Biological Computing in R: Silwood Masters (CMEE, EEC, EA, NHM)

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Chapter 0

Introduction

Donald Knuth, 1995: Science is what we understand well enough to explain to a computer. Art is everything else we do

0.1 What is this document all about?

This document contains the content of the Imperial College London Department of Life Sciences Msc/MRes Modules on Scientific Computing in R. The content will be updated over the week, with further sections and chapters added as we go along. This document is accompanied by data and code on which you can practice your skills in your own time and during the Practical sessions. these materials are available (and will be updated regularly) at: https://bitbucket.org/mhasoba/cmee2014masterepo/.

It is important that you work through the exercises and problems in each chapter/section. This document does not tell you every single thing you need to know to perform the exercises in it. In programming, you learn far more from trying to solve problems than from reading about how others have solved them — that is, you have license to google it! You will be provided guidelines for what makes good or efficient solutions. Later, when you have submitted your exercises and practicals (only relevant to the CMEEs, but the rest should have a go!), feedback will be provided on your solutions.

0.2 Outline of the this module

The content and structure of this week is geared towards the following objectives:

- Give you a introduction to R syntax and programming conventions, assuming you have never set your eyes on R or any other programming language before — we will breeze through this as you have already been introduced to R in the Stats Week!
- Teach you principles of clean and efficient programming in R, including delightful things like vectorization and debugging.
- Teach you how to generate publication quality graphics in R publication quality is thesis quality!
- Teach you how to develop reproducible data analyses "work flows" so (or anybody else) run and re-run your analyses, graphics outputs and all, in R.

You will use R a lot during the rest of your courses and probably your thesis and career — the aim is to lay down the foundations for you to become very comfortable with it!

0.3 Conventions used in this document

You will find all R commandline/console arguments, code snippets and output in colored boxes like this:

> ls()

Here > is the R prompt, and will type the commands/code that you see from this document into the R command line (or copy-paste, but not recommended!). I have aimed to make the content of this module computer platform (Mac, PC or Linux) independent because many of you are probably working (or later will be) with R on personal laptops or desktops. Indeed, platform-independence of data analyses is one of the main reasons why you are using R! Finally, note that:

* In all subsequent chapters, lines marked with a star like this are things for you to do.

0.4 A note on being organized

In this module, you will write plenty of R code, deal with different data files, and produce text and graphic outputs. Please keep all your code, data inputs and results outputs organized in separate directories named Code, Data, Results (or equivalent) respectively. The CMEEs are already implementing this along with version control in git (if you are intrigued, please look up CMEE Week 1 lectures) at https://bitbucket.org/mhasoba/cmee2014masterepo/.

Note that R, as in UNIX like systems (Mac, Linux), uses / instead of the \backslash used in Windows for directory path specification. Also, in general, we will be using relative paths throughout the exercises and practicals (more on this later).

0.5 Readings

(More will appear in different sections/chapters)

- Use the internet! Google "R tutorial", and plenty will pop up. Choose one that seems the most intuitive to you.
- Bolker, B. M.: Ecological Models and Data in R (eBook and Hardcover available).
- Beckerman, A. P. & Petchey, O. L. (2012) Getting started with R: an introduction for biologists. Oxford, Oxford University Press.
 Good, short, general introduction
- Crawley, R. (2013) The R book. 2nd edition. Chichester, Wiley.

 Excellent but enormous reference book, code and data available from www.bio.ic.ac.

 uk/research/mjcraw/therbook/index.htm

Chapter 1

Introduction to R

1.1 What is \mathbb{R} ?

R is a freely available statistical software with strong programming capabilities. R has become incredibly popular in biology due to several factors: i) many packages are available to perform all sorts of statistical and mathematical analyses; ii) it has been developed and scrutinised by top level academic statisticians; iii) it can produce beautiful, publication-quality graphics; iv) it has a very good support for matrix-algebra.

1.2 Would you ever need anything other than R?

Although we can technically program in R, the programming environment is not the greatest: especially the way types are managed is problematic (e.g., often your matrix will become a vector if it has only one column/row!), and the way errors and warnings are handled and displayed (often unintelligibly!).

Nevertheless, being able to program R means you can develop and automate your statistical analyses and the generation of figures into a reproducible work flow (there's that term again!). However, if your work also includes extensive numerical simulations, manipulation of very large matrices, bioinformatics, or complex workflows including databases, you will be much better off if you *also* know another programming language that is more versatile, computationally efficient (like python, PERL or C)).

But for most of you, R will do the job, so you may revel in that knowledge! In particular, python is recommended, as it is reasonably efficient and has very nice and clean syntax. With something like python, You can embed your R analysis work flow inside a more complex meta-workflow, for example, one that includes interfacing with the internet, manipulating/querying databases, and compiling Lagrange Lagrange and compiling co

1.3 Installing R

Linux/Ubuntu: run the following in terminal

\$ sudo apt-get install r-base r-base-dev

Mac OS X: download and install from

http://cran.r-project.org/bin/macosx/

Windows: download and install from

http://cran.r-project.org/bin/windows/base/

1.4 Getting started

Launch R (From Applications menu on Window or Mac, from terminal in Linux/Ubuntu) — it should look something like this (on Linux/Ubuntu or Mac terminal):

```
mhasoba@mhasoba-cha-lyaptop:~
mhasoba@mhasoba-cha-lyaptop:~$ R

R version 3.1.1 (2014-07-10) -- "Sock it to Me"
Copyright (C) 2014 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

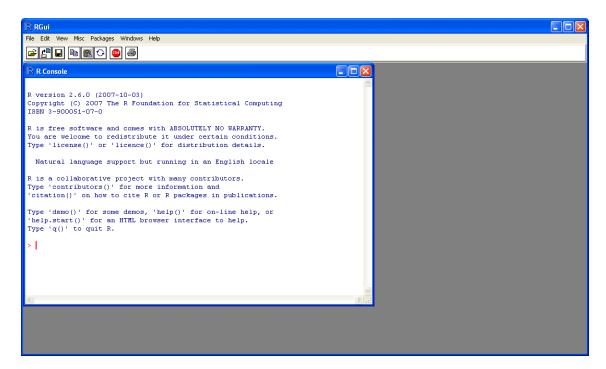
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.
```

Or like this (Windows "console", similar in Mac):



You can also use an IDE (Interactive Development Environment) that can offer delights like syntax highlighting (google it!), such as RStudio, geany, vim, etc.

1.5 Useful R commands

```
ls()
                   list all the variables in the work space
rm('a', 'b')
                   remove variable(s) a and b
rm(list=ls())
                   remove all variable(s)
getwd()
                   get current working directory
setwd('Path')
                   set working directory to Path
q()
                   quit R
                   show the documentation of Command
?Command
                   search the all packages/functions with Keyword, "fuzzy search"
??Keyword
```

1.6 Some Basics

Try out the following in the R console:

```
> a <- 4  # assignment
> a
[1] 4
> a*a  # product
[1] 16
> a_squared <- a*a
> sqrt(a_squared)  # square root
[1] 4
> v <- c(0, 1, 2, 3, 4)  # c: "concatenate"</pre>
```

c () (concatenate) is one of the most commonly used functions — Dont forget it! (try ?c) Note that any text after a "#" is ignored by R — handy for commenting. In general, please comment your code and scripts, for *everybody's* sake!

```
> v # Display the vector variable you created
[1] 0 1 2 3 4
> is.vector(v) # check if it's a vector
[1] TRUE
> mean(v) # mean
[1] 2
> var(v) # variance
[1] 2.5
> median(v) # median
[1] 2
> sum(v) # sum all elements
[1] 10
> prod(v + 1) # multiply
[1] 120
> length(v) # length of vector
[1] 5
```

1.6.1 Variable names and Tabbing

```
> wing.width.cm <- 1.2 #Using dot notation
> wing.length.cm <- c(4.7, 5.2, 4.8)</pre>
```

Using tabbing with dot notation can be handy. Type:

```
> wing.
```

And then hit the tab key. This is handy, but good style and readability is more important than just convenient variable names. Variable names should be as obvious as possible, not over-long!

