Scientific Programming with R

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September 22, 2020

Books and online help

- Introductory Statistics with `R` (Springer, Dalgaard).
- A first course in statistical programming with `R` (CUP, Braun and Murdoch).
- Computational Genome Analysis: An Introduction (Springer, Deonier, Tavaré and Waterman).
- `S` programming (Springer, Venables and Ripley).
- `R` programming for Bioinformatics (CRC Press, Gentleman).
- Scientific programming and simulation using `R` (CRC, Jones, Maillardet and Robinson).
- The art of R programming (No Starch Press, Matloff).
- Writing Scientific Software (WSS) (CUP, Oliveira and Stewart).
- `www.r-project.org`, `www.rseek.org`, `www.r-bloggers.com`
- `R` -help mailing list.

- Eglen (2009) `http://www.ploscompbiol.org/doi/pcbi.1000482`

Aims of course

This course aims to teach `R` as a general-purpose programming language. Issues specific to Computational Biology (e.g. Bioconductor packages) are covered in other course modules.

In part 1, topics to be mastered in this course include:

- Interactive use of `R` .
- Basic data types: `vector`, `matrix`, `list`, `data.frame`, `factor`, `character`.
- Writing scripts.
- Graphical facilities.
- Writing your own functions.
- File input/output.
- Control-flow statements, looping.
- Vectorization.
- Numerics issues.
- Debugging.

Part 2: Scientific computing issues

In part 2 of the course[1], we will explore various other topics, building on core knowledge of `R` .

- Numerical integration
- Phase plane analysis
- Handling large files/data bases
- String processing (e.g. for genomic data)
- Advanced graphing / presenting results
- Reproducible research
- Future directions (`R` and generally)
- (Object-oriented programming)
- (Package development)
- (`R` profiling)

[1]tentative

Outline

Scientific programming/software

- Different from software engineering (but should try to adhere to SE best practice, of course).
- Moving target.
- Domain scientists write the code (some argue this is a weakness).
- Has of course to be accurate, user-friendly (no GUI vs CLI ranting here), usable and useful, flexible, efficient and open, owned by the community, facilitate reproducible research.
- Contribute to users education (i.e not be a black box), in terms data requirements, the data processing and result interpret.
  Importance of documentation.

See Gentleman et al. `http://genomebiology.com/2004/5/10/R80` for an example of successful scientific software.

Trustworthy software

The complexity of the data processes and of the computations applied to them mean that those who receive the results of modern data analysis have limited opportunity to verify the results by direct observation. Users of the analysis have no option but to trust the analysis, and by extension the software that produced it. Both the data analyst and the software provider therefore have a strong responsibility to produce a result that is trustworthy, and, if possible, one that can be *shown* to be trustworthy.

This places an obligation on all creators of software to program in such a way that the computations can be understood and trusted.

John M. Chambers, *Software for Data Analysis* (Springer)

What is R ?

- Statistical computing environment, and programming language.
- Very popular in many areas of statistics, computational biology.
- "Programming with data" (Chambers)
- Approach: command-line for one-liners; interactive usage; write scripts/functions for larger work (edit/run cycle); develop package for consolidation and distribution.

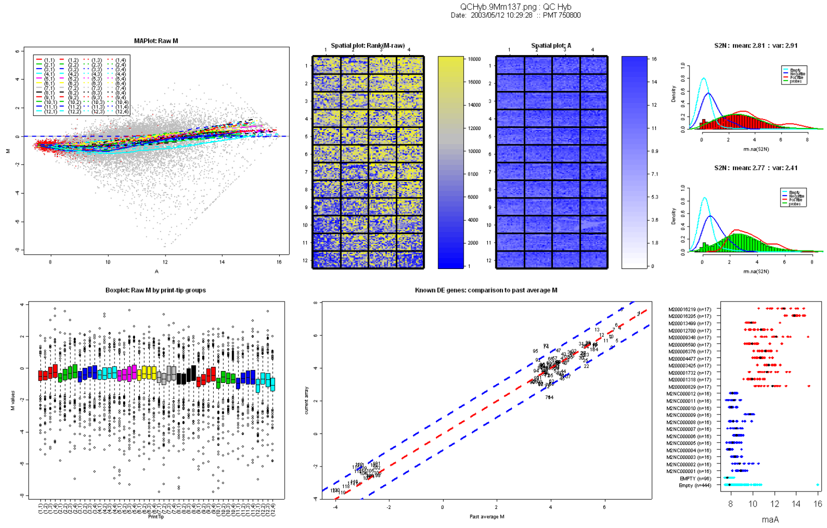
History

- `S` language came from Bell Labs (Becker, Chambers and Wilks). Commercial version S-plus (1988).
- `R` emerged as a combination of `S` and Scheme: Ross Ihaka and Robert Gentleman (NZ).
- 1993: first announcement.
- 1995: 0.60 release, now under GPL.
- 2020-09-18: release 4.0.2. Stable, multi-platform. Major release every April.
- R-core now 20 people, key researchers in field, including John Chambers. https://www.r-project.org/contributors.html

Strengths of R

- Freely available (under GPL) on many platforms.
- Excellent development team with yearly release cycle.
- Source always available to examine/edit.
- Fast for vectorized calculations.
- Foreign-language interface (C/Fortran) when speed crucial, or for interfacing with existing code.
- Good collection of numerical/statistical routines.
- Comprehensive R Archive Network (CRAN) $\sim$ 16,332 packages [2020-09-18] (cf 1000 in April 2007).
- On-line doc, with examples.
- High-quality graphics (pdf, postscript, quartz, x11, bitmaps). Often used just for plotting . . .

