Descriptive Statistics

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Exploratory Data Analysis

- Descriptive Statistics or Exploratory Data Analysis or (EDA) encompasses a set of techniques to quickly understand the nature of a data collection or dataset.
- The main goal of descriptive statistics is to explore the data to find some patterns that can be exploited to generate hypotheses.
- It was proposed by the statistician John Tukey.
- It is based mainly on two types of techniques: summary statistics and data visualization.
- In this class you will see both types of techniques, in addition to their application in R for some toy datasets.
- This class in partially based on chapter 3 of [Tan et al., 2016].

The Iris dataset

- We will work with a well-known dataset called Iris.
- The dataset consists of 150 observations of iris plant flowers.
- There are three types of iris flower classes: virginica, setosa and versicolor.
- There are 50 observations of each.
- The variables or attributes measured for each flower are:
 - The type of flower as a categorical variable.
 - The length and width of the petal in cm as numerical variables.
 - The length and width of the sepal in cm as numeric variables.



The Iris dataset







Figure: Virginica - Setosa - Versicolor

The dataset is available in R:

 In order to access the variables directly in our workspace we use the command attach (iris).

Summary Statistics

- Summary statistics are values that explain properties of the data.
- Some of these properties include: frequencies, measures of central tendency and dispersion.
- Example:
 - Central tendency: mean, median, mode.
 - Variation: measure the variability of the data, such as standard deviation, range, etc..
- Most summary statistics can be calculated by making a single pass through the data.

Frequency and Mode

- The absolute frequency of an attribute value is the number of times it is observed.
- The relative frequency is the absolute frequency divided by the total number of examples.
- In R we can count the frequencies of occurrence of each distinct value of a vector using the command table:

• Exercise: Calculate the relative frequencies of the above vector.

```
> table(vec)/length(vec) # Relative frequencies
vec
    0    1    2    3
0.2   0.3   0.1   0.4
```

Frequency and Mode (2)

- The mode of an attribute is the most frequent value observed.
- The mode function is not implemented natively in R, but it is easy to calculate using table and max:

```
my_mode<-function(var){
   frec.var<-table(var)
   value<-which(frec.var==max(frec.var))
   as.numeric(names(value))
}
> my_mode(vec)
[1] 3
> my_mode(iris$Sepal.Length)
[1] 5
```

• We generally use frequencies and mode to study categorical variables.

Central Tendency Measures

- These measures attempt to summarize the observed values into a single value associated with the centrally located value.
- The mean is the most common measure of central tendency for a numeric variable.
- If we have *n* observations it is calculated as the arithmetic mean or average.

$$\operatorname{mean}(x) = \overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

- The major problem with the mean is that it is very sensitive to outliers.
- We take a random vector of mean 20 and then add a random element that comes from a distribution of much larger mean. We see that the mean is strongly affected by noise:

```
> vec<-rnorm(10,20,10)
> mean(vec)
[1] 16.80036
> vec.noise<-c(vec,rnorm(1,300,100))
> mean(vec.noise)
[1] 35.36422
```

Central Tendency Measures (2)

- We can robust the mean by removing a fraction of the extreme values using the trimmed mean.
- In R we can give a second parameter to the function mean called trim that
 defines the fraction of extreme elements to discard.
- Example: We discard 10% of the extreme values in the previous example:

```
> mean(vec,trim=0.1)
[1] 17.78799
> mean(vec.noise,trim=0.1)
[1] 19.51609 # much more robust
```

Central Tendency Measures (3)

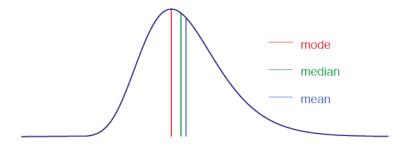
- The median represents the central ranking position of the variable that separates the lower half and the upper half of the observations.
- Intuitively, it consists of the value where for one half of the observations all values are greater than it, and for the other half all are less.

