

R FOR DATA SCIENCE: QUICK GUIDE.

GENNARO TEDESCO[†]

[†]gennarotedesco@gmail.com



The following is a quick reference guide to some of the R packages used in data science. It is by no means to be intended as exhaustive and the reader is assumed to be already familiar with the language. Errors in text and formulae may occur: I am grateful to anybody who will point them out.

CONTENTS

1	Introduction	3
2	Vectorised operations on data frames	4
2.1	apply	4
2.2	lapply and sapply	4
2.3	Vectorised assignments	5
3	The data.table package	6
3.1	Subsetting a data table upon constraints	6
3.2	Random and unique rows	8
3.3	Grouping by	9
3.4	Joining data tables	9
4	The dplyr package	11
4.1	Subsetting a data set upon constraints	11
4.2	Random and unique rows	12
4.3	Grouping by	13
4.4	Joining data sets	13
5	The reshape package	15
6	The ggplot2 package	18
6.1	General aesthetics	18
6.2	Error bars	18
6.3	Barplots	19
6.4	Boxplots	20
6.5	Data grouped by	20
6.6	Plotting functions	22
6.7	Histograms	23
6.8	Tiles	23
7	Data clustering	25
7.1	k-means clustering	26
8	Hypotheses tests	28
8.1	Normality tests and qq-plots	28
8.2	t-tests	29
8.3	Kruskal-Wallis test	31
8.4	Dunn's test	31
9	Date and time formats: lubridate	33
10	Writing and reading data	34
11	Text manipulation	35
A	Special functions	36
A.1	RXKCD	37
A.2	Colour palette	37

In the following a quick guide to common features of some R packages is shown. It is by no means intended to be a guide to the language, rather an introductory primer to some libraries useful in data science for the ones who are already familiar with the language. And still, no claim of completeness is assumed.

As best practice, the reader is always addressed to the official documentation; moreover, given any R function, the line `?<function>` prompts the corresponding definitions and in-built help.

A full list of functions according to the package they are defined in is available here.¹

Unless specified otherwise, minimal working examples are shown by making use of the sample datasets provided by R, in particular we will mainly refer to `data(iris)`, `data(mtcars)` and `data(morley)`. We will henceforth refer to a generic data frame as to `df`. Another set of data we will make use of is the following quark data set:

```
set.seed(1)
lab      <- sample(LETTERS[1:6], 100, replace = TRUE)
flavour  <- sample(c("up", "down", "charm", "strange",
                    "top", "bottom"), 100, replace = TRUE)
S_z      <- sample(c("1/2", "-1/2"), 100, replace = TRUE)
quarks   <- data.table(lab, flavour, S_z)

R: head(quarks, 5)
```

	lab	flavour	S_z
1:	B	strange	1/2
2:	C	charm	1/2
3:	D	down	-1/2
4:	F	bottom	1/2
5:	B	strange	1/2

¹ <http://www.rdocumentation.org/>

Given a data frame, the functions of the family `apply` allow to perform vectorised operations on rows and columns thereof, without having to manually access each entry to loop through.

2.1 *apply*

The general wrapper for such operations is the `apply` function, where rows and columns can be accessed specifying the labels (1, 2, ...) (and higher if any other multi-dimensional object is contained therein). It returns a vector (or a list) of values obtained by applying a function to the rows (columns, respectively) of a data frame, coerced to matrix first. The general syntax is `apply(df, margin, fun)`, with `margin` being 1, 2, ... and `function` being any function.

```
R> cars <- head(mtcars[,1:7],4)
R> cars
```

	mpg	cyl	disp	hp	drat	wt	qsec
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02
Datsun 710	22.8	4	108	93	3.85	2.320	18.61
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44

```
# choose 1 for rows
R> apply(cars, 1, mean)
```

	Mazda RX4	Mazda RX4 Wag	Datsun 710	Hornet 4 Drive
	45.71143	45.82786	36.08286	60.16214

```
# choose 2 for columns
R> apply(cars, 2, mean)
```

	mpg	cyl	disp	hp	drat	wt	qsec
	21.5500	5.5000	171.5000	105.7500	3.6825	2.7575	17.8825

In the simple cases of the function being the sum or the mean, specific operators exist as `colSums` and `colMeans`, and equivalently for rows:

```
R> colSums(cars)
```

	mpg	cyl	disp	hp	drat	wt	qsec
	86.20	22.00	686.00	423.00	14.73	11.03	71.53

```
R> rowMeans(cars)
```

	Mazda RX4	Mazda RX4 Wag	Datsun 710	Hornet 4 Drive
	45.71143	45.82786	36.08286	60.16214

2.2 *lapply* and *sapply*

`lapply` applies a function to each element of a list and returns a list back. Equivalently, `sapply` does the same job but returns a vector back instead. As a data frame can be seen as a list of columns, one can have

```
R> head(quarks)
```

	lab	flavour	S_z
1:	B	strange	1/2
2:	C	charm	1/2
3:	D	down	-1/2
4:	F	bottom	1/2
5:	B	strange	1/2
6:	F	down	-1/2

```
R> lapply(quarks, mode)
$lab
[1] "C"

$flavour
[1] "strange"
```

```
$S_z
[1] "1/2"

R: supply(quarks, mode)

lab    flavour      S_z
"C"    "strange"     "1/2"
```

2.3 Vectorised assignments

Vectorised assignments in R commute with functions, namely the operator `c` is such that `c(f) = f(c)`.

```
f <- function(x) sin(x) - cos(2*x)

set.seed(1234)
x <- f(c(rnorm(5)))

set.seed(1234)
y <- c(f(rnorm(5)))

x == y

[1] TRUE TRUE TRUE TRUE TRUE
```

Likewise, `ifelse` evaluates a given condition on each element of a vector, thus replacing an entire loop: the two examples below are indeed equivalent, the latter sparing memory and being faster

```
set.seed(1234)
x <- rnorm(5)

R: for(i in seq(1:length(x))) {
  if(x[i] < 0) {
    print("negative")
  } else {
    print("positive")
  }
}

[1] "negative"
[1] "positive"
[1] "positive"
[1] "negative"
[1] "positive"

R: ifelse(x < 0, "negative", "positive")

[1] "negative" "positive" "positive" "negative" "positive"
```

The function `cumsum` returns the cumulative sums of values element-wise, easily replacing a loop through:

```
set.seed(1234)
x <- rnorm(5)

R: x
[1] -1.2070657  0.2774292  1.0844412 -2.3456977  0.4291247

R: cumsum(x)
[1] -1.2070657 -0.9296365  0.1548047 -2.1908930 -1.7617683
```

As a more general result, given a vector of values, the operator `Reduce` applies a function on pairs of values at a time, defined as

```
Reduce(f, x) = ... f(f(f(x[1], x[2]), x[3]), ...)

set.seed(1234)
x <- rnorm(5)

R: x
[1] -1.2070657  0.2774292  1.0844412 -2.3456977  0.4291247

R: Reduce(max, x, accumulate = TRUE)
[1] -1.2070657  0.2774292  1.0844412  1.0844412  1.0844412
```

```
install.packages('data.table')
library('data.table')
```

A `data.table` is a `data.frame` plus additional features that allow to strongly simplify a large set of operations on data as subsetting according to constraints, grouping by specific categories, behaviours and functions as well as easy joins between them based on different common keys and values. As such, we recommend as best practice to always transform any set of data into such format first and then start performing anything, as they are the most memory efficient.

A `data.table` does not have row numbers because they are deprecated, as joins and subsets must occur on keys and common values insted. As such, one assigns:

```
iris <- data.table(iris)
R: key(iris)
NULL

R: setkey(iris , Species)
R: key(iris)
[1] "Species"

R: dim(iris)
[1] 150  5
```

Multiple keys can be set and the data table will be sorted accordingly (also refer here²). For instance:

```
R: setkey(iris , Species , Sepal.Length)
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1:	4.3	3.0	1.1	0.1	setosa
2:	4.4	2.9	1.4	0.2	setosa
3:	4.4	3.0	1.3	0.2	setosa
4:	4.4	3.2	1.3	0.2	setosa
5:	4.5	2.3	1.3	0.3	setosa

If we want the opposite (descending) order

```
R: setorder(iris , Species , -Sepal.Length)
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1:	5.8	4.0	1.2	0.2	setosa
2:	5.7	4.4	1.5	0.4	setosa
3:	5.7	3.8	1.7	0.3	setosa
4:	5.5	4.2	1.4	0.2	setosa
5:	5.5	3.5	1.3	0.2	setosa

Also note:

```
R: names(iris)
[1] "Sepal.Length" "Sepal.Width" "Petal.Length"
     "Petal.Width" "Species"

R: setnames(iris , c("Sepal.Length","Sepal.Width"),
             c("sep_length", "sep_width"))
R: names(iris)
[1] "sep_length"    "sep_width"     "Petal.Length"
     "Petal.Width" "Species"
```

3.1 Subsetting a data table upon constraints

The general syntax form for a data table is `dt[i, j, by = k]`, meaning to subset the rows using `i`, then apply `j` as a function grouped by `k`. The syntax is totally equivalent to the standard SQL, with `i, j` replacing `where` and `select` clauses, respectively. Any formal expression or function can be used as `j`.

