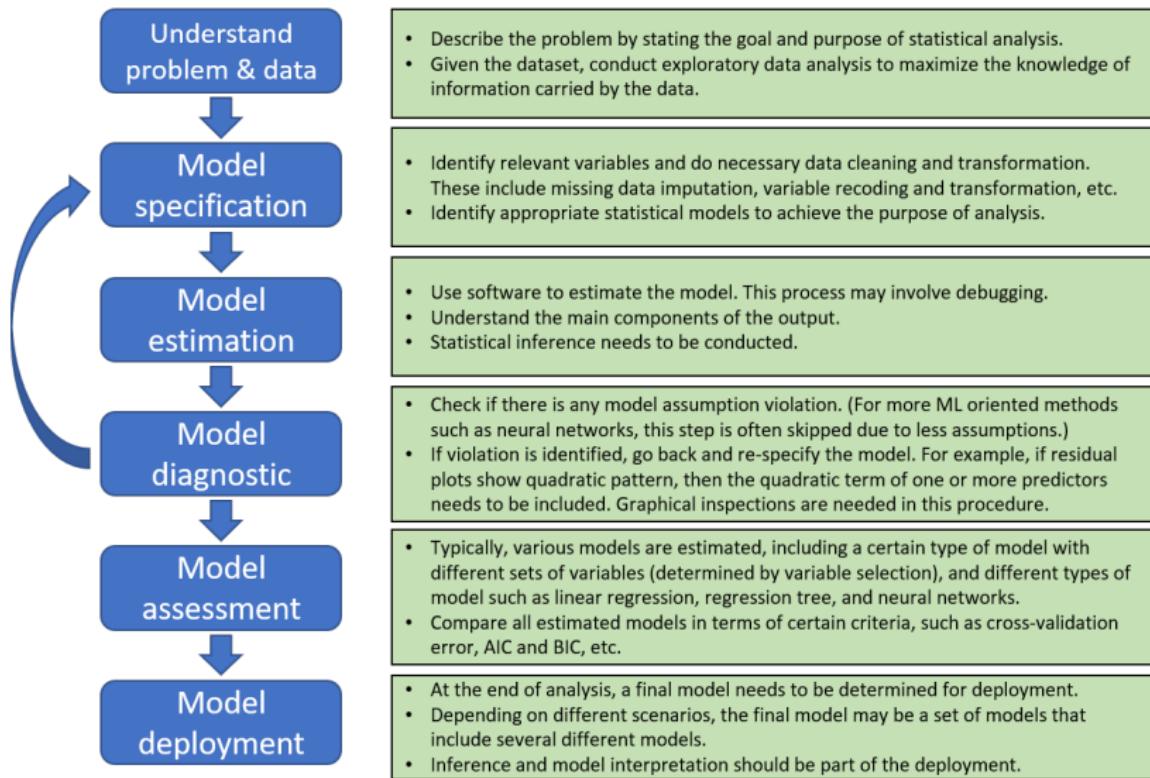
Normal Q-Q plot



Residual leverage plot



Model Building Process



- Resampling method
- A powerful tool to quantify uncertainty
 - standard error
 - confidence interval
- Random sampling with replacement
- The general procedure:
 - fit a model **B** times based on **B** bootstrap samples
 - store all the parameter estimates
 - calculate standard error and confidence interval