$$\mathrm{median}(x) = \left\{ \begin{array}{cc} x_{r+1} & \text{ If } |x| \text{ (vector length) is odd, } |x| = 2r+1 \\ \frac{1}{2}(x_r + x_{r+1}) & \text{ If } |x| \text{ is even, } |x| = 2r \end{array} \right.$$

 For the above example, we see that the median is more robust to noise than the mean:

```
> median(vec)
[1] 17.64805
> median(vec.noise)
[1] 17.64839
```

Comparison between mode, median and mean



Percentiles or Quantiles

- The k-th percentile of a numerical variable is a value such that k% of the observations are below the percentile and (100 k)% are above this value.
- Quantiles are equivalent to percentiles but expressed in fractions instead of percentages.
- In R they are calculated with the command quantile:

```
# All percentiles
quantile(Sepal.Length,seq(0,1,0.01))
```

- In addition it is very common to talk about the quartiles which are three specific percentiles:
 - The first quartile Q_1 (lower quartile) is the percentile with k = 25.
 - The second quartile Q_2 is with k = 50 which is equivalent to the median.
 - The third quartile Q_3 (upper quartile) is with k = 75.

Summarizing a Data Frame

- In R we can summarize various summary statistics of a variable or of a data.frame using the command summary.
- For numerical variables it gives us the minimum, the quartiles, the mean and the maximum.
- For categorical variables it gives us the frequency table.

```
> summarv(iris)
Sepal.Length Sepal.Width Petal.Length
                                          Petal Width
Min. :4.300 Min. :2.000
                            Min. :1.000
                                           Min. :0.100
1st Ou.:5.100
              1st Ou.:2.800
                             1st Ou.:1.600
                                           1st Ou.:0.300
Median :5.800 Median :3.000
                            Median :4.350
                                           Median :1.300
Mean :5.843 Mean :3.057
                            Mean :3.758
                                           Mean :1.199
3rd Ou.:6.400 3rd Ou.:3.300
                            3rd Ou.:5.100
                                           3rd Ou.:1.800
Max. :7.900
              Max. :4.400
                            Max. :6.900
                                           Max. :2.500
```

Species setosa :50 versicolor:50 virginica :50

Exercise

- Using the command tapply analyze the mean, median and quartiles for the three species of Iris for the four variables.
- Do you notice any differences in the different species?

```
tapply(iris$Petal.Length,iris$Species,summary)
tapply(iris$Petal.Width,iris$Species,summary)
tapply(iris$Sepal.Length,iris$Species,summary)
tapply(iris$Sepal.Width,iris$Species,summary)
```

Variability Measures

- Variability mesaures or dispersion measures tell us how different or similar the observations tend to be with respect to a particular value. Usually this value refers to some measure of central tendency.
- The range is the difference between the maximum and minimum value:

```
> max(Sepal.Length) -min(Sepal.Length)
[1] 3.6
```

 The standard deviation is the square root of the variance that measures the mean squared differences of the observations from the mean.

$$var(x) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \overline{x})^2$$

$$sd(x) = \sqrt{var(x)}$$

```
> var(Sepal.Length)
[1] 0.6856935
> sd(Sepal.Length)
[1] 0.8280661
```

Variability Measures (2)

- Like the mean, the standard deviation is sensitive to outliers.
- The most robust measures are usually based on the median.
- Let m(x) be a measure of central tendency of x (usually the median), we define the average absolute deviation (AAD) as:

$$AAD(x) = \frac{1}{n} \sum_{i=1}^{n} |x_i - m(x)|$$

 Exercise: Program the function add in R, as a function that receives a vector x and a central mean function fun. The absolute value is calculated with the command abs:

```
aad<-function(x, fun=median) {
  mean(abs(x-fun(x)))
}
> aad(Sepal.Length)
[1] 0.6846667
> aad(Sepal.Length, mean)
[1] 0.6875556
```

Variability Measures (3)