² <http://stackoverflow.com/a/20057411/5017267>

Columns in a data table can be accessed by name or by position reference: the two methods below are indeed equivalent in the result (notice `with = FALSE` in the latter)

```
R: iris[, .(Species, Petal.Width, Petal.Length)]
R: iris[, c(5,4,3), with = FALSE]
```

	Species	Petal.Width	Petal.Length
1:	setosa	0.2	1.4
2:	setosa	0.2	1.4
3:	setosa	0.2	1.3
4:	setosa	0.2	1.5
5:	setosa	0.2	1.4

Equivalently, new columns can be defined and added with

```
R: iris[, .(new_value = Sepal.Length/Sepal.Width, Species)]
```

	new_value	Species
1:	1.457143	setosa
2:	1.633333	setosa
3:	1.468750	setosa
4:	1.483871	setosa
5:	1.388889	setosa

and can be deleted as `iris[, c('Petal.Width', 'Petal.Length') := NULL]`.

Rows can be subset according to constraints:

```
subset(iris,
       Species == 'virginica'
       & (Petal.Width > 2.3 | Sepal.Width < 3))

subset(iris,
       Species %in% c('virginica', 'setosa'))
```

The `not in` operator in R is obtained by negating the variable instead of negating the set it belongs to, i. e. `subset(iris, !Species %in% c('virginica', 'setosa'))` gives the subset of variable whose Species are neither *virginica* nor *setosa*. The above are equivalent to directly impose the subset on the rows as

```
R: iris[Species == 'virginica']
R: iris[Species %in% c('virginica', 'setosa')]
R: iris[!Species %in% c('virginica', 'setosa')]
```

The `.I` operator shows the row number in correspondence of a matching constraint, should we want the data to be grouped by some other variables. For example

```
R: iris[, .I[Petal.Length = max(Petal.Length)],
         by = Species]
```

	Species	V1
1:	setosa	1
2:	versicolor	55
3:	virginica	106

The variable `V1` contains the actual row number at the match, which in turn can be plugged in the data table again, by reference, to have back the entire rows in correspondence thereof

```
R: iris[iris[, .I[Petal.Length = max(Petal.Length)],
              by = Species]$V1]
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1:	5.1	3.5	1.4	0.2	setosa
2:	6.5	2.8	4.6	1.5	versicolor
3:	7.6	3.0	6.6	2.1	virginica

Simple frequencies counts per group can be obtained via the `.N` operator.

```
R: iris[, .N, by = Species]
```

	Species	N
1:	setosa	50
2:	versicolor	50
3:	virginica	50

The `.SD` operator creates a data table whose values are the original values except the variables grouped by. Such new data table can be accessed on the fly to perform operations upon:

```
R: iris[, lapply(.SD, sd), by = Species]
```

	Species	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
1:	setosa	0.3524897	0.3790644	0.1736640	0.1053856
2:	versicolor	0.5161711	0.3137983	0.4699110	0.1977527
3:	virginica	0.6358796	0.3224966	0.5518947	0.2746501

The `[]` operator can be used in sequence to allow partial groupings as in the example below:

```
# simple use would be:
```

```
groups <- quarks[,
  .N,
  keyby = c("flavour", "lab")
]
```

```
R: head(groups)
```

	flavour	lab	N
1:	bottom	B	3
2:	bottom	C	3
3:	bottom	D	2
4:	bottom	E	4
5:	bottom	F	6
6:	charme	A	1

```
# we can normalise each count N to
```

```
# the overall number of counts per
```

```
# flavour, piping the []
```

```
groups <- quarks[,
  .N,
  keyby = c("flavour", "lab")
][,
  c("flavour_sum", "lab_freq") :=
    list(sum(N), N/sum(N)),
  by = "flavour"
]
```

```
R: head(groups)
```

	flavour	lab	N	flavour_sum	lab_freq
1:	bottom	B	3	18	0.16666667
2:	bottom	C	3	18	0.16666667
3:	bottom	D	2	18	0.11111111
4:	bottom	E	4	18	0.22222222
5:	bottom	F	6	18	0.33333333
6:	charme	A	1	17	0.05882353

3.2 Random and unique rows

In order to show the power of random and distinct sampling we will make use of the `quarks` data table as defined in (1). Random samples are easily obtained:

```
R: set.seed(1)
```

```
R: quarks[sample(.N, 10)]
```

	lab	flavour	S_z
1:	A	strange	1/2
2:	E	strange	-1/2
3:	B	strange	1/2
4:	B	bottom	1/2


```

5:  E strange  1/2
6:  B  down   1/2
7:  C    up    1/2
8:  B bottom  1/2
9:  D    up    1/2
10: F  down  -1/2

```

The function `unique(dt, by = c(first, second))` allows to fetch the *first occurrence* of unique row according to the variables “first, second”.

```

R: unique(quarks, by = c("flavour"))

  lab flavour S_z
1:  A strange 1/2
2:  B bottom 1/2
3:  B  down 1/2
4:  C    up 1/2

R: unique(quarks, by = c("flavour", "S_z"))

  lab flavour S_z
1:  A strange 1/2
2:  E strange -1/2
3:  B bottom 1/2
4:  B  down 1/2
5:  C    up 1/2
6:  F  down -1/2

```

3.3 Grouping by

Variables can be grouped by according to the following grammar:

```

R: iris[,.(width = mean(Petal.Width), dev = sd(Petal.Width), .N),
        by = Species]

  Species mean      dev N
1:  setosa 0.246 0.1053856 50
2: versicolor 1.326 0.1977527 50
3:  virginica 2.026 0.2746501 50

R: quarks[,.(observations = .N),
            keyby = c("lab", "flavour")]

  lab flavour observations
1:  A  charme             1
2:  A  down              3
3:  A strange            5
4:  A  top               2
5:  B bottom            3
6:  B  charme            3

```

3.4 Joining data tables

Inner joins

Given two data tables having at least one common variable, the syntax `merge(first, second, by = c('var1', 'var2'))` performs inner join based on the variables “var1, var2”. In the following example different laboratories perform measures of the spin projections of different quarks. We want to find what each lab has measured when the same quark has appeared:

```

set.seed(10)
first <- quarks[sample(.N, 10)]

set.seed(20)
second <- quarks[sample(.N, 10)]

  first | second
-----|-----
 lab flavour S_z | lab flavour S_z

```

1:	D	bottom	1/2		C	down	1/2
2:	E	charm	-1/2		F	strange	1/2
3:	C	strange	-1/2		F	strange	-1/2
4:	C	strange	1/2		A	top	1/2
5:	D	strange	-1/2		D	up	-1/2
6:		

```
R: merge(first, second, by = c("lab", "flavour"))
```

	lab	flavour	S_z.x	S_z.y
1:	B	strange	1/2	-1/2
2:	C	strange	-1/2	1/2
3:	C	strange	1/2	1/2
4:	C	strange	1/2	1/2
5:	D	bottom	1/2	1/2
6:	F	bottom	1/2	1/2

The above can equivalently be obtained with the syntax `first[second, nomatch=0]` once we set the variables we want to join on as keys. In fact

```
R: setkey(first, lab, flavour)
R: setkey(second, lab, flavour)
R: first[second, nomatch = 0]
```

	lab	flavour	S_z	i.S_z
1:	B	strange	1/2	-1/2
2:	C	strange	-1/2	1/2
3:	C	strange	1/2	1/2
4:	C	strange	1/2	1/2
5:	D	bottom	1/2	1/2
6:	F	bottom	1/2	1/2

gives the same results, as also `second[first, nomatch=0]`. The condition `nomatch=0` ensures the inner join as all the non-matching rows get discarded.

Left joins

The two equivalent give the same results:

```
# notice all.x = TRUE
R: merge(first, second, by = c("lab", "flavour"),
        all.x = TRUE)[order(flavour)]

# notice nomatch = 0 has been taken off
R: second[first]
```

	lab	flavour	S_z	i.S_z
1:	D	bottom	1/2	1/2
2:	F	bottom	1/2	1/2
3:	B	charm	NA	1/2
4:	C	charm	NA	-1/2
5:	E	charm	NA	-1/2
6:	B	strange	-1/2	1/2
7:	C	strange	1/2	-1/2
8:	C	strange	1/2	1/2
9:	C	strange	1/2	1/2
10:	D	strange	NA	-1/2

The advantage of the latter is that ordering is automatically performed on keys.

Full joins

Full joins are given by `merge(first, second, by = c("flavour", "S_z"), all = TRUE)`

Cartesian products

In order to perform cartesian products we refer to the non-in-built function shown in (A) `cross.join(first, second)`.

