R FOR DATA SCIENCE: QUICK GUIDE.

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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.

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1 INTRODUCTION

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:

¹ http://www.rdocumentation.org/

2 VECTORISED OPERATIONS ON DATA FRAMES

Given a data frame, the functions of the family apply allow to perform vectorised operations on rows and columns thereof, without having the 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
                45.82786
                               36.08286 60.16214
45.71143
# choose 2 for columns
R: apply(cars, 2, mean)
                       disp
                                   hp
              cvl
                                           drat
                                                       wt
                                                               asec
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
  C charme 1/2
2:
   D
        down −1/2
3:
4: F bottom 1/2
  B strange 1/2
5:
  F down −1/2
R: lapply(quarks, mode)
$lab
[1] "C"
$flavour
[1] "strange"
```

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

R: sapply(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</pre>
```

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] < o){
        print("negative")
    } else {
        print("positive")
    }
}

[1] "negative"
[1] "positive"
[1] "positive"
[1] "negative"
[1] "positive"
[1] "negative"
[1] "negative"</pre>
R: ifelse(x < o, "negative", "positive")

[1] "negative" "positive" "negative" "positive"</pre>
```

The function cumsum returns the cumulative sums of values elementwise, 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</pre>
```

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
                     3.0 1.1 0.1
                                                 setosa
           4.3
 2:
                      2.9
                                 1.4
                                            o.2 setosa
            4 \cdot 4
                     3.0
                                 1.3
                                           0.2
                                                 setosa
 3:
           4.4
 4:
            4 \cdot 4
                      3.2
                                 1.3
                                            0.2
                                                  setosa
               2.3 1.3
                                                  setosa
                                         0.3
 5:
         4.5
```

If we want the opposite (descending) order

```
R: setorder(iris, Species, -Sepal.Length)
    Sepal.Length Sepal.Width Petal.Length Petal.Width
                                                   Species
        5.8
 1:
                      4.0 1.2 0.2
                                                   setosa
 2:
                                                   setosa
            5.7
                       4.4
                                  1.5
                                              0.4
                      3.8
                                  1.7
                                              0.3
                                                    setosa
 3:
            5.7
                       4.2
                                   1.4
                                              0.2
                                                    setosa
 4:
            5.5
                                              0.2
 5:
            5.5
                       3.5
                                   1.3
                                                    setosa
```

Also note:

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.

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)

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

```
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
      setosa
                  0.2
 2:
                               1.4
      setosa
setosa
                  0.2
 3:
                               1.3
                               1.5
  4:
 5: setosa 0.2
                             1.4
```

Equivalently, new columns can be defined and added with

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

Rows can be subset according to constraints:

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

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

Simple frequencies counts per group can be obtained via the $\,$. $\!$ 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[,
                              keyby = c("flavour", "lab")
R: head(groups)
      flavour lab N
      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[,
                              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 0.166666667

      3:
      bottom
      D 2
      18 0.11111111

      4:
      bottom
      E 4
      18 0.22222222

      5:
      bottom
      F 6
      18 0.333333333

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

3.3 Grouping by

Variables can by grouped by according to the following grammar:

```
R: iris[,.(width = mean(Petal.Width), dev = sd(Petal.Width), .N),
       by = Species]
     Species mean
                       dev N
     setosa 0.246 0.1053856 50
1:
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
    A
 2:
         down
                        3
 3: A strange
 4: A top
 5: B bottom
                        3
6: B charme
```

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:

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

lab flavour S<sub>-</sub>z.x S<sub>-</sub>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 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 = o]

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 ensure 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 = o 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 charme NA 1/2
4: C charme NA -1/2
5: E charme NA -1/2
 6: B strange -1/2 1/2
 7:
     C strange 1/2 -1/2
     C strange 1/2 1/2
 8:
 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).

4 THE DPLYR PACKAGE

