

Collaborative Research Centre Transregio
Munich - Frankfurt (TRR 267)
Non-coding RNA in the cardiovascular system
Make your paper figures professionally: Scientific data
analysis and visualization with R

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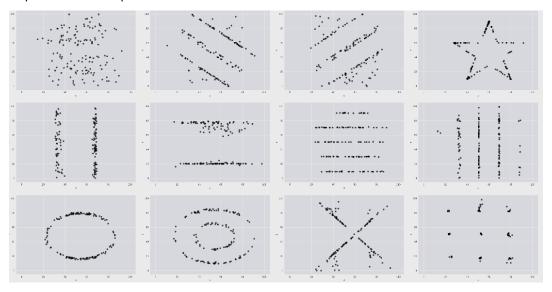
## **Chapter 1**

# Low dimensional visualizations

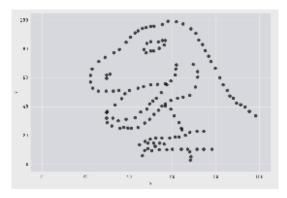
## 1.1 Why plotting?

With the increasing amounts of data, it's become increasingly difficult to manage and make sense of it all. It becomes nearly impossible for a single person to go through data line-by-line and see distinct patterns and make observations. In this context, data visualization becomes crucial for gaining insight into data that traditional descriptive statistics cannot. For instance, plotting can give hints about bugs in our code (or even in the data!) and can help us to develop and improve methods and models.

Do you see a pattern in these plots?



Maybe now?



All those plots, including the infamous datasaurus, actually share the same statistics!

X Mean: 54.26 Y Mean: 47.83 X SD : 16.76 Y SD : 26.93 Corr. : -0.06

When only looking at the statistics, we would have probably wrongly assumed that the datasets were identical. This illustration highlights why it is important to visualize data and not just rely on descriptive statistics.

We can consider another example given by a vector height containing (hypothetical) height measurements for 500 adults in Germany:

```
length(height)
```

```
## [1] 500
```

```
head(height, n = 20)
```

```
## [1] 1.786833 1.715319 1.789841 1.787259 1.748659 1.660702 1.688214 1.716738 
## [9] 1.729740 1.838209 1.764362 1.694045 1.678355 1.716974 1.716535 1.711482 
## [17] 1.741350 1.689864 1.749606 1.674311
```

Calculating the mean height returns the following output:

#### mean(height)

```
## [1] 2.056583
```

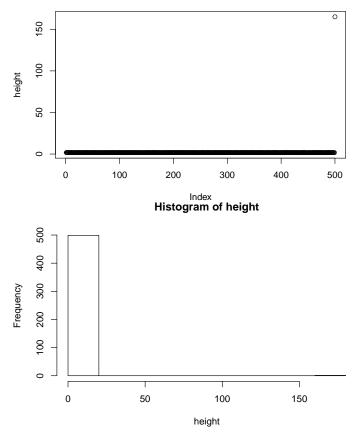
Wait... what?

What happened?

Assuming that adults in Germany are actually not exceptionally tall, we can plot the data for investigating this situation.

```
plot(height)
hist(height)
```

1.1. WHY PLOTTING?



Interestingly, there is an outlier in our data! One particular person seems to have a height above 150 meters that is obviously wrong. As a result, it inflates our mean giving us the false impression that Germans are exceptionally tall.

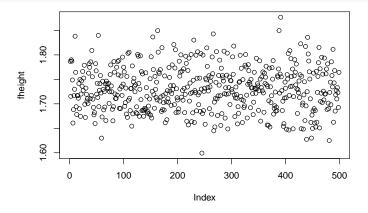
A quick way to fix our dataset is to remove our outlier.

```
fheight <- height[height < 3]</pre>
```

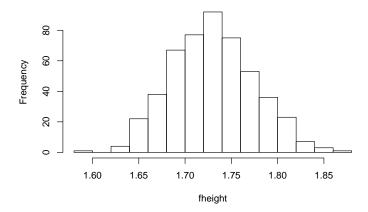
Now our plotted data seems more realistic and the mean height makes sense.

```
mean(fheight)
```

```
## [1] 1.730043
plot(fheight)
hist(fheight)
```



#### Histogram of fheight

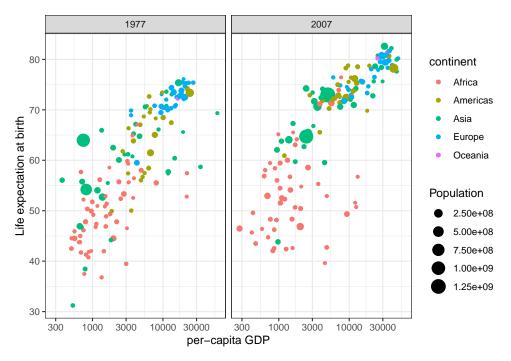


## 1.2 Grammar of graphics

Plotting with the help of the package ggplot2 has become widely used by R programmers. The plotting logic of ggplot2 is known as the grammar of graphics. The grammar of graphics is a visualization theory developed by Leland Wilkinson in 1999. It has influenced the development of graphics and visualization libraries alike and is based on 3 key principles:

- Separation of data from aesthetics (e.g. x and y-axis, color-coding)
- Definition of common plot/chart elements (e.g. scatter plots, box-plots, etc.)
- Composition of these common elements (one can combine elements as layers)

Now let's try to create a sophisticated example based on the R package ggplot2 for visualizing the relationship of between the per-capita GDP gdpPercap and the life expectancy at birth lifeExp for every country from the dataset gapminder. We want to compare this relationship for the years 1977 and 2007:



We may, for instance, use such visualization to find differences in the life expectancy of each country and each continent.

Now... how do we create such a sophisticated plot step by step? First, we will introduce the major components of grammar of graphics that will allow us to create and understand the previous example.

#### 1.2.1 Major components of the grammar of graphics

The following components are considered in the context of the grammar of graphics:

Data: data.table (or data.frame) object where columns correspond to variables

Aesthetics: visual characteristics that represent data (aes) - e.g. position, size, color, shape, transparency, fill

Layers: geometric objects that represent data (geom\_) - e.g. points, lines, polygons, ...