```
install.packages('dplyr')
library('dplyr')
```

`dplyr` allows pretty much the same operations as `data.table`, only with a different grammar. We will exploit its features showing the equivalent `data.table` syntax for comparison.

4.1 Subsetting a data set upon constraints

Data sets can be ordered by columns values as follows:

```
dplyr
R: arrange(iris, Species, desc(Sepal.Length))

data.table
R: setorder(iris, Species, -Sepal.Length)
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.8	4.0	1.2	0.2	setosa
2	5.7	4.4	1.5	0.4	setosa
3	5.7	3.8	1.7	0.3	setosa
4	5.5	4.2	1.4	0.2	setosa
5	5.5	3.5	1.3	0.2	setosa

Columns in a data set can be accessed by name or position reference:

```
dplyr
R: select(iris, Species, Petal.Width, Petal.Length)
R: select(iris, c(5,4,3))

data.table
R: iris[, .(Species, Petal.Width, Petal.Length)]
R: iris[, c(5,4,3), with = FALSE]
```

	Species	Petal.Width	Petal.Length
1	setosa	0.2	1.4
2	setosa	0.2	1.4
3	setosa	0.2	1.3
4	setosa	0.2	1.5
5	setosa	0.2	1.4

New columns can be defined and added as

```
dplyr
R: mutate(iris, new_value = Sepal.Length/Sepal.Width)
R: select(iris, new_values, Species)

# to only keep the new variables use
R: transmute(iris, new_value = Sepal.Length/Sepal.Width, Species)

data.table
R: iris[, .(new_value = Sepal.Length/Sepal.Width, Species)]
```

	new_value	Species
1:	1.457143	setosa
2:	1.633333	setosa
3:	1.468750	setosa
4:	1.483871	setosa
5:	1.388889	setosa

and can be deleted as `select(iris, -Petal.Width, -Petal.Length)`.

Rows can be subset according to constraints

```
dplyr
R: filter(iris,
  Species == 'virginica'
  & (Petal.Width > 2.3 | Sepal.Width < 3))

R: filter(iris,
  !Species %in% c("virginica", "setosa"))
```

```

data.table
R: subset(iris ,
  Species == 'virginica'
  & (Petal.Width > 2.3 | Sepal.Width < 3))

R: subset(iris ,
  !Species %in% c("virginica", "setosa"))

```

The rows in correspondence of a match can be extracted with

```

dplyr
R: iris %>%
  group_by(Species) %>%
  filter(Petal.Length == max(Petal.Length))

data.table
R: iris[
  iris[,
    .I[Petal.Length = max(Petal.Length)],
    by = Species]$V1
]

Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1:           5.1         3.5         1.4         0.2    setosa
2:           6.5         2.8         4.6         1.5 versicolor
3:           7.6         3.0         6.6         2.1  virginica

```

Simple frequencies counts per group can be obtained via the count function

```

dplyr
R: iris %>%
  count(Species)

data.table
R: iris[,
  .N,
  by = Species
]

Species n
1    setosa 50
2 versicolor 50
3  virginica 50

```

The equivalent of `lapply(.SD, fun)` is:

```

dplyr
R: iris %>%
  group_by(Species) %>%
  summarise_each(funs(sd))

data.table
R: iris[,
  lapply(.SD, sd),
  by = Species
]

Species Sepal.Length Sepal.Width Petal.Length Petal.Width
1    setosa    0.3524897    0.3790644    0.1736640    0.1053856
2 versicolor    0.5161711    0.3137983    0.4699110    0.1977527
3  virginica    0.6358796    0.3224966    0.5518947    0.2746501

```

4.2 Random and unique rows

Random rows can be easily subset with

```

dplyr
R: set.seed(1)
R: sample_n(quarks, 10)

data.table
R: set.seed(1)
R: quarks[sample(.N, 10)]

```

Unlike `data.table`, the package `dplyr` allows for sampling in percentage as fractions of the number of elements of the initial data set: `sample_frac(df, size = 0.3)` does the job, for example. Unique values can be fetched on constraints as

```
dplyr
R: quarks %>%
  distinct(flavour, S_z)

data.table
R: unique(quarks, by = c("flavour", "S_z"))
```

4.3 Grouping by

Variables can be grouped by according to the following grammar:

```
dplyr
R: iris %>%
  group_by(Species) %>%
  summarise(mean = mean(Petal.Width), dev = sd(Petal.Width))

R: iris[,
  .(mean = mean(Petal.Width), dev = sd(Petal.Width)),
  by = Species
]

  Species  mean      dev
1:   setosa 0.246 0.1053856
2: versicolor 1.326 0.1977527
3:   virginica 2.026 0.2746501
```

4.4 Joining data sets

Joins in `dplyr` can be performed using straightforward although verbose syntax, as shown in the following.

Inner joins

Given two data sets with at least one common variable, inner joins are performed using the following expression:

```
set.seed(10)
first <- sample_n(quarks, 10)

set.seed(20)
second <- sample_n(quarks, 10)

R: inner_join(first, second, by = c("lab", "flavour"))

  lab flavour S_z.x S_z.y
1   B strange  1/2  -1/2
2   C strange -1/2   1/2
3   C strange  1/2   1/2
4   C strange  1/2   1/2
5   D bottom  1/2   1/2
6   F bottom  1/2   1/2
```

Left joins

Equivalently for left joins

```
R: left_join(first, second, by = c("lab", "flavour"))

  lab flavour S_z.x S_z.y
1   B charme  1/2   NA
2   B strange  1/2  -1/2
3   C charme -1/2   NA
4   C strange -1/2   1/2
5   C strange  1/2   1/2
6   C strange  1/2   1/2
```

7	D	bottom	1/2	1/2
8	D	strange	-1/2	NA
9	E	charme	-1/2	NA
10	F	bottom	1/2	1/2

Unlike the `X[Y]` method in `data.table`, columns are here not automatically sorted after having been merged.

Full joins

Along the same lines:

```
R: full_join(first, second, by = c("lab", "flavour"))
```

	lab	flavour	S_z.x	S_z.y
1	C	strange	-1/2	1/2
2	C	strange	1/2	1/2
3	D	strange	-1/2	<NA>
4	E	charme	-1/2	<NA>
5	D	bottom	1/2	1/2
6	B	charme	1/2	<NA>
7	C	charme	-1/2	<NA>
...				

Anti-joins

The anti-joins returns all the rows in the first data sets not present in the second one

```
R: anti_join(first, second, by = c("lab", "flavour"))
```

	lab	flavour	S_z
1	B	charme	1/2
2	C	charme	-1/2
3	D	strange	-1/2
4	E	charme	-1/2

```
install.packages('reshape2')
library('reshape2')
```

The library `reshape` is mainly based on two functions: `dcast` and `melt` to reshape the data. The former transforms a *long* data frame into a *wide* one and the latter does viceversa.

A long data frame is such when one (or more variables) are arranged as row entries rather than columns instead. If so, those variables can be re-arranged back into columns whose values will be function of other chooses ones. For instance, given the `quarks` data table, we can calculate the mode (making use of the function in A) for each quark in each laboratory. The syntax is `dcast(dt, col1 + ... + colN ~ variable, fun.aggregate = fun)`

```
R: dcast(quarks, lab ~ flavour, fun.aggregate = mode)
```

Using `S_z` as value column. Use the `value` argument to cast to override this choice `lab` bottom charme down strange top up

	lab	bottom	charme	down	strange	top	up
1	A	<NA>	1/2	1/2	1/2	-1/2	<NA>
2	B	1/2	1/2	1/2	1/2	1/2	<NA>
3	C	1/2	1/2	1/2	1/2	1/2	1/2
4	D	1/2	1/2	1/2	-1/2	1/2	1/2
5	E	1/2	-1/2	-1/2	-1/2	1/2	-1/2
6	F	1/2	1/2	-1/2	-1/2	<NA>	-1/2

`dcast` does not work when more than a value is present per variable: a function must be provided (mode in the example above). To illustrate the converse behaviour we are using the in-built data set `airquality`.

```
R: head(airquality)
```

	Ozone	Solar.R	Wind	Temp	Month	Day
1	41	190	7.4	67	5	1
2	36	118	8.0	72	5	2
3	12	149	12.6	74	5	3
4	18	313	11.5	62	5	4
5	NA	NA	14.3	56	5	5
6	28	NA	14.9	66	5	6

One may want to make some of the columns row entries instead, keeping just some others as fixed. For instance we fix “Month” and “Day” and melt the rest accordingly

```
melt(airquality, id.vars = c("Month", "Day"))
```

```
R: head(melt(airquality, id.vars = c("Month", "Day")))
```

	Month	Day	variable	value
1	5	1	Ozone	41
2	5	2	Ozone	36
3	5	3	Ozone	12
4	5	4	Ozone	18
5	5	5	Ozone	NA
6	5	6	Ozone	28

```
R: tail(melt(airquality, id.vars = c("Month", "Day")))
```

	Month	Day	variable	value
607	9	25	Temp	63
608	9	26	Temp	70
609	9	27	Temp	77
610	9	28	Temp	75
611	9	29	Temp	76
612	9	30	Temp	68

```
R: data.table(melt(airquality, id.vars =
  c("Month", "Day")))[sample(.N, 5)]
```