```
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:

```
R: arrange(iris, Species, desc(Sepal.Length))
             data.table
R: setorder(iris, Species, -Sepal.Length)
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
         5.8
                                         o.2 setosa
                   4.0
                              1.2
                                        o.4 setosa
         5.7
                   4.4
                              1.5
                  3.8
                                        o.3 setosa
3
         5.7
                             1.7
                   4.2
                               1.4
                                         0.2
                                             setosa
4
         5.5
                                   0.2 setosa
         5.5 3.5 1.3
```

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

New columns can be defined and added as

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

Rows can be subset according to constraints

The rows in correspondence of a match can be extracted with

```
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
setosa
               3.5
           5.1
                                  1.4 0.2
2:
                      2.8
                                             1.5 versicolor
           6.5
                                  4.6
                                       2.1 virginica
                   3.0
```

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:

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)]
```

and unique values can be fetched on constraints as

4.3 Grouping by

Variables can by grouped by according to the following grammar:

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</pre>
```

Left joins

Equivalently for left joins

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

lab flavour S_z.x S_z.y

B charme 1/2 NA

B strange 1/2 -1/2

C charme -1/2 NA

C strange -1/2 1/2

C strange 1/2 1/2

C strange 1/2 1/2

D bottom 1/2 1/2

D strange -1/2 NA

E charme -1/2 NA

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

C strange -1/2 1/2

C strange 1/2 1/2

D strange -1/2 NA>

E charme -1/2 NA>

D bottom 1/2 1/2

B charme 1/2 NA>

C charme -1/2 NA>

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('reshape')
library('reshape')
```

The library reshape is mainly based on two functions: cast 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 choses 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 cast(dt, col1 + ... + colN variable, fun.aggregate = fun)

```
R: cast(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
        NA = 1/2  1/2  1/2  1/2  1/2  NA 
 1/2  1/2  1/2  1/2  NA 
       <NA>
        1/2 1/2 1/2
   C
                            1/2 1/2 1/2
               1/2 1/2
                           -1/2 1/2 1/2 -1/2 1/2 -1/2
   D
        1/2
         1/2
   Ε
               -1/2 -1/2
   F 1/2 1/2 -1/2 -1/2 NA> -1/2
```

cast 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
       190 7.4 67 5 1
   41
    36
          118 8.0
                   72
                  74 5 3
62 5 4
56 5 5
   12
          149 12.6
3
    18
          313 11.5
4
          NA 14.3
    NA
   28 NA 14.9
```

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
     5 1
5 2
              Ozone
                       41
2
              Ozone
                        36
     5 3 Ozone
                       12
3
     5 4
              Ozone
                       18
              Ozone
                       NA
     5 5
5
              Ozone
                       28
R: tail(melt(airquality, id.vars = c("Month", "Day")))
   Month Day variable value
                 Temp
607
       9 25
                         63
608
       9 26
                 Temp
                          70
609
       9 27
                 Temp
                          77
       9 28
610
                 Temp
                          75
611
       9 29
                 Temp
                          76
       9 30
                 Temp
                          68
612
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

