Session regression I: simple linear regression

Learning outcomes

- understand simple linear regression model incl. terminology and mathematical notations
- estimate model parameters and their standard error
- use model for checking the association between x and y
- use model for prediction
- asses model accuracy with RSE and R^2
- check model assumptions
- to be able to use `lm` function in R for model fitting, obtaining confidence interval and predictions

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Introduction

Quiz: What do we already know about `simple linear regression`?

Description

- Simple linear regression is a statistical method that allows us to summarize and study relationships between two continuous (quantitative, numerical) variables
  - one variable, denoted `x` is regarded as the *predictor*, *explanatory*, or *indepedent variable*, e.g. body weight (kg)
  - the other variable, denoted `y`, is regarded as the *response*, *outcome*, or *dependent variable*, e.g. plasma volume (liters)
- It is used to estimate the best-fitting straight line to describe the association

Used for to answer questions such as:

- is there a relationship between `x` exposure (e.g. body weight) and `y` outcome (e.g. plasma volume)?
- how strong is the relationship between the two variables?
- what will be a predicted value of the `y` outcome given a new set of exposure values?
- how accurately can we predict the outcome?

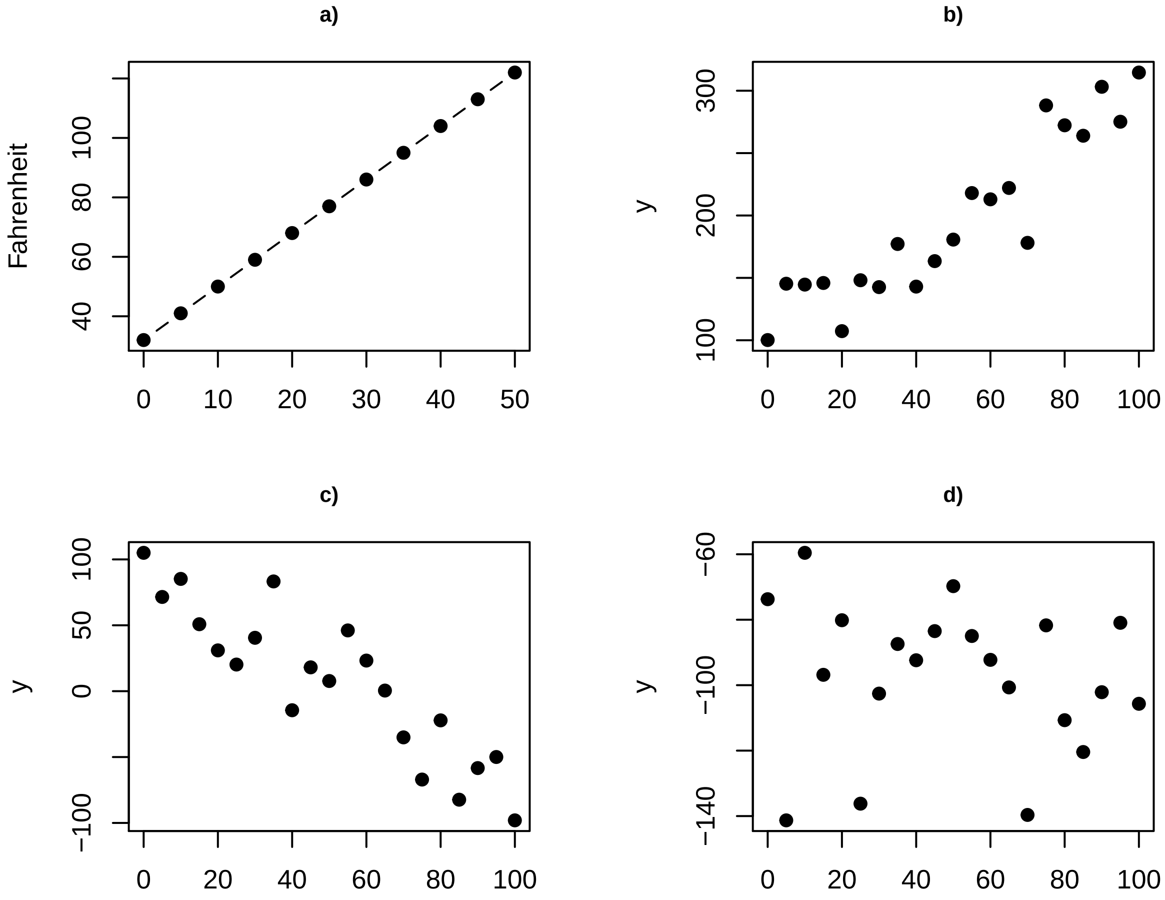


Figure 1: Determinisitc vs. statistical relationship: a) deterministic: equation exactly describes the relationship between the two variables e.g. $Fahrenheit = 9/5 * Celcius + 32$; b) statistical relationship between x and y is not perfect (increasing), c) statistical relationship between x and y is not perfect (decreasing), d) random signal

Example data

Example data contain the body weight (kg) and plasma volume (liters) for eight healthy men.

```
weight <- c(58, 70, 74, 63.5, 62.0, 70.5, 71.0, 66.0) # body weight (kg)
plasma <- c(2.75, 2.86, 3.37, 2.76, 2.62, 3.49, 3.05, 3.12) # plasma volume (liters)
```

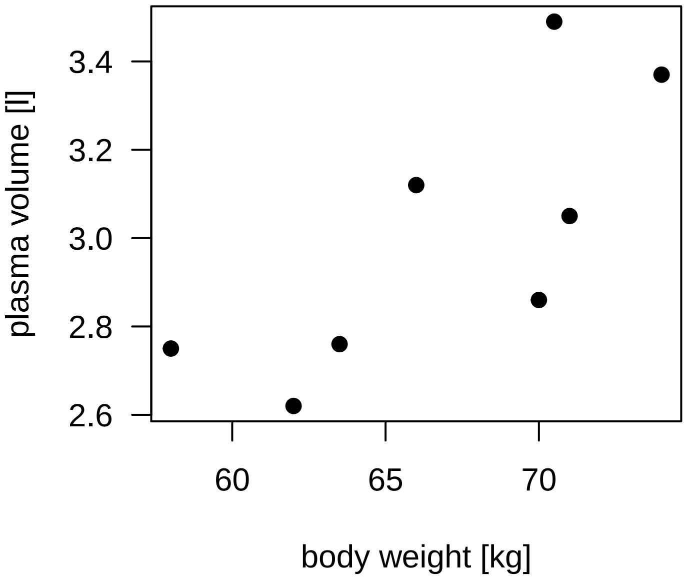


Figure 2: Scatter plot of the data shows that high plasma volume tends to be associated with high weight and *vice verca*.

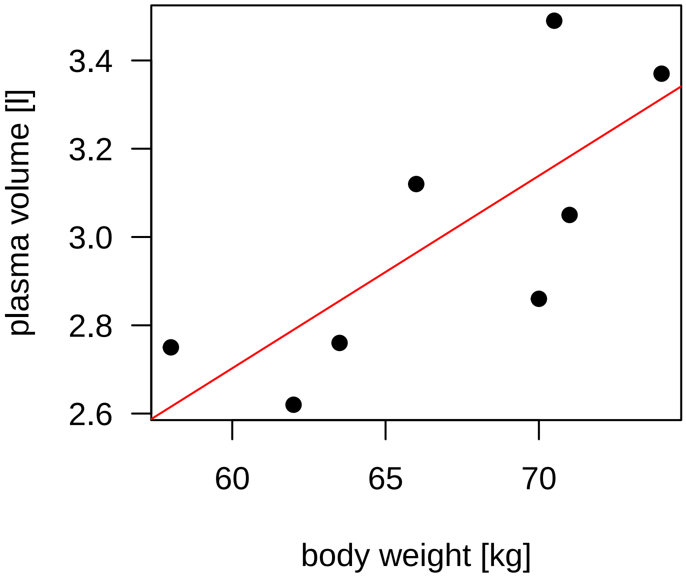


Figure 3: Scatter plot of the data shows that high plasma volume tends to be associated with high weight and *vice verca*. Linear regrssion gives the equation of the straight line that best describes how the outcome changes (increase or decreases) with a change of exposure variable (in red)