	Month	Day	variable	value
1:	9	14	Wind	10.9

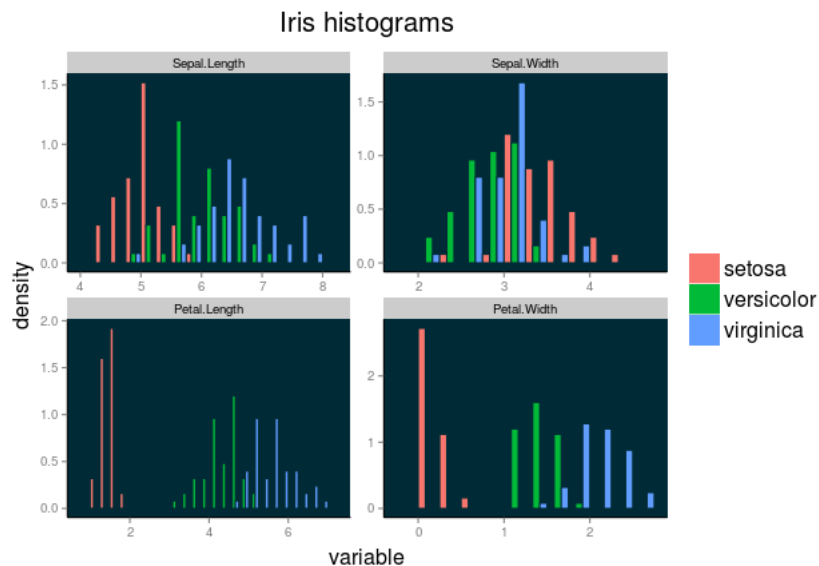
```
2:      7   13  Solar.R 175.0
3:      5   18    Temp  57.0
4:      5    7   Ozone  23.0
5:      8   21    Temp  77.0
```

Molten data are meant to be used to plot statistics in groups, especially histograms for each molten variable. The below is an example:

```
R> iris.molten <- melt(iris, id.vars = "Species")
R> iris.molten <- data.table(iris.molten)
R> iris.molten[sample(.N,5)]

   Species    variable  value
1: virginica Sepal.Width    2.9
2: versicolor Sepal.Width    2.5
3: virginica Petal.Width    2.0
4: versicolor Sepal.Length    6.1
5:   setosa Sepal.Length    4.5

p <- ggplot(iris.molten, aes(x=value, fill = Species))
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text=element_text(size=16),
               legend.title=element_blank(),
               axis.title.x = element_text(vjust=0, size=16),
               axis.title.y = element_text(vjust=1, size=16),
               plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_histogram(aes(y = ..density..), position = "dodge",
                        binwidth = 0.25, colour = "#002b36")
p <- p + facet_wrap(~ variable, scales="free")
p <- p + guides(fill = guide_legend(override.aes =
                                   list(colour = NULL)))
p <- p + labs(title = "Iris histograms")
p <- p + labs(x = "variable")
p <- p + labs(y = "density")
show(p)
```



Molten data set histograms

Obviously, if we cast the molten data table back, we obtain the data we started with, by definition.


```
R: dcast(melt(airquality , id.vars = c("Month", "Day")),
         Month + Day ~ variable)
```

	Month	Day	Ozone	Solar.R	Wind	Temp
1	5	1	41	190	7.4	67
2	5	2	36	118	8.0	72
3	5	3	12	149	12.6	74
4	5	4	18	313	11.5	62
5	5	5	NA	NA	14.3	56
6	5	6	28	NA	14.9	66

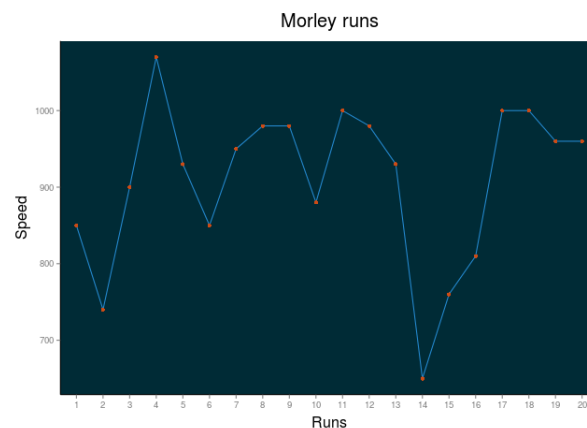
```
install.packages('ggplot2')
library('ggplot2')
```

The package `ggplot2` allows to produce graphs, plots and visual representations constructing the aesthetics step by step, incrementally adding different layers at the graphs. It is highly customisable due to this particular feature; we are going to show some of its main characteristics in the below.

6.1 General aesthetics

Given a data frame, `ggplot` is invoked as `p <- ggplot(df)`, which corresponds to the basic underlying plot object where we will construct the rest of the layers upon, incrementally. Each additional layer is given by a set of points to be represented in the form of aesthetics that can be plotted as points, lines, bars and so on and so forth. Background colour is set by the option `panel.background = element_rect(fill = '#002b36')` within the `theme` aesthetics. General syntax is:

```
morley <- head(morley, 20)
p <- ggplot(morley, aes(x=Run))
p <- p + theme(panel.grid.major = element_blank(),
              panel.grid.minor = element_blank(),
              panel.background = element_rect(fill = '#002b36'),
              axis.line = element_line(colour = "black"),
              legend.title = element_text(size=16),
              axis.title.x = element_text(vjust=0, size=16),
              axis.title.y = element_text(vjust=1, size=16),
              plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_line(aes(y=Speed), colour = '#268bd2')
p <- p + geom_point(aes(y=Speed), colour = '#cb4b16')
p <- p + scale_x_discrete(breaks = morley$Run)
p <- p + labs(title = "Morley runs")
p <- p + labs(x = "Runs")
p <- p + labs(y = "Speed")
show(p)
```

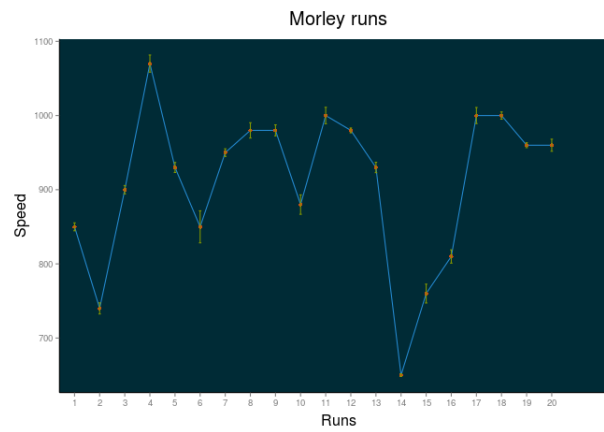


Simple plot

6.2 Error bars

If we want to add error bars we just have to add

```
error <- 10*runif(20)
dodge <- position_dodge(width=0.9)
p <- p + geom_errorbar(aes(ymin= Speed - error,
                          ymax = Speed + error), position = dodge,
                      colour="blue", width=.1)
```

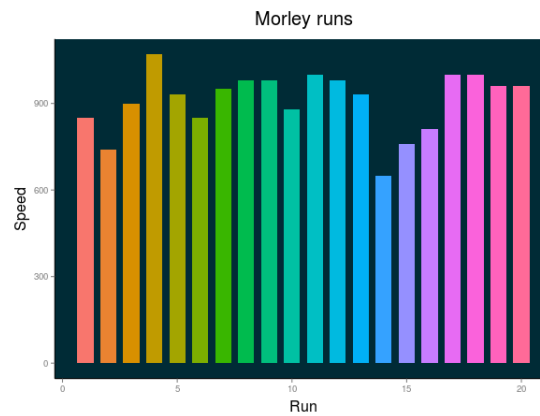


Error bars

6.3 Barplots

If, instead, we want to have a barplot thereof, just replace `geom_line` (`geom_point` respectively) with

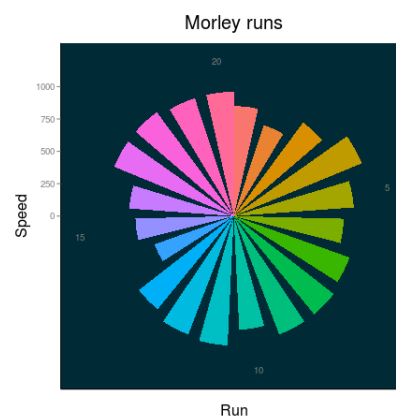
```
p <- p + geom_bar(aes(y=Speed), stat='identity', width=.7,
  fill='#657b83', color= '#6c71c4')
```



Barplot

How about we unfold the bars in polar coordinates instead?

```
p <- p + coord_polar()
```