1.6.2 R likes E Notation

```
> 1E4

[1] 10000

> 1e4

[1] 10000

> 5e-2

[1] 0.05
```

R uses *E* notation to print very large or small numbers:

```
> 1E4 ^ 2
[1] 1e+08
> 1 / 3 / 1e8
[1] 3.333333e-09
```

1.6.3 Operators

The usual operators are available in R (slight differences from python):

```
Addition
              Subtraction
              Multiplication
              Division
              Power
              Modulo
응응
응/응
              Integer division
              Equals
==
              Differs
              Greater
>
              Greater or equal
>=
              Logical and
&
              Logical or
              Logical not
```

1.7 Sequences

The: operator creates vectors of sequential integers:

```
> years <- 1990:2009
> years
[1] 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999
[11] 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009

> years <- 2009:1990 # or in reverse order
> years
[1] 2009 2008 2007 2006 2005 2004 2003 2002 2001 2000
[11] 1999 1998 1997 1996 1995 1994 1993 1992 1991 1990
```

For sequences of fractional numbers, you have to use seq():

```
> seq(1, 10, 0.5)
[1] 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0
[16] 8.5 9.0 9.5 10.0
```

You can also seq(from=1, to=10, by=0.5) OR seq(from=1, by=0.5, to=10) with the same effect (try it) — this explicit, "argument matching" approach is partly why R is so popular.

1.8 Strings and Pasting

R's string handling ain't elegant or pretty (unlike python!), but it works:

```
> species.name <- "Quercus robur" #double quotes
> species.name
[1] "Quercus robur"
> species.name <- 'Fraxinus excelsior' #single quotes
> species.name
[1] "Fraxinus excelsior"
> paste("Quercus", "robur")
[1] "Quercus robur"
> paste("Quercus", "robur", sep = "") #Get rid of space
"Quercusrobur"
> paste("Quercus", "robur", sep = ", ") #insert comma to separate
```

And as is the case with so many R functions, pasting works on vectors:

```
> paste('Year is:', 1990:2000)

[1] "Year is: 1990" "Year is: 1991" "Year is: 1992" "Year is: 1993"

[5] "Year is: 1994" "Year is: 1995" "Year is: 1996" "Year is: 1997"

[9] "Year is: 1998" "Year is: 1999" "Year is: 2000"
```

Note that this last example creates a vector of 11 strings.

1.9 Indices and Indexing

Every element of a vector in R has an order: the first value, second, third, etc. To illustrate this, type:

```
> MyVar <- c('a', 'b', 'c', 'd', 'e') # create a simple vector
```

Then, square brackets extract values based on their position in the order:

```
> MyVar[1] # Show element in first position
[1] "a"
> MyVar[4]
[1] "d" # Show element in fourth position
```

The values in square brackets are called "indices" — they give the index (position) of the required value. We can also select sets of values in different orders, or repeat values:

```
> MyVar[c(3,2,1)] # reverse order
[1] "c" "b" "a"
MyVar[c(1,1,5,5)] # repeat indices
[1] "a" "a" "e" "e"
```

So you can manipulate vectors by indexing:

```
> v <- c(0, 1, 2, 3, 4) # Re-create the vector variable v 
> v[3] # access one element 
[1] 2 
> v[1:3] # access sequential elements 
[1] 0 1 2 
> v[-3] # remove elements 
[1] 0 1 3 4 
> v[c(1, 4)] # access non-sequential 
[1] 0 3
```

1.10 Basic vector-matrix operations

```
> v2 <- v
> v2 <- v2*2 # whole-vector operation
[1] 0 2 4 6 8
> v * v2 # product element-wise
[1] 0 2 8 18 32
> t(v) # transpose the vector
[,1] [,2] [,3] [,4] [,5]
      0
> v %*% t(v) # matrix/vector product
[,1] [,2] [,3] [,4] [,5]
[1,]
      0
          0
[2,] 0 1 2
                    3 4
[3,] 0 2 4 6 8
[4,] 0 3 6 9 12
[5,] 0 4 8 12 16
> v3 <- 1:7 # assign using sequence
> v3
[1] 1 2 3 4 5 6 7
> v4 <- c(v2, v3) # concatenate vectors
> v4
[1] 0 2 4 6 8 1 2 3 4 5 6 7
> q() # quit
```

1.11 Data types

Like python (why python? Ask the CMEEs!), R comes with data-types. Mastering these will help you write better, more efficient programs and also handle diverse between datasets. Now get back into R (if you quit R using q()), and type:

1.11.1 Vectors

```
> a <- 5
> is.vector(a)
[1] TRUE
```

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```
> v1 <- c(0.02, 0.5, 1)
> v2 <- c("a", "bc", "def", "ghij")
> v3 <- c(TRUE, TRUE, FALSE)
```

1.11.2 Matrices and arrays

R has many functions to manipulate matrices (two-dimensional vectors) and arrays (multi-dimensional vectors).

```
> m1 <- matrix(1:25, 5, 5)
> m1
[,1] [,2] [,3] [,4] [,5]
         6 11
[1,]
     1
                  16
                        21
      2
              12
                   17
                        22
[2,]
[3,]
              13
                   18
                        23
[4,]
     4 9
             14 19
                        24
[5,] 5 10 15
                  20
                        25
> m1 <- matrix(1:25, 5, 5, byrow=TRUE)
> m1
[,1] [,2] [,3] [,4] [,5]
                  4
[1,] 1 2 3
                        5
          7
      6
               8
                   9
                        10
[2,]
         12
[3,] 11
              13
                   14
                        15
     16
         17
              18
                   19
                        20
[4,]
         22 23
[5,]
     21
                  24
> dim(m1)
[1] 5 5
> m1[1,2]
[1] 2
> m1[1,2:4]
[1] 2 3 4
> m1[1:2,2:4]
[,1] [,2] [,3]
[1,] 2 3
[2,] 7 8
> arr1 <- array(1:50, c(5, 5, 2))
> arr1
[,1] [,2] [,3] [,4] [,5]
[1,] 1 6 11
                   16
                        21
     2 7
             12
                   17
                        22
[2,]
                  18
[3,] 3 8 13
                        23
    4 9
5 10
                   19
[4,]
              14
                        24
[5,]
               15
                  20
, , 2
[,1] [,2] [,3] [,4] [,5]
[1,]
      26
          31
               36
                   41
                        46
               37
      27
          32
[2,]
                   42
                        47
[3,]
      28
          33
              38
                  43
                        48
[4,]
     29
          34
               39
                  44
                        49
[5,]
     30
         35
               40
                   45
                        50
```

1.11.3 Data frames

This is a very important data type that is peculiar to R. It is great for storing your data. Basically, it's a two-dimensional table in which each column can contain a different data type (e.g., numbers, strings, boolean). You can think of a dataframe as a spreadsheet. Data frames are great for plotting your data, performing regressions and such. Later (Chapter 2) you will see that fancy plotting using gaplot demands the use of dataframes. Now try the following:

```
> Col1 <- 1:10
> Col1
[1] 1 2 3 4 5 6 7 8 9 10
> Col2 <- LETTERS[1:10]
> Co12
 [1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J"
> Col3 <- runif(10) # 10 random num. from uniform</pre>
 [1] 0.29109 0.91495 0.64962 0.95503 0.26589 0.02482 0.59718
 [8] 0.99134 0.98786 0.86168
> MyDF <- data.frame(Col1, Col2, Col3)</pre>
> MyDF
Coll Col2
              Col3
    1 A 0.2910981
     2 B 0.9149558
    3 C 0.6496248
    4 D 0.9550331
5
    5 E 0.2658936
    6 F 0.0248217
7
     7 G 0.5971868
    8 н 0.9913407
8
9 9 I 0.9878679
10 10 J 0.8616854
> names(MyDF) <- c("A.name", "another", "another.one")</pre>
> MyDF
A.name another another.one
    1 A 0.2910981
2 B 0.9149558
       3
               C 0.6496248
3
              D 0.9550331
            E 0.2658936
F 0.0248217
G 0.5971868
H 0.9913407
      5
5
      6
6
7
      7
      8
              I 0.9878679
      9
     10 J 0.8616854
10
> MyDF$A.name
[1] 1 2 3 4 5 6 7 8 9 10
> MyDF[,1]
[1] 1 2 3 4 5 6 7 8 9 10
> MyDF[c("A.name", "another")]
A.name another
      1
            A
               В
3
       3
               С
4
       4
               D
5
       5
               Ε
               F
8
       8
               Н
9
       9
               I
10
      10
               J
```

1.11.4 Lists

A list is simply an ordered collection of objects (that can be other variables) (a bit like python lists!). You can build lists of lists too.

```
> 11 <- list(names=c("Fred","Bob"), ages=c(42, 77, 13, 91))
> 11
$names
[1] "Fred" "Bob"

$ages
[1] 42 77 13 91

> 11[[1]]
[1] "Fred" "Bob"
> 11[[2]]
[1] 42 77 13 91

> 11[["ages"]]
[1] 42 77 13 91
> 11$ages
[1] 42 77 13 91
```

1.12 The Working Directory

Before we go any further, let's get ourselves organized. In R, type:

```
> getwd()
```

This tells you what the current "working directory" is.

In using R for an analysis, you will likely use and create several files. This means that it is sensible to create a folder (directory) to keep all code files together. You can then set R to work from this directory, so that files are easy to find and run — this will be your working directory. So now do the following:

- * Create a directory called Week5 in an appropriate location (For CMEEs, in CMEECourseWork for others, some place you can remember!
- \star Create subdirectories within CMEECourseWork/Week5 called Code, Data, and Results You can create directories using dir.create() within R

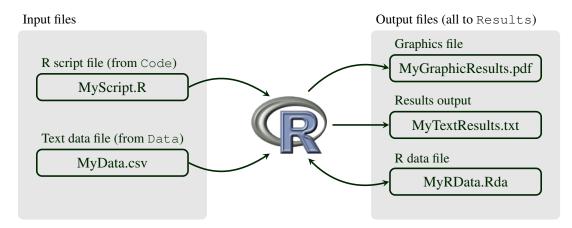
Use relative paths Using relative paths in in your R scripts and code will make your code computer independent and your life better! For example, in R, ../Data/mydata.txt specifies a file named mydata.txt located in the "parent" of the current directory. Now, set the working directory to be Week5/Code:

```
> setwd("FullPathUptoHere/Week5/Code")
> dir()
```

Note that FullPathUptoHere is not to be taken literally and entered! For example, if you created Week5 in H:, you would use setwd(\H:/MyICStatsModules/Code")
For CMEE, it would be setwd(\FullPathUptoHere/CMEECourseWork/Week5/Code")

1.13 The R analysis workflow

Your typical R analysis workflow will be as follows:



Some details on each kind of file:

R script files These are plain text files containing all the R code needed for an analysis. These should always be created with a simple text editor like Notepad (Windows), TextEdit (MacOS) or Geany (Linux) and saved with the extension *.R. We will use the built-in editor in R in this class. Alternatively, if RStudio is a good option because it also works across platforms. Try it. A big advantage of something like RStudio is that you will get syntax highlighting, which is very handy and will make R programming far more convenient and error-free. You should *never* use Word to save or edit these files as R can only read code from plain text files.

Text data files These are files of data in plain text format containing one or more columns of data (numbers, strings, or both). Although there are several format options, we will tyoucally be using csv files, where the entries are separated by commas. These are easy to create and export from Excel (if that's what you use...).¹

Results output files These are a plain text files contain your results, such the summary of output of a regression or ANOVA analysis. Typically, you will putput your results in a table format where the columns are separated by commas (csv) or tabs (tab-delimited)

Graphics files R can export graphics in a wide range of formats. This can be done automatically from R code and we will look at this later but you can also select a graphics window and click 'File ▷ Save as...'

Rdata files You can save any data loaded or created in R, including model outputs and other things, into a singleRdata file. These are not plain text and can only be read by R, but can hold all the data from an analysis in a single handy location. I never use these, but you can, if you want.

¹If you are using a computer from elsewhere in the EU, Excel may use a comma ($\pi = 3,1416$) instead of a decimal point ($\pi = 3.1416$). In this case, *csv* files may use a semi-colon to separate columns and you can use the alternative function *read.csv2()* to read them into R.

1.14 Importing and Exporting Data

Now we are ready to see how to import and export data in R, typically the first step of your analysis. The best option is to have your data in a comma separated value text file or in a tab separated file. Then, you can use the function read.csv (or read.table) to import your data (note the relative paths!):

```
> MyData <- read.csv("../Data/trees.csv")
> head(MyData) # Have a quick look at the data frame
> str(MyData) # Have a quick look at the column types
> MyData <- read.csv("../Data/trees.csv", header = TRUE) # with headers
> MyData <- read.table("../Data/trees.csv", sep = ',',
header = TRUE) # A more general way
> head(MyData)
> MyData <- read.csv("../Data/trees.csv", skip = 5) # skip first 5 lines</pre>
```

Note that the resulting MyData in your workspace is a R dataframe. You can also save your data frames using write.table or write.csv:

```
> write.csv(MyData, "../Results/MyData.csv")
> dir("../Results/") # Check if it worked
> write.table(MyData[1,], file = "../Results/MyData.csv", append=TRUE) # append
> write.csv(MyData, "../Results/MyData.csv", row.names=TRUE) # write row names
> write.table(MyData, "../Results/MyData.csv", col.names=FALSE) # ignore col names
```

1.15 Control statements

In R, you can write if, then, else statements, and for and while loops like any programming language. However, loops are slow in R, so use them sparingly.

* Type the following in a script file called control.R (save it in your Code directory)

