Introduction to R.

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Overview

What is R?

R is a powerful statistical environment and programming language for the analysis and visualization of data. The associated Bioconductor and CRAN package repositories provide many additional R packages for statistical data analysis for a wide array of research areas. The R software is free and runs on all common operating systems.

Why Using R?

- Complete statistical environment and programming language
- Efficient functions and data structures for data analysis
- Powerful graphics
- Access to fast growing number of analysis packages
- Most widely used language in bioinformatics
- Is standard for data mining and biostatistical analysis
- Technical advantages: free, open-source, available for all OSs

Books and Documentation

- simpleR Using R for Introductory Statistics (John Verzani, 2004) URL
- Bioinformatics and Computational Biology Solutions Using R and Bioconductor (Gentleman et al., 2005) - URL
- More on this see "Finding Help" section in UCR Manual URL

R Working Environments

R Projects and Interfaces

Some R working environments with support for syntax highlighting and utilities to send code to the R console:

- RStudio: excellent choice for beginners (Cheat Sheet)
- Basic R code editors provided by Rguis
- gedit, Rgedit, RKWard, Eclipse, Tinn-R, Notepad++, NppToR
- Vim-R-Tmux: R working environment based on vim and tmux
- Emacs (ESS add-on package)

Example: RStudio

New integrated development environment (IDE) for R. Highly functional for both beginners and advanced.

RStudio IDE

Some userful shortcuts: Ctrl+Enter (send code), Ctrl+Shift+C (comment/uncomment), Ctrl+1/2 (switch window focus)

Example: Vim-R-Tmux

Terminal-based Working Environment for R: Vim-R-Tmux

Vim-R-Tmux IDE for R

R Package Repositories

- CRAN (>11,000 packages) general data analysis URL
- Bioconductor (>1,100 packages) bioscience data analysis URL
- Omegahat (>90 packages) programming interfaces URL

Installation of R Packages

- 1. Install R for your operating system from CRAN.
- 2. Install RStudio from RStudio.
- 3. Install CRAN Packages from R console like this:

```
install.packages(c("pkg1", "pkg2"))
install.packages("pkg.zip", repos=NULL)
```

4. Install Bioconductor packages as follows:

```
source("http://www.bioconductor.org/biocLite.R")
library(BiocInstaller)
BiocVersion()
biocLite()
biocLite(c("pkg1", "pkg2"))
```

5. For more details consult the Bioc Install page and BiocInstaller package.

Getting Around

Startup and Closing Behavior

- Starting R: The R GUI versions, including RStudio, under Windows and Mac OS X can be opened by double-clicking their icons. Alternatively, one can start it by typing R in a terminal (default under Linux).
- Startup/Closing Behavior: The R environment is controlled by hidden files in the startup directory: .RData, .Rhistory and .Rprofile (optional).
- Closing R:

```
q()
```

Save workspace image? [y/n/c]:

• Note: When responding with y, then the entire R workspace will be written to the .RData file which can become very large. Often it is sufficient to just save an analysis protocol in an R source file. This way one can quickly regenerate all data sets and objects.

Navigating directories

Create an object with the assignment operator \leftarrow or =

```
object <- ...
```

List objects in current R session

```
ls()
```

Return content of current working directory

```
dir()
```

Return path of current working directory

```
getwd()
```

Change current working directory

```
setwd("/home/user")
```

Basic Syntax

General R command syntax

```
object <- function_name(arguments)
object <- object[arguments]</pre>
```

Finding help

?function_name

Load a library/package

```
library("my_library")
```

List functions defined by a library

```
library(help="my_library")
```

Load library manual (PDF or HTML file)

```
vignette("my_library")
```

Execute an R script from within R

```
source("my_script.R")
Execute an R script from command-line (the first of the three options is preferred)
$ Rscript my_script.R
$ R CMD BATCH my_script.R
$ R --slave < my_script.R</pre>
Data Types
Numeric data
Example: 1, 2, 3, ...
x \leftarrow c(1, 2, 3)
## [1] 1 2 3
is.numeric(x)
## [1] TRUE
as.character(x)
## [1] "1" "2" "3"
Character data
Example: "a", "b", "c", ...
x <- c("1", "2", "3")
## [1] "1" "2" "3"
is.character(x)
## [1] TRUE
as.numeric(x)
```

Complex data

[1] 1 2 3

Example: mix of both

```
c(1, "b", 3)
## [1] "1" "b" "3"
Logical data
Example: TRUE of FALSE
x < -1:10 < 5
   [1] TRUE TRUE TRUE TRUE FALSE FALSE FALSE FALSE FALSE
!x
   [1] FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE TRUE
which(x) # Returns index for the 'TRUE' values in logical vector
## [1] 1 2 3 4
Data objects
Object types
Vectors (1D)
Definition: numeric or character
myVec <- 1:10; names(myVec) <- letters[1:10]</pre>
myVec[1:5]
## a b c d e
## 1 2 3 4 5
myVec[c(2,4,6,8)]
## b d f h
## 2 4 6 8
myVec[c("b", "d", "f")]
## b d f
## 2 4 6
```

Factors (1D)

Definition: vectors with grouping information

```
factor(c("dog", "cat", "mouse", "dog", "dog", "cat"))
## [1] dog
            cat
                   mouse dog
                                dog
                                      cat
## Levels: cat dog mouse
Matrices (2D)
Definition: two dimensional structures with data of same type
myMA <- matrix(1:30, 3, 10, byrow = TRUE)
class(myMA)
## [1] "matrix"
myMA[1:2,]
        [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
## [1,]
                     3
                                5
                                     6
                                          7
## [2,]
          11
               12
                    13
                          14
                               15
                                    16
                                         17
                                              18
                                                          20
myMA[1, , drop=FALSE]
```

Data Frames (2D)

Definition: two dimensional objects with data of variable types

3

[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]

6

5

```
myDF <- data.frame(Col1=1:10, Col2=10:1)
myDF[1:2, ]</pre>
```

```
## Col1 Col2
## 1 1 10
## 2 2 9
```

Arrays

[1,]

Definition: data structure with one, two or more dimensions

Lists

Definition: containers for any object type

```
myL <- list(name="Fred", wife="Mary", no.children=3, child.ages=c(4,7,9))
myL</pre>
```

```
## $name
## [1] "Fred"
##
## $wife
## [1] "Mary"
##
## $no.children
## [1] 3
##
## $child.ages
## [1] 4 7 9
myL[[4]][1:2]
```