Barplot in polar coordinates

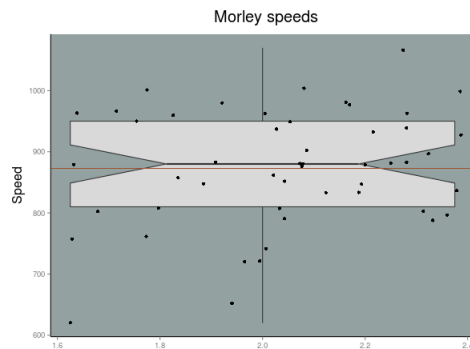
6.4 Boxplots

A boxplot is obtained as follows (theme is kept as before):

```
p <- ggplot(morley, aes(x=2, y=morley$Speed))
p <- p + geom_boxplot(outlier.colour = "blue", fill="grey85")
p <- p + labs(title = "Morley_speeds")
p <- p + labs(y = "Speed")
p <- p + labs(x = "")
show(p)
```

where the values of the x axis is irrelevant. Additional options can be included with

```
p <- p + geom_boxplot(notch = TRUE)
p <- p + geom_jitter()
p <- p + geom_hline(aes(yintercept=mean(morley$Speed)),
  colour="sienna")
```



Boxplot with jitters and notches

6.5 Data grouped by

Should we have data belonging to different groups, it would be convenient to represent each one of them with different colours, lines and bars. Here is how:

```
library(data.table)
iris <- data.table(iris)
groups <- iris[, .(length = mean(Sepal.Length)),
  by = c("Species", "Sepal.Width")]

p <- ggplot(groups, aes(x=Sepal.Width, y=length,
  group = Species, colour= Species))
p <- p + theme(panel.grid.major = element_blank(),
  panel.grid.minor = element_blank(),
  panel.background = element_rect(fill = '#002b36'),
  axis.line = element_line(colour = "black"),
  legend.text=element_text(size=16),
  legend.title=element_blank(),
  axis.title.x = element_text(vjust=0, size=16),
  axis.title.y = element_text(vjust=1, size=16),
  plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_point()
p <- p + geom_line()
p <- p + scale_colour_discrete()
p <- p + labs(title = "Iris_species")
p <- p + labs(x = "Sepal_width")
p <- p + labs(y = "Sepal_length")
show(p)
```

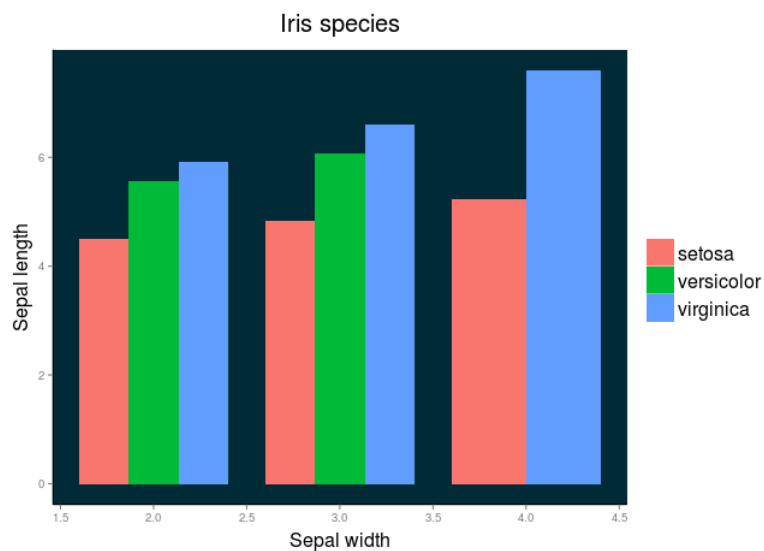
Equivalently with barplots

```
iris <- data.table(iris)
iris$Sepal.Width <- round(iris$Sepal.Width)
groups <- iris[, .(length = mean(Sepal.Length)),
  by = c("Species", "Sepal.Width")]
```



Data grouped by distinguished by colours

```
p <- ggplot(groups, aes(x=Sepal.Width, y=length))
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text=element_text(size=16),
               legend.title=element_blank(),
               axis.title.x = element_text(vjust=0, size=16),
               axis.title.y = element_text(vjust=1, size=16),
               plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_bar(aes(fill=Species), width = 0.8,
                  position = "dodge", stat = "identity")
p <- p + scale_colour_discrete()
p <- p + labs(title = "Iris species")
p <- p + labs(x = "Sepal width")
p <- p + labs(y = "Sepal length")
show(p)
```



Barplot of data grouped by

The option `position = "dodge"` ensures that the bars lie by one other. Taking that off would make a stacked barplot instead. Adding the option `facet_grid` allows to move different groups to different windows of the graph `p <- p + facet_grid(Species ~)`

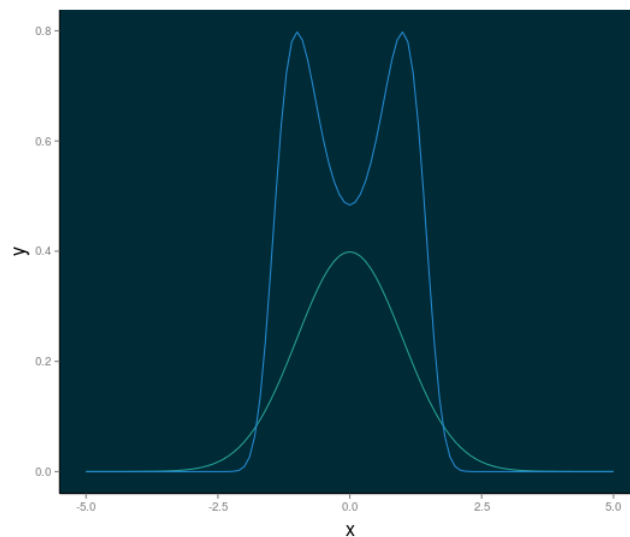


Barplots in different windows

6.6 Plotting functions

In order to plot several functions on the same graph

```
p <- ggplot(data.frame(x = c(-5, 5)), aes(x))
p <- p + stat_function(fun = dnorm, colour = "#2aa198")
p <- p + stat_function(fun = function(x) 2*dnorm(x^2-1),
                      colour = "#268bd2")
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text = element_text(size=16),
               legend.title = element_blank(),
               axis.title.x = element_text(vjust=0, size=16),
               axis.title.y = element_text(vjust=1, size=16),
               plot.title = element_text(vjust=1.5, size=20))
show(p)
```



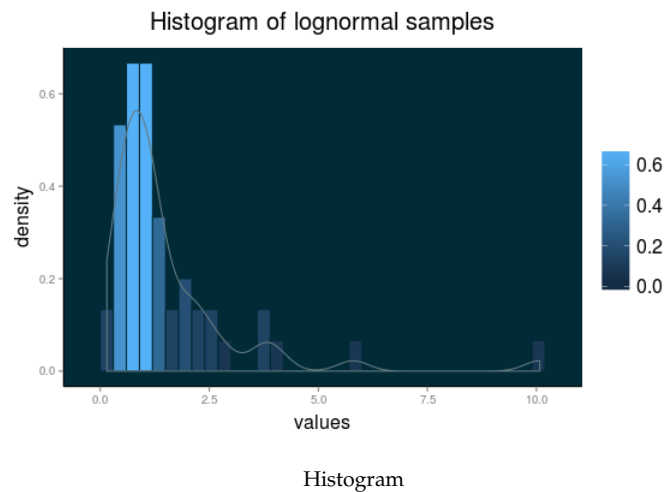
Plot of more than one function

6.7 Histograms

`geom_histogram` does the job. The values have to nevertheless be made into a data table format, that has to be invoked as first argument of `ggplot`

```
dt <- data.table(values = rlnorm(50))

p <- ggplot(dt, aes(x=values))
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text=element_text(size=16),
               legend.title=element_blank(),
               axis.title.x = element_text(vjust=0, size=16),
               axis.title.y = element_text(vjust=1, size=16),
               plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_histogram(aes(y=..density.., fill = ..density..),
                       colour="#002b36", binwidth = 0.3)
p <- p + geom_density(color = "#657b83")
# the below is to manually set the gradient
# p <- p + scale_fill_gradient(low = "red", high = "green")
p <- p + labs(title = "Histogram of normal samples")
show(p)
```



6.8 Tiles

```
install.packages(scale)
library(scale)
```

A powerful visualisation method for many variables at a time is provided by `geom_tile`, where different values of each variable are represented by different tiles filled on gradient according to the value: the set of data must be molten first and then the variables values have to be scaled between $[0,1]$ so that one can assign standard gradient fillings. The example below clarifies the issue:

```
cars <- data.table(mtcars)
cars$carnames <- rownames(mtcars)
cars.molten <- melt(cars)

R: cars.molten <- data.table(cars.molten)
R: cars.molten[sample(.N,5)]
```

	carnames	variable	value
1:	Merc 230	qsec	22.90
2:	Honda Civic	am	1.00
3:	Merc 240D	drat	3.69
4:	Lincoln Continental	mpg	10.40
5:	Merc 450SL	am	0.00