The equation of the regression line is:

$$y = \beta_0 + \beta_1 x$$

or mathematically using matrix notation

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

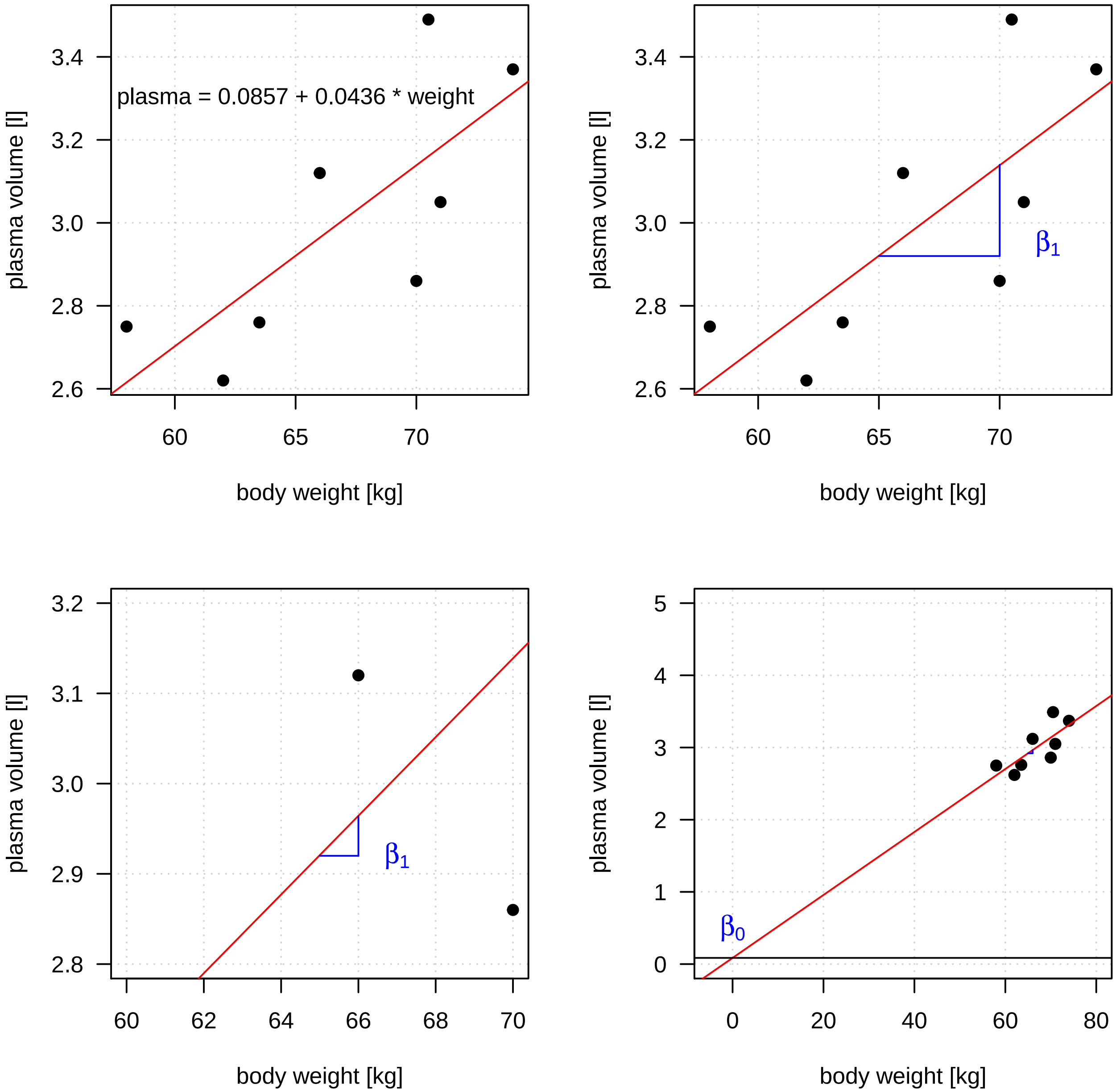
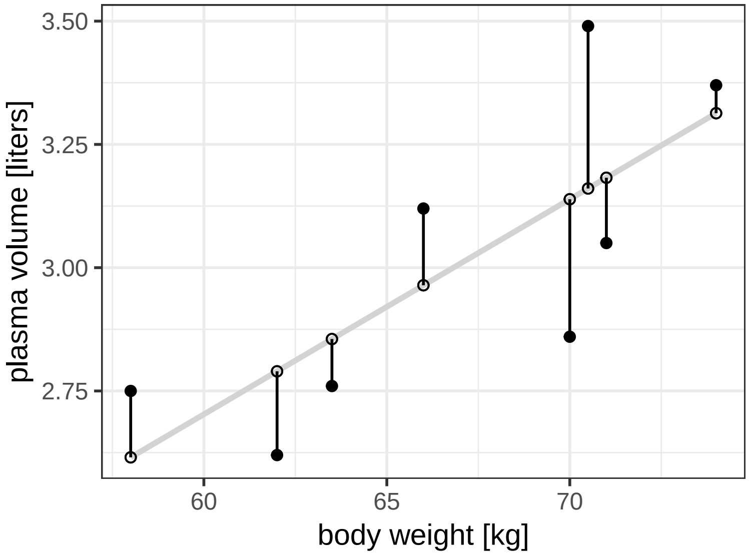