Graphics example



Jean YH Yang; gpQuality

http://bioinf.wehi.edu.au/marray/ibc2004/lect1b-quality.pdf

Weaknesses of R

- Loops are slow. Learn how to vectorize solutions.
- No fast compiler yet, and unlikely to happen due to nature of language. Byte compiler available in **compiler** package.
- No (decent) endorsed GUI built-in to R . Tk is available within base R , and packages for other graphical tooklits (e.g. Gtk2, Qt) are also available.
  "Programming Graphical User Interfaces with R ", M. F. Lawrence and J. Verzani

Brief comparison to matlab

- Flexible language, similar to matlab, but definitely not "everything is a matrix". Frames, lists, vectors . . .
- From matlab to `R` : `http://cran.r-project.org/doc/contrib/R-and-octave.txt`
- Comprehensive matlab and `R` guide: `http://www.math.umaine.edu/faculty/hiebeler/comp/matlabR.html`
- Use `x[i]` not `x(i)` for indexing vectors.
- Making vectors: `x <- c(10, 9, 5, 1)`
- Assignment: advised to use `<-` rather than `=`.

Using R

- Start-up: type 'R' at command line.
- Type commands interactively, and get results.
- Type commands into a file; source('myfile.R'); edit file ...
- Mac/Win has a GUI for interactive use, with internal editors.
- All platforms have a command-line interface
- Many external editors have support for R , including
    - Emacs through ESS (`http://ess.r-project.org`),
    - Eclipse IDE (`http://www.walware.de/goto/statet`),
    - Rstudio (`http://www.rstudio.org`),
    - Jupyter (https://irkernel.github.io/)
    - ...

My very first R session

```r
x <- rnorm(50, mean=4)
x
mean(x)
range(x)
hist(x)
## check help -- how to change title?
?hist
hist(x, main="my first plot")
q()
```

Interacting with `R`

- Can use up/down arrow keys to go through command history. Within a command, use left/right arrow keys to edit.
- History can be saved over sessions (`?history`).
- Multiple commands can be put onto one line, using `;` as separator between lines, e.g. `x<-10; y<-3; a <- 5`.
- `TAB` can do object/file completion.

Objects and Functions

`R` manipulates objects. Each object has a name and a type (`vector`, `matrix`, `list`, `...`)
Name of an object: letters (upper/lower case are distinct), digits, period. Start with a letter.
Objects set by way of assignment. Use the `<-` assignment operator rather than = wherever possible. (Does `i = i+1` make sense?)

Objects and Functions

```
> x <- 200
> half.x <- x/2
> threshold <- 95.0
> age <- c(15, 19, 30)
> age[2]       ## [] for accessing element.

[1] 19

> length(age) ## () for calling function.

[1] 3
```

What's up with the assignment and underscore? (Advanced)

Historically, underscore was used in `S` for assignment (because an old system keyboard had a key equivalent to the ASCII underscore that generated a back arrow). Hence underscore was not used within variables.
More recently, = is now available as an assignment operator (similar to languages like `C`), but is frowned upon as it can be confusing.
What does `i = i+1` imply mathematically?
Better to stick to `i <- i + 1` and use equals just within calls to functions, e.g. `runif(max=3)`.
Note also that assignments return values:

```
> y <- 1 + ( x <- 9 )
> a <- b <- 0
```

http://developer.r-project.org/equalAssign.html

Outline

Vectors

Vectors are a fundamental object for `R` . Scalars are treated as vector of length 1.

```
> y <- c(10, 20, 40)
> y[2]

[1] 20

> length(y)

[1] 3

> x <- 5
> length(x)

[1] 1
```

Vectors

Some operations work element by element, others on the whole vector, compare:

```
> y <- c(20, 49, 16, 60, 100)
> min(y)

[1] 16

> range(y)

[1]  16 100

> sqrt(y)

[1]  4.472136  7.000000  4.000000  7.745967 10.000000

> log(y)

[1] 2.995732 3.891820 2.772589 4.094345 4.605170
```

Generating vectors

Many short hand methods for regular sequences; `c()` for irregular.

```
> x <- seq(from=1, to=9, by=2)
> y <- seq(from=2, by=7, length=3)
> z <- 4:8
> a <- seq.int(5)  ## fast for integers
> b <- c(3, 9, 2)
> d <- c(a, 10, b)
> e <- rep( c(1,2), 3)
> f <- integer(7)
```

Accessing and setting elements

```
> x <- seq(from=100, by=1, length=20)
> x[3]         ## just element 3.

[1] 102

> x[c(12,14)] ## element 12 and 14

[1] 111 113

> x[1:5]

[1] 100 101 102 103 104

> bad <- 1:4
> x[-bad]      ## exclude elements

 [1] 104 105 106 107 108 109 110 111 112 113 114 115 116 117
[15] 118 119
```

Accessing and setting elements

Can also provide a logical vector of same length as vector (logical values explained later).

```
> x <- c(5, 2, 9, 4)
> v <- c(TRUE, FALSE, FALSE, TRUE)
> x[v]

[1] 5 4
```

Accessing and setting elements

Elements can be set in several ways

```
> x <- rep(0,10)
> x[1:3] <- 2
> x[5:6] <- c(-5, NA)
> x[7:10] <- c(1,9) ## recycling.
```

Recycling rule (Advanced)