```
## If statement
  a <- TRUE
 if (a == TRUE) {
      print ("a is TRUE")
  } else {
      print ("a is FALSE")
  ## On a single line
  z <- runif(1) ##random number</pre>
 if (z \le 0.5) {
  print ("Less than a quarter") }
  ## For loop using a sequence
  for (i in 1:100) {
15
      j <- i * i
      print(paste(i, " squared is", j ))
17
  ## For loop over vector of strings
 for (species in c ('Heliodoxa rubinoides',
                    'Boissonneaua jardini',
                    'Sula nebouxii'))
23
   print(paste('The species is', species))
```

```
## for loop using a vector
v1 <- c("a","bc","def")
for (i in v1) {
    print(i)
    }

## While loop
i <- 0
while (i<100) {
    i <- i+1
    print(i^2)
}
</pre>
```

1.16 Running R code

You can run the code you wrote in blocks to test and understand it:

* Place the cursor on the first line of code and run it by pressing the keyboard shortcut (PC: ctrl+R, Mac: command+enter, Linux: ctrl+enter if you are using geany).

Of course, you write code so that you can just "run" it, which runs your full analysis and outputs all the results. The way to run \star . R script/code from the command line is to source it. This causes R to accept code input from a named file and run it:

```
> source("control.R") # Assuming you are in Code directory!
```

Note that you will need to add the directory path to the file name (control.R in the above example), if the file is not in your working directory. For example, ../Code/control.R if you are in, say, Data.

1.17 Type Conversion and Special Values

There are different kinds of data variable types such as integer, float (including real numbers), and string (e.g., text words). Beware of the difference between NA (Not Available) and NaN (Not a Number).

```
> as.integer(3.1)
[1] 3
> as.real(4)
[1] 4
> as.roman(155)
[1] CLV
> as.character(155)
[1] "155"
> as.logical(5)
[1] TRUE
> as.logical(0)
[1] FALSE
> b <- NA
> is.na(b)
[1] TRUE
> b < - 0./0.
> b
[1] NaN
```

```
> is.nan(b)
[1] TRUE
> b <- 5/0
> b
[1] Inf
> is.nan(b)
[1] FALSE
> is.infinite(b)
[1] TRUE
> is.finite(b)
[1] TRUE
> is.finite(b)
[1] FALSE
```

1.18 Writing Functions

R lets you write your own functions. The syntax is quite simple, with each function accepting arguments and returning a value:

```
MyFunction <- function(Arg1, Arg2) {

## statements involving Arg1, Arg2

return (ReturnValue)

7 }</pre>
```

* Type the following in a script file called TreeHeight.R, save it in your Code directory and run it using source:

```
This function calculates heights of trees
 # from the angle of elevation and the distance
  # from the base using the trigonometric formula
4 # height = distance * tan(radians)
 # Arguments:
 8
  # The height of the tree, same units as "distance"
12
  TreeHeight <- function(degrees, distance)</pre>
14
   radians <- degrees * pi / 180
   height <- distance * tan(radians)</pre>
16
   print(paste("Tree height is:", height))
   return (height)
18
20
  TreeHeight (37, 40)
```

1.19 Practical 2.1

Modify the script TreeHeight . R so that it does the following:

- * Loads trees.csv and calculates tree heights for all trees in the data. Note that the distances have been measured in meters. (Hint: use relative paths))
- * Creates a csv output file called TreeHts.csv in Results that contains the calculated tree heights along with the original data in the following format (only first two rows and headers shown):

```
"Species", "Distance.m", "Angle.degrees", "Tree.Height.m"

"Populus tremula", 31.6658337740228, 41.2826361937914, 25.462680727681

"Quercus robur", 45.984992608428, 44.5359166583512, 46.094124200205
```

1.20 Useful R Functions

Mathematical

```
log(x)
                 Natural logarithm
                 Logarithm in base 10
log10(x)
exp(x)
                 Absolute value
abs(x)
                 Largest integer < x
floor(x)
                 Smallest integer > x
ceiling(x)
                 \pi
рi
                 \sqrt{x}
sqrt(x)
                 Sinus function
sin(x)
```

Strings

```
strsplit(x,';')
nchar(x)
toupper(x)
tolower(x)
paste(x1,x2,sep=';')
Split the string according to ';'
Number of characters
Set to upper case
Set to lower case
Join the strings inserting ';'
```

Statistical

mean(x)	Compute mean (of a vector or matrix)
sd(x)	Standard deviation
var(x)	Variance
median(x)	Median
quantile $(x, 0.05)$	Compute the 0.05 quantile
range(x)	Range of the data
min(x)	Minimum
max(x)	Maximum
sum(x)	Sum all elements

Random number distributions

Draw 10 normal random numbers with mean 0 and s.d. 1
Density function
Cumulative density function
Twenty random numbers from uniform [0,2]
Twenty random numbers from $Poisson(\lambda)$

1.21 Vectorize it!

R is very slow at running cycles (for and while loops). This is because R is a "nimble" language: at execution time R does not know what you'are going to perform until it "reads" the code

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to perform. Compiled languages such as \mathbb{C} , know exactly what the flow of the program is, as the code is compiled before execution. As a metaphor, \mathbb{C} is a musician playing a score she has seen before – optimizing each passage, while R is playing it "a prima vista" (i.e., at first sight).

Hence, in R you should try to avoid loops like the plague. In practical terms, sometimes it is much easier to throw in a for loop, and then optimize the code to avoid the loop if the running time is not satisfactory. R has several functions that can operate on entire vectors and matrices.

* For example, type (save in Code) in Vectorize1.R and run it (it sums all elements of a matrix):

```
M <- matrix(runif(1000000),1000,1000)

SumAllElements <- function(M) {
    Dimensions <- dim(M)

    Tot <- 0
    for (i in 1:Dimensions[1]) {
        for (j in 1:Dimensions[2]) {
            Tot <- Tot + M[i,j]
        }
    }

return (Tot)
}

## This on my computer takes about 1 sec
print(system.time(SumAllElements(M)))
## While this takes about 0.01 sec
print(system.time(sum(M)))</pre>
```

Both approaches are correct, and will give you the right answer. However, one is 100 times faster than the other!

Fortunately, R offers several ways of avoiding loops. Here are the main ones:

```
# applying the same function to rows/colums of a matrix
  ## Build a random matrix
 M <- matrix(rnorm(100), 10, 10)</pre>
  ## Take the mean of each row
 RowMeans <- apply(M, 1, mean)</pre>
  print (RowMeans)
  ## Now the variance
  RowVars <- apply(M, 1, var)</pre>
 print (RowVars)
  ## By column
 ColMeans <- apply(M, 2, mean)</pre>
13
  print (ColMeans)
15
  ## You can use it to define your own functions
 ## (What does this function do?)
  SomeOperation <- function(v) {</pre>
   if (sum(v) > 0){
19
      return (v * 100)
21
    return (v)
23
  print (apply(M, 1, SomeOperation))
25
  ## by:
27 ## apply the function to a dataframe, using some factor
```

```
## to define the subsets
29
  ## import some data
31
  attach(iris)
  print (iris)
  ## use colMeans (as it is better for dataframes)
35 by(iris[,1:2], iris$Species, colMeans)
  by(iris[,1:2], iris$Petal.Width, colMeans)
37
  ## There are many other methods: lapply, sapply, eapply, etc.
39 ## Each is best for a given data type (lapply -> lists)
41 ## replicate:
  ## this is quite useful to avoid a loop for function that typically
43 ## involve random number generation
  print(replicate(10, runif(5)))
```

1.22 Practical 2.2

Non-CMEE students can ignore this one!

The Ricker model is a classic discrete population model which was introduced in 1954 by Ricker to model recruitment of stock in fisheries. It gives the expected number (or density) N_{t+1} of individuals in generation t+1 as a function of the number of individuals in the previous generation t:

$$N_{t+1} = N_t e^{r\left(1 - \frac{N_t}{k}\right)} \tag{1.1}$$

Here r is intrinsic growth rate and k as the carrying capacity of the environment. Try this script that runs it:

```
Ricker <- function(N0=1, r=1, K=10, generations=50)

{
    # Runs a simulation of the ricker model
    # Returns a vector of length generations

6    N <- rep(NA, generations)  # Creates a vector of NA

8    N[1] <- N0
    for (t in 2:generations)

10    {
        N[t] <- N[t-1] * exp(r*(1.0-(N[t-1]/K)))

12    }
    return (N)

14 }

plot(Ricker(generations=10), type="l")</pre>
```

Now open and run the script Vectorize2.R (available on the bitbucket Git repository). This is the stochastic Ricker model (compare with the above script to see where the stochasticity (random error) enters. Now modify the script to complete the exercise given. CMEEs, As always, bring your functional code and data under version control!

1.23 Packages

The main strength of R is that users can easily build packages and share them through cran. r-project.org. There are packages to do most statistical and mathematical analysis you

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might conceive, so check them out before reinventing the wheel! Visit cran.r-project.org and go to Packages to see a list and a brief description. To install a package, within R type install.packages() and choose the package to install.

1.24 Readings

- The Use R! series (the yellow books) by Springer are really good. In particular, consider: "A Beginner's Guide to R", "R by Example", "Numerical Ecology With R", "ggplot2" (we'll see this in Chapter 2), "A Primer of Ecology with R", "Nonlinear Regression with R", "Analysis of Phylogenetics and Evolution with R".
- For more focus on dynamical models: Soetaert & Herman. 2009 "A practical guide to ecological modelling: using R as a simulation platform".
- There are excellent websites besides cran. In particular, check out www.statmethods.net and http://en.wikibooks.org/wiki/R_Programming.

Chapter 2

Plotting and graphics in R

2.1 Basic plotting

R can produce beautiful graphics, without the time consuming and fiddly methods that you might have used in Excel or equivalent (it's not you, it's Excel!). Later, you can explore how the package ggplot2, can allow the rapid creation of truly elegant publication-grade graphics. However, in many cases you just want to quickly plot the data for exploratory analysis of your data. Here are the basic plotting commands:

plot(x,y) Scatterplot

plot $(y \sim x)$ Scatterplot with y as a response variable

hist(mydata) Histogram barplot(mydata) Bar plot

points (y1~x1) Add another series of points

boxplot $(y \sim x)$ Boxplot

Let's try some basic plotting. As a case study, we will use a simplified version of a dataset on predator-prey body mass ratios taken from the Ecological Archives of the ESA (Barnes *et al.* 2008, Ecology 89:881).



These data should be in your Data directory. Let's import the data:

```
> MyDF <- read.csv(".../Data/EcolArchives-E089-51-D1.csv")</pre>
> dim(MyDF)
[1] 34931
> MyDF$
MyDF$Record.number
                                   MyDF$Predator.mass
MyDF$In.refID
                                   MyDF$Prey
MyDF$IndividualID
                                   MyDF$Prey.common.name
MyDF$Predator
                                  MyDF$Prey.taxon
MyDF$Predator.common.name
                                  MyDF$Prey.mass
MyDF$Predator.taxon
                                   MyDF$Prey.mass.unit
MyDF$Predator.lifestage
                                   MyDF$Location
MyDF$Type.of.feeding.interaction
```

2.1.1 Scatter Plot

Let's start by plotting Predator mass vs. Prey mass:

```
> plot(MyDF$Predator.mass,MyDF$Prey.mass)
```

That doesn't look very nice! Let's try taking logarithms (why?).

```
> plot(log(MyDF$Predator.mass),log(MyDF$Prey.mass))
```

We can change almost any aspect of the resulting graph; lets change the symbols by specifying the plot characters using pch:

2.1.2 Histograms

Now plot a histogram of Predator body masses:

2.1.3 Subplots

We can also plot both predator and prey body masses in different sub-plots using par

2.1.4 Overlaying plots

Better still, we would like to see if the predator mass and prey mass distributions are similar by overlaying them.

2.1.5 Exercise

We can do a lot more beautification! As an exercise, try adjusting the bin widths to make them same for the predator and prey, and making the x and y labels larger and in boldface.

2.1.6 Saving your graphics

And you can also save the figure in a vector graphics format (important to learn to do this!). PDF is a good option:

```
> pdf("../Results/Pred_Prey_Overlay.pdf", # Open blank pdf page
    11.7, 8.3) # These numbers are page dimensions in inches
> hist(log(MyDF$Predator.mass), # Plot predator histogram (note 'rgb')
    xlab="Body Mass (kg)", ylab="Count",
    col = rgb(1, 0, 0, 0.5),
    main = "Overlay")
> hist(log(MyDF$Prey.mass), # Plot prey weights
    col = rgb(0, 0, 1, 0.5),
    add = T) # Add to same plot = TRUE
> legend('topleft',c('Predators','Prey'), # Add legend
    fill=c(rgb(1, 0, 0, 0.5), rgb(0, 0, 1, 0.5)))
> dev.off()
```

You can also try other graphic output formats. For example, png () (a raster format) instead of pdf ().

2.1.7 Boxplots

Now, let's try plotting boxplots instead of histograms. These are useful for getting a visual summary of your data (note that we are using a \sim symbol though it may not appear so):

```
> boxplot(log(MyDF$Predator.mass) ~ MyDF$Location, # Why the tilde?
xlab = "Location", ylab = "Predator Mass",
main = "Predator mass by location")
```

That's a lot of locations! Let's try boxplots by feeding interaction type:

```
> boxplot(log(MyDF$Predator.mass) ~ MyDF$Type.of.feeding.interaction,
xlab = "Location", ylab = "Predator Mass",
main = "Predator mass by feeding interaction type")
```

2.1.8 Practical 3.1

You can also make lattice graphs to avoid the somewhat laborious par () approach above. For this, you will need:

```
> library(lattice)
```

A lattice plot of the above data for predator mass could look like Fig. 2.1: This was generated using (and printing to a pdf with particular dimensions):