• Let b be a constant we define the **median absolute deviation** as:

$$\mathsf{MAD}(x) = b \times \mathsf{median}(|x_i - \mathsf{m}(x)|)$$

 In R is calculated with the command mad with the parameters center as a function measuring the central tendency of the variable and constant as the constant b. By default the median and the value 1.482 is used.

```
> mad(Sepal.Length)
[1] 0.7
```

• Finally, the interquartile range (IQR) is defined as the difference between the third and the first quartile $(Q_3 - Q_1)$.

```
IQR(Sepal.Length)
[1] 1.3
```

Multivariate Summary Statistics

- To compare how one variable varies with respect to another, we use multivariate measures.
- The covariance cov(x, y) measures the degree of joint linear variation of a pair of variables x, y:

$$cov(x,y) = \frac{1}{n-1} \sum_{i=1}^{n} (x - \overline{x})(y - \overline{y})$$

- Where cov(x, x) = var(x)
- In R it is computed with the command cov:

```
> cov(Sepal.Length, Sepal.Width)
[1] -0.042434
```

 If we give it a matrix or a data.frame of numeric variables, it computes a covariance matrix:

Multivariate Summary Statistics (2)

- If two variables are independent of each other, their covariance is zero.
- A measure of relationship that does not depend on the scale of each variable is the linear correlation.
- The linear correlation or **Pearson's** correlation coefficient r(x, y) is defined as:

$$r(x,y) = \frac{cov(x,y)}{sd(x)sd(y)}$$

■ The linear correlation varies between -1 to 1.

Multivariate Summary Statistics (3)

- A value close to 1 indicates that as one variable grows the other also grows in a linear proportion.
- A value close to -1 indicates an inverse relationship (one is growing and the other is decreasing).
- If the correlation is close to zero we have linear independence.
- Note that a correlation of zero does not imply that there cannot be a non-linear relationship between the variables.
- In R, the correlation is calculated with the command cor.

Contingency Tables

- To analyze the relationship between categorical variables we use contingency tables.
- The table is filled with the marginal frequencies of all pairs of values between two categorical variables.
- In R they are created using the command table that we used before for computing frequencies, but now giving two vectors as input:

Skweness and Kurtosis

There are other two summary statistics that focus on more complex properties of the data distribution called skeweness and kurtosis [Pipis, 2020].

Skeweness

Skeweness is a measure of the asymmetry of the probability distribution.

skewness(x) =
$$\frac{\sum_{i=1}^{n} (x_i - \overline{x})^3}{(n-1)sd(x)^3}$$

- It indicates how much our underlying distribution deviates from the normal distribution since the normal distribution has skewness 0.
- Generally, we have three types of skewness:
 - Symmetrical: the skewness is close to 0 and the mean is almost the same as the median.
 - 2 Negative skew: the majority of the observations are concentrated on the right tail (the median is greater than the mean).
 - Positive skew: the majority of the observations are concentrated on the left tail (the median is less than the mean).

Skweness

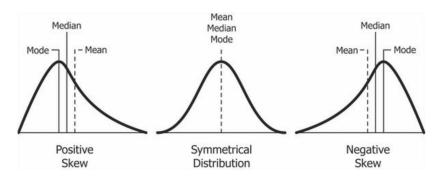


Figure: Source: Wikipedia

Skweness

 In R, we can calculate skweness with the formula skewness from the library moments:

```
> library(moments)
#positive skew
> skewness(c(1,1,2,3))
[1] 0.4933822
#symmetrical
> skewness(c(1,2,3))
[1] 0
#negative skew
> skewness(c(1,2,3,3))
[1] -0.4933822
```

Kurtosis

• The Kurtosis describes the "tailedness" of a distribution [Westfall, 2014].

$$kurtosis(x) = \frac{\sum_{i=1}^{n} (x_i - \overline{x})^4}{(n-1)sd(x)^4}$$

- Let's see the main three types of kurtosis.
 - **Mesokurtic**: This is the normal distribution (kurtosis \approx 3)
 - Leptokurtic: This distribution has fatter tails than a normal distribution (kurtsosis > 3). Consequently, outliers are more likely to occur than in a normal distribution.
 - Platykurtic: The distribution has thinner tails than a normal distribution (kurtosis < 3). Consequently, outliers are less likely to occur than in a normal distribution.