Recycling is convenient, but dangerous; when vectors are of different lengths, the shorter one is often recycled to make a vector of the same length.

```
> a <- c(1,5) + 2
> x <- c(1,2); y <- c(5,3,9,2)
> x + y

[1]  6  5 10  4

> x + c(y,1)  ## odd recycling, warning.

Warning in x + c(y, 1):  longer object length is not a
multiple of shorter object length

[1]  6  5 10  4  2
```

Recycling rule (Advanced)

```
> x <- 1:10
> y <- x * 2
> z <- x^2
> y + z
> x + 1:2
> x + 1:3
```

Recycling rule (Advanced)

```
> x <- 1:10
> y <- x * 2
> z <- x^2
> y + z

 [1]   3   8  15  24  35  48  63  80  99 120

> x + 1:2

 [1]  2  4  4  6  6  8  8 10 10 12

> x + 1:3

Warning in x + 1:3:  longer object length is not a multiple
of shorter object length

 [1]  2  4  6  5  7  9  8 10 12 11
```

Naming indexes of a vector

```
> joe <- c(24, 1.70)
> joe

[1] 24.0  1.7

> names(joe)

NULL

> names(joe) <- c("age", "height") ## replacement function
> joe

   age height
  24.0    1.7
```

Naming indexes of a vector

```
> joe["height"] == joe[2]

height
  TRUE
```

Refering to index by name rather than by position can make code more readable, and flexible. Cannot do things like `x[1:4]` easily though, since you need to name all four elements you want.
Although extremly useful, names have a cost when processing large objects.

Note: in second use of `names()` above, we are actually using the *replacement function* `names<-`, see later.

Common functions for vectors

- `length()`
- `rev()`
- `sum()`, `cumsum()`, `prod()`, `cumprod()`
- `mean()`, `sd()`, `var()`, `median()`
- `min()`, `max()`, `range()`, `summary()`
- `exp()`, `log()`, `sin()`, `cos()`, `tan()` (radians, not degrees)
- `round()`, `ceiling()`, `floor()`, `signif()`
- `sort()`, `order()`, `rank()`
- `which()`, `which.max()`
- `any()`, `all()`

Functions as function args

Functions can be called within function calls; the following are equivalent:

```
> x <- c(3, 2, 9, 4)
>
> y <- exp(x); z1 <- which(y > 20) ## case 1
> z2 <- which ( exp(x) > 20)       ## case 2
>
> all.equal(z1, z2)

[1] TRUE
```

Outline

Default values for function arguments

A function will error if not all required arguments are provided. Some functions have both required and optional arguments. If the optional arguments are not provided, they are either ignored, or they take a default value.

```
Usage:
     round(x, digits = 0)
```

Default values for function arguments

```
> x <- c(2.091, 4.126, 7.925)
> round()         ## required arg is missing

Error in eval(expr, envir, enclos):  0 arguments passed to
'round' which requires 1 or 2 arguments

> round(x)

[1] 2 4 8

> round(x, digits = 2)

[1] 2.09 4.13 7.92
```

Let's see how this works in more detail.

Argument matching

R has a flexible method for specifying arguments to function. We can either provide an actual value for a formal argument, or give arguments as key=value (or formal=actual).
As an example, let's look at help for seq:

```
seq(from = 1, to = 1, by = ((to - from)/(length.out - 1)),
    length.out = NULL, along.with = NULL, ...)
```

(NB: in seq(from=x), from is the **formal argument** of the function, and here x is the actual value.)

The ... notation allows for other arguments to be passed, which are not used by this function.

Argument matching

Typical calls are as follows:

```
> seq(1, 3, 0.5)         ## positional matching
[1] 1.0 1.5 2.0 2.5 3.0
> seq(1, 5,length.out=3) ## can skip args (e.g. by)
[1] 1 3 5
> seq(to=5)              ## order not important.
[1] 1 2 3 4 5
> seq(f=5,t=1)           ## abbrev tags.
[1] 5 4 3 2 1
> seq(len=5, 1,2)        ## tags removed before positional matching
[1] 1.00 1.25 1.50 1.75 2.00
```

. . . in function calls (Advanced)

Why do some functions, like `sqrt`, require only one argument, yet others take many arguments?
Functions like `c`, `cbind`, have `...` in the arguments:

```
Usage:

     c(..., recursive=FALSE)

Arguments:

     ...: objects to be concatenated.
```

The `...` indicate any number of objects may be passed, not just (say) one or two.
The result of `c()` is to combine them all into one long vector, taking into account if the keyword “recursive” is provided (when args are first flattened).
The `...` can also indicate that other arguments can be provided which are not processed directly by this function, but may be useful for other functions (e.g. popular when plotting).

Replacement functions (Advanced)

```
> x <- 1:5
> x

[1] 1 2 3 4 5

> length(x)

[1] 5

> length(x) <- 2
> x

[1] 1 2
```

Replacement functions (Advanced)

Normally `length(x)` would return a value, rather than you assigning a value to the function! These are **replacement functions**, see help page:

```
Usage:

     length(x)
     length(x) <- value
```

Getting help: key commands

- `help(hist)` to see help file (or `?hist`).
- `args(hist)` to see arguments of a function.
- `example(boxplot)` run examples in help page.
- `options(help_type="html")` will then use web-browser for help.
- `help.search("histogram")`
- `demo()` to list all demos, e.g. `demo(graphics)`

NB: In the `R` terminal `?command` works as shorthand for `help("command")` except for a small number of commands, e.g. `if`, `while`. Use the longhand for these.