**Scales:** for each aesthetic, describes how visual characteristic is converted to display values (scale\_) - e.g. log scales, color scales, size scales, shape scales, . . .

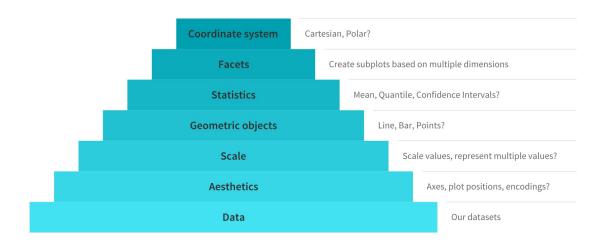
Facets: describes how data is split into subsets and displayed as multiple subgraphs (facet\_)

**Stats:** statistical transformations that typically summarize data (stat) - e.g. counts, means, medians, regression lines, . . .

**Coordinate system:** describes 2D space that data is projected onto (coord\_) - e.g. Cartesian coordinates, polar coordinates, map projections, ...

The following illustration represents the abstraction of grammar of graphics:

## **Major Components of the Grammar of Graphics**



#### 1.2.2 Defining the data and layers

In our example, we consider the gapminder dataset, which serves as the data component of our visualization. First, we have a quick look at the data. We want to plot the variable lifeExp against the variable gdpPercap so we better have a look at the first lines of the data:

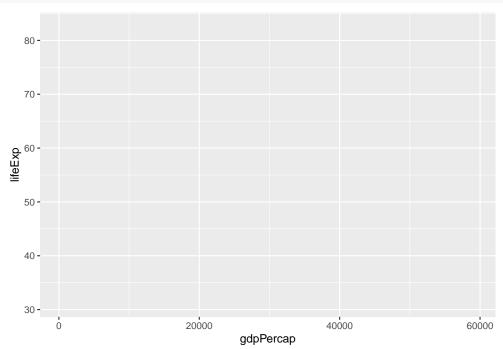
```
head(gm_dt[, .(country, continent, gdpPercap, lifeExp, year)])
##
         country continent gdpPercap lifeExp year
## 1: Afghanistan
                   Asia 786.1134 38.438 1977
## 2: Afghanistan
                     Asia 974.5803 43.828 2007
         Albania Europe 3533.0039 68.930 1977
## 3:
## 4:
         Albania Europe 5937.0295
                                     76.423 2007
## 5:
         Algeria
                   Africa 4910.4168
                                     58.014 1977
         Algeria
                   Africa 6223.3675 72.301 2007
```

For starting with the visualization we initiate a ggplot object which generates a plot with background:

ggplot()

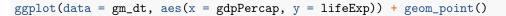
Next, we can define the data to be plotted, which needs to be a  $\mathtt{data.table}$  (or  $\mathtt{data.frame}$ ) object and the  $\mathtt{aes}()$  function. This  $\mathtt{aes}()$  function defines which columns in the  $\mathtt{data.table}$  object map to  $\mathtt{x}$  and  $\mathtt{y}$  coordinates and if they should be colored or have different shapes and sizes based on the values in a different column. These elements are called "aesthetic" elements, which we observe in the plot.

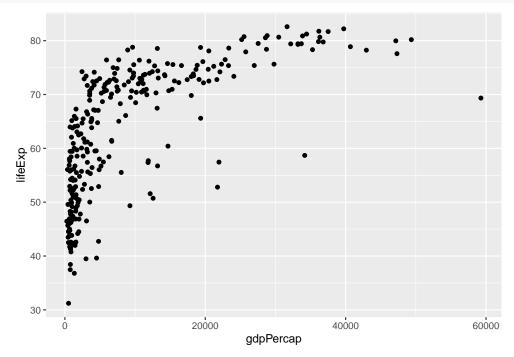
ggplot(data = gm\_dt, aes(x = gdpPercap, y = lifeExp))



As we can see, we obtain a plot with labeled axis and ranges. We want to visualize the data with a simple **scatter plot**. In a scatter plot, the values of two variables are plotted along two axes. Each pair of values is represented as a point. In R, a scatter plot can be plotted with ggplot2 using the function geom\_point. We want to construct a scatter plot containing the gdpPercap on the x-axis and the lifeExp on the y-axis. For this we combine the function geom\_point() to the previous line of code with the operator +:

names(p)





One of the advantages of plotting with ggplot is that it returns an object which can be stored (e.g. in a variable called p). The stored object can be further edited.

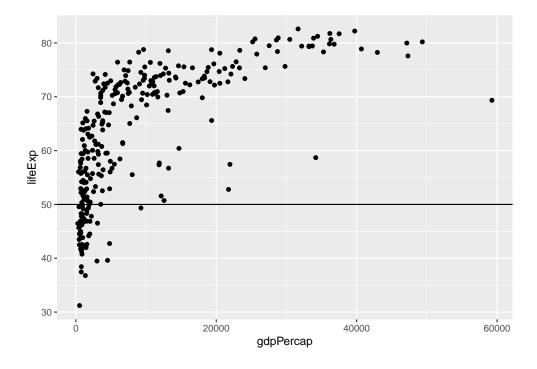
```
p <- ggplot(data = gm_dt, aes(x = gdpPercap, y = lifeExp)) + geom_point()</pre>
```

We can inspect the names of elements of the stored object with names():

```
## [1] "data" "layers" "scales" "mapping" "theme" ## [6] "coordinates" "facet" "plot_env" "labels"
```

We can also save the ggplot object with the help of the function saveRDS(). Then, we can read the saved object again with the help of the function readRDS() and add a horizontal line at y=50 to the plot:

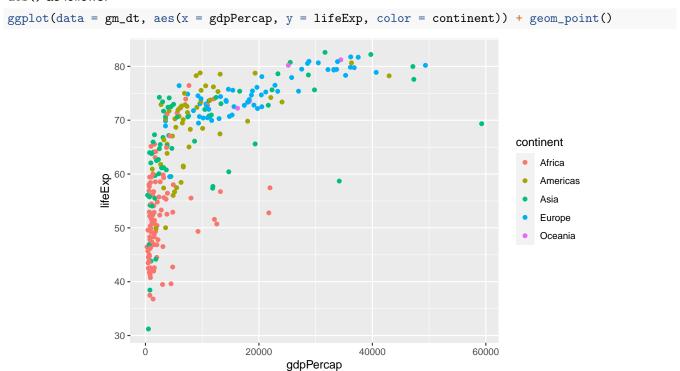
```
saveRDS(p, "../extdata/my_first_plot.rds")
p <- readRDS("../extdata/my_first_plot.rds")
p + geom_hline(yintercept = 50)</pre>
```



### 1.2.3 Mapping of aesthetics

#### 1.2.3.1 Mapping of color, shape and size

We can easily map variables to different colors, sizes or shapes depending on the value of the specified variable. To assign each point to its corresponding continent, we can define the variable continent as the color attribute in aes() as follows:



American color or British colour are both acceptable as the argument specification.

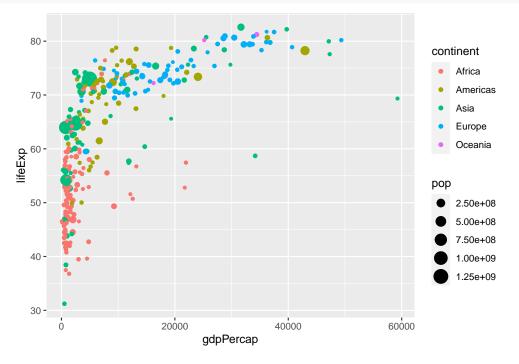
Instead of color, we can also use different shapes for characterizing the different continents in the scatter plot. For this we specify the shape argument in aes() as follows:

ggplot(data = gm\_dt, aes(x = gdpPercap, y = lifeExp, shape = continent)) + geom\_point() 80 -70 continent Africa lifeExp <sub>09</sub> Americas Asia Europe 50 Oceania 40 30 -60000 Ö 20000 40000

Additionally, we distinguish the population of each country by giving a size to the points in the scatter plot:

gdpPercap

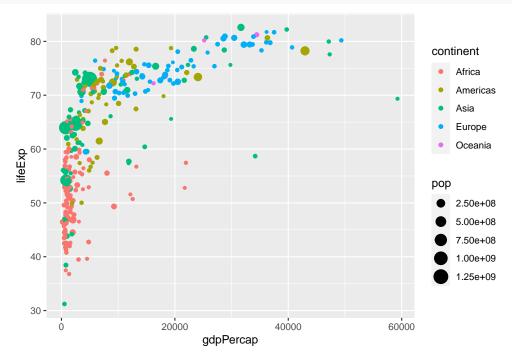
ggplot(data = gm\_dt, aes(x = gdpPercap, y = lifeExp, color = continent, size = pop)) +
 geom\_point()



#### 1.2.3.2 Global versus individual mapping

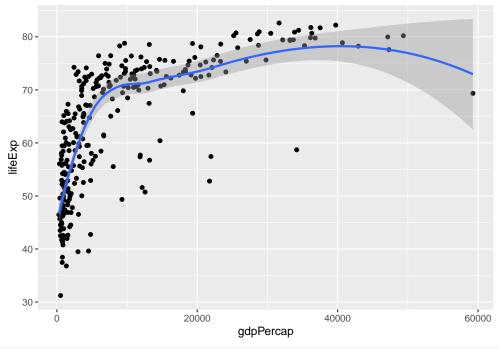
Mapping of aesthetics in aes() can be done globally or at individual layers.

For instance, in the previous plot we define the variables gdpPercap and lifeExp in the aes() function inside ggplot() for a **global** definition. Global mapping is inherited by default to all geom layers (geom\_point in the previous example), while mapping at **individual** layers is only recognized at that layer. For example, we define the aes(x=gdpPercap, y=lifeExp) globally, but the color attributes only locally for the layer geom\_point:

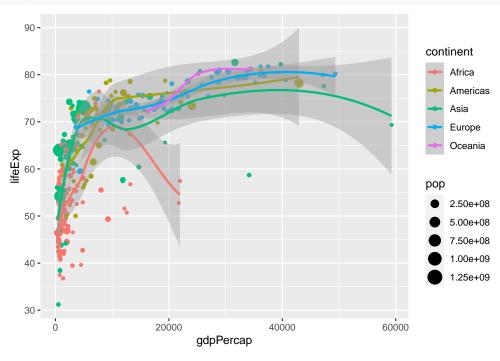


Note that individual layer mapping cannot be recognized by other layers. For instance, we can add another layer for smoothing with stat\_smooth().

```
# this doesn't work as stat_smooth didn't know aes(x , y)
ggplot(data = gm_dt) + geom_point(aes(x = gdpPercap, y = lifeExp)) + stat_smooth()
## Error: stat_smooth requires the following missing aesthetics: x and y
# this would work but too redundant
ggplot(data = gm_dt) + geom_point(aes(x = gdpPercap, y = lifeExp)) + stat_smooth(aes(x = gdpPercap, y = lifeExp))
```



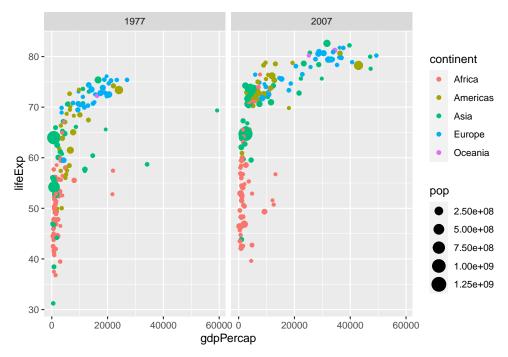
```
# the common aes(x, y) shared by all the layers can be put in the ggplot()
ggplot(data = gm_dt, aes(x = gdpPercap, y = lifeExp, color = continent)) + geom_point(aes(size = pop)) +
    stat_smooth()
```



#### 1.2.4 Facets, axes and labels

For comparing the data from the year 1977 with the data from 2007, we can add a facet with facet\_wrap():