[1] 4 7

Functions

Definition: piece of code

```
myfct <- function(arg1, arg2, ...) {
    function_body
}</pre>
```

Subsetting of data objects

(1.) Subsetting by positive or negative index/position numbers

```
myVec <- 1:26; names(myVec) <- LETTERS
myVec[1:4]

## A B C D
## 1 2 3 4</pre>
```

(2.) Subsetting by same length logical vectors

```
myLog <- myVec > 10
myVec[myLog]
```

```
## K L M N O P Q R S T U V W X Y Z ## 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
```

(3.) Subsetting by field names

```
myVec[c("B", "K", "M")]
```

```
## B K M
## 2 11 13
```

(4.) Subset with \$ sign: references a single column or list component by its name

```
iris$Species[1:8]
## [1] setosa setosa setosa setosa setosa setosa setosa
## Levels: setosa versicolor virginica
Important Utilities
Combining Objects
The c function combines vectors and lists
c(1, 2, 3)
## [1] 1 2 3
x <- 1:3; y <- 101:103
c(x, y)
## [1]
             2
                 3 101 102 103
iris$Species[1:8]
## [1] setosa setosa setosa setosa setosa setosa setosa
## Levels: setosa versicolor virginica
The cbind and rbind functions can be used to append columns and rows, respecively.
ma <- cbind(x, y)</pre>
##
## [1,] 1 101
## [2,] 2 102
## [3,] 3 103
rbind(ma, ma)
##
        \mathbf{x}
            у
## [1,] 1 101
## [2,] 2 102
## [3,] 3 103
## [4,] 1 101
```

Accessing Dimensions of Objects

[5,] 2 102 ## [6,] 3 103

Length and dimension information of objects

```
length(iris$Species)
## [1] 150
dim(iris)
```

Accessing Name Slots of Objects

[1] 150

Accessing row and column names of 2D objects

```
rownames(iris)[1:8]

## [1] "1" "2" "3" "4" "5" "6" "7" "8"

colnames(iris)

## [1] "Sepal.Length" "Sepal.Width" "Petal.Length" "Petal.Width" "Species"

Return name field of vectors and lists

names(myVec)

## [1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J" "K" "L" "M" "N" "O" "P" "Q" "R" "S" "T" "U" "V" "W" "X" "#" [25] "Y" "Z"

names(myL)
```

Sorting Objects

[1] "name"

The function sort returns a vector in ascending or descending order

"wife"

[1] 14 9 39 43 42 4 7 23 48 3 30 12

```
## [1] 1 2 3 4 5 6 7 8 9 10

The function order returns a sorting index for sorting an object

sortindex <- order(iris[,1], decreasing = FALSE)
sortindex[1:12]</pre>
```

"no.children" "child.ages"

```
iris[sortindex,][1:2,]
##
      Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 14
               4.3
                          3.0
                                       1.1
                                                   0.1 setosa
## 9
               4.4
                           2.9
                                        1.4
                                                    0.2 setosa
sortindex <- order(-iris[,1]) # Same as decreasing=TRUE</pre>
Sorting multiple columns
iris[order(iris$Sepal.Length, iris$Sepal.Width),][1:2,]
      Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 14
              4.3
                          3.0
                                       1.1
                                                   0.1 setosa
               4.4
                                       1.4
## 9
                          2.9
                                                   0.2 setosa
Operators and Calculations
Comparison Operators
Comparison operators: ==, !=, <, >, <=, >=
1==1
## [1] TRUE
Logical operators: AND: &, OR: |, NOT: !
x <- 1:10; y <- 10:1
x > y & x > 5
   [1] FALSE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE
Basic Calculations
To look up math functions, see Function Index here
x + y
   [1] 11 11 11 11 11 11 11 11 11 11
sum(x)
```

[1] 55

```
mean(x)
## [1] 5.5
apply(iris[1:6,1:3], 1, mean)
## 1 2 3 4 5 6
## 3.333333 3.100000 3.066667 3.066667 3.333333 3.666667
```

Reading and Writing External Data

Import of tabular data

Import of a tab-delimited tabular file

```
myDF <- read.delim("myData.xls", sep="\t")</pre>
```

Import of Excel file. Note: working with tab- or comma-delimited files is more flexible and preferred.

```
library(gdata)
myDF <- read.xls"myData.xls")</pre>
```

Import of Google Sheets. The following example imports a sample Google Sheet from here. Detailed instructions for interacting from R with Google Sheets with the required googlesheets package are here.

```
library("googlesheets"); library("dplyr"); library(knitr)
gs_auth() # Creates authorizaton token (.httr-oauth) in current directory if not present
sheetid <-"1U-32UcwZP1k3saKeaH1mbvEAOfZRdNHNkWK2GI1rpPM"
gap <- gs_key(sheetid)
mysheet <- gs_read(gap, skip=4)
myDF <- as.data.frame(mysheet)
myDF</pre>
```

Export of tabular data

```
write.table(myDF, file="myfile.xls", sep="\t", quote=FALSE, col.names=NA)
```

Line-wise import

```
myDF <- readLines("myData.txt")</pre>
```

Line-wise export

```
writeLines(month.name, "myData.txt")
```

Copy and paste into R

On Windows/Linux systems

```
read.delim("clipboard")
```

On Mac OS X systems

```
read.delim(pipe("pbpaste"))
```

Copy and paste from R

On Windows/Linux systems

```
write.table(iris, "clipboard", sep="\t", col.names=NA, quote=F)
```

On Mac OS X systems

```
zz <- pipe('pbcopy', 'w')
write.table(iris, zz, sep="\t", col.names=NA, quote=F)
close(zz)</pre>
```

Homework 3A

Homework 3A: Object Subsetting Routines and Import/Export

Useful R Functions

Unique entries

Make vector entries unique with unique

```
length(iris$Sepal.Length)
## [1] 150
```

```
length(unique(iris$Sepal.Length))
```