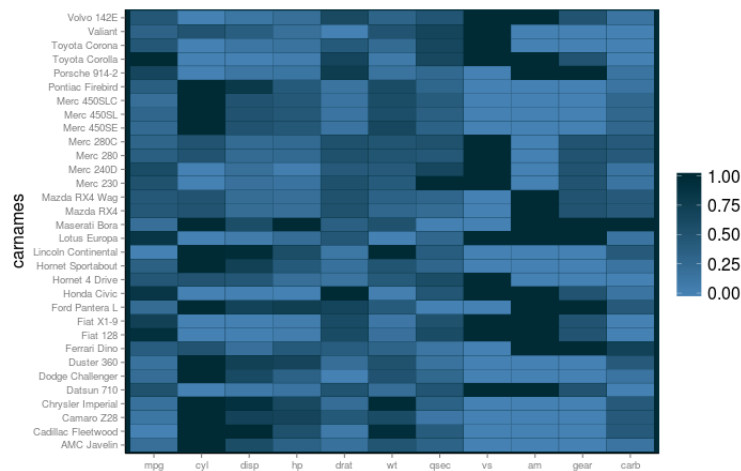
We now make use of the `rescale` function in the `scale` package as:

```
cars.molten <- ddply(cars.molten, .(variable), transform,
  rescale = rescale(value))
R: cars.molten <- data.table(cars.molten)
R: cars.molten[sample(.N,5)]

      carnames variable value  rescale
1:      Camaro Z28    mpg  13.3 0.1234043
2:      Merc 450SE    mpg  16.4 0.2553191
3:      Camaro Z28    disp 350.0 0.6956847
4: Lincoln Continental hp  215.0 0.5759717
5:      Merc 280C     qsec  18.9 0.5238095

p <- ggplot(cars.molten, aes(x=variable, y = carnames,
  fill = rescale))
p <- p + theme(panel.grid.major = element_blank(),
  panel.grid.minor = element_blank(),
  panel.background = element_rect(fill
    = '#002b36'),
  axis.line = element_line(colour = "black"),
  legend.text=element_text(size=16),
  legend.title=element_blank(),
  axis.title.x = element_text(vjust=0,
    size=16),
  axis.title.y = element_text(vjust=1, size=16),
  plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_tile(colour = "#002b36")
p <- p + scale_fill_gradient(low = "steelblue",
  high = "#002b36")
p <- p + labs(x = "")
show(p)
```

Tiled results are shown in the plot below, with the row names arranged on the *y* axis and the variables displayed horizontally instead.



Tiled heatmap

Hierarchical clustering and dendograms

Hierarchical clustering pairwise groups variables according to the minimum distances, and so on and so forth until the entire data set is reconstructed and tree shaped. Distances between points can be calculated using any distance $d(x,y)$ via `dist(df, method = <method>)`, the data frame containing the rows as points whose distances one wants to calculate.

As an example we can hierarchically cluster a subset of the `mtcars` data starting from calculating its euclidean distances among different rows (which, in turn, represent the different points that we want to cluster)

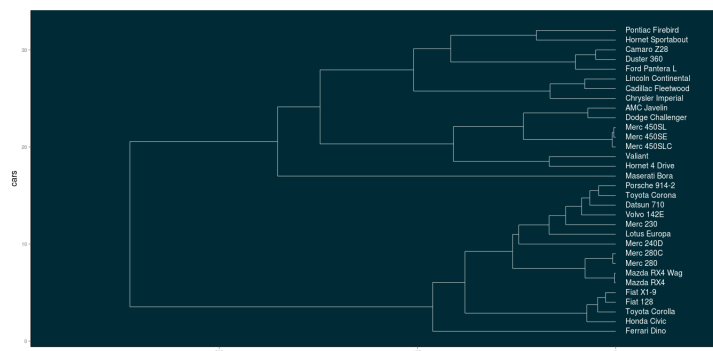
```
distances <- dist(iris, method = "euclidean")
dendog <- hclust(distances, method = "ave")
```

The function `hclust` pairwise couples the points according to the minimum distance, going up in pairs until the whole data set is exhausted. The dendrogram can be plotted making use of the following packages:

```
library("ggplot2")
install.packages("ggdendro")
library("ggdendro")
```

```
# dendro_data extracts the dendrogram
# objects numerical data
dendog <- dendro_data(dendog, type = "rectangle")

p <- ggplot(segment(dendog))
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text = element_text(size = 16),
               legend.title = element_blank(),
               axis.title.x = element_text(vjust = 0, size = 16),
               axis.title.y = element_text(vjust = 1, size = 16),
               plot.title = element_text(vjust = 1.5, size = 20))
p <- p + geom_segment(aes(x = x, y = y,
                          xend = xend, yend = yend),
                      colour = "white", alpha = 0.7)
p <- p + geom_text(data = label(dendog), colour = "white",
                   aes(x = x + 0.5, y = -5, label = label),
                   vjust = 1.2, hjust = 0)
p <- p + coord_flip()
p <- p + scale_y_reverse(expand = c(0.2, 0))
p <- p + labs(x = "cars")
p <- p + labs(y = "")
show(p)
```



Hierarchical clustering dendrogram

7.1 *k*-means clustering

k -means clustering groups the data in clusters according to the shortest distances to the centres of the cluster, whose number may be manually set. How to properly calculate the correct number of clusters and their centres will not be investigated here and we refer the reader to standard literature for that.

kmeans needs a set of data whose rows represent different point, whose coordinates are in turn given as column entries; all the provided values must be in numerical format. Different methods to calculate the clusters can be specified as additional arguments and options parameters.

```
# storing the names
names <- iris[,5]
iris <- iris[-5]

cluster <- kmeans(iris , centers = 3)

# coordinates of the centres
R: cluster$centers

  Sepal.Length Sepal.Width Petal.Length Petal.Width
1    5.006000    3.428000    1.462000    0.246000
2    5.901613    2.748387    4.393548    1.433871
3    6.850000    3.073684    5.742105    2.071053

# dimensions of the clusters
R: cluster$size

[1] 50 62 38

# each labelled row belongs to the specified cluster
R: cluster$cluster

  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1...
 [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 3 2 2 2 2...
 [75] 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2...
[112] 3 3 2 2 3 3 3 3 2 3 2 3 2 3 3 2 2 3 3 3...
[149] 3 2
```

Additional information can be gained investigating the outcome values of the function `kmeans`. However, row names can be placed back against the clusters labels as

```
R> table(names, cluster$cluster)
```

names	1	2	3
setosa	50	0	0
versicolor	0	48	2
virginica	0	14	36

Clustering can be made use of to spot possible outliers in the set of data, as those point having the furthest distances from any of the clusters centres.

```
centres <- cluster$centers[cluster$cluster,]
distances <- sqrt(rowSums((iris-centres)^2))

outliers <- head(iris[order(distances, decreasing = TRUE),])

R: outliers
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
99	5.1	2.5	3.0	1.1
58	4.9	2.4	3.3	1.0
94	5.0	2.3	3.3	1.0
61	5.0	2.0	3.5	1.0
119	7.7	2.6	6.9	2.3
118	7.7	3.8	6.7	2.2

The above can be made into a function, such that, given a data set, one can return the first M outliers once a clustering around N groups has been performed:

```

outlier.by.clustering <- function(df,N,M){
  cluster <- kmeans(df, centers = N)
  centres <- cluster$centers[cluster$cluster,]
  distances <- sqrt(rowSums((df-centres)^2))
  outliers <- head(df[order(distances,
                             decreasing = TRUE),],M)
  return(outliers)
}

```

```
R: outlier.by.clustering(iris,3,5)
```

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
99	5.1	2.5	3.0	1.1
58	4.9	2.4	3.3	1.0
94	5.0	2.3	3.3	1.0
61	5.0	2.0	3.5	1.0
119	7.7	2.6	6.9	2.3

8.1 Normality tests and qq-plots

Hypotheses tests *against* the normal Gaussian distribution can be performed starting with the `shapiro.test(values)`. The sample size affects the results of the normality test:

```
set.seed(1)
x <- rlnorm(20, 0, .4)
y <- rlnorm(100, 0, .4)

R: shapiro.test(x)
R: shapiro.test(y)

Shapiro-Wilk normality test

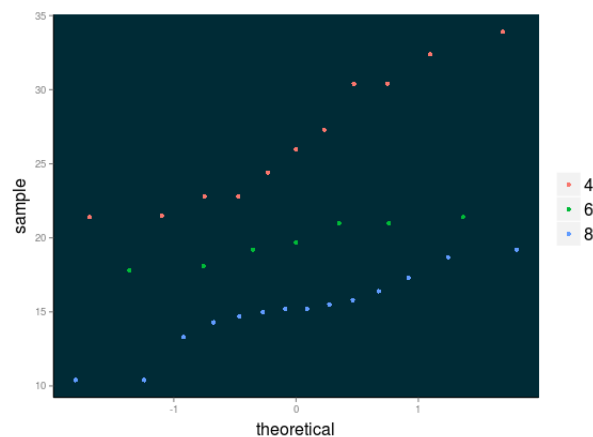
data:  x | data: y
W = 0.98049, p-value = 0.9403 | W = 0.91864, p-value = 1.193e-05
```

In small sample sizes, even big departures from normality are not detected. QQ-plots help us to represent deviations from normality, as in the example below:

```
R: mtcars[, .(p.value = shapiro.test(mpg)[2]),
             by = "cyl"]

   cyl  p.value
1:   6 0.3251776
2:   4 0.2605931
3:   8 0.3228563

p <- ggplot(mtcars, aes(sample = mpg, colour = factor(cyl)))
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text = element_text(size = 16),
               legend.title = element_blank(),
               axis.title.x = element_text(vjust = 0, size = 16),
               axis.title.y = element_text(vjust = 1, size = 16),
               plot.title = element_text(vjust = 1.5, size = 20))
p <- p + stat.qq()
show(p)
```



QQ-plot for data grouped by

Let us define a function that shows the rejection tests against the normal distribution for a set of grouped data, once an initial p -value is set.