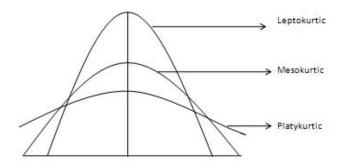
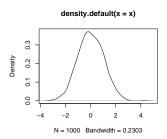


Figure: Source: tutorialspoints

- In R, we can calculate kurtosis with the formula kurtosis from the library moments.
- Let's calculate kurtosis for normal data:

```
> x <- rnorm(1000, 0,1)
> plot(density(x))
> kurtosis(x)
[1] 2.946869
```

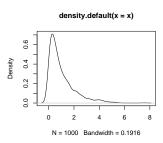
As expected we got a value close to 3.



Now using random data generated with an exponential long-tailed distribution:

```
> x<-rexp(1000)
> plot(density(x))
> kurtosis(x)
[1] 6.839485
```

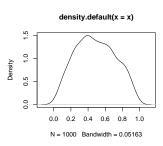
 As expected we get a positive excess kurtosis (i.e. greater than 3) since the distribution has fatter tails (Leptokurtic).



 Now using data generated with a thinner-tailed Beta distribution with hyperparameters 2, 2:

```
> x <-rbeta(1000,2,2)
> plot(density(x))
> kurtosis(x)
[1] 2.1046
```

 As expected we get a negative excess kurtosis (i.e. less than 3) since the distribution has thinner tails (Platykurtic).



Data Visualization

- Data visualization is the transformation of a dataset into a visual format that allows people to identify the characteristics and relationships between examples in the dataset.
- Visualization allows people to recognize patterns or trends based on their judgment or expertise in the particular domain.



Representation

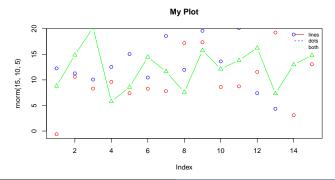
- Representation is understood as the mapping of data into a visual format
- Examples, their attributes and relationships are translated into graphical elements such as points, lines, shapes and colors.
- Examples are usually represented as points.
- Attribute values are represented as the position of the points or the characteristics of the points, e.g. color, size and shape.
- When using position to represent values it is simple to detect if groups of objects are formed or the presence of outliers.

Plotting in R

- In R the most frequent display function is plot.
- t is a generic function whose result depends on the nature of the variables given as input.
- To all plots we can add additional parameters such as: main for the title, xlab and ylab for the name of the x-axis and y-axis.
- Other properties are: col to define the color, type to define the chart type: (p) for points or (l) for lines.
- We can also add new layers to a plot with the command lines.
- To save an image to a file we can use Rstudio's export button.
- To do it from the R command line:

```
png("image.png")
plot(1:10)
dev.off()
```

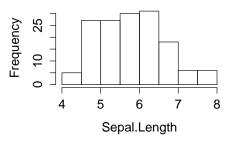
Example



Histograms

- They show the distribution of the values of a variable.
- The values of the elements are divided into bins and bar charts are created for each of them.
- The height of each bar indicates the number of examples in the corresponding bin.
- In R they are created with the command hist.
 - > hist (Sepal.Length)

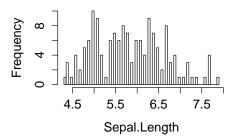
Histogram of Sepal.Length



Histograms (2)

- The shape of the histogram depends on the number of bins.
- In R this number can be defined with the parameter nclass.
 - > hist(Sepal.Length,nclass=100)

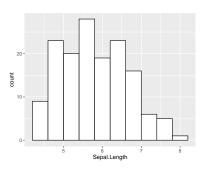
Histogram of Sepal.Length



Histograms (3)

- A very popular library for making visualizations in R, which is part of tidyverse, is ggplot2.
- It is based on the idea of decomposing the plot into semantic components such as scales and layers.