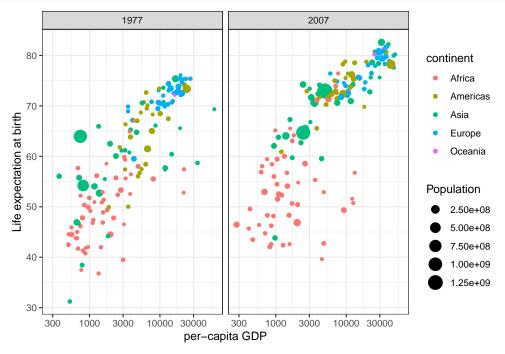
```
ggplot(data = gm_dt, aes(x = gdpPercap, y = lifeExp, color = continent, size = pop)) +
    geom_point() + facet_wrap(~year)
```



For a better visualization of the data points, we can consider log scaling, which we will describe more in detail later. Finally, we can adapt the axes labels of the plot with labs() and define a theme of our plot:

```
mysize <- 15
mytheme <- theme(axis.title = element_text(size = mysize), axis.text = element_text(size = mysize),
    legend.title = element_text(size = mysize), legend.text = element_text(size = mysize)) +
    theme_bw()

ggplot(data = gm_dt, aes(x = gdpPercap, y = lifeExp)) + geom_point(aes(color = continent,
    size = pop)) + facet_grid(~year) + scale_x_log10() + labs(x = "per-capita GDP",
    y = "Life expectation at birth", size = "Population") + mytheme</pre>
```



We remark here that ggplot2 allows many further adaptions to plots, such as specifying axis breaks and limits. Some of these are covered in the appendix at the end of this script.

### 1.3 Different types of one- and two-dimensional plots

In the previous examples, we had a look at scatter plots which are suitable for plotting the relationship between two continuous variables. However, there are many more types of plots (e.g. histograms, boxplots) which can be used for plotting in different scenarios. Mainly, we distinguish between plotting one or two variables and whether the variables are continuous or discrete.

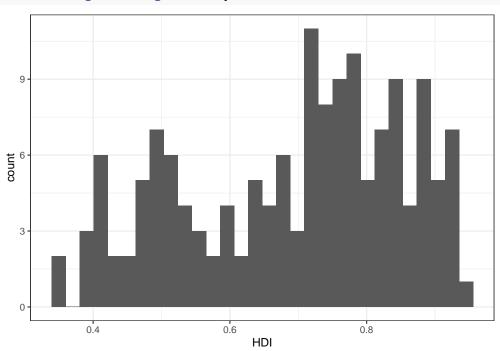
#### 1.3.1 Plots for one single continuous variable

#### 1.3.1.1 Histograms

A histogram represents the frequencies of values of a variable bucketed into ranges. It takes as input numeric variables only. A histogram is similar to a bar plot but the difference is that it groups the values into continuous ranges. Each bar in a histogram represents the height of the number of values present in that range. Each bar of the histogram is called a bin.

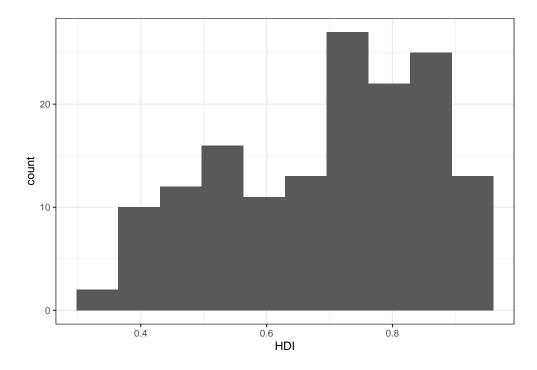
We can construct a histogram of the Human Development Index (HDI) in the ind dataset with the function geom\_histogram():

ggplot(ind, aes(HDI)) + geom\_histogram() + mytheme



By default, the number of bins in ggplot2 is 30. We can simply change this by defining the number of desired bins in the bins argument of the geom\_histogram() function:

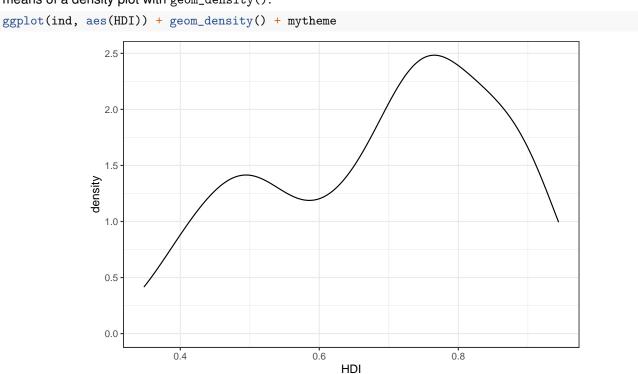
```
ggplot(ind, aes(HDI)) + geom_histogram(bins = 10) + mytheme
```



#### 1.3.1.2 Density plots

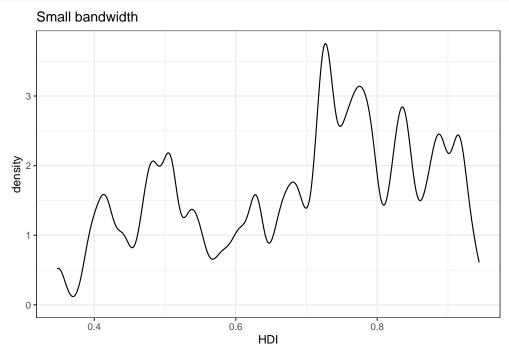
Histograms are sometimes not optimal to investigate the distribution of a variable due to discretization effects during the binning process. A variation of histograms is given by density plots. They are used to represent the distribution of a numeric variable. These distribution plots are typically obtained by kernel density estimation to smoothen out the noise. Thus, the plots are smooth across bins and are not affected by the number of bins, which helps create a more defined distribution shape.

