Topic 2 – Exploratory Data Analysis (EDA)

ENVX1002 Introduction to Statistical Methods

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Topic 2 - Exploratory Data Analysis

- Summary statistics:
  - measures of centre;
  - measures of spread (dispersion).
- Graphical summaries:
  - bar chart;
  - histogram;
  - boxplot.

Learning Outcomes

- At the end of this topic students should able to:
  - Calculate “by hand” summary statistics for simple datasets;
  - Manually draw graphical summaries (boxplots and histograms) for simple datasets;
  - Demonstrate proficiency in the use of R and Excel for calculating summary statistics and generating graphical summaries;
  - Describe key features of their data using summary statistics and graphical summaries.

Types of data

- Numerical:
  - Continuous: yield, weight
  - Discrete: weeds per m^2
- Categorical:
  - Binary: 2 mutually exclusive categories
  - Ordinal: categories ranked in order
  - Nominal: qualitative data

Presentation of data

Tables: Experimental data

Table 1 Yields of cabbage (mean fresh weight per head in kg) for 24 plots (Source: Mead, Curnow & Hasted (2003)).

Irrigation	Spacing	Field A	Field B	Field C
Frequent	1 (21 in)	1.11	1.03	0.94
Frequent	2 (18 in)	1.00	0.82	1.00
Frequent	3 (15 in)	0.89	0.80	0.95
Frequent	4 (12 in)	0.87	0.65	0.85
Rare	1 (21 in)	0.97	0.86	0.92
Rare	2 (18 in)	0.80	0.91	0.68
Rare	3 (15 in)	0.57	0.72	0.77
Rare	4 (12 in)	0.60	0.69	0.51

Presentation of data

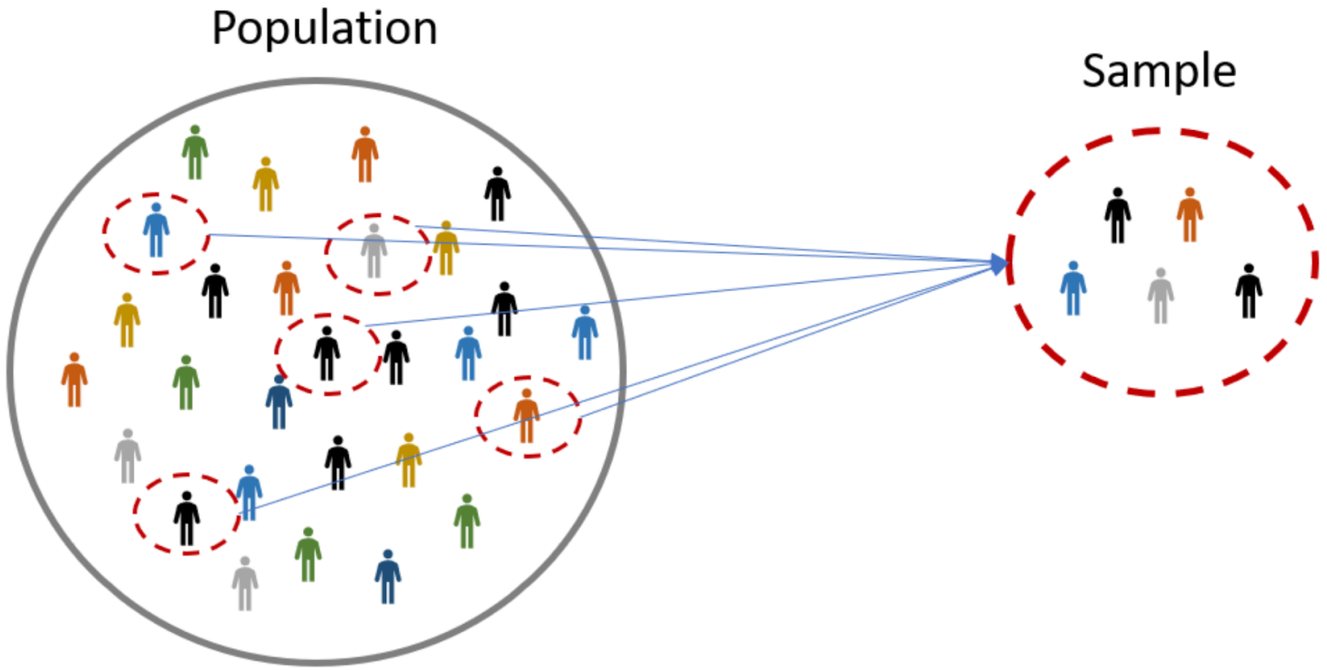
Tables: Observational data

ID	Eastings	Northings	Yield
1	508562	235514	4.00
2	508533	235469	2.33
3	508562	235591	4.16
……	……	……	……
99981	508722	235521	3.88
99982	508706	235590	3.76

Population versus Sample

Before we go calculate averages, we need to think about the difference between population and sample

- We take a sample from a larger population
- What information does the sample give about the population and how reliable is that information?