Figure 4: Scatter plot of the data shows that high plasma volume tends to be associated with high weight and *vice verca*. Linear regrssion gives the equation of the straight line that best describes how the outcome changes (increase or decreases) with a change of exposure variable (in red). Parameters explanation

Quiz: regression model parameters

Estimating model coefficients

In practice, β_0 and β_1 are usually unknown. The best-fitting line is derived using the method of **least squares**, i.e. by finding the values of the parameters β_0 and β_1 tht minimize the sum of the squared vertical distances of the points from the line.



Let $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$ represent n observation pairs, each of which consists of a measurement of X and Y, e.g. in our example we have 8 pairs of observations, e.g. (58, 2.75), (70, 2.86) etc.

```r
weight <- c(58, 70, 74, 63.5, 62.0, 70.5, 71.0, 66.0) # body weight (kg)
plasma <- c(2.75, 2.86, 3.37, 2.76, 2.62, 3.49, 3.05, 3.12) # plasma volume (liters)
```

We seek to find coefficients estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ such that liner model fits the available data well, i.e. such that the resulting line is as close as possible to the 8 data points.

There are a number of ways of measuring *closeness*. By far the most common approach involves minimizing the *least squares* criterion.

Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction Y based on the ith value of X. Then $\epsilon_i = y_i - \hat{y}_i$ represents the ith *residual*, i.e. the difference between the ith observed response value and the ith response value that is predicted by the linear model.

RSS, the *residual sum of squares* is defined as:

$$RSS = \epsilon_1^2 + \epsilon_2^2 + ...\epsilon_n^2$$

or equivalently as:

$$RSS = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + ... + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2$$

The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. With some calculus one gets:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$$

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

where $\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ are the sample means.