```
> densityplot(~log(Predator.mass) | Type.of.feeding.interaction, data=MyDF)
```

Look up http://www.statmethods.net/advgraphs/trellis.html and the lattice package help.

In this practical, you will write script that draws and save three lattice graphs by feeding interaction type: one of predator mass , one of prey mass and one of the size ratio of prey mass over predator mass. Note that you would want to use logarithms of masses (or mass-ratios) for all three plots. In additon, the script will calculate the mean and median predator, prey and predator-prey size-ratios to a csv file. The workflow would be:

* Write a script file called PP_Lattice and save it in the Code directory — sourcing or running this script should result in three files called Pred_Lattice.pdf, Prey_Lattice.pdf, and SizeRatio_Lattice.pdf being saved in the Results directory (the names are self-explanatory, I hope).

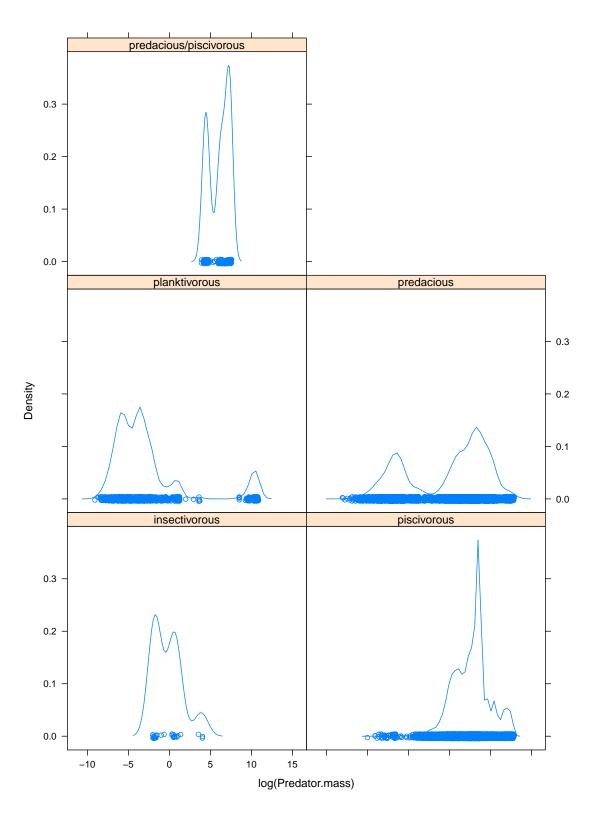


Figure 2.1: Write a script that generates this figure.

- * In addition, the script should calculate the mean log predator mass, prey mass, and predatorprey size ratio, and save it as a single csv output table called PP_Results.csv to the Results directory. The table should have appropriate headers (e.g.,). (Hint: you will have to initialize a new dataframe in the script to first store the calculations)
- * The script should be self-sufficient and not need any external inputs it should import the above predator-prey dataset from the appropriate directory, and save the graphic plots to the appropriate directory (Hint: use relative paths).

2.2 Publication-quality figures in R

R can produce beautiful graphics, but it takes a lot of work to obtain the desired result. This is because the starting point is pretty much a "bare" plot, and adding features commonly required for publication-grade figures (legends, statistics, regressions, etc.) can be quite involved. Moreover, it is very difficult to switch from one representation of the data to another (i.e., from boxplots to scatterplots), or to plot several dataset together. To overcome these issues, the R package ggplot2 is very powerful. It can can be used to produce truly high-quality graphics for papers, theses and reports.

ggplot2 differs from other approaches as it attempts to provide a "grammar" for graphics in which each layer is the equivalent of a verb, subject etc. and a plot is the equivalent of a sentence. All graphs start with a layer showing the data, other layers and commands are added to modify the plot.

For a complete reference, please see the book "ggplot2: Elegant Graphics for Data Analysis", by H. Wickham. Also, a great resource is represented by the website ggplot2.org. To install ggplot2, open a session of R and type (launch R using sudo R) in Linux first):

```
> install.packages("ggplot2")
> install.packages("reshape") #A handy additional package
```

2.2.1 Basic graphs with aplot

qplot stands for quick plot, and is the basic plotting function provided by ggplot2. It can be used to quickly produce graphics for exploratory data analysis, and as a base for more complex graphics.

In ggplot2, it is very important to use data frames to store the data. Again we can start plotting the Predator.mass vs Prey.mass.

```
> require(ggplot2) ## Load the package
Loading required package: ggplot2
> qplot(Prey.mass, Predator.mass, data = MyDF)
```

This graph is very basic. Let's transform everything in logarithms:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF)
```

Now, color the points according to the type of feeding interaction:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
colour = Type.of.feeding.interaction)
```

The same as above, but changing the shape:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
shape = Type.of.feeding.interaction)
```

To manually set a color or a shape, you have to use I () (meaning "Identity"):

```
> qplot(log(Prey.mass), log(Predator.mass),
data = MyDF, colour = I("red"))
> qplot(log(Prey.mass), log(Predator.mass),
data = MyDF, shape= I(3))
```

Because there are so many points, we can make them semi-transparent:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
colour = Type.of.feeding.interaction, alpha = I(1/5))
```

Now add a smoother to the points.

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
geom = c("point", "smooth"))
```

If we want to have a linear regression, we can specify the method 1m:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
geom = c("point", "smooth"), method = "lm")
```

We can add a smoother for each type of interaction:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
geom = c("point", "smooth"), method = "lm",
colour = Type.of.feeding.interaction)
```

To extend the lines to the full range, use fullrange = TRUE:

```
> qplot(log(Prey.mass), log(Predator.mass), data = MyDF,
geom = c("point", "smooth"), method = "lm",
colour = Type.of.feeding.interaction,
fullrange = TRUE)
```

Now we want to see how the ratio between prey and predator mass changes according to the type of interaction:

```
> qplot(Type.of.feeding.interaction,
log(Prey.mass/Predator.mass), data = MyDF)
```

Because there are so many points, we can "jitter" them to get a better idea of the spread:

```
> qplot(Type.of.feeding.interaction,
log(Prey.mass/Predator.mass), data = MyDF,
geom = "jitter")
```

Or we can draw a boxplot of the data:

```
> qplot(Type.of.feeding.interaction,
log(Prey.mass/Predator.mass), data = MyDF,
geom = "boxplot")
```

Let's draw an histogram of predator-prey mass ratios:

```
> qplot(log(Prey.mass/Predator.mass), data = MyDF,
geom = "histogram")
```

Color the histogram according to the interaction type:

```
> qplot(log(Prey.mass/Predator.mass), data = MyDF,
geom = "histogram", fill = Type.of.feeding.interaction)
```

To make it easier to read, we can plot the smoothed density of the data:

```
> qplot(log(Prey.mass/Predator.mass), data = MyDF,
geom = "density", fill = Type.of.feeding.interaction)
```

Using colour instead of fill draws only the edge of the curve:

```
> qplot(log(Prey.mass/Predator.mass), data = MyDF,
geom = "density", colour = Type.of.feeding.interaction)
```

Similarly, geom = \bar" produces a barplot, geom = \line" a series of points joined by a line, etc.

An alternative way of displaying data belonging to different classes is the so-called "faceting". A simple example:

```
> qplot(log(Prey.mass/Predator.mass),
facets = Type.of.feeding.interaction ~ .,
data = MyDF, geom = "density")
```

A more elegant way of drawing logarithmic quantities is to set the logarithm for the axes:

```
> qplot(Prey.mass, Predator.mass, data = MyDF, log="xy")
```

Let's add a title and labels:

```
> qplot(Prey.mass, Predator.mass, data = MyDF, log="xy",
main = "Relation between predator and prey mass",
xlab = "Prey mass (g)",
ylab = "Predator mass (g)")
```

Adding + theme_bw () makes it suitable for black and white printing.

```
> qplot(Prey.mass, Predator.mass, data = MyDF, log="xy",
main = "Relation between predator and prey mass",
xlab = "Prey mass (g)",
ylab = "Predator mass (g)") + theme_bw()
```

Finally, let's save a pdf file of the figure.

2.3. VARIOUS GEOM 29

```
> pdf("MyFirst-ggplot2-Figure.pdf")
> print(qplot(Prey.mass, Predator.mass, data = MyDF,log="xy",
main = "Relation between predator and prey mass",
xlab = "Prey mass (g)",
ylab = "Predator mass (g)") + theme_bw())
> dev.off()
```

Adding the command print ensures that the whole command is kept together and that you can use the command in a script.