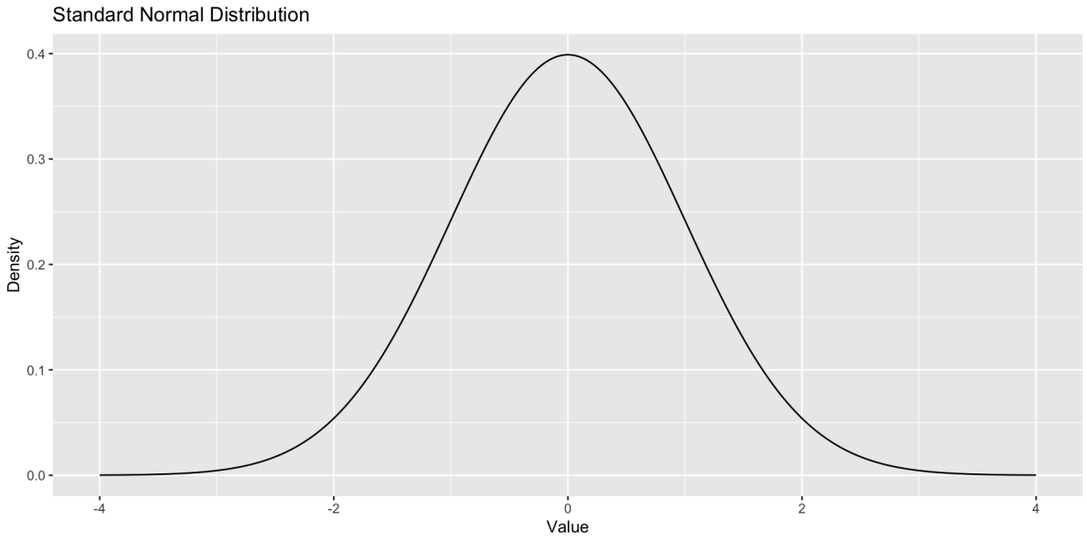


Source: https://www.omniconvert.com/what-is/sample-size/

Descriptive statistics

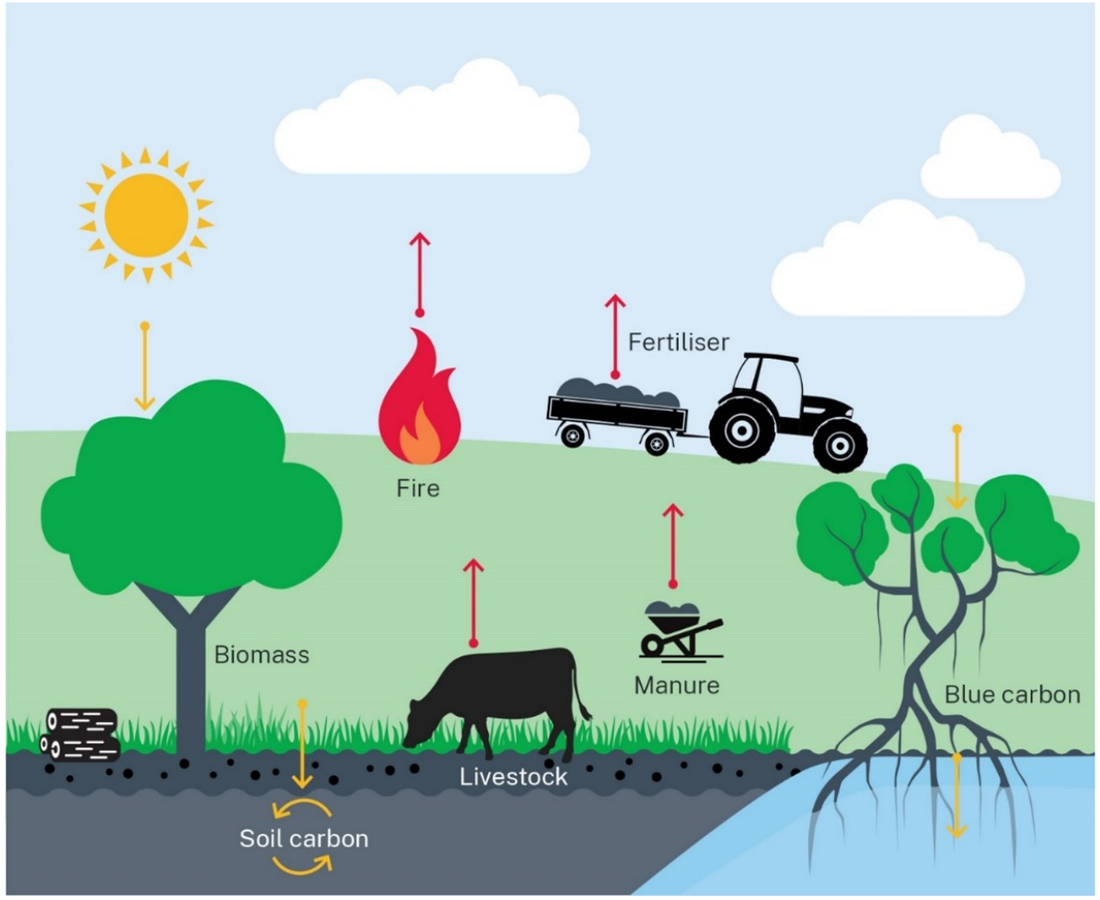
- Measures of central tendency
  - Mean
  - Median
  - Mode
- Measures of spread or dispersion
  - Range
  - Interquartile range
  - Standard deviation / Variance

```r
library(ggplot2)
library(tidyverse)

# Generate a normal distribution
normal_dist <- tibble(x = seq(-4, 4, by = 0.01)) %>%
  mutate(y = dnorm(x))

# Plot the distribution
ggplot(normal_dist, aes(x = x, y = y)) +
  geom_line() +
  ggtitle("Standard Normal Distribution") +
  xlab("Value") +
  ylab("Density")
```