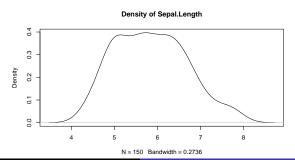
```
>install.packages("ggplot2")
>library(ggplot2)
>ggplot(iris, aes(x=Sepal.Length))
+ geom_histogram(bins = 10, color="black", fill="white")
```



Density

- Another way to visualize how the data are distributed is to estimate a density.
- These are calculated using nonparametric statistical techniques called kernel density estimation.
- The density is a smoothed version of the histogram and allows us to determine more clearly if the observed data behaves like a known density e.g., Gaussian.
- In R they are created with the command density, and then visualized with the command plot.

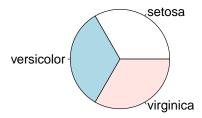
plot(density(iris\$Sepal.Length), main=""Density of Sepal.Length")



Pie Charts

- The pie charts represent the frequency of the elements in a circle.
- Each category has a share proportional to its relative frequency.
- They are generally used for categorical variables:

```
pie(table(iris$Species))
```



 Many people consider pie charts to be misleading and recommend using histograms as a better alternative [Poldrack, 2019].

Boxplots

- Boxplots are built from the percentiles.
- A rectangle is constructed between the first and third quartiles (Q_1 and Q_3).
- The height of the rectangle is the interquartile range IQR $(Q_3 Q_1)$.
- The median is a line that divides the rectangle.
- Each end of the rectangle is extended with a line or arms of length Q1 - 1.5*IQR for the lower line and Q3 + 1.5*IQR for the upper line.
- Values more extreme than the length of the arms are considered outliers.
- The boxplot gives us information about the symmetry of the data distribution.
- If the median is not in the center of the rectangle, the distribution is not symmetrical.
- They are useful to detect the presence of outliers.

Boxplots (2)

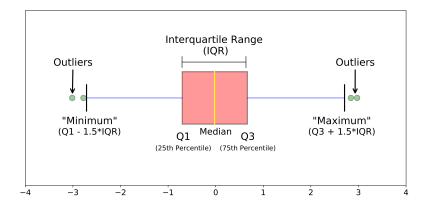
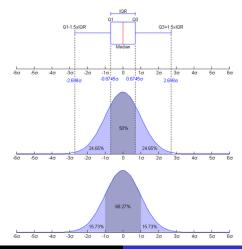


Figure: https://www.laboneconsultoria.com.br/wp-content/uploads/2018/07/Boxplot-04.png

Boxplots (3)

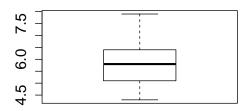
 The length of the arms as well as the criteria for identifying outliers is based on the behavior of a normal distribution.



Boxplots (4)

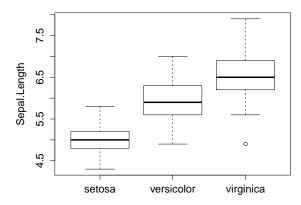
- In R boxplots are plotted with the command boxplot:
 - > boxplot (Sepal.Length, main="Boxplot Sepal.Length")

Boxplot Sepal.Length



Boxplots (4)

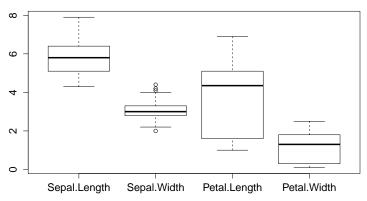
- If we have a factor variable we can create a boxplot for each category as follows:
 - > boxplot(Sepal.Length~Species, ylab="Sepal.Length")



Boxplots (5)

- We can also compare several boxplots in the same plot:
 - > boxplot(x=iris[,1:4],main="Boxplots Iris")