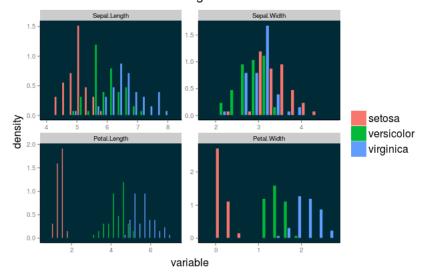
4: 5 7 Ozone 23.0

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
       setosa Sepal.Length
5:
                               4.5
p <- ggplot(iris.molten, aes(x=value, fill = Species))</pre>
p <- p + theme(panel.grid.major = element_blank(),</pre>
                panel.grid.minor = element_blank()
                panel.background = element_rect(fill
                                                  = '#oo2b36'),
                axis.line = element_line(colour = "black"),
                legend.text=element_text(size=16),
                legend.title=element_blank(),
                axis.title.x = element_text(vjust=o, size=16),
                axis.title.y = element_text(vjust=1, size=16),
plot.title = element_text(vjust=1.5, size=20))
p \leftarrow 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)
```

Iris histograms



Molten data set histograms

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

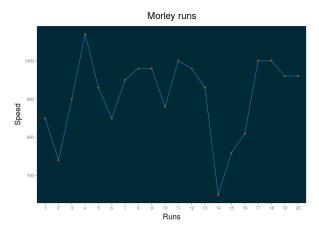
```
install.packages('ggplot2')
library('ggplot2')
```

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:

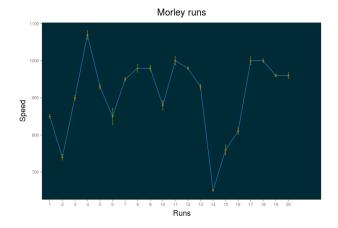
```
morley <- head (morley,20)
p <- ggplot(morley, aes(x=Run))</pre>
p <- p + theme(panel.grid.major = element_blank(),
                panel.grid.minor = element_blank(),
                panel.background = element_rect(fill = '#002b36'),
                axis.line = element_line(colour = "black"),
                legend.text=element_text(size=16),
                legend.title=element_blank(),
                axis.title.x = element_text(vjust=o, size=16),
                axis.title.y = element_text(vjust=1, size=16),
                plot.title = element_text(vjust=1.5, size=20))
p \leftarrow 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 \leftarrow p + labs(x = "Runs")
p \leftarrow p + labs(y = "Speed")
show(p)
```



Simple plot

6.2 Error bars

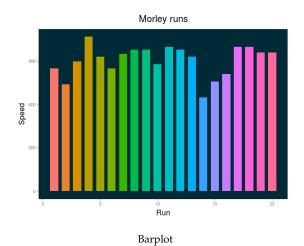
If we want to add error bars we just have to add



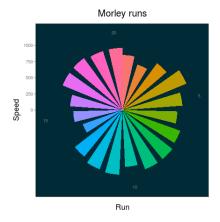
Error bars

6.3 Barplots

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



How about we unfold the bars in polar coordinates instead? $p \leftarrow p + coord_polar()$

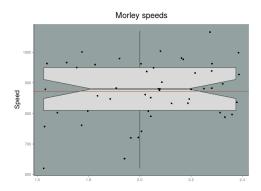


Barplot in polar coordinates

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)</pre>
```

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



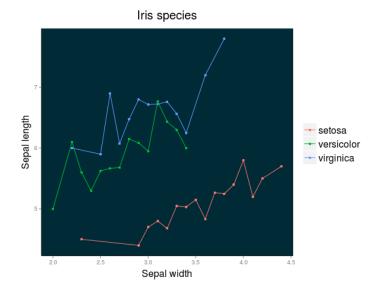
Boxplot with jitters and notches

6.5 Data grouped by

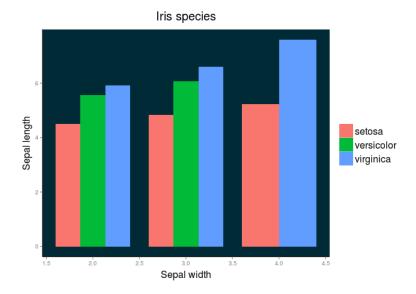
Should we have data belonging to different groups, it would be convenient to represent each one of them with different colours, lines and bars. Here is how:

```
library (data.table)
iris <- data.table(iris)</pre>
groups <- iris[, .(length = mean(Sepal.Length)),</pre>
              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=o, 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 \leftarrow p + labs(x = "Sepal_width")
p <- p + labs(y = "Sepal_length")
show(p)
```