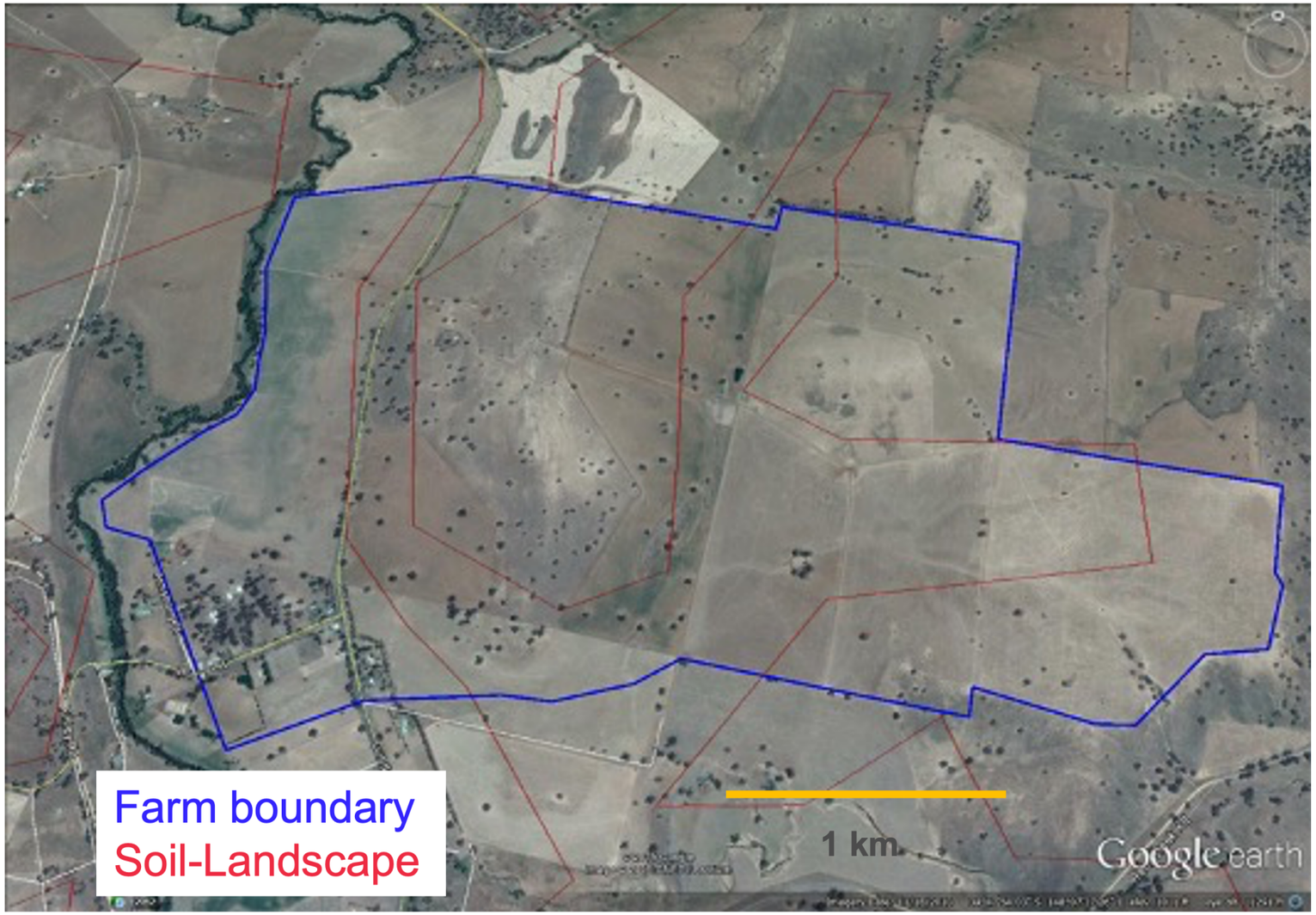
Motivating example

- Sequestered soil carbon is worth $35/tonne if measured (1 Tonne of Carbon = 1 Australian Carbon Credit Unit = $AU35 See Clean Energy Regulator)
- It costs $100 to collect and analyse one soil sample for soil carbon
- The farmer needs an estimate of carbon stored on the property.
- How many samples are needed to give a good estimate of carbon on the property? Is it worth measuring soil carbon for a land holder?



Source: https://www.energy.nsw.gov.au/business-and-industry/programs-grants-and-schemes/primary-industries-carbon-farming

Motivating example



Google earth image with farm and soil-landscape boundaries

Motivating example

- Soil carbon content was measured at 6 points across a farm
  - The amount at each location was 48, 56, 90, 78, 86, 271 (t/ha)
- We will now get into some formulas and calculations ;o)

Sigma notation

- Σ, is the greek capital letter called sigma, refers to the sum
- It is a convenient way to represent long sums

$$\Sigma_{i=1}^{n} = x_1 + x_2 + x_3 + ... + x_n$$

 - `sum(c(48, 56, 78, 86, 90, 271))`

```r
total_c <- sum(c(48, 56, 78, 86, 90, 271))
print(total_c)
```

```
[1] 629
```

 - `=SUM(A1:A6)`

Centre: Arithmetic mean

- Population mean (μ): sum of all values of a variable divided by the number of objects in the population;

$$\mu = \frac{\sum_{i=1}^{N} y_i}{N}$$

- Sample mean $(\overline{y})$ is based on a subset of n objects from a population of size N

$$\overline{y} = \frac{\sum_{i=1}^{n} y_i}{n}$$

 - `mean(c(48, 56, 78, 86, 90, 271))`

```r
mean_c <- mean(c(48, 56, 78, 86, 90, 271))
print(mean_c)
```

```
[1] 104.8333
```

 - `=AVERAGE(A1:A6)`

Centre: Median

- Median is the middle number of a set of ordered observations
- Population median M: sum of all values of a variable divided by the number of objects in the population;

Population median: $M = \left(\frac{N+1}{2}\right) th$ sorted value

Sample median: $\tilde{y} = \left(\frac{n+1}{2}\right) th$ sorted value

 - `median(c(48, 56, 78, 86, 90, 271))`

```r
median_c <- median(c(48, 56, 78, 86, 90, 271))
print(median_c)
```

```
[1] 82
```

 - `=MEDIAN(A1:A6)`

Centre: Mode

Mode is the most commonly occurring number in a set of observations

-

```r
mode_function <- function(x) {
  uniq_x <- unique(x)
  uniq_x[which.max(tabulate(match(x, uniq_x)))]
}
data_vector <- c(1, 2, 4, 4, 3, 5, 4)
mode_value <- mode_function(data_vector)
print(mode_value)
```

```
[1] 4
```

- `=MODE.SNGL(A1:A7)`

Spread: Range

- Difference between largest and smallest observations in a group of data
- Note that we also refer to spread as measures of dispersion

- `max(c(48, 56, 78, 86, 90, 271)) - min(c(48, 56, 78, 86, 90, 271))`

```r
range_c <- max(c(48, 56, 78, 86, 90, 271)) - min(c(48, 56, 78, 86, 90, 271))
print(range_c)
```

```
[1] 223
```

- `=MAX(A1:A6) - MAX(A1:A6)`

Spread: Inter-quartile range (IQR)

- Median divides dataset into 2, quartile divides it into 4:
  - 25% observations ≤ 1st quartile (Q1)
  - 50% observations ≤ Median (Q2)
  - 75% observations ≤ 3rd quartile (Q3)

Let’s take an easy example

1 2 3 4 5 6 7 8 9

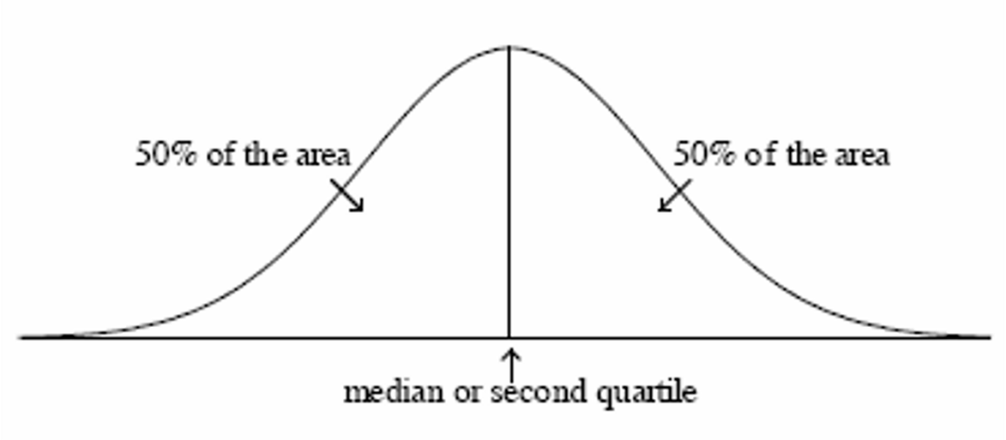
What is Q1, Median, Q3?