Other important options to keep in mind:

```
xlim limits for x axis: xlim = c(0,12).
ylim limits for y axis.
log log transform variable log = \x", log = \y", log = \xy".
main title of the plot main = \My Graph".
xlab x-axis label.
ylab y-axis label.
asp aspect ratio asp = 2, asp = 0.5.
margins whether or not margins will be displayed.
```

2.3 Various geom

Try the following:

```
1 # load the package
  require(ggplot2)
  # load the data
 MyDF <- as.data.frame(</pre>
   read.csv("../Data/EcolArchives-E089-51-D1.csv"))
  # barplot
  qplot (Predator.lifestage,
       data = MyDF, geom = "bar")
11
  # boxplot
  qplot(Predator.lifestage, log(Prey.mass),
13
        data = MyDF, geom = "boxplot")
  # density
  qplot(log(Predator.mass),
        data = MyDF, geom = "density")
19
  # histogram
 qplot(log(Predator.mass),
21
        data = MyDF, geom = "histogram")
  # scatterplot
25 qplot(log(Predator.mass), log(Prey.mass),
        data = MyDF, geom = "point")
```

2.4 Exercise

Write a script called Prob-9-1. R that draws a pdf file of Figure 2.4.

2.5 Advanced plotting: ggplot

The command qplot allows you to use only a single dataset and a single set of "aesthetics" (x, y, etc.). To make full use of gqplot2, we need to use the command gqplot. We need:

- The data to be plotted, in a data frame;
- Aesthetics mappings, specifying which variables we want to plot, and how;
- The geom, defining how to draw the data;
- (Optionally) some stat that transform the data or perform statistics using the data.

To start a graph, we can specify the data and the aesthetics:

```
> p <- ggplot(MyDF, aes(x = log(Predator.mass),
y = log(Prey.mass),
colour = Type.of.feeding.interaction ))</pre>
```

Now try to plot the graph:

```
> p
Error: No layers in plot
```

In fact, we have to specify a geometry in order to see the graph:

```
> p + geom_point()
```

We can use the "plus" sign to concatenate different commands:

```
> p <- ggplot(MyDF, aes(x = log(Predator.mass),
y = log(Prey.mass),
colour = Type.of.feeding.interaction ))
> q <- p + geom_point(size=I(2), shape=I(10)) + theme_bw()
> q
```

Let's remove the legend:

```
> q + opts(legend.position = "none")
```

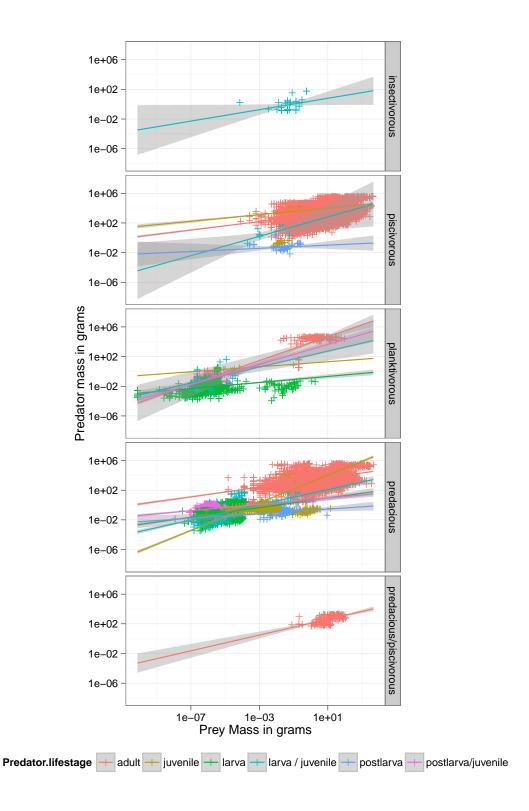


Figure 2.2: Write a script that generates this figure.

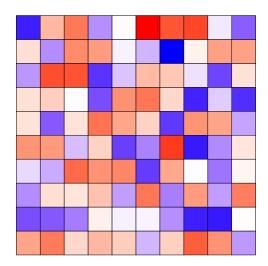


Figure 2.3: Random matrix with values sampled from uniform distribution.

2.6 Case study 1: plotting a matrix

In this section we will plot a matrix of random values taken from a normal distribution $\mathscr{U}[0,1]$. Our goal is to produce the plot in Figure 2.3. Because we want to plot a matrix, and ggplot2 accepts only dataframes, we use the package reshape that can "melt" a matrix into a dataframe:

```
require(ggplot2)
require(reshape)
GenerateMatrix <- function(N) {</pre>
M \leftarrow matrix(runif(N * N), N, N)
return(M)
> M <- GenerateMatrix(10)
> M[1:3, 1:3]
[,1] [,2]
                   [,3]
[1,] 0.2700254 0.8686728 0.7365857
[2,] 0.1744879 0.8488169 0.4165879
[3,] 0.3980783 0.7727821 0.4271121
> Melt <- melt(M)
> Melt[1:4,]
X1 X2
        value
  1 1 0.2700254
  2 1 0.1744879
  3 1 0.3980783
4 4 1 0.3196671
> ggplot(Melt, aes(X1, X2, fill = value)) + geom_tile()
# adding a black line dividing cells
> p <- ggplot(Melt, aes(X1, X2, fill = value))</pre>
```

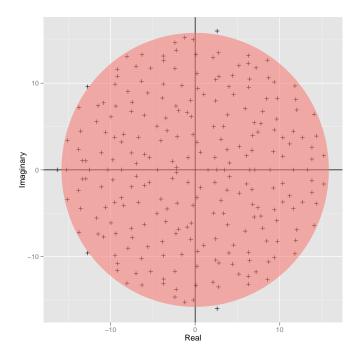


Figure 2.4: Girko's circular law.

```
> p <- p + geom_tile(colour = "black")</pre>
# removing the legend
  q <- p + opts(legend.position = "none")
# removing all the rest
> q <- p + opts(legend.position = "none",</pre>
panel.background = theme_blank(),
axis.ticks = theme_blank(),
panel.grid.major=theme_blank(),
panel.grid.minor=theme_blank(),
axis.text.x = theme_blank(),
axis.title.x=theme_blank(),
 axis.text.y = theme_blank(),
axis.title.y=theme_blank())
# exploring the colors
> q + scale_fill_continuous(low = "yellow",
high = "darkgreen")
> q + scale_fill_gradient2()
> q + scale_fill_gradientn(colours = grey.colors(10))
> q + scale_fill_gradientn(colours = rainbow(10))
 q + scale_fill_gradientn(colours =
c("red", "white", "blue"))
```