Equivalently with barplots

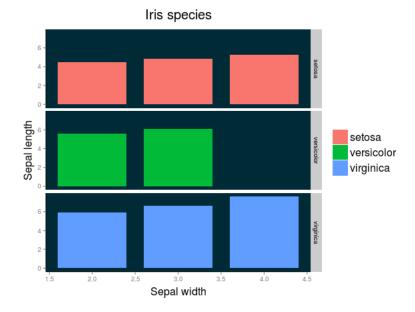


Data grouped by distinguished by colours



Barplot of data grouped by

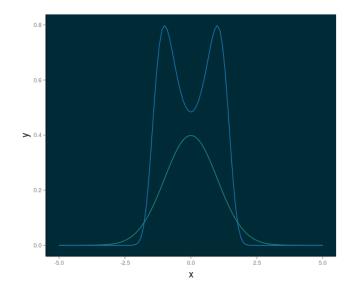
The option position = "dodge" ensures that the bars lie by one other. Taking that off would make a stacked barplot instead. Adding the option faced_grid allows to move different groups to different windows of the graph $p <-p + facet_grid(Species \div)$



Barplots in different windows

6.6 Plotting functions

In order to plot several functions on the same graph

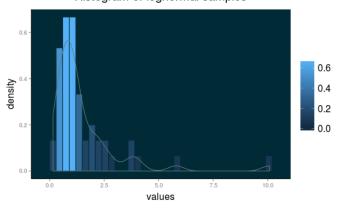


Plot of more than one function

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))</pre>
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 \leftarrow p + geom_histogram(aes(y=..density.., fill = ..density..),
                          colour = "#oo2b36", binwidth = o.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")</pre>
show(p)
```

Histogram of lognormal samples



Histogram

6.8 Tiles

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

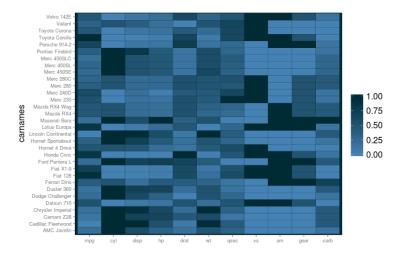
A powerful visualisation method for many variables at a time is provided by <code>geom_tile</code>, where different values of each variable are represented by different tiles filled on gradient according to the value: the set of data must be molten first and then the variables values have to be scaled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

```
<- data.table(mtcars)
cars$carnames <- rownames(mtcars)</pre>
cars.molten <- melt(cars)</pre>
R: cars.molten <- data.table(cars.molten)
R: cars.molten[sample(.N,5)]
              carnames variable value
                          qsec 22.90
1:
              Merc 230
2:
           Honda Civic
                             am 1.00
                            drat 3.69
             Merc 240D
3:
4: Lincoln Continental
                            mpg 10.40
           Merc 450SL
                             am 0.00
5:
```

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

```
cars.molten <- ddply(cars.molten, .(variable), transform,</pre>
                 rescale = rescale(value))
R: cars.molten <- data.table(cars.molten)
R: cars.molten[sample(.N,5)]
               carnames variable value
                                          rescale
             Camaro Z28
                          mpg 13.3 0.1234043
mpg 16.4 0.2553191
1:
2:
             Merc 450SE
            Camaro Z28
                             disp 350.0 0.6956847
3:
4: Lincoln Continental
                             hp 215.0 0.5759717
              Merc 28oC
                             qsec 18.9 0.5238095
5:
p <- ggplot(cars.molten, aes(x=variable, y = carnames,</pre>
                                         fill = rescale))
p <- p + theme(panel.grid.major = element_blank(),
                panel.grid.minor = element_blank(),
                panel.background = element_rect(fill
                                               = '#oo2b36'),
                axis.line = element_line(colour = "black"),
                legend.text=element_text(size=16),
                legend.title=element_blank(),
                axis.title.x = element_text(vjust=o,
                                        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 = "#oo2b36")</pre>
p <- p + scale_fill_gradient(low = "steelblue",
                               high = "#002b36")
p \leftarrow p + labs(x = "")
show(p)
```

Tiled results are shown in the plot below, whit 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 $\mathtt{dist}(\mathtt{df}, \mathtt{method} = \mathtt{method})$, the data frame containing the rows as points whose distances one wants to calculate.

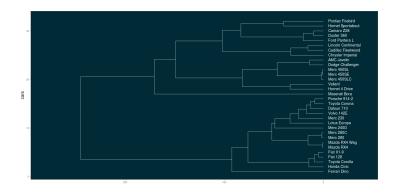
As an example we can hierarchically cluster a subset of the mtcars data starting from calculating its euclidean distances among different rows (which, in turn, represent the different points that we want to cluster)

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

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

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