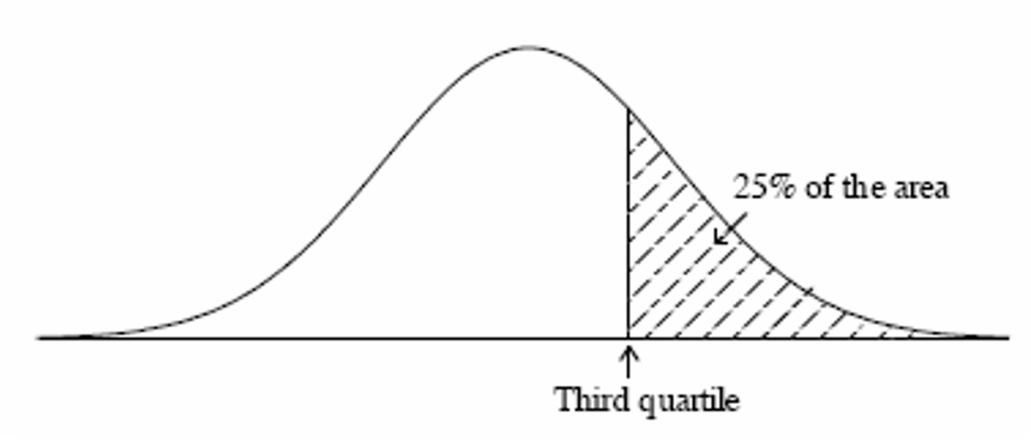
```
1 quantile(c(1,2,3,4,5,6,7,8,9))
```

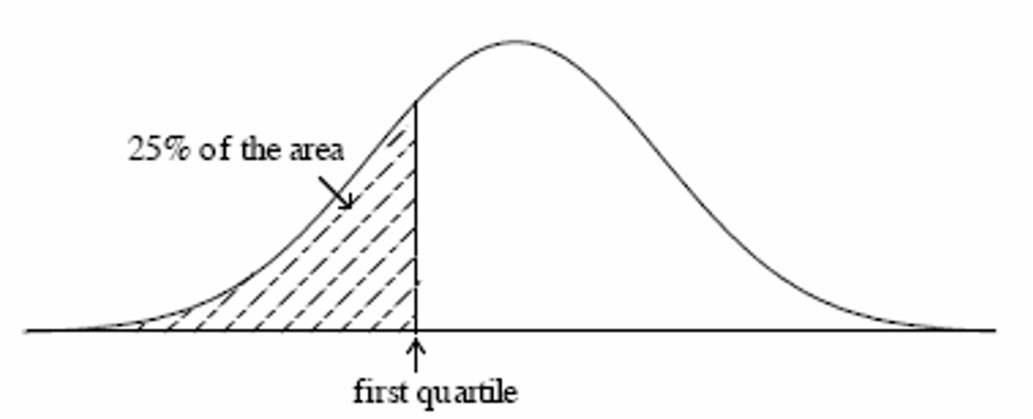
```
  0%  25%  50%  75% 100% 
   1    3    5    7    9 
```

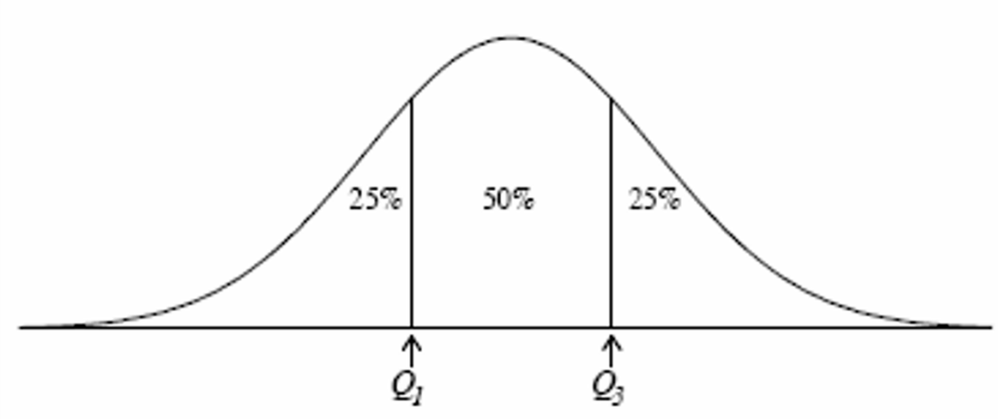
Spread: Inter-quartile range (IQR)

- $IQR = Q_3 - Q_1$









Source: Nicholas (1999)

Spread: Inter-quartile range (IQR)

Quartiles

- `quantile(c(48, 56, 78, 86, 90, 271))`

```r
quant_c <- quantile(c(48, 56, 78, 86, 90, 271))
print(quant_c)
```

```
   0%   25%   50%   75%  100%
 48.0  61.5  82.0  89.0 271.0
```

- `=QUARTILE.INC(A1:A6, 1)` - first quartile

Spread: Inter-quartile range (IQR)

IQR

- `IQR(c(48, 56, 78, 86, 90, 271))`

```r
iqr_c <- IQR(c(48, 56, 78, 86, 90, 271))
print(iqr_c)
```

```
[1] 27.5
```

- `=QUARTILE.INC(A1:A6, 3)-QUARTILE.INC(A1:A6, 1)` - third quartile - first quartile

Spread: Variance

- Describes variability around the arithmetic mean

Population variance: $\sigma^2 = \frac{\sum_{i=1}^{N}(y_i - \mu)^2}{N}$

Sample variance: $\backslash s^2 = \frac{\sum_{i=1}^{n}(y_i - \bar{y})^2}{n}$

- `var(c(48, 56, 78, 86, 90, 271))`

```r
var_c <- var(c(48, 56, 78, 86, 90, 271))
print(var_c)
```

```
[1] 6904.167
```

- `=VAR.S(A1:A6)`

Spread: Standard deviation

- Describes variability around the **arithmetic mean**
  - Variance is in $units^2$ as it is based on squared deviations from the mean
  - Standard deviation describes variability around the mean in original units
  - Standard deviation \sqrt of the variance

Population standard deviation: $\sigma^2 = \sqrt{\frac{\sum_{i=1}^{N}(y_i-\mu)^2}{N}}$

Sample variance: $s^2 = \sqrt{\frac{\sum_{i=1}^{n}(y_i-\overline{y})^2}{n-1}}$

Spread: Standard deviation

- R's sd function always calculates the sample standard deviation
- The denominator of sample standard is n−1 (Bessel's correction) this is an important concept in statistics. A key property is that it gives a more accurate estimate of the population variance and standard deviation when working with a sample.