Help pages

- What you can expect to find:
  - Description – one line summary
  - Usage – formal arguments
  - Arguments – interpretation of arguments
  - Details – what the function does
  - Value – return value.
  - References – documentation
  - See also – helps you find related pages
  - Examples – guaranteed to run: `example(hist)`

Numbers and special values

- `numeric` (floating-point, double): 12, 4.92, 1.5e3 – `is.numeric()` (integers converted to f.p.)
- `integers` 1L – `is.integer()`
- `complex`: 3+2i – `is.complex()`

```
> typeof(1)

[1] "double"

> typeof(1L)

[1] "integer"

> is.integer(1)

[1] FALSE

> is.integer(1L)

[1] TRUE
```

Numbers and special values

Special values:

- `NA`: not available. (Often used to represent missing data point) – `is.na()`
- `NaN`: not a number. e.g. $0/0$ – `is.nan()`
- `Inf`, `-Inf`: $\pm\infty$ – `is.finite()`

You will also meet:

- `NULL`: often, list of zero length – `is.null()`

Numbers and special values

```
> typeof(NA)

[1] "logical"

> typeof(NaN)

[1] "double"

> typeof(Inf)

[1] "double"

> typeof(NULL)

[1] "NULL"
```

Operator precedence ?Syntax

```
> 3 * 4 + 2 != 3 * (4 + 2)
> 2^3+1  != 2^(3+1)
> 1:5-1
```

Operator precedence ?Syntax

```
> 3 * 4 + 2 != 3 * (4 + 2)
[1] TRUE
> 2^3+1  != 2^(3+1)
[1] TRUE
> 1:5-1
[1] 0 1 2 3 4
```

Operator precedence ?Syntax

Subset taken from `?Syntax`, see that page for full list. Highest precedence at top.

`'[ [['`	`indexing`
`'$ @'`	`component / slot extraction`
`'^'`	`exponentiation (right to left)`
`'- +'`	`unary minus and plus`
`':'`	`sequence operator`
`'%any%'`	`special operators`
`'* /'`	`multiply, divide`
`'+ -'`	`(binary) add, subtract`
`'< > <= >= == !='`	`ordering and comparison`
`'!'`	`negation`
`'&  &&'`	`and`
`'| ||'`	`or`
`'<- <<-'`	`assignment (right to left)`
`'?'`	`help (unary and binary)`

Bottom line: use parentheses to order preference.

Operators

Most operators will be familiar, but some may not:

```
x <- 10
x == 4      ## test for equality
x != 10     ## not equal?
7 %/% 2     ## division, ignoring remainder. (3)
7 %% 2      ## remainder (1)
x <- 9      ## assignment
x <<- 9     ## assign x to 9 in the global env. (BAD)
## Raising to a power can be done in two ways.
all.equal( 10.1 ** 2.5, 10.1^2.5 )
```

When things go wrong

Syntax errors are those where you've just made a typing mistake.
Logical errors are harder to find!

Common problems:

- missing close bracket leads to continuation line.

  ```
  > x <- (1 + (2 * 3)
  +
  ```

  Hit `Ctrl C` (below) or keep typing!
- too many parens:

  ```
  2 + (2*3))
  ```

- wrong/mismatched brackets (see next slide).
- Likewise, do not mix double quotes and single quotes.
  (Unless you need to quote within quotes.)
- ...
- wrong variable name (not syntax error)
- When things seem to take too long, try `C-c` [Ctrl and C, together]

Types of parentheses

- `f(3,4)` – call the function `f`, with `arg1=3`, `arg2=4`.
- `a + (b*c)` – use to enforce order over which statements are executed.
- `{ expr1; expr2; ...; exprn }` – group a set of expressions into one compound expression. Value returned is value of last expression; used in looping/conditionals.
- `x[4]` – get the 4^{th} element of the vector `x`.
- `l[[3]]` – get the 3^{rd} element of some list `l`, and return it. (compare with `l[3]` which returns a list with just the 3^{rd} element inside – will see `list` objects later).

From interactive to source files

- Typing in commands interactively is good for one-liners, but soon you will want to switch to putting your sequence of commands into a script file, and then ask R to run (source) those commands.
- This leaves to a rapid edit–run–edit cycle.
- e.g. type these commands into a file trig.R:

```r
x <- seq(from=0, to=2*pi, length=100)
y <- sin(x)
z <- cos(2*x)
z ## will not appear when source'd
print(y[1:10]) ## should use print()
plot(x, y, type='l')
lines(x, z, type='l', col='red')
```

- Eval within R using source('trig.R').

Outline

Scripts

- Use `source('trig.R', echo=TRUE)` to see commands and output. Or use `print(x)` to print an object within a script.
- Keep your code open in the editor in one window, and keep `R` running in another window.
- Are you in the right directory? Check that you can see your script file in the same directory as where `R` is currently. Check `dir()`, and `setwd`, see later.
- On unix, the initial directory is the directory from where you started `R` . On windows, the initial directory might be "My Documents". You may need to change directory (`setwd`) first.
- Use a good editor that helps you spot mistakes (e.g. paren matching, syntax highlighting). Examples: Emacs/ESS, gedit, Rstudio.
- Use `.R` or `.r` as the filename suffix. Avoid any temptation to put spaces (although `R` does not mind) in your filenames!

Why are scripts a good thing?

- You don't have to remember what commands you ran, they are saved in the file.
- This corresponds to the "source is real" philosophy of using `S` and `R` .
- You can easily give your work to others, by passing them the file.
- You can eventually run your scripts in BATCH, i.e. non-interactively. Good for long jobs which you can leave overnight.