```
# dendro_data extracts the dendogram
# objects numerical data
        <- dendro_data(dendog, type = "rectangle")</pre>
dendog
p <- ggplot(segment(dendog))</pre>
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=o, size=16),
                axis.title.y = element_text(vjust=1, size=16),
                plot.title = element_text(vjust=1.5, size=20))
p \leftarrow 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 \leftarrow p + scale_y_reverse(expand = c(0.2, 0))
p \leftarrow p + labs(x = "cars")
p \leftarrow p + labs(y = "")
show(p)
```



Hierarchical clustering dendogram

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 \langle -iris[-5]
cluster <- kmeans(iris, centers = 3)</pre>
# coordinates of the centres
R: cluster$centers
  Sepal. Length Sepal. Width Petal. Length Petal. Width

      5.006000
      3.428000
      1.462000
      0.246000

      5.901613
      2.748387
      4.393548
      1.433871

     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
  [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

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))</pre>
outliers <- head(iris[order(distances, decreasing = TRUE),])</pre>
R: outliers
    Sepal.Length Sepal.Width Petal.Length Petal.Width
99
        5.1 2.5 3.0 1.1
                                   3.3
58
                       2.4
                                                1.0
            4.9
           5.0
5.0
7.7
                      2.4
2.3
2.0
2.6
                                   3·3
3·5
94
                                               1.0
61
                                               1.0
119
                                    6.9
                                               2.3
                     3.8
118
                                    6.7
                                               2.2
           7.7
```

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:

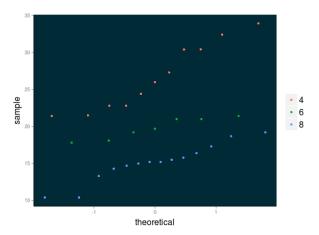
```
outlier.by.clustering <- function(df,N,M){
    cluster <- kmeans(df, centers = N)
centres <- cluster$centers[cluster$cluster,]</pre>
    distances <- sqrt(rowSums((df-centres)^2))
    outliers <- head(df[order(distances,
                         decreasing = TRUE),],M)
    return(outliers)
R: outlier.by.clustering(iris,3,5)
    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
61
              5.0
                            2.3
                                                         1.0
                                           3.3
               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:

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
     8 0.3228563
3:
p <- ggplot(mtcars, aes(sample = mpg, colour = factor(cyl)))</pre>
p <- p + theme(panel.grid.major = element_blank(),
               panel.grid.minor = element_blank(),
               panel.background = element_rect(fill = '#oo2b36'),
               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 \leftarrow 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 <- 'o.o5'
   if(shapiro.test(my.column)[2] < my.p.value){
      return("rejected")
   } else {
      return("not_rejected")</pre>
```

```
}
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
2: versicolor not rejected not rejected not rejected
3: virginica not rejected not rejected not rejected
```

8.2 *t-tests*

Student's t-test can be performed againts 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

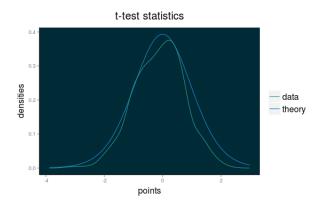
```
set.seed(1)
tt <- t.test(rnorm(10), rnorm(10))
        Welch Two Sample t-test
data: rnorm(10) and rnorm(10)
t = -0.27858, df = 16.469, p-value = 0.784
alternative hypothesis: true difference
in means is not equal to o
95 percent confidence interval:
 -1.0022169 0.7689325
sample estimates:
mean of 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