- `sd(c(48, 56, 78, 86, 90, 271))`

```r
sd_c <- sd(c(48, 56, 78, 86, 90, 271))
print(sd_c)
```

```
[1] 83.09132
```

- `=STDEV.S(A1:A6)`

Spread: Coefficient of variation

- Let’s take an example where we measured both nitrogen and carbon in our soil such that:

Soil nitrogen (%): 2 16 22 45 65 93

- How could we find out which measurements have a greater spread given they have very different units (% versus t/ha)?
- It turns out we can use the CV

$$CV = \left(\frac{s}{\bar{y}}\right) \times 100$$

Spread: Coefficient of variation

- Looking at the calculations below, which is more variable, Carbon or Nitrogen?

 - `sd(c(48, 56, 78, 86, 90, 271))`

```
cv_c <- sd(c(48, 56, 78, 86, 90, 271))/mean(c(48, 56, 78, 86, 90, 271))*100
print(cv_c)
```

```
[1] 79.2604
```

```
cv_n <- sd(c(2, 16, 22, 45, 65, 93))/mean(c(2, 16, 22, 45, 65, 93))*100
print(cv_n)
```

```
[1] 84.10661
```

 - `=(STDEV.S(A1:A6)/AVERAGE(A1:A6))*100`

Robustness (to outliers)

- Which summary statistics should I use to describe centre?
  - Example: 48, 56, 8, 86, 90, 27
  - Example: 48, 56, 8, 86, 90, 271

mean - $\overline{y}$:

```
1 mean(c(48, 56, 8, 86, 90, 27))
```

```
[1] 52.5
```

```
1 mean(c(48, 56, 8, 86, 90, 271))
```

```
[1] 93.16667
```

median - $\tilde{y}$:

```
1 median(c(48, 56, 8, 86, 90, 27))
```

```
[1] 52
```

```
1 median(c(48, 56, 8, 86, 90, 271))
```

```
[1] 71
```

Robustness (to outliers)

- Which summary statistics should I use to describe spread?
  - Example: 48, 56, 8, 86, 90, 27
  - Example: 48, 56, 8, 86, 90, 271

variance - s:

```
1  var(c(48, 56, 8, 86, 90, 27))
```

```
[1] 1038.3
```

```
1  var(c(48, 56, 8, 86, 90, 271))
```

```
[1] 8472.167
```

Inter quartile range - IQR:

```
1  IQR(c(48, 56, 8, 86, 90, 27))
```

```
[1] 46.25
```

```
1  IQR(c(48, 56, 8, 86, 90, 271))
```

```
[1] 39
```

Categorical data

- Different types with examples:
  - Binary: We spray insects and see how many die
  - Nominal: We count how animals, and their species, are in a forest
  - Ordinal: Different disease levels for a plant, no disease, moderate, severe
- We can count the number observations belonging to each class, called frequency, f.
  - Can present as a frequency table

Plant disease severity	Frequency
None	3
Moderate	5
Severe	2

Graphical summaries

- Visualisation of data is useful for identifying
  - outliers
  - shape and distribution
  - communicating results
  - suggest modelling strategies
- Bar chart
- Strip chart
- Boxplot
- Histogram

Bar chart

- We first tabulate the data

```r
# Load necessary library
library(ggplot2)

# Your disease data
disease <- c("None", "Moderate", "None", "Severe", "Moderate", "Moderate", "Severe", "Moderate", "None", "Moderate")

# Order factors from no disease to severe disease
disease = factor(disease, levels = c("None", "Moderate", "Severe"))

# Create a frequency table
disease_tbl <- table(disease)
print(disease_tbl)
```

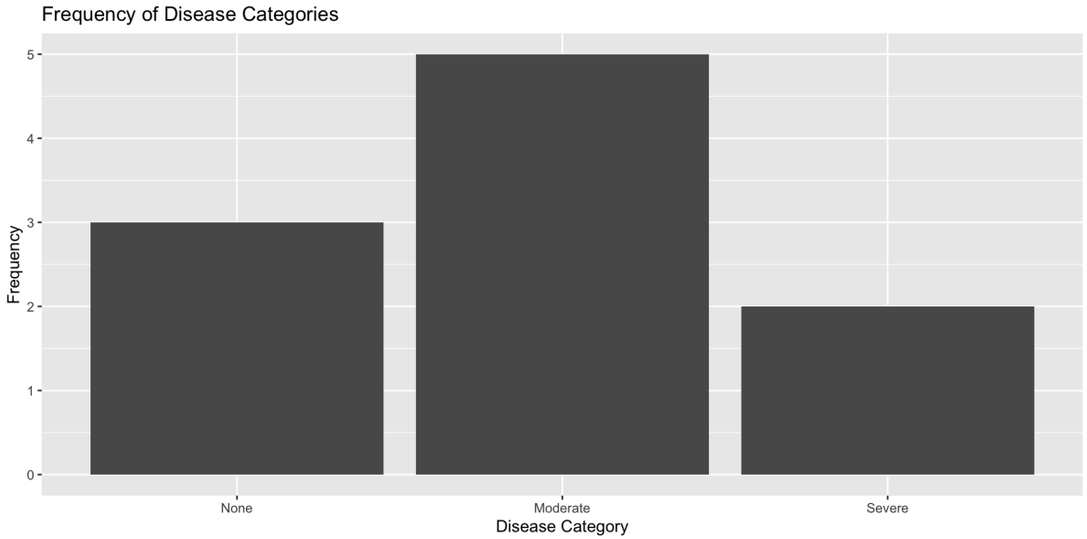
```
disease
    None Moderate   Severe
       3        5        2
```

Bar chart

- We then plot the table in ggplot

```r
# Convert the table to a data frame for ggplot2
disease_df <- as.data.frame(disease_tbl)

# Rename the columns appropriately
names(disease_df) <- c("Disease", "Frequency")

# Create the bar plot
p <- ggplot(disease_df, aes(x = Disease, y = Frequency)) +
  geom_bar(stat = "identity") +
  ggtitle("Frequency of Disease Categories") +
  xlab("Disease Category") +
  ylab("Frequency")
```