Running scripts in batch (Advanced)

- At the command line, type `R CMD BATCH trig.R`. `R` will start up, process your commands and then quit.
- Output is stored in the file trig.Rout
- If there were no errors, the last line of the output file shows the time taken to run the script.
- Any output is not shown on the screen but sent to a PDF called `Rplots.pdf`.
- This is a GREAT way of testing your scripts, since `R` starts with an empty workspace, you will see if you have all the steps needed.
- Aim to always leave your scripts in a working state at the end of a session, so that a few days later you don't have to remember why it wasn't working!

Rscript

- `Rscript` works as an interpreter. It is quicker to start than `R` (fewer packages are loaded?).
- Can use interactively or for standalone scripts.

```
$ Rscript -e 'round(runif(10))'
 [1] 0 1 0 0 1 0 1 1 0 0
```

```r
#!/usr/bin/env Rscript
args <- commandArgs(TRUE)

stopifnot(length(args)==3)
args = as.numeric(args)
n = args[1]; mean = args[2]; sd = args[3]
rnorm(n, mean, sd)
```

```
$ ./simple_rnorm.R 5 10 2
[1]  8.651807 13.372094 10.063347 10.703155  6.351886
```

Commenting your work

- Do not be shy when putting comments into your code.
- Meaningful variable names help, but do document. At a bare minimum, each file should state at the top what the purpose of the file. Important variables and functions should be clearly documented.
- You may think it obvious how your code works, but try looking at it a week or a month later and then see if you clearly understand it. If in doubt, document it.
- Describe *what* your code is doing, not *how* it is doing it (WSS, p79). Compare the following two:

```
> s <- s + 1   ## prepare to process next subject
> j <- j + 1   ## increment j by 1.
```

- Comments can be put before commands, if you temporarily do not want to run that command; remove the comments when you want to run the command again, or delete the line.

```
> ## x <- c(x, c(1,2,3))
```

Line wrapping

- Line-wrapping. Do not write beyond around column 72, for readability. You can break long expressions at suitable points.
- End of line shold not look like end of an expression. Compare:

```
x <- sqrt(  c(100, 200, 300, 400, 500) ) + 10
x <- sqrt(  c(100, 200, 300, 400, 500) )
+ 10
x <- sqrt(  c(100, 200, 300, 400, 500) ) +
10
x <- sqrt(  c(100, 200, 300, 400, 500) ) +
     10
```

Line wrapping

```
> ## 1: ok - all fits onto one line, just.
> (x <- sqrt(  c(100, 200, 300, 400, 500) ) + 10)

[1] 20.00000 24.14214 27.32051 30.00000 32.36068

> ## 2: not okay -- first line is seen as complete.
> x <- sqrt(  c(100, 200, 300, 400, 500) )
> + 10

[1] 10

> x

[1] 10.00000 14.14214 17.32051 20.00000 22.36068
```

Line wrapping

```
> ## 3: solved, by moving the operator (+) up.
> x <- sqrt(  c(100, 200, 300, 400, 500) ) +
+ 10
> x

[1] 20.00000 24.14214 27.32051 30.00000 32.36068

> ## 4: as 3, but indentation makes it clearer.
> x <- sqrt(  c(100, 200, 300, 400, 500) ) +
+      10
> x

[1] 20.00000 24.14214 27.32051 30.00000 32.36068
```

Outline

Matrices

A matrix is just a vector with some additional markup to reformat it. Matrix stored in column-major order (like fortran, unlike C).

```
> x <- 1:6
> is.matrix(x)

[1] FALSE

> dim(x) <- c(2,3)
> is.matrix(x)

[1] TRUE

> x

     [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6

> dim(x)

[1] 2 3
```

Matrices

```
> x[2,2] ## extracting a value.

[1] 4

> x[1,]  ## extracting row

[1] 1 3 5

> x[1:2, 2:3]

     [,1] [,2]
[1,]    3    5
[2,]    4    6

> x[,2]  ## not column vector!

[1] 3 4
```

Matrices

```
> x[, 2, drop=TRUE]  ## default

[1] 3 4

> x[, 2, drop=FALSE] ## gotcha!

     [,1]
[1,]    3
[2,]    4
```

Typical matrix construction methods

- `matrix()`
- `cbind()`
- `rbind()`

```
> m <- matrix( floor(runif(6, max=50)), nrow=3)
> x <- rbind( c(1,4,9), c(2,6,8), c(3,2,1))
> y <- cbind( c(1,2,3), 5, c(4,5,6))
```

Typical matrix construction methods

```
> matrix( floor(runif(6, max = 50)), nrow = 3 )  ## ncol = 2

     [,1] [,2]
[1,]   46   23
[2,]   35   30
[3,]    6   34
```

Typical matrix construction methods

```
> rbind( c(1,4,9), c(2,6,8), c(3,2,1) )

     [,1] [,2] [,3]
[1,]    1    4    9
[2,]    2    6    8
[3,]    3    2    1
```

Typical matrix construction methods

```
> cbind( c(1,2,3), 5, c(4,5,6) )  ## recycling again

     [,1] [,2] [,3]
[1,]    1    5    4
[2,]    2    5    5
[3,]    3    5    6
```

Typical matrix construction methods

Note that matrix indices can also be named:

```
> dimnames(m) <- list(student = c("ann", "bob", "joe"),
+                     exam = c("math", "french"))
> m

       exam
student math french
    ann   36     11
    bob   30     30
    joe    5      0

> m["bob", ]  ## get bob's scores

  math french
    30     30
```

Common matrix operations

- diagonal: `diag(x)` – watch if x matrix or scalar!
- matrix multiplication: `%*%` vs `*` (element-wise)

```
> x <- matrix(1:4, 2,2)
> i <- diag(2) ## 2 x 2 identity matrix
> x %*% i      ## should be x

     [,1] [,2]
[1,]    1    3
[2,]    2    4

> x  *  i      ## not x!

     [,1] [,2]
[1,]    1    0
[2,]    0    4
```