```
shapiro.p.value <- function(my.column) {
  my.p.value <- '0.05'
  if (shapiro.test(my.column)[2] < my.p.value) {
    return("rejected")
  } else {
    return("not_rejected")
  }
}
```

```

    }
  }
}

R: iris[, lapply(.SD, shapiro.p.value), by = Species]

      Species Sepal.Length Sepal.Width Petal.Length Petal.Width
1:   setosa not rejected not rejected not rejected not rejected
2: versicolor not rejected not rejected not rejected not rejected
3:  virginica not rejected not rejected not rejected not rejected

```

8.2 *t*-tests

Student's *t*-test can be performed against two sets of values to have the null hypothesis that their means and variances to be the same, under the underlying assumption for both samples to come from a normal distribution. If this were true, then the *t*-test statistic $t = \frac{(\bar{x} - \mu_0)}{(s/\sqrt{n})(\sigma/\sqrt{n})}$ would follow a Student's *t*-distribution with $n_1 + n_2 - 2$ degrees of freedom, n_1, n_2 being the samples sizes. For additional references, please see³

As an example we consider two normal samples and test the *t*-statistic obtained after *N* *t*-tests. Given two sets of data *x, y* then

```

set.seed(1)
tt <- t.test(rnorm(10), rnorm(10))

R: tt

      Welch Two Sample t-test

data:  rnorm(10) and rnorm(10)
t = -0.27858, df = 16.469, p-value = 0.784
alternative hypothesis: true difference
in means is not equal to 0
95 percent confidence interval:
 -1.0022169  0.7689325
sample estimates:
mean of x mean of y
0.1322028 0.2488450

R: names(tt)
[1] "statistic" "parameter" "p.value" "conf.int"
[6] "estimate" "null.value" "alternative" "method"
[10] "data.name"

```

where we are interested in the `statistic` parameter. Therefore

```

N <- 10000
tstat <- replicate(N, t.test(rnorm(10), rnorm(10))$statistic)

points <- seq(range(tstat)[1], range(tstat)[2], length=100)

# theoretical values of the t-distribution
theory <- dt(points, df = 10+10-2)
# density values of the obtained t-statistics.
num <- density(tstat, n=100)$y

data <- data.table(points = points, theory = theory,
                   num = num)

p <- ggplot(data, aes(x=points))
p <- p + theme(panel.grid.major = element_blank(),
              panel.grid.minor = element_blank(),
              panel.background = element_rect(fill = '#002b36'),
              axis.line = element_line(colour = "black"),
              legend.text = element_text(size=16),
              legend.title = element_blank(),
              axis.title.x = element_text(vjust=0, size=16),
              axis.title.y = element_text(vjust=1, size=16),
              plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_line(aes(y=theory, colour = "theory"))

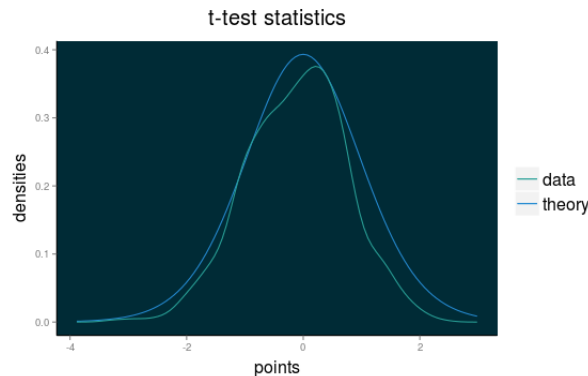
```

³ <http://statistics.berkeley.edu/computing/r-t-tests>

```

p <- p + geom_line(aes(y=num, colour = "data"))
p <- p + scale_colour_manual(values=c("#2aa198", "#268bd2"))
p <- p + labs(title = "t-test statistics")
p <- p + labs(y = "densities")
show(p)

```



t-test statistics densities

Another way to compare two densities is with a quantile-quantile plot. In this type of plot the quantiles of two samples are calculated at a variety of points in the range $[0, 1]$, and then are plotted against each other. If the two samples came from the same distribution with the same parameters, we would see a straight line through the origin with unit slope; in other words, we are testing to see if various quantiles of the data are identical in the two samples. If the two samples came from similar distributions, but their parameters were different, we would still see a straight line, but not through the origin.

We will get `qqplot` to perform the necessary calculations and then use `ggplot2` to display them.

```

x <- rnorm(100)
y <- rnorm(100)

dt <- as.data.table(qqplot(x, y, plot.it=FALSE))

p <- ggplot(dt)
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#002b36'),
               axis.line = element_line(colour = "black"),
               legend.text=element_text(size=16),
               legend.title=element_blank(),
               axis.title.x = element_text(vjust=0, size=16),
               axis.title.y = element_text(vjust=1, size=16),
               plot.title = element_text(vjust=1.5, size=20))
p <- p + geom_point(aes(x=x, y=y, colour = "QQ-plot"))
p <- p + geom_abline(aes(colour="ideal"),
                    intercept = 0, slope = 1)
p <- p + scale_colour_manual(values=c("#2aa198", "#268bd2"))
p <- p + labs(title = "t-test statistics")
p <- p + labs(y = "densities")
show(p)

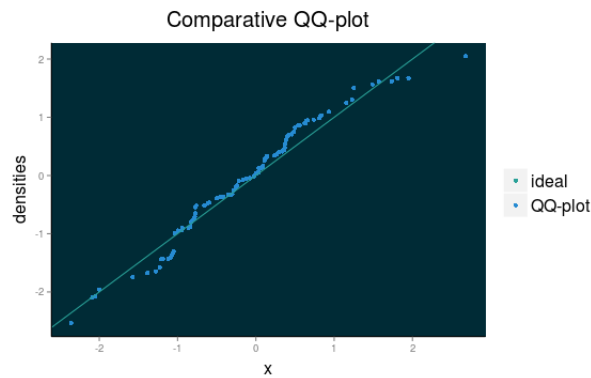
```

Equivalently, if the null hypothesis were true, namely if the two sets of data came from the same distribution, the p -value distribution would be uniform. Doing so on the above analysis we have

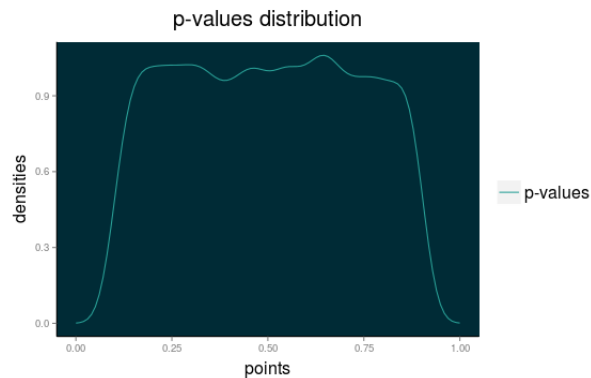
```

N <- 10000
tpstat <- replicate(N, t.test(rnorm(10), rnorm(10))$p.value)
points <- seq(range(tpstat)[1], range(tpstat)[2], length=100)
# density values of the obtained p-values.
num <- density(tpstat, n=100)$y
data <- data.table(points = points, num = num)

```



QQ-plots to compare two distributions



p -value uniform distribution

8.3 Kruskal-Wallis test

A collection of data samples are independent if they come from unrelated populations and the samples do not affect each other. Using the Kruskal-Wallis Test, we can decide whether the population distributions are identical without assuming them to follow the normal distribution.

As a matter of example we can test whether the petal width in the `iris` data set come from different distributions, according the species. The null hypothesis is that they are identical populations:

```
R: kruskal.test(Petal.Width ~ Species, data = iris)
```

```
Kruskal-Wallis rank sum test
```

```
data: Petal.Width by Species
```

```
Kruskal-Wallis chi-squared = 131.19, df = 2, p-value < 2.2e-16
```

It is therefore very *unlikely* (p -value < 0.05) the populations are identical.

8.4 Dunn's test

After having found out that a certain sets of data come from dissimilar distributions, it is possible to pairwise compare them to realise which specific couplings disturb the entire set. The above is obtained by means of the Dunn's test.