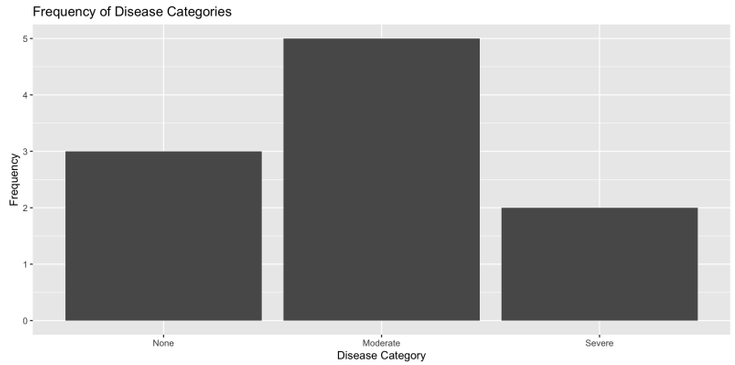
```r
print(p)
```



Bar chart

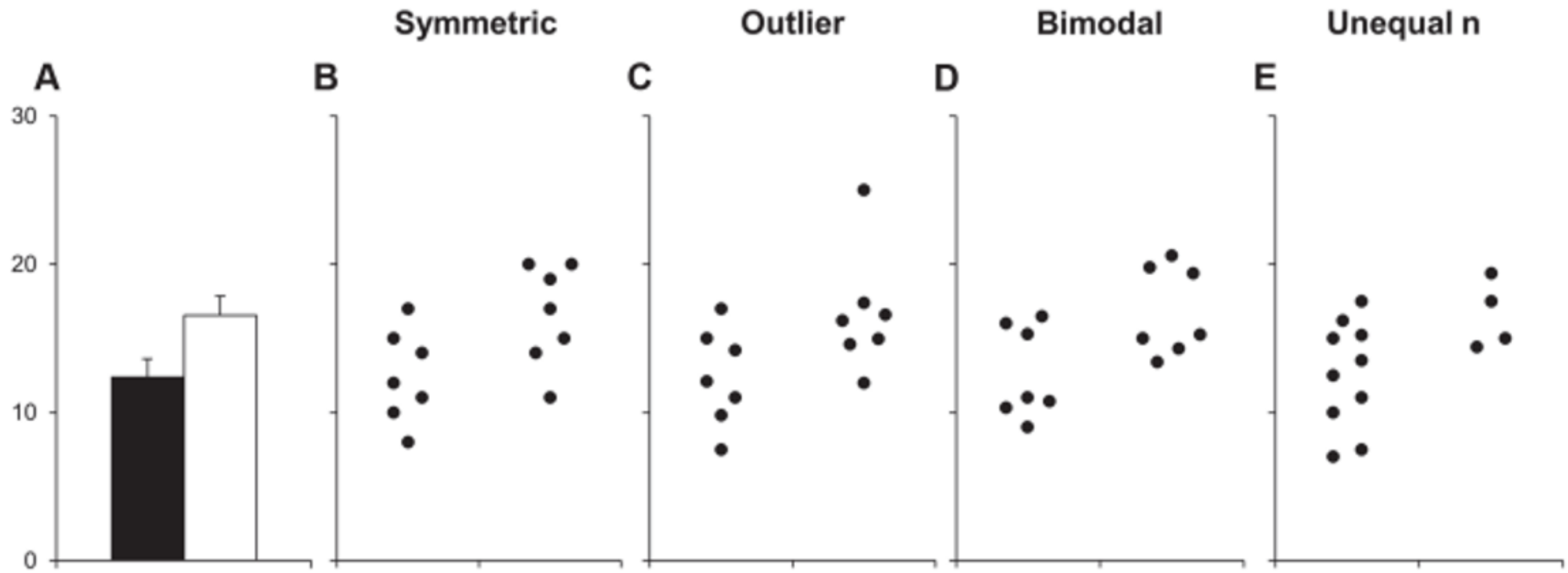
- Using `tidyverse`

```r
# Load necessary libraries
library(tidyverse)

# Your disease data
disease <- c("None", "Moderate", "None", "Severe", "Moderate", "Moderate", "Severe", "Moderate", "None", "Moderate")

# Convert to tibble and count occurrences
disease_data <- tibble(disease) %>%
  mutate(disease = factor(disease, levels = c("None", "Moderate", "Severe"))) %>%
  count(disease, name = "Frequency")

# Create the bar plot
ggplot(disease_data, aes(x = disease, y = Frequency)) +
  geom_bar(stat = "identity") +
  ggtitle("Frequency of Disease Categories") +
  xlab("Disease Category") +
  ylab("Frequency")
```



Bar chart

- NOTE: Bar charts should generally not used for continuous numerical data



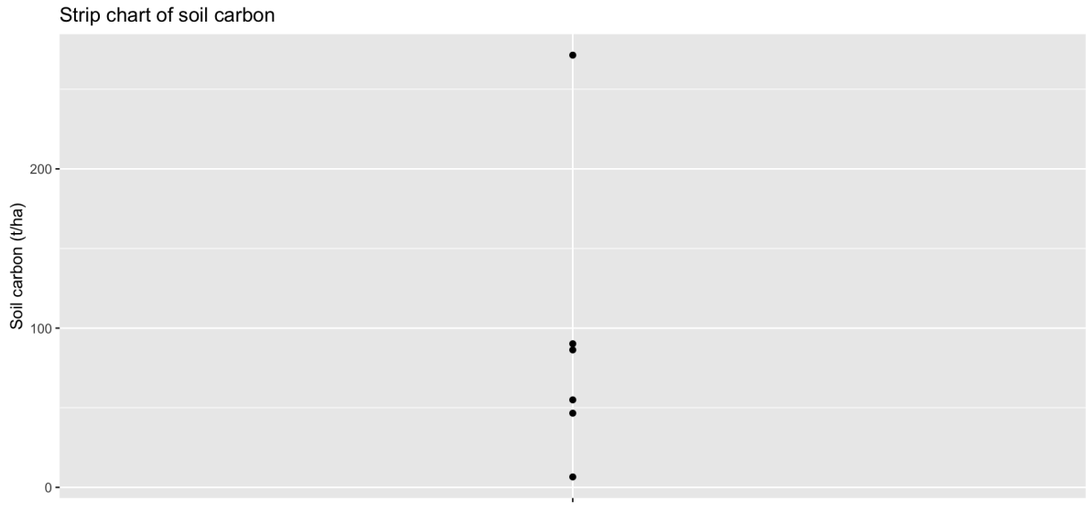
Source: Weissgerber at al. (2015)

Strip chart

- Often if we have a small data set (1-5 data points), we can use a stripchart to visualise our data. We will demonstrate using our soil carbon data set.
- What do we notice from the plot?