[1] 35

Count occurrences

Count occurrences of entries with table

table(iris\$Species)

```
## setosa versicolor virginica
## 50 50 50
```

Aggregate data

Compute aggregate statistics with aggregate

```
aggregate(iris[,1:4], by=list(iris$Species), FUN=mean, na.rm=TRUE)
```

```
##
       Group.1 Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1
                       5.006
                                   3.428
                                                1.462
## 2 versicolor
                       5.936
                                   2.770
                                                4.260
                                                            1.326
## 3 virginica
                       6.588
                                   2.974
                                                5.552
                                                            2.026
```

Intersect data

Compute intersect between two vectors with %in%

```
month.name %in% c("May", "July")
```

[1] FALSE FALSE FALSE FALSE TRUE FALSE TRUE FALSE FALSE FALSE FALSE FALSE

Merge data frames

Join two data frames by common field entries with merge (here row names by.x=0). To obtain only the common rows, change all=TRUE to all=FALSE. To merge on specific columns, refer to them by their position numbers or their column names.

```
frame1 <- iris[sample(1:length(iris[,1]), 30), ]
frame1[1:2,]</pre>
```

```
## Sepal.Length Sepal.Width Petal.Length Petal.Width Species ## 110 7.2 3.6 6.1 2.5 virginica ## 60 5.2 2.7 3.9 1.4 versicolor
```

```
dim(frame1)
```

```
## [1] 30 5
```

```
my_result <- merge(frame1, iris, by.x = 0, by.y = 0, all = TRUE)
dim(my_result)</pre>
```

```
## [1] 150 11
```

SQLite Databases

SQLite is a lightweight relational database solution. The RSQLite package provides an easy to use interface to create, manage and query SQLite databases directly from R. Basic instructions for using SQLite from the command-line are available here. A short introduction to RSQLite is available here.

Loading data into SQLite databases

The following loads two data.frames derived from the iris data set (here mydf1 and mydf2) into an SQLite database (here test.db).

```
library(RSQLite)
mydb <- dbConnect(SQLite(), "test.db") # Creates database file test.db
mydf1 <- data.frame(ids=paste0("id", seq_along(iris[,1])), iris)
mydf2 <- mydf1[sample(seq_along(mydf1[,1]), 10),]
dbWriteTable(mydb, "mydf1", mydf1)

## [1] TRUE

dbWriteTable(mydb, "mydf2", mydf2)

## [1] TRUE</pre>
```

List names of tables in database

```
dbListTables(mydb)
## [1] "mydf1" "mydf2"
```

Import table into data.frame

```
dbGetQuery(mydb, 'SELECT * FROM mydf2')
##
        ids Sepal.Length Sepal.Width Petal.Length Petal.Width
                                                                  Species
## 1
       id8
                     5.0
                                 3.4
                                              1.5
                                                           0.2
                                                                   setosa
## 2
       id28
                     5.2
                                 3.5
                                               1.5
                                                           0.2
                                                                   setosa
## 3 id111
                     6.5
                                 3.2
                                              5.1
                                                           2.0 virginica
## 4
      id65
                     5.6
                                 2.9
                                               3.6
                                                           1.3 versicolor
## 5
       id92
                     6.1
                                 3.0
                                              4.6
                                                           1.4 versicolor
## 6 id108
                     7.3
                                 2.9
                                              6.3
                                                           1.8 virginica
## 7 id140
                     6.9
                                 3.1
                                              5.4
                                                           2.1 virginica
## 8
       id37
                     5.5
                                 3.5
                                              1.3
                                                           0.2
                                                                   setosa
## 9 id101
                                                           2.5 virginica
                     6.3
                                 3.3
                                              6.0
## 10 id118
                     7.7
                                              6.7
                                                           2.2 virginica
                                 3.8
```

Query database

dbGetQuery(mydb, 'SELECT * FROM mydf1 WHERE "Sepal.Length" < 4.6')</pre>

```
##
      ids Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1 id9
                   4.4
                               2.9
                                             1.4
                                                         0.2 setosa
## 2 id14
                   4.3
                               3.0
                                             1.1
                                                         0.1
                                                              setosa
                               3.0
                                             1.3
## 3 id39
                   4.4
                                                         0.2
                                                              setosa
## 4 id42
                   4.5
                               2.3
                                             1.3
                                                         0.3
                                                              setosa
## 5 id43
                   4.4
                               3.2
                                             1.3
                                                         0.2 setosa
```

Join tables

The two tables can be joined on the shared ids column as follows.

```
dbGetQuery(mydb, 'SELECT * FROM mydf1, mydf2 WHERE mydf1.ids = mydf2.ids')
```

##		ids	Sepal.Length	Sepal.Widt	h Petal	$. \\ \texttt{Length}$	Petal.	Width	Species	ids	Sepal.Length
##	1	id8	5.0	3.	4	1.5		0.2	setosa	id8	5.0
##	2	id28	5.2	3.	5	1.5		0.2	setosa	id28	5.2
##	3	id37	5.5	3.	5	1.3		0.2	setosa	id37	5.5
##	4	id65	5.6	2.	9	3.6		1.3	versicolor	id65	5.6
##	5	id92	6.1	3.	0	4.6		1.4	versicolor	id92	6.1
##	6	id101	6.3	3.	3	6.0		2.5	virginica	id101	6.3
##	7	id108	7.3	3 2.	9	6.3		1.8	virginica	id108	7.3
##	8	id111	6.5	3.	2	5.1		2.0	virginica	id111	6.5
##	9	id118	7.7	3.	8	6.7		2.2	virginica	id118	7.7
##	10	id140	6.9			5.4		2.1	virginica	id140	6.9
##		Sepal.	.Width Petal.	Length Peta	l.Width	Spe	cies				
##	1		3.4	1.5	0.2	set	tosa				
##	2		3.5	1.5	0.2	set	tosa				
##	3		3.5	1.3	0.2	set	tosa				
##	4		2.9	3.6	1.3	versic	olor				
##	5		3.0	4.6	1.4	versic	olor				
##	6		3.3	6.0	2.5	virgi	nica				
##	7		2.9	6.3	1.8	virgi	nica				
##	8		3.2	5.1	2.0	virgi	nica				
##	9		3.8	6.7	2.2	virgi	nica				
##	10		3.1	5.4	2.1	virgi	nica				

Graphics in R

Advantages

- Powerful environment for visualizing scientific data
- Integrated graphics and statistics infrastructure
- Publication quality graphics
- Fully programmable
- Highly reproducible
- Full LaTeX and Markdown support via knitr and R markdown
- Vast number of R packages with graphics utilities

Documentation for R Graphics

General

- Graphics Task Page URL
- R Graph Gallery URL
- R Graphical Manual URL
- Paul Murrell's book R (Grid) Graphics URL

Interactive graphics

- rggobi' (GGobi) URL
- iplots URL
- Open GL (rgl) URL

Graphics Environments

Viewing and saving graphics in R

- On-screen graphics
- postscript, pdf, svg
- jpeg, png, wmf, tiff, ...