2.7 Case study 2: plotting two dataframes

According to Girko's circular law, the eigenvalues of a matrix M of size $N \times N$ are approximately contained in a circle in the complex plane with radius \sqrt{N} . We are going to draw a simulation displaying this result (Figure 2.4).

```
require(ggplot2)
  # function that returns an ellipse
  build_ellipse <- function(hradius, vradius){</pre>
   npoints = 250
    a \leftarrow seq(0, 2 * pi, length = npoints + 1)
   x <- hradius * cos(a)
    y <- vradius * sin(a)
    return (data.frame (x = x, y = y))
11
  # Size of the matrix
13 N <- 250
  # Build the matrix
15 M <- matrix(rnorm(N * N), N, N)</pre>
  # Find the eigenvalues
eigvals <- eigen(M) $values</pre>
  # Build a dataframe
19 eigDF <- data.frame("Real" = Re(eigvals),</pre>
                        "Imaginary" = Im(eigvals))
21
  # The radius of the circle is sqrt(N)
23 my_radius <- sqrt(N)
  # Ellipse dataframe
25 ellDF <- build_ellipse(my_radius, my_radius)</pre>
  # rename the columns
27 names(ellDF) <- c("Real", "Imaginary")</pre>
29 # Now the plotting:
  # plot the eigenvalues
31 p <- ggplot(eigDF, aes(x = Real, y = Imaginary))</pre>
  p <- p +
   geom_point(shape = I(3)) +
    opts(legend.position = "none")
35
37 # now add the vertical and horizontal line
  p <- p + geom_hline(aes(intercept = 0))</pre>
39 p <- p + geom_vline(aes(intercept = 0))</pre>
41 # finally, add the ellipse
  p <- p + geom_polygon(data = ellDF,</pre>
43
                          aes(x = Real,
                              y = Imaginary,
                               alpha = 1/20,
45
                              fill = "red"))
47 pdf ("Girko.pdf")
  print(p)
49 dev.off()
```

2.8 Case study 3: annotating the plot

In the plot in Figure 2.5, we use the geometry "text" to annotate the plot.

```
require(ggplot2)

filename <- "Results.txt"
```

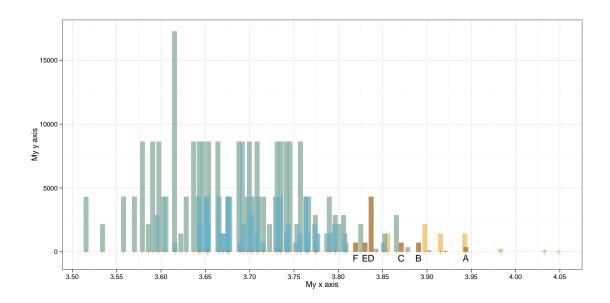


Figure 2.5: Overlay of three lineranges and a text geometry.

```
4 a <- read.table(filename, header = TRUE)</pre>
  # here's how the data looks like
 print(a[1:3,])
  print(a[90:95,])
  # append a col of zeros
10 a$ymin <- rep(0, dim(a)[1])</pre>
# print the first linerange
  p <- ggplot(a)
p <- p + geom_linerange(data = a, aes(</pre>
                              x = x,
                              ymin = ymin,
16
                              ymax = y1,
18
                              size = (0.5)
                              ),
                            colour = "#E69F00",
20
                            alpha = 1/2, show_guide = FALSE)
22
  # print the second linerange
  p <- p + geom_linerange(data = a, aes(</pre>
24
                              x = x,
                              ymin = ymin,
26
                              ymax = y2,
                              size = (0.5)
28
                              ),
                            colour = "#56B4E9",
30
                            alpha = 1/2, show_guide = FALSE)
32
  # print the third linerange
 p <- p + geom_linerange(data = a, aes(</pre>
34
                              x = x,
                              ymin = ymin,
36
                              ymax = y3,
                              size = (0.5)
38
```

```
colour = "#D55E00",
40
                           alpha = 1/2, show_guide = FALSE)
42
  # annotate the plot with labels
p \leftarrow p + geom_text(data = a,
                      aes (x = x, y = -500, label = Label))
  # now set the axis labels,
48 # remove the legend, prepare for bw printing
  p <- p + scale_x_continuous("My x axis",</pre>
                               breaks = seq(3, 5, by = 0.05)
50
    scale_y_continuous("My y axis") + theme_bw() +
52
    opts(legend.position = "none")
54
56 # Finally, print in a pdf
  pdf("MyBars.pdf", width = 12, height = 6)
58 print (p)
  dev.off()
```

2.9 Case study 4: mathematical display

In Figure 2.6, you can see the mathematical annotation of the axis and on the plot.

```
require(ggplot2)
  # create an "ideal" linear regression data!
4 \times - seq(0, 100, by = 0.1)
  y < -4. + 0.25 * x +
   rnorm(length(x), mean = 0., sd = 2.5)
  # now a dataframe
  my_data <- data.frame(x = x, y = y)
  # perform a linear regression
my_lm <- summary(lm(y ~ x, data = my_data))</pre>
14 # plot the data
  p \leftarrow ggplot(my_data, aes(x = x, y = y,
16
                            colour = abs(my_lm$residual))
   geom_point() +
18
    scale_colour_gradient(low = "black", high = "red") +
   opts(legend.position = "none") +
20
    scale_x_continuous(
     expression(alpha^2 * pi / beta * sqrt(Theta)))
24 # add the regression line
  p <- p + geom_abline(</pre>
   intercept = my_lm$coefficients[1][1],
   slope = my_lm$coefficients[2][1],
  colour = "red")
28
  # throw some math on the plot
30 p \leftarrow p + geom_text(aes(x = 60, y = 0,
                         label = "sqrt(alpha) * 2* pi"),
                          parse = TRUE, size = 6,
32
                          colour = "blue")
```

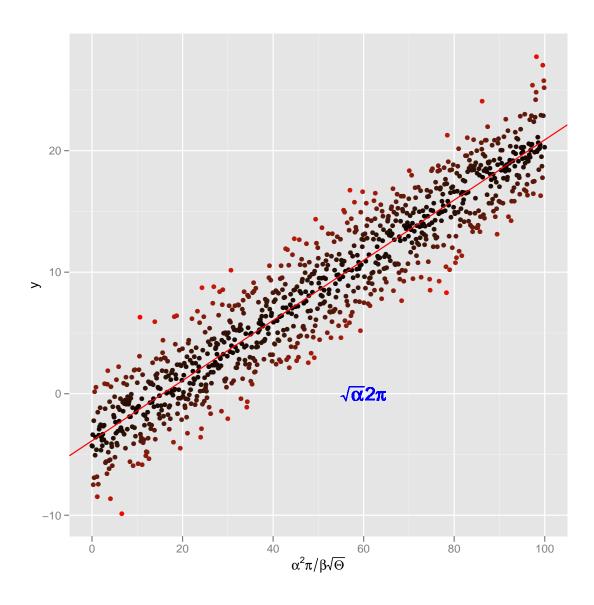


Figure 2.6: Linear regression with colors expressing residuals and mathematical annotations.

```
# print in a pdf
pdf("MyLinReg.pdf")
print(p)
dev.off()
```

2.10 Readings

- The classic Tufte www.edwardtufte.com/tufte/books_vdqi (btw, check out what Tufte thinks of PowerPoint!)

 Available in the Central Library, I have also added extracts and a related book in pdf (on Blackboard)
- Rolandi et al. "A Brief Guide to Designing Effective Figures for the Scientific Paper", doi:10.1002/adma.201102518 (on Blackboard)
- Lauren et al. "Graphs, Tables, and Figures in Scientific Publications: The Good, the Bad, and How Not to Be the Latter", doi:10.1016/j.jhsa.2011.12.041 (on Blackboard)
- Effective scientific illustrations: www.labtimes.org/labtimes/issues/lt2008/lt05/lt_2008_05_52_53.pdf (on Blackboard)
- https://web.archive.org/web/20120310121708/http://addictedtor.free.fr/graphiques/thumbs.php
- Make xkcd style graphs in R: http://xkcd.r-forge.r-project.org/