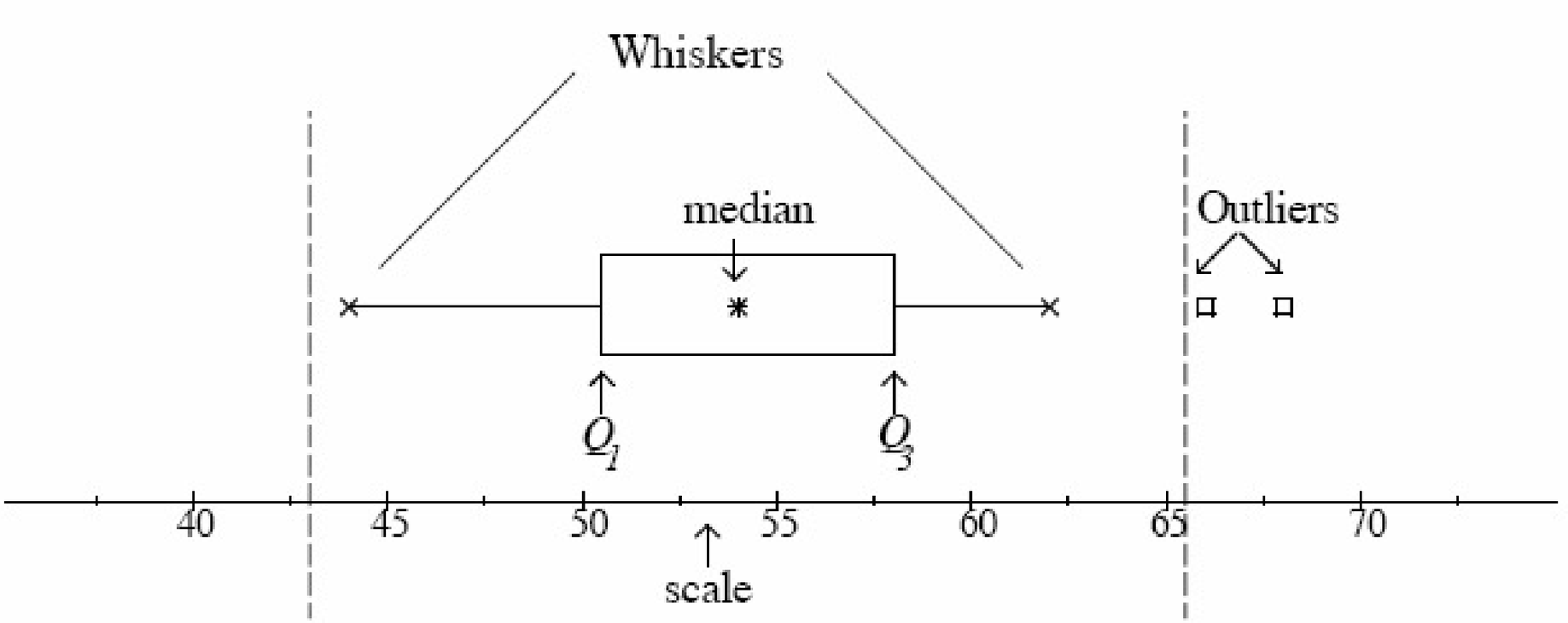
```r
# Load necessary library
library(ggplot2)

# Your data
soil_c <- c(48, 56, 8, 86, 90, 271)

# Convert to a data frame
soil_c_df <- data.frame(Value = soil_c)

# Create the strip chart
p <- ggplot(soil_c_df, aes(x = "", y = Value)) +
  geom_jitter(width = 0) +
  ggtitle("Strip chart of soil carbon") +
  xlab("") +
  ylab("Soil carbon (t/ha)")
```

```r
print(p)
```



Boxplot

- We can overlay our strip chart with a boxplot. This shows use the min/max, quartiles and median and can also show outliers.
- We generally use boxplots when we have more than 5 data points.
- See lecture notes for creating boxplot by hand.



Nicholas 1999

Boxplot

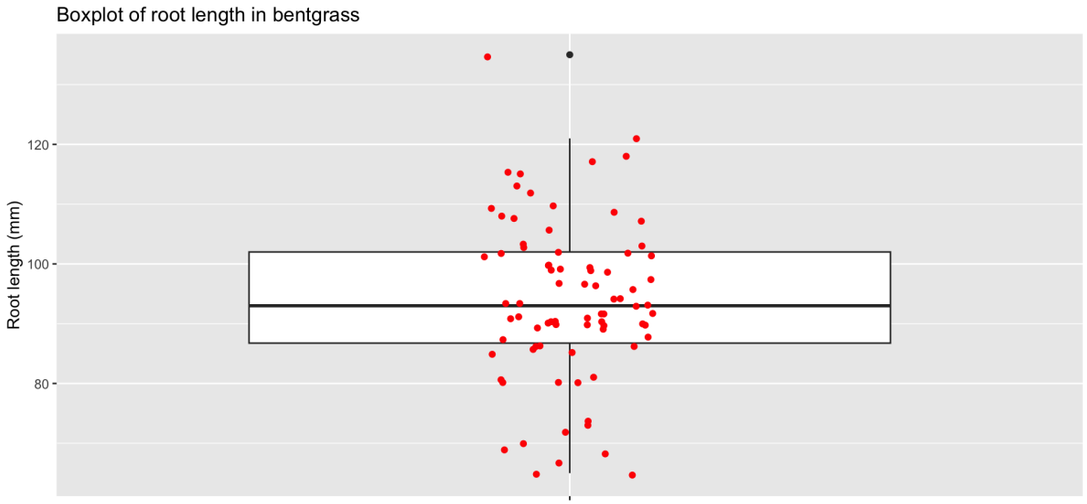
- Here is a slightly larger data set from a trial where creeping bentgrass turf was laid in an experiment to assess root growth. Eighty (80) “plugs” were randomly sampled 4 weeks after laying. Root growth was measured by averaging the length (mm) of the ten longest roots in each plug.

```
root_length <- c(108, 102, 100, 135, 113, 109, 92, 97, 73, 65,
68, 74, 93, 97, 118, 121, 103, 99, 90, 90,
99, 102, 106, 90, 92, 97, 100, 92, 80, 99,
103, 103, 115, 85, 96, 86, 85, 86, 91, 90,
94, 93, 93, 99, 109, 115, 110, 94, 107, 88,
101, 89, 117, 91, 112, 101, 91, 81, 80, 67,
69, 80, 86, 81, 65, 90, 99, 93, 90, 102,
72, 70, 90, 90, 87, 89, 90, 96, 108, 86)
```

Boxplot

- The follow produces a boxplot and also includes the jittered data points (red coloured)
- Note that there is on outlier which is the black data pointat the top of the plot