Four major graphic environments

- (a) Low-level infrastructure
- R Base Graphics (low- and high-level)
- grid: Manual
- (b) High-level infrastructure \begin{itemize}
 - lattice: Manual, Intro, Book
 - ggplot2: Manual, Intro, Book

Base Graphics: Overview

Important high-level plotting functions

- plot: generic x-y plotting
- barplot: bar plots
- boxplot: box-and-whisker plot
- hist: histograms
- pie: pie charts
- dotchart: cleveland dot plots
- image, heatmap, contour, persp: functions to generate image-like plots
- qqnorm, qqline, qqplot: distribution comparison plots
- pairs, coplot: display of multivariant data

Help on graphics functions

- ?myfct
- ?plot
- ?par

Preferred Object Types

- Matrices and data frames
- Vectors
- Named vectors

Scatter Plots

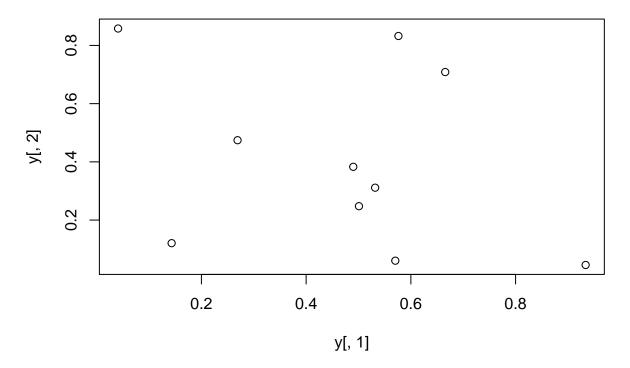
Basic Scatter Plot

Sample data set for subsequent plots

```
set.seed(1410)
y <- matrix(runif(30), ncol=3, dimnames=list(letters[1:10], LETTERS[1:3]))</pre>
```

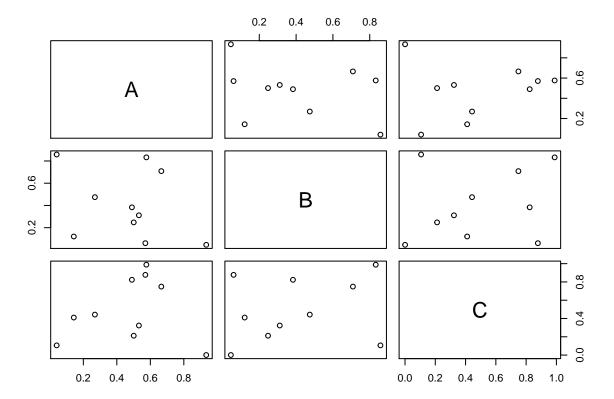
Plot data

```
plot(y[,1], y[,2])
```



All pairs

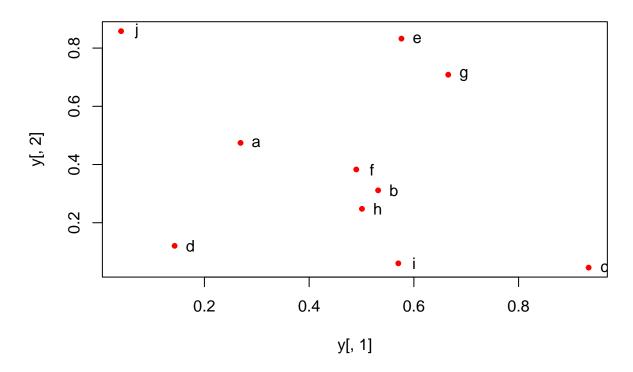
```
pairs(y)
```



With labels

```
plot(y[,1], y[,2], pch=20, col="red", main="Symbols and Labels")
text(y[,1]+0.03, y[,2], rownames(y))
```

Symbols and Labels

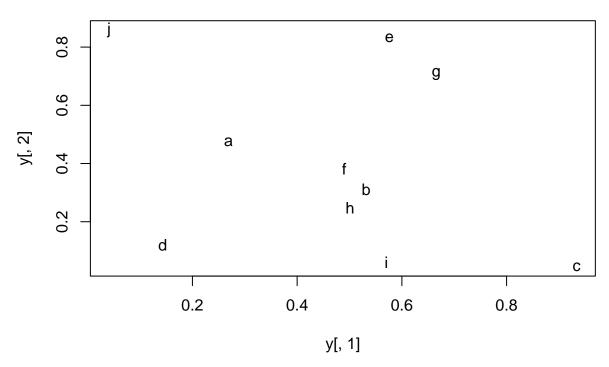


More examples

Print instead of symbols the row names

```
plot(y[,1], y[,2], type="n", main="Plot of Labels")
text(y[,1], y[,2], rownames(y))
```

Plot of Labels



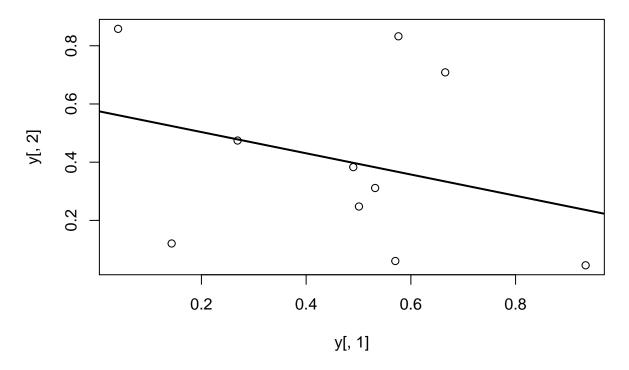
Usage of important plotting parameters

__Important arguments_

- mar: specifies the margin sizes around the plotting area in order: c(bottom, left, top, right)
- col: color of symbols
- pch: type of symbols, samples: example(points)
- lwd: size of symbols
- cex.*: control font sizes
- For details see ?par