Pen and Paper exercise: Estimating model coefficients

Hypothesis testing

Accuracy of the coefficient estimates

- The calculated $\hat{\beta}_0$ and $\hat{\beta}_1$ are estimates of the population values of the intercept and slope and are, therefore, subject to sampling variation
- Their precision is measure by their standard errors

$$s.e(\hat{\beta}_0) = s * \sqrt{[\frac{1}{n} + \frac{x_i^2}{\sum_{i=1}^{n}(x_i - \overline{x})^2}]}$$

$$s.e(\hat{\beta}_1) = \frac{s}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}}$$

where, s is the *standard deviation of the points about the line.* It has $(n-2)$ degrees of freedom, i.e. the sample size minus the number of regression coefficients

$$s = \sqrt{[\frac{\sum_{i=1}^{n}(y_i - \overline{y})^2 - \overline{\beta_1}\sum_{i=1}^{n}(x_i - \overline{x})^2}{n-2}]}$$

Pen and Paper exercise: Accuracy of the coefficient estimates

Confidence interval

- Standard errors can be used to compute `confidence interval`.
- A 95% confidence interval is defined as a range of values such that with 95% probability, the range will contain the true unknown value of the parameter.
- The range is defined in terms of lower and upper limits computed from the data. For linear regression, the 95% confidence intervals takes form:

$$[\hat{\beta}_1 - 2 * s.e.(\hat{\beta}_1), \hat{\beta}_1 + 2 * s.e.(\hat{\beta}_1)]$$

and

$$[\hat{\beta}_1 - 2 * s.e.(\hat{\beta}_0), \hat{\beta}_1 + 2 * s.e.(\hat{\beta}_0)]$$

Hypothesis testing

- Standard errors can also be used to perform `hypothesis testing` on the coefficients.
- The most common hypothesis test involves testing the `null hypothesis` of:

H_0 : There is no relationship between X and Y

versus the `alternative hypothesis`

H_0 : There is some relationship between X and Y

Mathematically, this corresponds to testing

$$H_0 : \beta_1 = 0$$

versus

$$H_0 : \beta_1 \neq 0$$

since if

$$\beta_1 = 0$$

then the model

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

reduces to

$$Y = \beta_0 + \epsilon$$

To test the null hypothesis we need to determine whether $\hat{\beta}_1$, our estimate of β_1, is sufficiently far from zero that we can be confident that β_1 is non-zero.

How far is far enough? This depends on the accuracy of $\hat{\beta}_1$, that is standard error $s.e.(\hat{\beta}_1)$. If $s.e.(\hat{\beta}_1)$ is small, then small values of $\hat{\beta}_1$ may provide strong evidence that $\hat{\beta}_1 \neq 0$ and *vice verca*. In practice, we compute a `t-statistics` given by

$$t = \frac{\hat{\beta}_1 - 0}{s.e.(\hat{\beta}_1)}$$

which measures the standard deviations that $\hat{\beta}_1$ is away from 0.

If there really is no relationship between X and Y, then we this will have a t-distribution with $n - 2$ degrees of freedom. From previous sessions, we now know how to compute probability of observing any value equal to $|t|$. We call this probability the $p - value$.

We can interpret the $p - value$ as follows: a small p-value indicates that it is unlikely to observe such a substantial association between X and Y due to chance, i.e. in the absence of any real association. We therefore can `reject the null hypothesis`.

Typical p-value cutoffs for rejecting the null hypothesis are 5 or 1%. Pen and Paper exercise: Hypothesis testing

Live coding demo

```
# Data
weight <- c(58, 70, 74, 63.5, 62.0, 70.5, 71.0, 66.0)
plasma <- c(2.75, 2.86, 3.37, 2.76, 2.62, 3.49, 3.05, 3.12)

# Plot
plot(weight, plasma)

# Regression
reg <- lm(plasma~weight)
summary(reg)

# Coefficients
coef(reg)

# Confidence intervals
confint(reg)

# Add regression line to the plot
abline(reg)
```