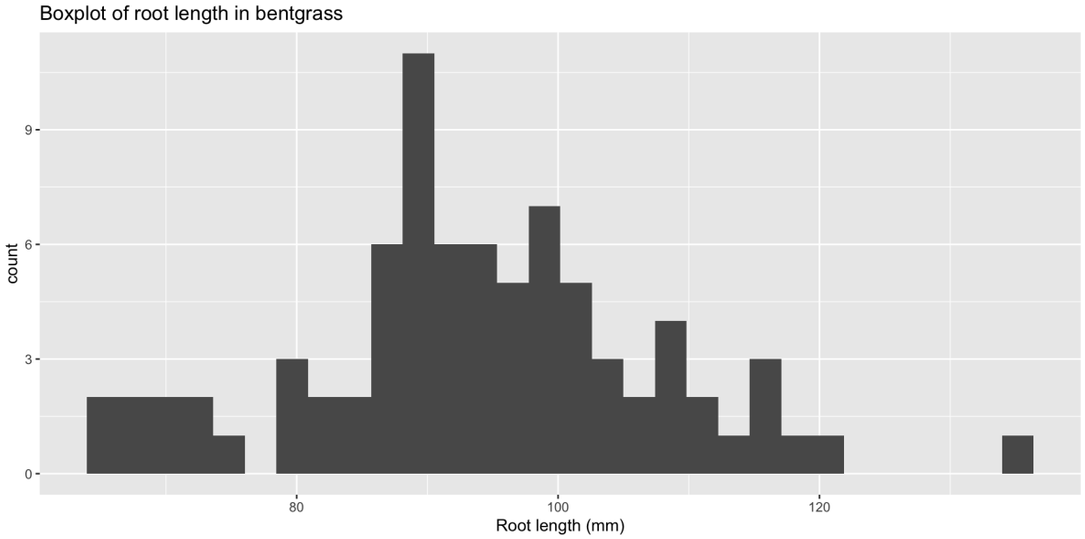
```r
# Load necessary library
library(ggplot2)

# Convert to a data frame
root_length_df <- data.frame(Value = root_length)

# Create the strip chart
ggplot(root_length_df, aes(x = "", y = Value)) +
  geom_boxplot() +
  geom_jitter(width = 0.1, col = "red") +
  ggtitle("Boxplot of root length in bentgrass") +
  xlab("") +
  ylab("Root length (mm)")
```



Histogram

- Based on frequency table
  - Height of each bar proportional to frequency - need to group data
  - We can use histograms to describe the shape of distributions for continuous data sets that are larger than 20 data points.

```r
# Load necessary library
library(ggplot2)

# Convert to a data frame
root_length_df <- data.frame(Value = root_length)

# Create the strip chart
ggplot(root_length_df, aes(Value)) +
  geom_histogram() +
  ggtitle("Boxplot of root length in bentgrass") +
  xlab("Root length (mm)")
```



Summary

- The following is a rough guide for plotting *continuous* data

observations	graphics	R function
1-5	raw data	stripchart
6-20	boxplot	boxplot
20+	histogram	hist

- Remember for *categorical* data we use **Tables** and **Bar Charts**

Symmetry

- Throughout this unit you will be assessing the shape of distributions, in particular you will be looking at whether the distribution (histogram) of the data is symmetrical in shape;
- For small data sets, you will generally compare the mean and median;
  - if the mean and the median are similar it indicates that the data is symmetrical.
  - if the mean and the median are not similar it indicates that the data is skewed.

```
1 mean(soil_c)
```

```
[1] 93.16667
```

```
1 median(soil_c)
```

```
[1] 71
```

- What can we conclude from the mean and median of our soil carbon data?

Symmetry

- For larger data sets, we can look at the mean, median and the histogram to determine if it is symmetrical.

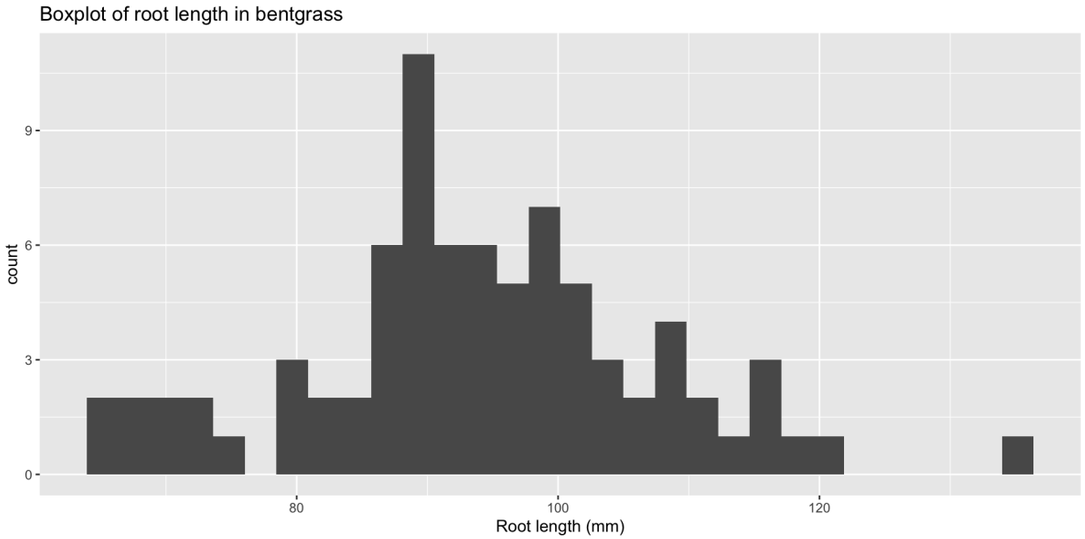
```
1  mean(root_length)
```

```
[1] 93.8625
```

```
1  median(root_length)
```

```
[1] 93
```

```
1  # Create the strip chart
2  ggplot(root_length_df, aes(Value)) +
3    geom_histogram() +
4    ggtitle("Boxplot of root length in bentgrass") +
5    xlab("Root length (mm)")
```



Symmetry

- We can also calculate skewness using the following equation

$$g_1 = \frac{n}{(n-1)(n-2)} \sum_{i=1}^{n} \left(\frac{y_i - \bar{y}}{s} \right)^3$$

- in RStudio, we can use the `skewness` function found in the `e1071` package

```
1 library(e1071)
2 skewness(root_length)
```

```
[1] 0.08316635
```

- if $|g_1| < 1.0$ then the dataset is approximately symmetrical. If $g_1 > 1.0$ then the data is positively skewed and if $g_1 < -1.0$ then the data is negatively skewed

Reading

- Canvas site
- Notes
- Quinn & Keough (2002)
  - Chapter 2. Sections 2.1-2.2, p. 14-17.
  - Chapter 4. Sections 4.1, p. 58-61 (stop at scatterplot)
- Mead et al. (2002).
  - Chapter 1.
  - Chapter 2. Sections 2.1-2.3, p. 9-19

References

- J. Nicholas (1999). Introduction to descriptive statistics. Mathematics Learning Centre, University of Sydney.
- T. L. Weissgerber, N. M. Milic, S. J. Winham and V. D. Garovic (2015). Beyond bar and line graphs: time for a new data presentation paradigm. PLOS Biology. 13. e1002128.

Thanks!

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