Add regression line

```
plot(y[,1], y[,2])
myline <- lm(y[,2]~y[,1]); abline(myline, lwd=2)</pre>
```



summary(myline)

```
##
## Call:
## lm(formula = y[, 2] ~ y[, 1])
##
## Residuals:
##
       Min
                 1Q
                     Median
                                   3Q
## -0.40357 -0.17912 -0.04299 0.22147 0.46623
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                0.5764
                           0.2110
                                    2.732
                                            0.0258 *
                           0.3959 -0.921
                                            0.3839
## y[, 1]
               -0.3647
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3095 on 8 degrees of freedom
## Multiple R-squared: 0.09589, Adjusted R-squared:
                                                       -0.01712
## F-statistic: 0.8485 on 1 and 8 DF, p-value: 0.3839
```

Log scale

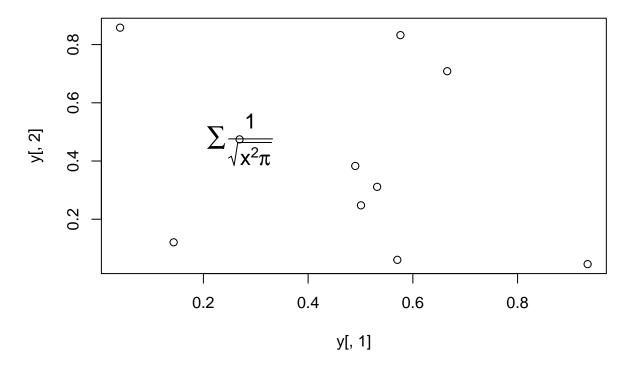
Same plot as above, but on log scale

```
plot(y[,1], y[,2], log="xy")
```



Add a mathematical expression

plot(y[,1], y[,2]); text(y[1,1], y[1,2], expression(sum(frac(1,sqrt(x^2*pi)))), cex=1.3)

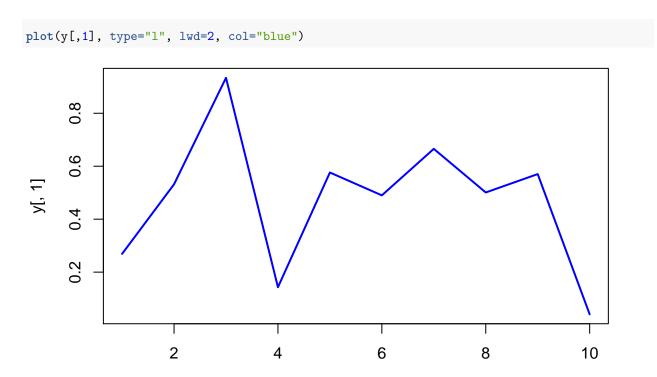


Homework 3B

Homework 3B: Scatter Plots

Line Plots

Single data set



Many Data Sets

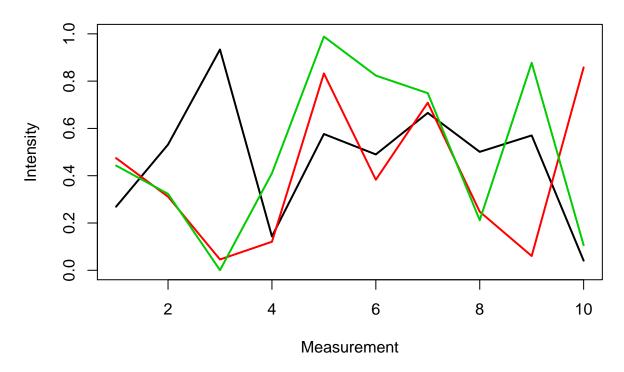
Plots line graph for all columns in data frame y. The split.screen function is used in this example in a for loop to overlay several line graphs in the same plot.

Index

```
split.screen(c(1,1))

## [1] 1

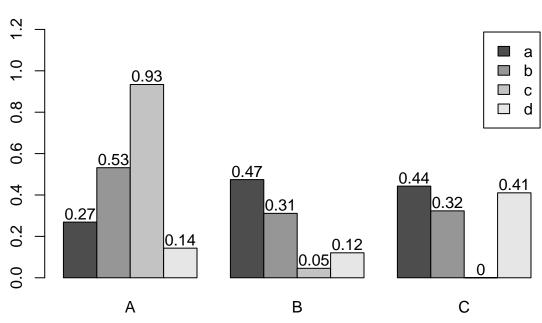
plot(y[,1], ylim=c(0,1), xlab="Measurement", ylab="Intensity", type="l", lwd=2, col=1)
for(i in 2:length(y[1,])) {
    screen(1, new=FALSE)
    plot(y[,i], ylim=c(0,1), type="l", lwd=2, col=i, xaxt="n", yaxt="n", ylab="", xlab="", main="", bty
}
```



close.screen(all=TRUE)

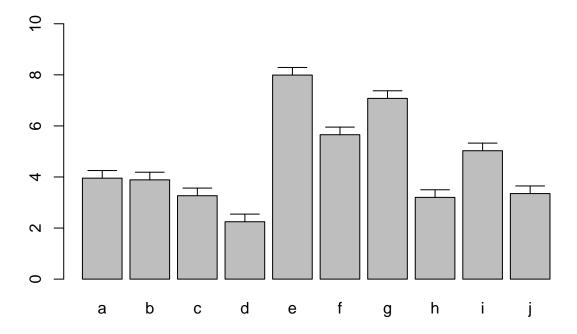
Bar Plots

Basics



Error Bars

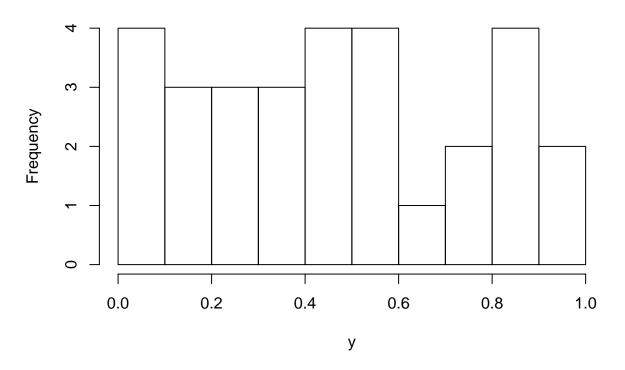
```
bar <- barplot(m <- rowMeans(y) * 10, ylim=c(0, 10))
stdev <- sd(t(y))
arrows(bar, m, bar, m + stdev, length=0.15, angle = 90)</pre>
```