```
tstat <- replicate(N, t.test(rnorm(10),rnorm(10))$statistic)</pre>
points <- seq(range(tstat)[1], range(tstat)[2], length=100)</pre>
# theoretical values of the t-distribution
theory \leftarrow dt(points, df = 10+10-2)
# density values of the obtained t-statistics.
      <- density(tstat, n=100)$y</pre>
       <- data.table(points = points, theory = theory,
data
                      num = num)
p <- ggplot(data, aes(x=points))</pre>
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)</pre>
```



t-test statistics densities

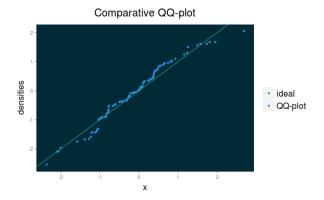
Another way to compare two densities is with a quantile-quantile plot. In this type of plot the quantiles of two samples are calculated at a variety of points in the range [0,1], and then are plotted against each other. If the two samples came from the same distribution with the same parameters, we would 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.

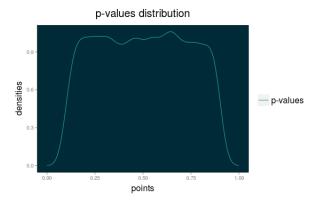
```
x \leftarrow rnorm(100)
y <- rnorm(100)
dt <- as.data.table(qqplot(x, y, plot.it=FALSE))</pre>
p <- ggplot(dt)</pre>
p <- p + theme(panel.grid.major = element_blank(),
                panel.grid.minor = element_blank(),
                panel.background = element_rect(fill = '#oo2b36'),
                axis.line = element_line(colour = "black"),
                legend.text=element_text(size=16),
                legend.title=element_blank(),
                axis.title.x = element_text(vjust=o, size=16),
                axis.title.y = element_text(vjust=1, size=16),
                plot.title = element_text(vjust=1.5, size=20))
p \leftarrow p + geom_point(aes(x=x, y=y, colour = "QQ-plot"))
p <- p + geom_abline(aes(colour="ideal"),
                      intercept = o, slope = 1)
p <- p + scale_colour_manual(values=c("#2aa198","#268bd2"))
p <- p + labs(title = "t-test_statistics")
p <- p + labs(y = "densities")</pre>
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)</pre>
```



QQ-plots to compare two distributions



p-value uniform distribution

8.3 Kruskal-Wallist 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
```

c 1 M	(No ad	on of x by ljustment)	group		
Col Mean- Row Mean	•	versicol			
versicol	7.787706 0.0000				
virginic	5.374419	-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 here⁴. Also, the function strptime converts between character representations and objects obigf classes "POSIXIt" 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.package(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</pre>
```

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 \leftarrow 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
           4 3 3.23 | 1: 440.0
4 4 3.92 | 2: 167.6
1: 440.0
                                         4 3 3.23
2: 167.6
                                           4
                                                 4 3.92
3: 275.8 3 3.07 3: 275.8 3 3.07
4: 120.1 1 3.70 4: 120.1 1 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 tailing 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!"</pre>
```

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", "!")

[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 standars procedure is to split their letters and sort them alphabetically to match them.

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"</pre>
```

- nazzero:

```
 \begin{array}{c} \text{nazzero} < - \text{ function}(x) \; \{ \\ x[] < - \text{ lapply}(x, \text{function}(x) \{ x[\text{is.na}(x)] < - \text{ o; } x \}) \\ x \\ \} \end{array}
```

- Cartesian product

- Shapiro p-value rejections

```
shapiro.p.value <- function(my.column) {
         my.p.value <- 'o.o5'
         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
2: versicolor not rejected not rejected
3: virginica not rejected not rejected</pre>
```

- 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</pre>
```

- Outliers by clustering

```
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")

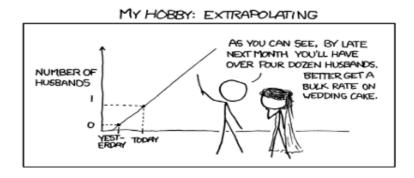


Figure 1: XKCD strip fetched in R

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