As an example, we can visualize the distribution of the Human Development Index (HDI) in the ind dataset by means of a density plot with geom\_density():



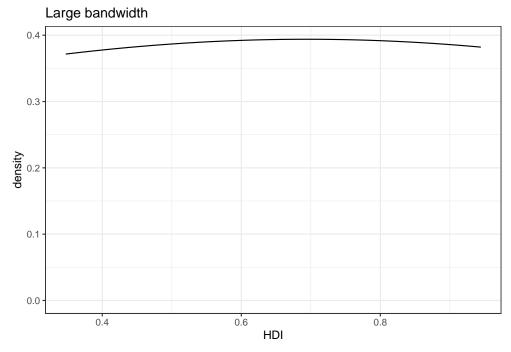
The bw argument of the geom\_density() function allows to tweak the bandwidth of a density plot manually. The default option is a bandwidth rule, which is usually a good choice.

Setting a small bandwidth on the previous plot has a huge impact on the plot:



Setting a large bandwidth has also a huge impact on the plot:

ggplot(ind, aes(HDI)) + geom\_density(bw = 1) + ggtitle("Large bandwidth") + mytheme



Thus, we should be careful when changing the bandwidth, since we can get a wrong impression from the distribution of a continuous variable.

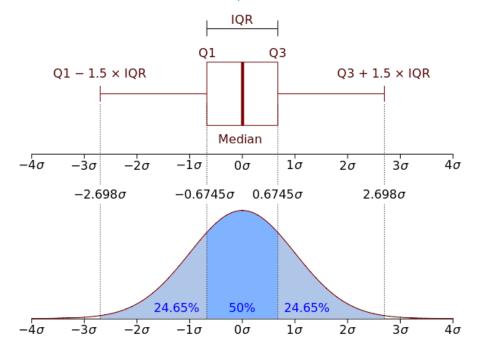
#### 1.3.1.3 Boxplots

Box plots can give a good graphical insight into the distribution of the data. They show the median, quantiles, and how far the extreme values are from most of the data.

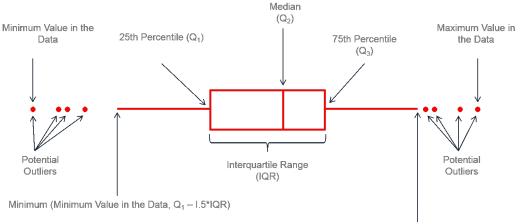
Five values are essential for constructing a boxplot:

- the median: the center of the data, middle value of a sorted list, 50% quantile of the data
- the first quantile (Q1): 25% quantile of the data
- the third quantile (Q3): 75% quantile of the data
- the interquantile range (IQR): the distance between Q1 and Q3

Every boxplot has lines at Q1, the median, and Q3, which together build the box of the boxplot. The other major feature of a boxplot is its whiskers. The whiskers are determined with the help of the IQR. Here, we compute  $1.5 \times IQR$  below Q1 and  $1.5 \times IQR$  above Q3. Anything outside of this range is called an outlier. We then draw lines at the smallest and largest point within this subset (Q1 -  $1.5 \times IQR$  to Q3 +  $1.5 \times IQR$ ) from the dataset. These lines define our whiskers which reach the most extreme data point within  $\pm 1.5 \times IQR$ .

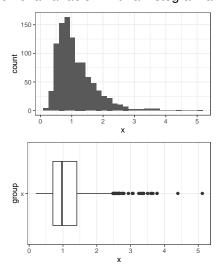


It is possible to not show the outliers in boxplots, as seen in the visualization before. However, we strongly recommend keeping them. Outliers can reveal interesting data points (discoveries "out of the box") or bugs in data preprocessing.



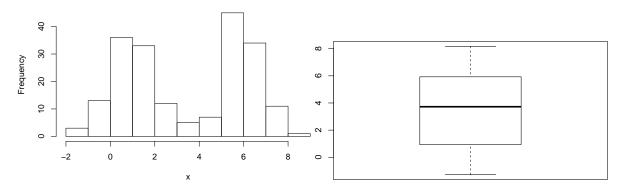
Maximum (Maximum Value in the Data, Q<sub>3</sub> + I.5\*IQR)

For instance, we can plot the distribution of a variable x with a histogram and visualize the corresponding boxplot:



Boxplots are particularly suited for plotting non-gaussian symmetric and non-symmetric data and for plotting exponentially distributed data. However, boxplots are not well suited for bimodal data, since they only show one mode (the median). In the following example, we see a bimodal distribution in the histogram and the corresponding boxplot, which does not properly represent the distribution of the data.



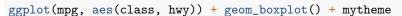


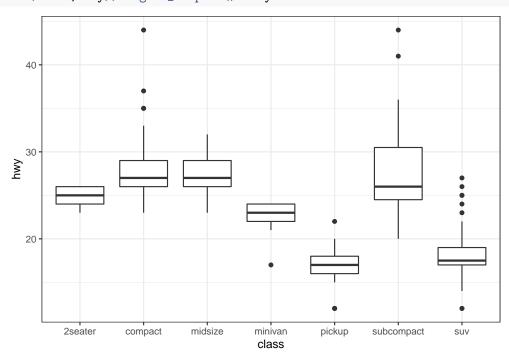
#### 1.3.2 Plots for two variables: one continuous, one discrete

#### 1.3.2.1 Boxplots by category

As illustrated before, boxplots are well suited for plotting one continuous variable. However, we can also use boxplots to show distributions of continuous variables with respect to some categories. This can be particularly interesting for comparing the different distributions of each category.

For instance, we want to visualize the highway miles per gallon hwy for every one of the 7 vehicle classes (compact, SUV, minivan, etc.). For this, we define the categorical class variable on the x axis and the continuous variable hwy on the y axis.



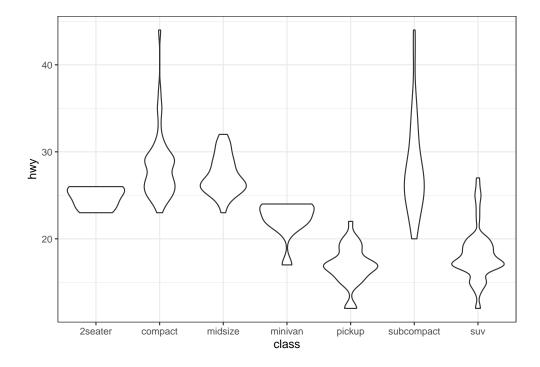


#### 1.3.2.2 Violin plots

A violin plot is an alternative to the boxplot for visualizing either one continuous variable (grouped by categories). An advantage of the violin plot over the boxplot is that it also shows the entire distribution of the data. This can be particularly interesting when dealing with multimodal data.