Histograms

```
hist(y, freq=TRUE, breaks=10)
```

Histogram of y



Density Plots

```
plot(density(y), col="red")
```

density.default(x = y)



Pie Charts

```
pie(y[,1], col=rainbow(length(y[,1]), start=0.1, end=0.8), clockwise=TRUE)
legend("topright", legend=row.names(y), cex=1.3, bty="n", pch=15, pt.cex=1.8,
col=rainbow(length(y[,1]), start=0.1, end=0.8), ncol=1)
```



Color Selection Utilities

Default color palette and how to change it

```
palette()

## [1] "black" "red" "green3" "blue" "cyan" "magenta" "yellow" "gray"

palette(rainbow(5, start=0.1, end=0.2))
palette()

## [1] "#FF9900" "#FFBF00" "#F2FF00" "#CCFF00"

palette("default")
```

The gray function allows to select any type of gray shades by providing values from 0 to 1

```
gray(seq(0.1, 1, by= 0.2))
```

```
## [1] "#1A1A1A" "#4D4D4D" "#808080" "#B3B3B3" "#E6E6E6"
```

Color gradients with colorpanel function from gplots library'

```
library(gplots)
colorpanel(5, "darkblue", "yellow", "white")
```

```
## [1] "#00008B" "#808046" "#FFFF00" "#FFFF80" "#FFFFFF"
```

Much more on colors in R see Earl Glynn's color chart here

Saving Graphics to File

After the pdf() command all graphs are redirected to file test.pdf. Works for all common formats similarly: jpeg, png, ps, tiff, . . .

```
pdf("test.pdf")
plot(1:10, 1:10)
dev.off()
```

Generates Scalable Vector Graphics (SVG) files that can be edited in vector graphics programs, such as InkScape.

```
library("RSvgDevice")
devSVG("test.svg")
plot(1:10, 1:10)
dev.off()
```

Homework 3C

Homework 3C: Bar Plots

Analysis Routine

Overview

The following exercise introduces a variety of useful data analysis utilities in R.

Analysis Routine: Data Import

- Step 1: To get started with this exercise, direct your R session to a dedicated workshop directory and download into this directory the following sample tables. Then import the files into Excel and save them as tab delimited text files.
 - MolecularWeight_tair7.xlsTargetP_analysis_tair7.xls

Import the tables into R

Import molecular weight table

```
my_mw <- read.delim(file="MolecularWeight_tair7.xls", header=T, sep="\t")
my_mw[1:2,]</pre>
```

Import subcelluar targeting table

```
my_target <- read.delim(file="TargetP_analysis_tair7.xls", header=T, sep="\t")
my_target[1:2,]</pre>
```

Online import of molecular weight table

```
my_mw <- read.delim(file="http://faculty.ucr.edu/~tgirke/Documents/R_BioCond/Samples/MolecularWeight_ta
my_mw[1:2,]</pre>
```

```
## Sequence.id Molecular.Weight.Da. Residues
## 1 AT1G08520.1 83285 760
## 2 AT1G08530.1 27015 257
```

Online import of subcelluar targeting table

```
my_target <- read.delim(file="http://faculty.ucr.edu/~tgirke/Documents/R_BioCond/Samples/TargetP_analys
my_target[1:2,]</pre>
```

```
## GeneName Loc cTP mTP SP other
## 1 AT1G08520.1 C 0.822 0.137 0.029 0.039
## 2 AT1G08530.1 C 0.817 0.058 0.010 0.100
```

Merging Data Frames

• Step 2: Assign uniform gene ID column titles

```
colnames(my_target)[1] <- "ID"
colnames(my_mw)[1] <- "ID"</pre>
```

• Step 3: Merge the two tables based on common ID field

```
my_mw_target <- merge(my_mw, my_target, by.x="ID", by.y="ID", all.x=T)</pre>
```

• Step 4: Shorten one table before the merge and then remove the non-matching rows (NAs) in the merged file

```
my_mw_target2a <- merge(my_mw, my_target[1:40,], by.x="ID", by.y="ID", all.x=T) # To remove non-matchi my_mw_target2 <- na.omit(my_mw_target2a) # Removes rows containing "NAs" (non-matching rows).
```

- Homework 3D: How can the merge function in the previous step be executed so that only the common rows among the two data frames are returned? Prove that both methods the two step version with na.omit and your method return identical results.
- Homework 3E: Replace all NAs in the data frame my_mw_target2a with zeros.

Filtering Data

• Step 5: Retrieve all records with a value of greater than 100,000 in 'MW' column and 'C' value in 'Loc' column (targeted to chloroplast).

```
query <- my_mw_target[my_mw_target[, 2] > 100000 & my_mw_target[, 4] == "C", ]
query[1:4,]
##
                  ID Molecular. Weight. Da. Residues Loc
                                                             cTP
                                                                   mTP
                                                                           SP other
## NA
                                                  NA <NA>
                                                              NA
                                                                    NA
                                                                           NA
                                                                                 NA
                < NA >
                                        NA
## NA.1
                <NA>
                                                  NA <NA>
                                                              NA
                                                                    NA
                                                                           NA
                                        NA
                                                                                 NA
## NA.2
                <NA>
                                                  NA <NA>
                                                              NΑ
                                                                    NΑ
                                                                           NΑ
                                        NΑ
                                                                                 NA
## 219 AT1G02730.1
                                    132588
                                                1181
                                                         C 0.972 0.038 0.008 0.045
dim(query)
```

```
## [1] 1092 8
```

• Homework 3F: How many protein entries in the my_mw_target data frame have a MW of greater then 4,000 and less then 5,000. Subset the data frame accordingly and sort it by MW to check that your result is correct.