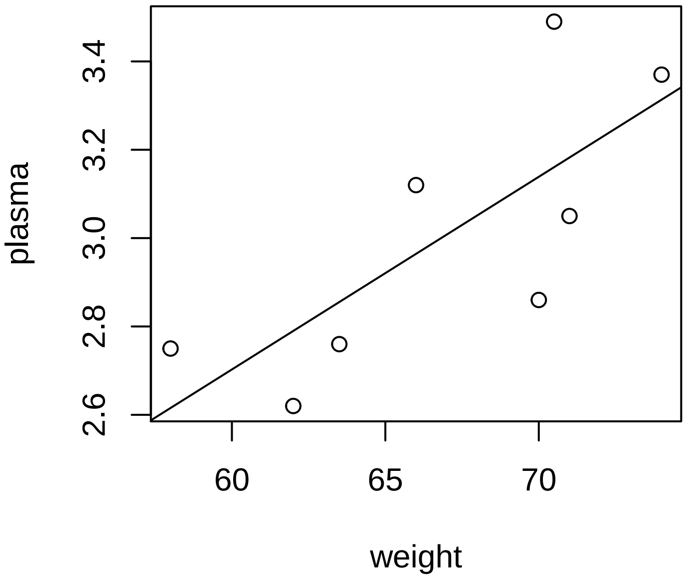


Figure 5: Body weight vs. plasma volume

```
##
## Call:
## lm(formula = plasma ~ weight)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.27880 -0.14178 -0.01928  0.13986  0.32939
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.08572    1.02400   0.084   0.9360
## weight       0.04362    0.01527   2.857   0.0289 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2188 on 6 degrees of freedom
## Multiple R-squared:  0.5763, Adjusted R-squared:  0.5057
## F-statistic:  8.16 on 1 and 6 DF,  p-value: 0.02893
##
## (Intercept)      weight
##  0.08572428  0.04361534
##                   2.5 %     97.5 %
## (Intercept) -2.419908594 2.59135716
## weight       0.006255005 0.08097567
```

Prediction

Sometimes it may be useful to use the regression equation to predict the value of y_i for a particular value of x_i, say x_it. The `predicted value` is:

$$y_i' = \hat{\beta}_0 + \hat{\beta}_1 x_i'$$

and its standard error is:

$$s.e.(y_i') = s\sqrt{[1 + \frac{1}{n} + \frac{(x_i - \overline{x_i})^2}{\sum_{i=1}^{n}(x_i - \overline{x_i})^2}]}$$

The standard error is least when x_it' is close to the mean, $\overline{x}$

In general, one should be recluctant to use the regression line for predicting values outside the range of x in the original data, as the linear relationship will not necessarily hold true beyond the range over which it has been fitted.

Prediction interval

There is also a concept called `prediction interval`. Here, we look at any specific value of x_i, and find an interval around the predicted value y_i' for x_i such that there is a 95% probability that the real value of y (in the population) corresponding to x_i is within this interval.

Prediction interval regression vs. confidence interval

- 95% condifence interval: there is 95% probability that the true best fit-line for the population lies within the confidence interval
- 95% prediction interval: 95% of the y values found for a certain x value will be within the interval range around the linear regression line
- prediction interval > than a confidence interval, as it must account for both the uncertainty in knowing the value of the population mean, plus data scatter.

The 95% prediction interval of the forecasted value y_i':

Live coding demo

```
# Prediction
predict(reg, data.frame(weight=60))
```

```
##        1
## 2.702645
```

```
predict(reg, data.frame(weight=c(60, 70)))
```

```
##        1        2
## 2.702645 3.138798
```

```
# Prediction with confidence intervals
predict(reg, data.frame(weight=66), interval="prediction")
```

```
##        fit      lwr      upr
## 1 2.964337 2.395511 3.533162
```

Asesssing the Accuracy of the Model & Correlation

Assumptions