For a direct comparison, we show a violin plot for the hwy grouped by class as before with the help of the function geom\_violin():

```
ggplot(mpg, aes(class, hwy)) + geom_violin() + mytheme
```

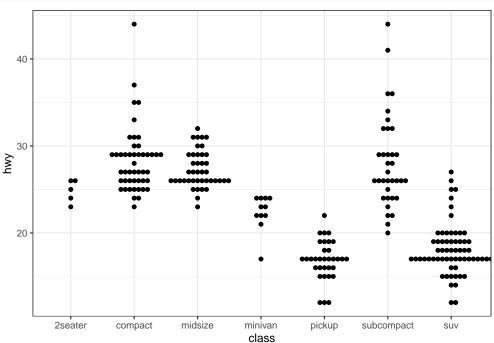


#### 1.3.2.3 Beanplots

Another alternative to the popular boxplot is the beanplot. In a beanplot, the individual observations are shown as small lines in a one-dimensional scatter plot. Moreover, the estimated density of the distributions is visible in a beanplot. It is easy to compare different groups of data in a beanplot and to see if a group contains enough observations to make the group interesting from a statistical point of view.

For creating beanplots in R, we can use the package ggbeeswarm. We use the function geom\_besswarm() to create a beanplot to visualize once again the hwy grouped by class:

```
# install.packages('ggbeeswarm')
library(ggbeeswarm)
ggplot(mpg, aes(class, hwy)) + geom_beeswarm() + mytheme
```



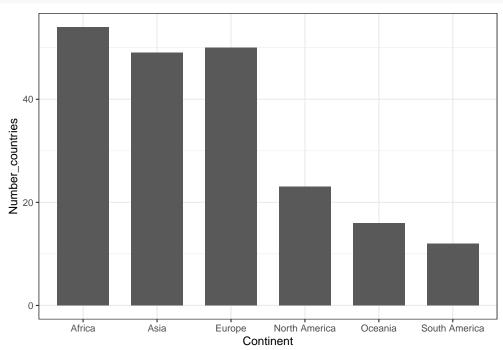
We remark that beanplots are useful only up to a certain number of data points. The creation of beanplots for larger datasets may become too expensive.

#### 1.3.2.4 Barplots

Barplots are often used to highlight individual quantitative values per category. Bars are visual heavyweights compared to dots and lines. In a barplot, we can combine two attributes of 2-D location and line length to encode quantitative values. In this manner, we can focus the attention primarily on individual values and support the comparison of one to another.

For creating a barplot with ggplot2 we can use the function geom\_bar(). In the next example, we visualize the number of countries (defined in the y axis) per continent (defined in the x axis).

```
ggplot(countries_dt, aes(Continent, Number_countries)) + geom_bar(stat = "identity",
    width = 0.7) + mytheme
```



#### 1.3.2.5 Barplots with errorbars

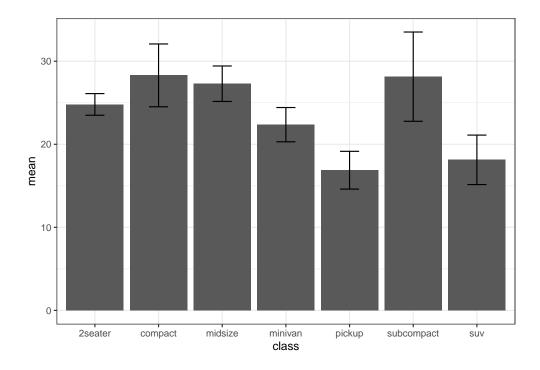
Visualizing uncertainty is important, otherwise, barplots with bars as a result of an aggregation can be misleading. One way to visualize uncertainty is with error bars.

As error bars, we can consider the standard deviation (SD) and the standard error of the mean (SEM). We remark that SD and SEM are completely different concepts. On the one hand, SD indicates the variation of quantity in the sample. On the other hand, SEM represents how well the mean is estimated.

The central limit theorem implies that:  $SEM = SD/\sqrt{(n)}$  , where n is the sample size (number of observations). With large n, SEM tends to 0.

In the following example, we plot me average highway miles per gallon hwy per vehicle class class including error bars computed as the average plus/minus standard devation of hwy:

```
as.data.table(mpg) %>% .[, .(mean = mean(hwy), sd = sd(hwy)), by = class] %>% ggplot(aes(class, mean, ymax = mean + sd, ymin = mean - sd)) + geom_bar(stat = "identity") + geom_errorbar(width = 0.3) mytheme
```

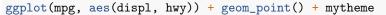


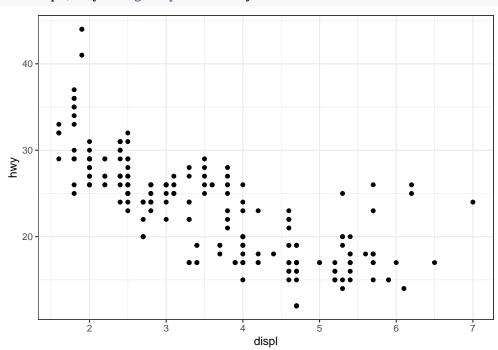
#### 1.3.3 Plots for two continuos variables

#### 1.3.3.1 Scatter plots

Scatter plots are a useful plot type for easily visualizing the relationship between two continuous variables. Here, dots are used to represent pairs of values corresponding to the two considered variables. The position of each dot on the horizontal (x) and vertical (y) axis indicates values for an individual data point.