String Substitutions

• Step 6: Use a regular expression in a substitute function to generate a separate ID column that lacks the gene model extensions. <>=

```
my_mw_target3 <- data.frame(loci=gsub("\\..*", "", as.character(my_mw_target[,1]), perl = TRUE), my_mw_target3[1:3,1:8]</pre>
```

```
##
                         ID Molecular.Weight.Da. Residues Loc cTP mTP SP
## 1 AT1G01010 AT1G01010.1
                                           49426
                                                       429 <NA>
                                                                     NA NA
                                                                 NΑ
## 2 AT1G01020 AT1G01020.1
                                                                     NA NA
                                           28092
                                                       245 <NA>
                                                                 NA
## 3 AT1G01020 AT1G01020.2
                                           21711
                                                       191 <NA>
                                                                     NA NA
                                                                 NΑ
```

• Homework 3G: Retrieve those rows in my_mw_target3 where the second column contains the following identifiers: c("AT5G52930.1", "AT4G18950.1", "AT1G15385.1", "AT4G36500.1", "AT1G67530.1"). Use the %in% function for this query. As an alternative approach, assign the second column to the row index of the data frame and then perform the same query again using the row index. Explain the difference of the two methods.

Calculations on Data Frames

• Step 7: Count the number of duplicates in the loci column with the table function and append the result to the data frame with the cbind function.

```
mycounts <- table(my_mw_target3[,1])[my_mw_target3[,1]]
my_mw_target4 <- cbind(my_mw_target3, Freq=mycounts[as.character(my_mw_target3[,1])])</pre>
```

• Step 8: Perform a vectorized devision of columns 3 and 4 (average AA weight per protein)

```
data.frame(my_mw_target4, avg_AA_WT=(my_mw_target4[,3] / my_mw_target4[,4]))[1:2,5:11]
```

```
## Loc cTP mTP SP other Freq.Var1 Freq.Freq
## 1 <NA> NA NA NA NA AT1G01010 1
## 2 <NA> NA NA NA NA AT1G01020 2
```

• Step 9: Calculate for each row the mean and standard deviation across several columns

```
mymean <- apply(my_mw_target4[,6:9], 1, mean)
mystdev <- apply(my_mw_target4[,6:9], 1, sd, na.rm=TRUE)
data.frame(my_mw_target4, mean=mymean, stdev=mystdev)[1:2,5:12]</pre>
```

```
## Loc cTP mTP SP other Freq.Var1 Freq.Freq mean
## 1 <NA> NA NA NA NA AT1G01010 1 NA
## 2 <NA> NA NA NA NA AT1G01020 2 NA
```

Plotting Example

• Step 10: Generate scatter plot columns: 'MW' and 'Residues'

```
plot(my_mw_target4[1:500,3:4], col="red")
```



Export Results and Run Entire Exercise as Script

• Step 11: Write the data frame my_mw_target4 into a tab-delimited text file and inspect it in Excel.

```
write.table(my_mw_target4, file="my_file.xls", quote=F, sep="\t", col.names = NA)
```

• Homework 3H: Write all commands from this exercise into an R script named exerciseRbasics.R, or download it from here. Then execute the script with the source function like this: source("exerciseRbasics.R"). This will run all commands of this exercise and generate the corresponding output files in the current working directory.

source("exerciseRbasics.R")

R Markdown

Overview

R Markdown combines markdown (an easy to write plain text format) with embedded R code chunks. When compiling R Markdown documents, the code components can be evaluated so that both the code and its output can be included in the final document. This makes analysis reports highly reproducible by allowing to automatically regenerate them when the underlying R code or data changes. R Markdown documents (.Rmd files) can be rendered to various formats including HTML and PDF. The R code in an .Rmd document is processed by knitr, while the resulting .md file is rendered by pandoc to the final output formats (e.g. HTML or PDF). Historically, R Markdown is an extension of the older Sweave/Latex environment. Rendering of mathematical expressions and reference management is also supported by R Markdown using embedded Latex syntax and Bibtex, respectively.

Quick Start

Install R Markdown

```
install.packages("rmarkdown")
```

Initialize a new R Markdown (Rmd) script

To minimize typing, it can be helful to start with an R Markdown template and then modify it as needed. Note the file name of an R Markdown scirpt needs to have the extension .Rmd. Template files for the following examples are available here:

- R Markdown sample script: sample.Rmd
- Bibtex file for handling citations and reference section: bibtex.bib

Users want to download these files, open the sample.Rmd file with their preferred R IDE (e.g. RStudio, vim or emacs), initilize an R session and then direct their R session to the location of these two files.

Metadata section

The metadata section (YAML header) in an R Markdown script defines how it will be processed and rendered. The metadata section also includes both title, author, and date information as well as options for customizing the output format. For instance, PDF and HTML output can be defined with pdf_document and html_document, respectively. The BiocStyle:: prefix will use the formatting style of the BiocStyle package from Bioconductor.

```
title: "My First R Markdown Document"
author: "Author: First Last"
date: "Last update: 13 April, 2017"
output:
    BiocStyle::html_document:
    toc: true
    toc_depth: 3
    fig_caption: yes

fontsize: 14pt
bibliography: bibtex.bib
____
```

Render Rmd script

An R Markdown script can be evaluated and rendered with the following render command or by pressing the knit button in RStudio. The output_format argument defines the format of the output (e.g. html_document). The setting output_format="all" will generate all supported output formats. Alternatively, one can specify several output formats in the metadata section as shown in the above example.

```
rmarkdown::render("sample.Rmd", clean=TRUE, output_format="html_document")
```

The following shows two options how to run the rendering from the command-line.

```
$ echo "rmarkdown::render('sample.Rmd', clean=TRUE)" | R --slave
$ Rscript -e "rmarkdown::render('sample.Rmd', clean=TRUE)"
```

Alternatively, one can use a Makefile to evaluate and render an R Markdown script. A sample Makefile for rendering the above sample.Rmd can be downloaded here. To apply it to a custom Rmd file, one needs open the Makefile in a text editor and change the value assigned to MAIN (line 13) to the base name of the corresponding .Rmd file (e.g. assign systemPipeRNAseq if the file name is systemPipeRNAseq.Rmd). To execute the Makefile, run the following command from the command-line.

```
$ make -B
```

R code chunks

R Code Chunks can be embedded in an R Markdown script by using three backticks at the beginning of a new line along with arguments enclosed in curly braces controlling the behavior of the code. The following lines contain the plain R code. A code chunk is terminated by a new line starting with three backticks. The following shows an example of such a code chunk. Note the backslashes are not part of it. They have been added to print the code chunk syntax in this document.