Common matrix operations

- transpose: `t(x)`
- `dim`, `nrow`, `ncol`
- inverse: `solve(x)`,

```
> (x %*%  solve(x)) == diag(nrow(x))

     [,1] [,2]
[1,] TRUE TRUE
[2,] TRUE TRUE
```

Arrays

Arrays as extension of matrices to multiple dimensions.

```
> array(1:12, c(2,2,3))

, , 1

     [,1] [,2]
[1,]    1    3
[2,]    2    4

, , 2

     [,1] [,2]
[1,]    5    7
[2,]    6    8

, , 3

     [,1] [,2]
[1,]    9   11
[2,]   10   12
```

Outline

Boolean values – ?logical

Logical values TRUE/FALSE (avoid abbrev to T/F).

TRUE/FALSE equivalent to 1/0

```
> as.integer(TRUE)

[1] 1

> as.integer(FALSE)

[1] 0

> as.logical(1)

[1] TRUE

> as.logical(0)

[1] FALSE
```

Boolean values – ?logical

```
> d <- c(3.2, 1.0, 4.0, 9.2, 2.3, 8.1, 6.3)
> d > 5.0

[1] FALSE FALSE FALSE  TRUE FALSE  TRUE  TRUE

> d[d> 5.0]

[1] 9.2 8.1 6.3

> which(d>5.0)

[1] 4 6 7
```

Boolean values – ?logical

```
> d[which(d>5.0)]

[1] 9.2 8.1 6.3

> medium.sized <- (d > 3.0) & (d< 5.0)
> d[medium.sized]

[1] 3.2 4.0

> d[!medium.sized]

[1] 1.0 9.2 2.3 8.1 6.3

> ifelse(d > 3.0, 1.0, 0.0) ## same as as.numeric(d > 3)

[1] 1 0 1 1 0 1 1
```

Boolean values – ?logical

Key operators for handling boolean values:

```
> !TRUE                        ## negation: swap T -- F.

[1] FALSE

> TRUE  & FALSE                ## and: both must be true.

[1] FALSE

> FALSE | TRUE                 ## or: one must be true.

[1] TRUE

> xor(TRUE, TRUE)              ## xor: only one is true.

[1] FALSE
```

Boolean logic: issues

`a & b` (same for `a | b`) is an **elementwise** operation, with a result the same length as the longer of `a`, `b` (recycling is used if one vector is shorter).

`a && b` examines only the **first** element of `a` and `b`, returning one logical value. **Lazy evaluation** is used: we calculate only what's needed to determine result.

```
> TRUE || some.long.computation()

[1] TRUE

> TRUE && stop("no")

Error in eval(expr, envir, enclos):  no

> FALSE && stop("no")

[1] FALSE
```

Lazy (Advanced)

R uses *Lazy evaluation*, which delays the evaluation of an expression (here the argument) until its value is actually required [2]:

```
> f <- function(x) { 10 }
> system.time(f(Sys.sleep(3)))

   user  system elapsed
      0       0       0

> f <- function(x) { force(x); 10 }
> system.time(f(Sys.sleep(3)))

   user  system elapsed
  0.000   0.000   3.002
```

[2]example from Hadley Wickham's devtools

Boolean logic: issues

Comparing numbers: When testing numbers for equality, can use `x == y` when `x`, `y` are integers, otherwise use `all.equal(x,y)`. See later on numerics.

Avoid using `F`

```
> F <- 3
> F == FALSE

[1] FALSE
```

Outline

What is a list?

A list is used to collect a group of objects of different sizes and types. Very flexible. Often returned as the result of a complex function (e.g. model fit) to return all relevant information in one object.

```
> l <- list(who='joe', height=1.70, dob=c(1960, 12, 1))
> l

$who
[1] "joe"

$height
[1] 1.7

$dob
[1] 1960   12    1
```

What is a list?

```
> length(l)
[1] 3
> names(l)  ## show components
[1] "who"    "height" "dob"
> l$height  ## access an element.
[1] 1.7
```

What is a list?

List elements can either be accessed by name (e.g. `l$height` or `l[['height']]` – if named list) or by position (`l[[2]]`).

When using numbers to index list, compare `l[2]` (a list with one element) with `l[[2]]`. You can therefore do `l[2:3]` but not `l[[2:3]]`.

What is a list?

```
> unlist(l) ## opposite of list

   who height   dob1   dob2   dob3
 "joe"  "1.7" "1960"   "12"    "1"

> str(l) ## structure of l

List of 3
 $ who   : chr "joe"
 $ height: num 1.7
 $ dob   : num [1:3] 1960 12 1
```

Modifying lists (Advanced)

We can append new items to list either by making a new list from the old one (e.g. 1) , or directly by assigning new element (e.g. 2):

```
> l1 <- list(who="fred")
> l1 <- c(l1, height=1.8)         ## e.g. 1
> l1[["dob"]] <- c(1965, 10, 17) ## e.g. 2
```

Modifying lists (Advanced)

Deleting list items:

```
> l1["height"] <- NULL
> str(l1)

List of 2
 $ who: chr "fred"
 $ dob: num [1:3] 1965 10 17
```

Modifying lists (Advanced)

Finally, for completeness, here is a way to predefine a list of given length and gradually fill it in:

```
> empty <- vector("list", 3) ## Prealloc to given length.
> names(empty) <- c("who", "height", "dob")
> empty[["height"]] <- 1.8
```

Initialisation

Initialising R object (list, vectors, . . .) is **much** faster than creating and extending these objects on the fly

```
> n <- 1e4
> l <- list()
> system.time(for (i in 1:n) l[[i]] <- rnorm(1e3) )

   user  system elapsed
  0.680   0.010   0.691

> l <- vector("list", n)
> system.time(for (i in 1:n) l[[i]] <- rnorm(1e3) )

   user  system elapsed
  0.624   0.003   0.628
```

Data frames

A data frame is like a matrix, but each column can be of a different type.