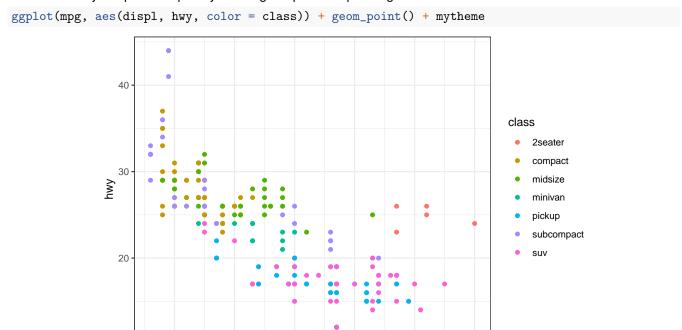
In the next example, we analyze the relationship between the engine displacement in liters displ and the highway miles per gallon hwy from the mpg dataset:





3

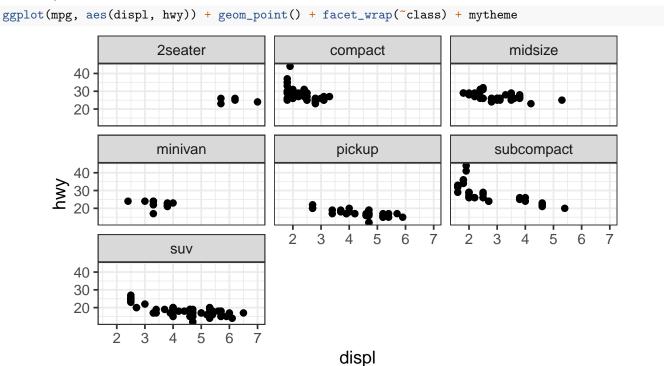
We can modify the previous plot by coloring the points depending on the vehicle class:



Sometimes, too many colors can be hard to distinguish. In such cases, we can use facet to separate them into different plots:

displ

5

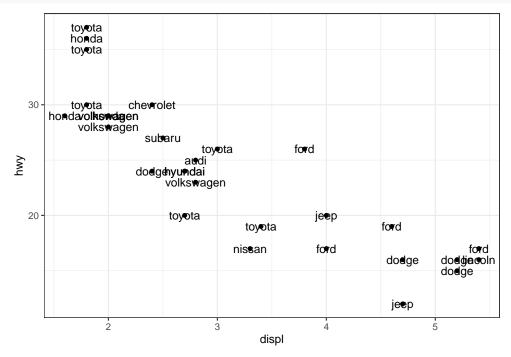


#### 1.3.3.1.1 Text labeling

For labeling the individual points in a scatter plot, ggplot2 offers the function geom\_text(). However, these labels tend to overlap. To avoid this, we can use the library ggrepel which offers a better text labeling through the function geom\_text\_repel().

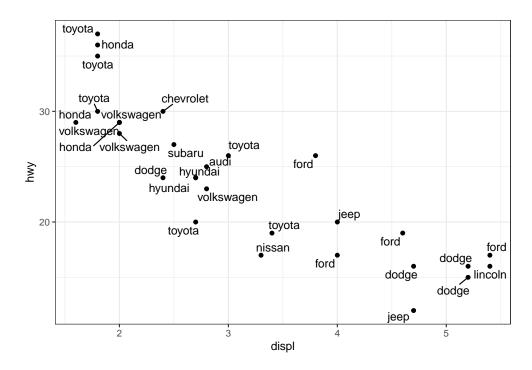
We first show the output of the classic text labeling with <code>geom\_text()</code> for a random subset of 40 observations of the dataset <code>mpg</code>. Here we plot the engine displacement in liters <code>displ</code> vs. the highway miles per gallon <code>hwy</code> and label by <code>manufacturer</code>:

```
set.seed(12)
mpg_subset <- mpg[sample(1:nrow(mpg), 30, replace = FALSE), ]
ggplot(mpg_subset, aes(displ, hwy, label = manufacturer)) + geom_point() + geom_text() +
    mytheme</pre>
```



As seen in the previous illustration, the text labels overlap. This complicates understanding the plot. Therefore, we exchange the function <code>geom\_text()</code> by <code>geom\_text\_repel()</code> from the library <code>ggrepel:</code>

```
library(ggrepel)
ggplot(mpg_subset, aes(displ, hwy, label = manufacturer)) + geom_point() + geom_text_repel() +
    mytheme
```

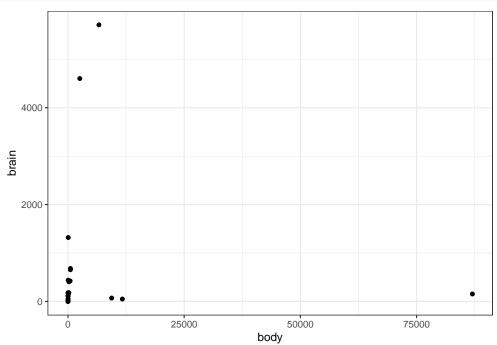


#### 1.3.3.1.2 Log scaling

We consider another example where we want to plot the weights of the brain and body of different animals using the dataset Animals. This is what we obtain after creating a scatterplot.

```
library(MASS) # to access Animals data sets
animals_dt <- as.data.table(Animals)

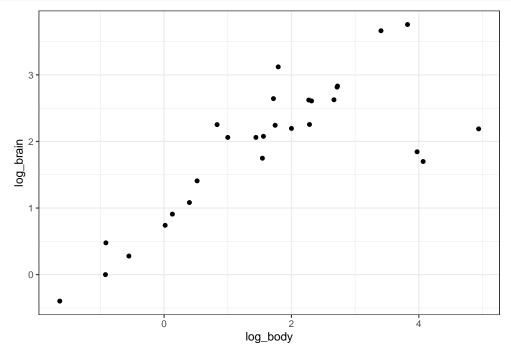
ggplot(animals_dt, aes(x = body, y = brain)) + geom_point() + mytheme</pre>
```



We can clearly see that there are a few points which are notably larger than most of the points. This makes it harder to interpret the relationships between most of these points. In such cases, we can consider **logarithmic** transformations and/or scaling. More precisely, a first idea would be to manually transform the values into a