The following lists the most important arguments to control the behavior of R code chunks:

- r: specifies language for code chunk, here R
- chode_chunk_name: name of code chunk; this name needs to be unique
- eval: if assigned TRUE the code will be evaluated
- warning: if assigned FALSE warnings will not be shown
- message: if assigned FALSE messages will not be shown
- cache: if assigned TRUE results will be cached to reuse in future rendering instances
- fig.height: allows to specify height of figures in inches
- fig.width: allows to specify width of figures in inches

For more details on code chunk options see here.

Learning Markdown

The basic syntax of Markdown and derivatives like kramdown is extremely easy to learn. Rather than providing another introduction on this topic, here are some useful sites for learning Markdown:

- Markdown Intro on GitHub
- Markdown Cheet Sheet
- Markdown Basics from RStudio
- R Markdown Cheat Sheet
- kramdown Syntax

Tables

There are several ways to render tables. First, they can be printed within the R code chunks. Second, much nicer formatted tables can be generated with the functions kable, pander or xtable. The following example uses kable from the knitr package.

```
library(knitr)
kable(iris[1:12,])
```

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
4.6	3.4	1.4	0.3	setosa
5.0	3.4	1.5	0.2	setosa
4.4	2.9	1.4	0.2	setosa
4.9	3.1	1.5	0.1	setosa
5.4	3.7	1.5	0.2	setosa
4.8	3.4	1.6	0.2	setosa

Figures

Plots generated by the R code chunks in an R Markdown document can be automatically inserted in the output file. The size of the figure can be controlled with the fig.height and fig.width arguments.

```
library(ggplot2)
dsmall <- diamonds[sample(nrow(diamonds), 1000), ]
ggplot(dsmall, aes(color, price/carat)) + geom_jitter(alpha = I(1 / 2), aes(color=color))</pre>
```



Sometimes it can be useful to explicitly write an image to a file and then insert that image into the final document by referencing its file name in the R Markdown source. For instance, this can be useful for time consuming analyses. The following code will generate a file named myplot.png. To insert the file in the final document, one can use standard Markdown or HTML syntax, e.g.: .

```
png("myplot.png")
ggplot(dsmall, aes(color, price/carat)) + geom_jitter(alpha = I(1 / 2), aes(color=color))
dev.off()

## pdf
## 2
```

Inline R code

To evaluate R code inline, one can enclose an R expression with a single back-tick followed by \mathbf{r} and then the actual expression. For instance, the back-ticked version of 'r 1+1' evaluates to 2 and 'r pi' evaluates to 3.1415927.

Mathematical equations

To render mathematical equations, one can use standard Latex syntax. When expressions are enclosed with single \$ signs then they will be shown inline, while enclosing them with double \$\$ signs will show them in display mode. For instance, the following Latex syntax $d(X,Y) = \sqrt{i}-y_{i}$ renders in display mode as follows:

$$d(X,Y) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

Citations and bibliographies

Citations and bibliographies can be autogenerated in R Markdown in a similar way as in Latex/Bibtex. Reference collections should be stored in a separate file in Bibtex or other supported formats. To cite a publication in an R Markdown script, one uses the syntax [@<id1>] where <id1> needs to be replaced with a reference identifier present in the Bibtex database listed in the metadata section of the R Markdown script (e.g. bibtex.bib). For instance, to cite Lawrence et al. (2013), one uses its reference identifier (e.g. Lawrence2013-kt) as <id1> (Lawrence et al. 2013). This will place the citation inline in the text and add the corresponding reference to a reference list at the end of the output document. For the latter a special section called References needs to be specified at the end of the R Markdown script. To fine control the formatting of citations and reference lists, users want to consult this the corresponding R Markdown page. Also, for general reference management and outputting references in Bibtex format Paperpile can be very helpful.

Session Info

sessionInfo()

```
## R version 3.3.3 (2017-03-06)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Ubuntu 14.04.5 LTS
##
## locale:
   [1] LC CTYPE=en US.UTF-8
##
                                   LC NUMERIC=C
                                                               LC TIME=en US.UTF-8
    [4] LC COLLATE=en US.UTF-8
                                   LC MONETARY=en US.UTF-8
                                                               LC MESSAGES=en US.UTF-8
   [7] LC_PAPER=en_US.UTF-8
##
                                    LC_NAME=C
                                                               LC_ADDRESS=C
  [10] LC_TELEPHONE=C
                                    LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
  [1] methods
##
                 stats
                           graphics utils
                                                datasets
                                                         grDevices base
##
## other attached packages:
## [1] knitr_1.14
                       gplots_3.0.1
                                        RSQLite_1.0.0
                                                        DBI_0.5-1
                                                                         ggplot2_2.1.0
                                                                                         limma_3.30.0
## [7] BiocStyle_2.2.0
##
## loaded via a namespace (and not attached):
   [1] Rcpp_0.12.7
##
                           magrittr_1.5
                                               munsell_0.4.3
                                                                   colorspace_1.2-7
                                                                                      highr_0.6
  [6] stringr_1.1.0
                           plyr 1.8.4
                                               caTools 1.17.1
                                                                   tools 3.3.3
                                                                                      grid 3.3.3
## [11] gtable_0.2.0
                           KernSmooth_2.23-15 htmltools_0.3.5
                                                                   gtools_3.5.0
                                                                                      yaml_2.1.13
## [16] assertthat_0.1
                           digest_0.6.10
                                               tibble_1.2
                                                                   formatR 1.4
                                                                                      codetools 0.2-15
                                               rmarkdown 1.1
                                                                                      gdata 2.17.0
## [21] bitops 1.0-6
                           evaluate 0.10
                                                                  labeling 0.3
                           scales 0.4.0
## [26] stringi 1.1.2
```

References

Lawrence, Michael, Wolfgang Huber, Hervé Pagès, Patrick Aboyoun, Marc Carlson, Robert Gentleman, Martin T Morgan, and Vincent J Carey. 2013. "Software for Computing and Annotating Genomic Ranges." *PLoS Comput. Biol.* 9 (8): e1003118. doi:10.1371/journal.pcbi.1003118.