```
R: dunn.test(iris$Sepal.Width, g = iris$Species)
```

```
Kruskal-Wallis rank sum test
```

```
data: x and group
```

```
Kruskal-Wallis chi-squared = 63.5711, df = 2, p-value = 0
```

Comparison of x by group (No adjustment)		
Col Mean— Row Mean	setosa	versicol
versicol	7.787706 0.0000	
virginic	5.374419 0.0000	-2.413287 0.0079

R: `dunn.test(iris$Sepal.Width, g = iris$Species)$P`

[1] 3.411812e-15 3.841494e-08 7.904669e-03

The pairwise p -values are smaller than any threshold, hence all three groups come from three dissimilar populations.

The function `as.Date` converts the most date formats given to *input* them into the rules of the ISO-8601 international standard, which expresses the dates as year-month-day. The format to be converted must correspond to the introduced date format:

```
date1 <- as.Date("19/02/87", format = "%d/%m/%y")
date2 <- as.Date("04-06-15", format = "%d-%m-%y")

R: date1
[1] "1987-02-19"

R: date1 > date2
[1] FALSE

R: year(date1)
[1] 1987

R: week(date1)
[1] 8
```

Different placeholders after the percentage sign % correspond to different date formats. A full list is available [here](#)⁴. Also, the function `strptime` converts between character representations and objects of classes "POSIXlt" and "POSIXct" representing calendar dates and times; consequently, it is used to *output* a given date in a different desired time format or representation. The functions `as.POSIXct` and `as.POSIXlt` give representation in the central (local, respectively) time stamp format as

```
R: as.POSIXct(Sys.Date())
[1] "2015-10-17 02:00:00 CEST"

R: as.POSIXlt(Sys.Date())
[1] "2015-10-17 UTC"
```

The package `lubridate` simplifies the date and time arithmetics as

```
install.packages(lubridate)
library(lubridate)

R: date1 + weeks(5)
[1] "1987-03-26"

R: date1 - years(2)
[1] "1985-02-19"
```

Also notice the additional functions giving back precise information on the weekday and position in the year as `ymd_hms` or

```
R: wday(Sys.Date())
[1] 7

R: wday(Sys.Date(), label = TRUE)
[1] Sat
```

and the function `isoweek`

```
date1 <- as.Date("2014-12-31")

R: isoweek(date1)
[1] 1

R: week(date1)
[1] 53
```

⁴ <https://stat.ethz.ch/R-manual/R-patched/library/base/html/strptime.html>

Below is an example on how to write out and read in data sets.

```
set.seed(10)
mtcars <- data.table(mtcars)
cars <- mtcars[sample(.N,5), sample(11,4), with = FALSE]

write.table(cars, file = "my_file.csv", sep = "\t",
            quote = FALSE, append = FALSE, na = "NA",
            dec = ".", row.names = FALSE)

read_cars <- read.table("my_file.csv", sep = "\t", quote = "",
                       header = TRUE, dec = ".", fill = FALSE,
                       na.strings = c("NA", "-"),
                       stringsAsFactors = FALSE)
```

R: cars		R: read_cars
	disp carb gear drat	disp carb gear drat
1: 440.0	4 3 3.23	1: 440.0 4 3 3.23
2: 167.6	4 4 3.92	2: 167.6 4 4 3.92
3: 275.8	3 3 3.07	3: 275.8 3 3 3.07
4: 120.1	1 3 3.70	4: 120.1 1 3 3.70
5: 108.0	1 4 3.85	5: 108.0 1 4 3.85

The option `na.strings = c("NA", "-")` decides which lines must be interpreted as NA. Likewise `fill = TRUE` allows to skip and continue whenever inconsistencies in the data are present: on the other hand `fill = FALSE` throws an error whenever so (and hence allows control on the inconsistent data). To trim leading and trailing space from unquoted strings use `strip.white = TRUE`.

The `data.table` package makes use of `fread` to read data file in, this being much faster (especially for large sets of data), while keeping the same syntax.

```
install.package(stringr)
library(stringr)
```

Use `str_trim` to trim leading and tailing white spaces:

```
s <- ' _Hello, _world! _'

R: str_trim(s, side = "left") | R: str_trim(s, side = "right")
[1] "Hello, _world! _"          | [1] "_Hello, _world!"

R: str_trim(s)                | R: str_trim("\n\nHello, _world!\t")
[1] "Hello, _world!"            | [1] "Hello, _world!"
```

In order to replace *all* white space (and likewise any other character) use `str_replace_all`.

```
R: str_replace_all(s, fixed("_"), "")

[1] "Hello, world!"

R: str_replace_all(s, "l", "i")
[1] "_He! !o, _wor!d! _"
```

The functions `tolower` and `toupper` do the job as named:

```
R: tolower(s) | R: toupper(s)
[1] "hello, _world!" | [1] "HELLO, _WORLD!"
```

Strings can be alphabetically sorted using the `sort` numerical function plus a little manipulation of the characters. This can be useful when checking whether a certain number of words having the same number of characters are anagrams of one other: the standard procedure is to split their letters and sort them alphabetically to match them.

```
sort.word <- function(x){
  x <- tolower(x)
  x <- str_replace_all(x, fixed("_"), "")
  x <- paste(sort(unlist(strsplit(x, ""))), collapse = "")
  return(x)
}

is.anagram <- function(x,y){
  return(sort.word(x) == sort.word(y))
}

first <- "Eleven_plus_Two"
second <- "Twelve_plus_One"
third <- "Ten_plus_three"

R: is.anagram(first, second) | R: is.anagram(first, third)
[1] TRUE | [1] FALSE
```

A SPECIAL FUNCTIONS

A collection of useful (non-in-built) functions.

- *Mode*:

```
mode <- function(x) {  
  ux <- unique(x)  
  ux[which.max(tabulate(match(x, ux)))]  
}  
  
R: mode(quarks$flavour)  
[1] "strange"
```

- *na2zero*:

```
na2zero <- function(x) {  
  x[] <- lapply(x, function(x){x[is.na(x)] <- 0; x})  
  x  
}
```

- *Cartesian product*

```
cross.join <- function(a, b) {  
  idx <- expand.grid(seq(length=nrow(a)),  
                    seq(length=nrow(b)))  
  cbind(a[idx[,1],], b[idx[,2],])  
}
```

- *Shapiro p-value rejections*

```
shapiro.p.value <- function(my.column) {  
  my.p.value <- '0.05'  
  if(shapiro.test(my.column)[2] < my.p.value){  
    return("rejected")  
  } else {  
    return("not_rejected")  
  }  
}  
  
R: iris[, lapply(.SD, shapiro.p.value), by = Species]  
      Species Sepal.Length Sepal.Width Petal.Length  
1:   setosa not rejected not rejected not rejected  
2: versicolor not rejected not rejected not rejected  
3:  virginica not rejected not rejected not rejected
```

- *Anagrams*

```
sort.word <- function(x){  
  x <- tolower(x)  
  x <- str_replace_all(x, fixed("_"), "")  
  x <- paste(sort(unlist(strsplit(x, ""))), collapse = "")  
  return(x)  
}  
  
is.anagram <- function(x,y){  
  return(sort.word(x) == sort.word(y))  
}  
  
first <- "Eleven_plus_Two"  
second <- "Twelve_plus_One"  
  
R: is.anagram(first, second)  
[1] TRUE
```

- *Outliers by clustering*

```
outlier.by.clustering <- function(df,N,M){  
  cluster <- kmeans(df, centers = N)  
  centres <- cluster$centers[cluster$cluster,]  
  distances <- sqrt(rowSums((df-centres)^2))  
  outliers <- head(df[order(distances,  
                             decreasing = TRUE),],M)  
  return(outliers)  
}
```

```
}
R: outlier.by.clustering(mtcars[,1:7], 5, 5)
```

	mpg	cyl	disp	hp	drat	wt	qsec
Maserati Bora	15.0	8	301	335	3.54	3.570	14.60
Cadillac Fleetwood	10.4	8	472	205	2.93	5.250	17.98
Lincoln Continental	10.4	8	460	215	3.00	5.424	17.82
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02
Pontiac Firebird	19.2	8	400	175	3.08	3.845	17.05

A.1 RXKCD

```
install.packages(RXKCD)
library(RXKCD)
```

The above fetches comic strips from XKCD⁵

```
R: getXKCD(which = "random")
```

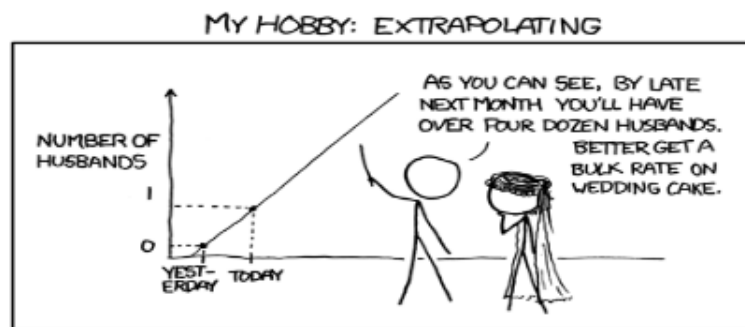


Figure 1: XKCD strip fetched in R

A.2 Colour palette

I have used the following colour palette (inspired from “Solarized”⁶)

- Background: #002b36
- Bars: #657b83
- Lines: #2aa198, #268bd2

⁵ <http://xkcd.com/>

⁶ <http://ethanschoonover.com/solarized>