Data frame is stored as a list, with each element a vector of same length.
Useful for reading in tabular data from a file (see `read.csv`).

```
> nms <- c("joe", "fred", "harry")
> a <- c(24, 19, 30)
> ht <- c(1.7, 1.8, 1.75)
> s <- c(TRUE, FALSE, TRUE)
```

Data frames

```
> cbind(a, ht)       ## matrix, preserves

      a   ht
[1,] 24 1.70
[2,] 19 1.80
[3,] 30 1.75

> class(cbind(a, ht))

[1] "matrix" "array"
```

Data frames

```
> cbind(nms, ht)  ## matrix, ht col becomes strings.

     nms     ht
[1,] "joe"   "1.7"
[2,] "fred"  "1.8"
[3,] "harry" "1.75"

> class(cbind(nms, ht))

[1] "matrix" "array"
```

Data frames

```
> d <- data.frame(name = nms,
+                 age = a,
+                 height = ht,
+                 student = s)
> class(d)

[1] "data.frame"
```

Data frames

```
> d$age ## same as d[, "age"]

[1] 24 19 30

> names(d)

[1] "name"    "age"     "height"  "student"

> d[2,] ## access 2nd row.

  name age height student
2 fred  19    1.8   FALSE
```

Data frames

Compare how a data frame (`d`) is printed, compared to printing `as.list(d)`.

```
> d

   name age height student
1   joe  24   1.70    TRUE
2  fred  19   1.80   FALSE
3 harry  30   1.75    TRUE

> as.list(d)

$name
[1] "joe"   "fred"  "harry"

$age
[1] 24 19 30

$height
[1] 1.70 1.80 1.75

$student
[1]  TRUE FALSE  TRUE
```

Outline

Factors (Advanced)

(Mostly seen when reading in data frames; abandoned in R 4.0.0)
"... in 2019, it was decided to move towards using stringsAsFactors = FALSE by default, ideally starting with the 4.0.0 release."
`https://developer.r-project.org/Blog/public/2020/02/16/stringsasfactors/`
Factors internally code categorical variables with a number. e.g. `1=Sunday`, `2=Monday`, ... `7=Saturday`. For large vectors, this is more efficient storage, especially when character strings repeat. Can also make code more readable.

Also useful in many statistical functions, using the formula interface.

Factors (Advanced)

```
> scores1 <- c('good', 'poor', 'bad', 'poor',
+              'bad', 'bad', 'good')
> scores <- factor(scores1)
> scores

[1] good poor bad  poor bad  bad  good
Levels: bad good poor

> levels(scores)

[1] "bad"  "good" "poor"

> as.integer(scores)   ## integer representation

[1] 2 3 1 3 1 1 2

> as.character(scores) ## show strings

[1] "good" "poor" "bad"  "poor" "bad"  "bad"  "good"
```

Factors (Advanced)

```
> which(scores1 == 'bad')

[1] 3 5 6

> ## Can do further comparisons with an ordered factor.
> ## Levels are now ordered, as shown by "<" in levels.
>
> s2 <- factor(scores1,
+              levels = c('poor', 'bad', 'good'),
+              ordered = TRUE)
> s2[1] > s2[2]

[1] TRUE
```

Outline

Strings / character arrays

Character arrays are vectors of strings.
Use single (') or double (") quotes to mark strings, but don't mix:

```
> x <- 'good'
> z <- "no'  # need to match"
> z <- "it's working"
```

Strings / character arrays

Within a script, easy way to generate output:

```
> cat("Now computing the steady-state\n")

Now computing the steady-state

> x <- 134
> cat("sqrt of", x, "is", sqrt(x), "\n")

sqrt of 134 is 11.57584

> cat("sqrt of", x, "is", sqrt(x), "\n", sep='__')

sqrt of__134__is__11.57584__
```

See also `message`, `warning` and `stop` for communicating diagnostic messages – `cat` and `print` are generally used when displaying an object.

Strings / character arrays

blackslash characters allow you to generate control characters, importantly: newline: $\backslash n$, tab: $\backslash t$.

```
> cat("5\t9\n_")

5 9

_
```

paste() returns a string, e.g. for assignment.

```
> x <- 1:5; exp.dir <- '/home/stephen/res'
> file <- paste(exp.dir, '/expt_res', x, '.dat', sep='')
> file

[1] "/home/stephen/res/expt_res1.dat"
[2] "/home/stephen/res/expt_res2.dat"
[3] "/home/stephen/res/expt_res3.dat"
[4] "/home/stephen/res/expt_res4.dat"
[5] "/home/stephen/res/expt_res5.dat"
```

paste0

Don't forget `paste0()` where sep=''.
(Humour): http://simplystatistics.org/2013/01/31/paste0-is-statistical-computings-most-influential-contributio

Strings

- Just as R stores vectors of numbers, it also stores vectors of strings.
- Pattern matching facilities are available, based on Unix terms (grep, regular expressions). These are worth learning:

```
> s <- c('apple', 'bee', 'cars', 'danish', 'egg')
> nchar(s)

[1] 5 3 4 6 3

> substr(s, 2,3)

[1] "pp" "ee" "ar" "an" "gg"
```