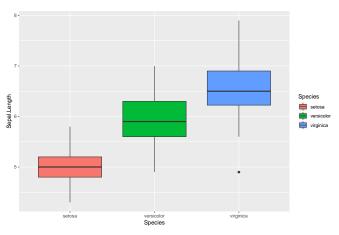
Boxplots Iris



Boxplots (6)

Now using ggplot2:

```
> ggplot(iris, aes(x = Species, y = Sepal.Length,
fill = Species)) + geom_boxplot()
```

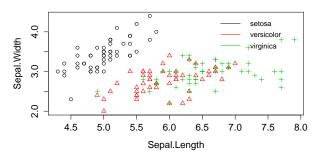


Scatter Plots

- Scatter plots use Cartesian coordinates to display the values of two numerical variables of the same length.
- The values of the attributes determine the position of the elements.
- Other attributes can be used to define the size, shape or color of objects.
- In R we can plot a scatterplot of two numeric variables using the command plot (x, y), which would be y vs x.
- We can also define formulas f(x) = y using the notation y^x .
- Thus, the command plot (y~x) is equivalent to plot (x, y).
- If we have a data.frame or a numerical matrix, we can see the scatterplots of all pairs using the command pairs (x).

Scatter Plots (2)

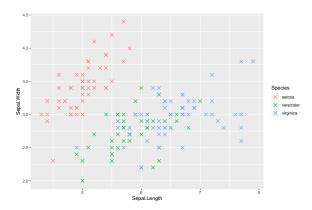
Examples:



Scatter Plots (3)

• The same using *ggplot2*:

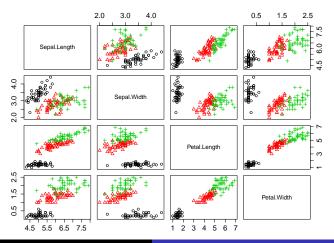
```
ggplot(iris, aes(x=Sepal.Length,
y=Sepal.Width, color=Species)) +
geom_point(size=3,shape=4)
```



Scatter Plots (4)

 All pairs of the 4 variables of the iris dataset using a different color and character for each species:

pairs(iris[,1:4],pch=as.numeric(iris\$Species),col=iris\$Species)



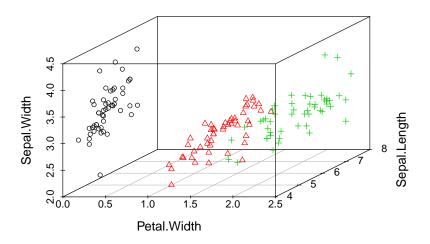
Scatter Plots (5)

- Three-dimensional scatterplots can also be created.
- The scatterplot3d library must be installed using the following command:

```
install.packages("scatterplot3d", dependencies=T)
```

- Then load the library by typing library (scatterplot3d).
- A 3d scatterplot for petal width, sepal length and sepal width:

Scatter Plots (6)



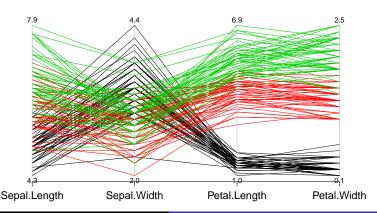
Parallel Coordinate Plots

- Parallel coordinate plots are another way to visualize multi-dimensional data.
- Instead of using perpendicular axes (x-y-z) we use several axes parallel to each other.
- Each attribute is represented by one of the parallel axes with its respective values.
- The values of the different attributes are scaled so that each axis has the same height.
- Each observation represents a line that joins the different axes according to their values.
- In this way, examples similar to each other tend to be grouped in lines with similar trajectory.
- In many occasions it is necessary to re-order the axes in order to visualize a pattern.

Parallel Coordinate Plots (2)

- In R we can create parallel coordinate graphs with the command parcoord from the MASS library.
- Example:

```
library(MASS)
parcoord(iris[1:4], col=iris$Species, var.label=T)
```



Conclusions

- We have learned how to describe a dataset using various metrics and visualizations.
- These techniques give us a general understanding of the data.

References I



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