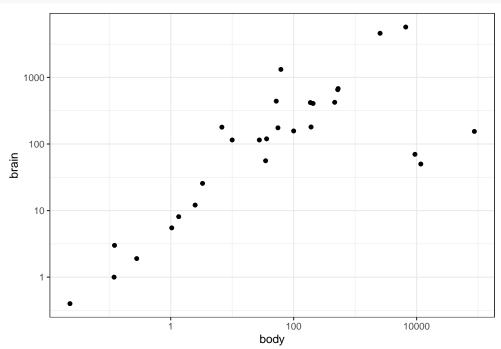
logarithmic space and plot the transformed values instead of the original values:

```
animals_dt[, `:=`(c("log_body", "log_brain"), list(log10(body), log10(brain)))]
ggplot(animals_dt, aes(x = log_body, y = log_brain)) + geom_point() + mytheme
```



Alternativelt, ggplot2 offers to simply scale the data without the need to transform. This can be done with the help of the functions  $scale_xlog10()$  and  $scale_ylog10()$  which allow appropriate scaling and labeling of the axes:

```
ggplot(animals_dt, aes(x = body, y = brain)) + geom_point() + scale_x_log10() + scale_y_log10() +
    mytheme
```

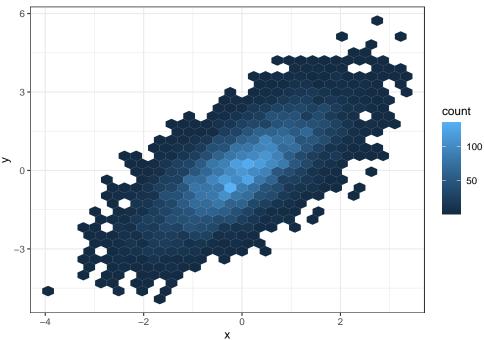


#### 1.3.3.2 Density plots in 2D

Using scatterplots can become problematic when dealing with a huge number of points. This is due to the fact that points may overlap and we cannot clearly see how many points are at a certain position. In such cases, a 2D density plot is particularly well suited. This plot counts the number of observations within a particular area of the 2D space.

The function <code>geom\_hex()</code> is particularly useful for creating 2D density plots in R:

```
x <- rnorm(10000)
y = x + rnorm(10000)
data.table(x, y) %>% ggplot(aes(x, y)) + geom_hex() + mytheme
```

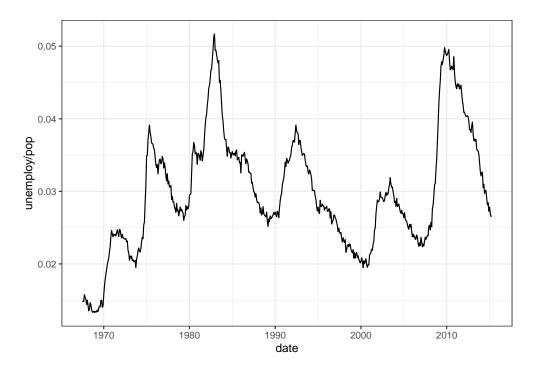


#### 1.3.3.3 Line plots

A line plot can be considered for connecting a series of individual data points or to display the trend of a series of data points. This can be particularly useful to show the shape of data as it flows and changes from point to point. We can also show the strength of the movement of values up and down through time.

As an example we show the connection between the individual datapoints of unemployment rate over the years:

```
ggplot(economics, aes(date, unemploy/pop)) + geom_line() + mytheme
```



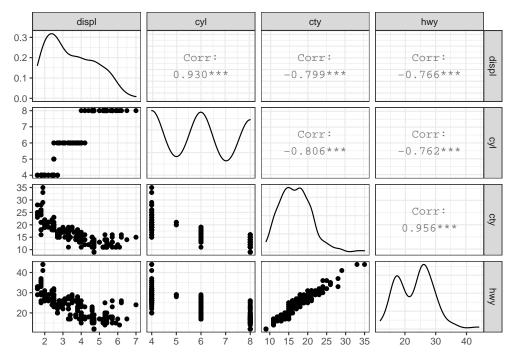
## 1.4 Further plots for low dimensional data

#### 1.4.1 Plot matrix

A so-termed plot matrix is useful for exploring the distributions and correlations of a few variables in a matrix-like representation. Here, for each pair of considered variables, a scatterplot is created and the correlation coefficient is computed. For every single variable, a histogram is created for showing the respective distribution.

We can use the function ggpairs() from the library GGally for constructing plot matrices. As an example, we analyze the variables displ, cyl, cty and hwyfrom the dataset mpg:

```
library(GGally)
ggpairs(mpg, columns = c("displ", "cyl", "cty", "hwy")) + mytheme
```

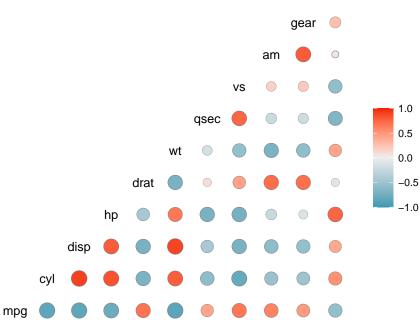


We remark that this plot is not well suited for comparing more than a few variables.

### 1.4.2 Correlation plot

A correlation plot is a graphical representation of a correlation matrix. It is useful to highlight the most correlated variables in a dataset. In this plot, correlation coefficients are colored according to the value. A correlation matrix can be also reordered according to the degree of association between variables.

Correlation plots are also called "corrgrams" or "correlograms". As an example, we visualize the correlation between the variables of the dataset mtcars with the help of the function ggcorr() from the library GGally:



## 1.5 Summary

This first chapter of data visualization covered the basics of the grammar of graphics and ggplot2 to plot low dimensional data. We introduced the different types of plots such as histograms, boxplots and barplots and discussed when to use which plot.

### 1.6 Resources

- · Plotting libraries:
  - http://www.r-graph-gallery.com/portfolio/ggplot2-package/
  - http://ggplot2.tidyverse.org/reference/
  - https://plot.ly/r/
  - https://plot.ly/ggplot2/
- · Udacity's Data Visualization and D3.js
  - https://www.udacity.com/courses/all
- · Graphics principles
  - https://onlinelibrary.wiley.com/doi/full/10.1002/pst.1912
  - https://graphicsprinciples.github.io/