Strings

```
> grep('e', s)
[1] 1 2 5
> grep('^e', s)    ## regexps...
[1] 5
>  sub('e', '_', s)
[1] "appl_"  "b_e"    "cars"   "danish" "_gg"
> gsub('e', '_', s)  ## global sub, watch "bee"
[1] "appl_"  "b__"    "cars"   "danish" "_gg"
```

Strings

```
> toupper(s)

[1] "APPLE"  "BEE"    "CARS"   "DANISH" "EGG"

> sprintf('name %s len %d', s, nchar(s)) ## C users!

[1] "name apple len 5"  "name bee len 3"
[3] "name cars len 4"   "name danish len 6"
[5] "name egg len 3"
```

Outline

Environments (Advanced)

An environment is a *frame*, or collection of named objects (variables), and a pointer to an *enclosing environment*.

The working environment of your interactive R session is the <R_GlobalEnv>.

```
> x <- 2
> ls()

[1] "x"

> ## current environment
> environment()

<environment: R_GlobalEnv>
```

```
> e <- new.env()
> e

<environment: 0x55aaa23cccf8>

> ls(e)

character(0)

> parent.env(e)

<environment: R_GlobalEnv>

> e$x <- 1
> ls(e)

[1] "x"

> e$x != x

[1] TRUE
```

Inspecting variables and the environment

```r
x <- 9
y<- c(2,4,5)
m <- matrix(2:5, 12,10)
objects()       ## what vars do I have?
ls()            ## shorthand for objects.
str(m)          ## Display compact representation
head(m)
tail(m)
rm(list = ls()) ## clear up the working environment
ls()
```

Converting an object from one type to another

Some ways of finding out what kind of object you have and converting.

```r
mode(y)
typeof(y)
class(y)
object.size(y)
is.vector(y)    ## is.xyz() check if type XYZ
is.matrix(y)
as.vector(m)    ## convert object to type XYZ
l <- list(x=c(1,4), y=c(6,9,12))
unlist(l)
```

What is an object?

- An object is typically either a variable or a function.
- You can use the same name for a function and a variable, and R uses context to decide which you mean:

```
> sum <- 3 + 4 + 5
> total <- sum(1:4)
> total

[1] 10

> sum

[1] 12

> sum(sum)  ## can get confusing!

[1] 12
```

OO programming in R

Data abstraction; object manipluation becomes independent of the implementation details.

There are several OO programming frameworks in R . The main ones, supported in base R are `S3`, `S4` and `S4 ReferenceClasses`. `S6` are lightweight reference classes.

Bioconductor provides many ad hoc classes to store, manipulate and process microarray, RNA Seq, proteomics, flow cytometry, . . . data.

It there is interest, we could have a session about OO programming at the end of the course.

Outline

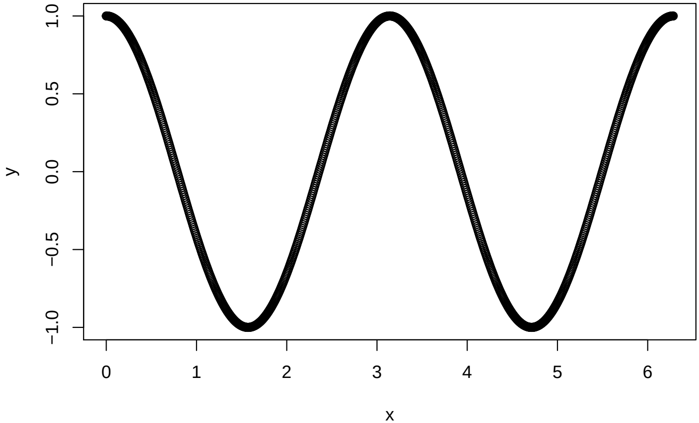
Basic plotting

- Basic x,y plots (scatter plots)
- Multiple plots in one figure
- Saving your plots

This section will just introduce the mechanics of making basic plots, rather than worry about interpreting them.

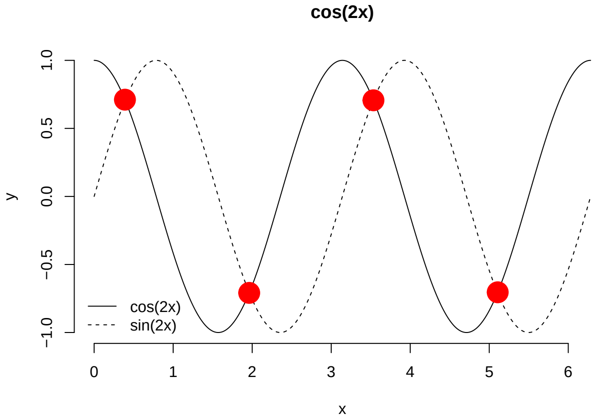
Basic plotting

```
> x <- seq(from=0, to=2*pi, len=1000)
> y <- cos(2*x)
> plot(x,y) ## just provide data; sensible labelling
```



Basic plotting

```
> ## Expand on previous plot ...
> plot(x,y, main='cos(2x)', type='l', lty=1, bty='n')
> y2 <- sin(2*x)
> lines(x,y2, type='l', lty=2)
> same <- which( abs(y - y2) < 0.01)
> points(x[same], y[same], pch=19, col='red', cex=3)
> legend('bottomleft', c("cos(2x)", "sin(2x)"), bty='n', lty=c(1,2))
```



Options controlling the plot

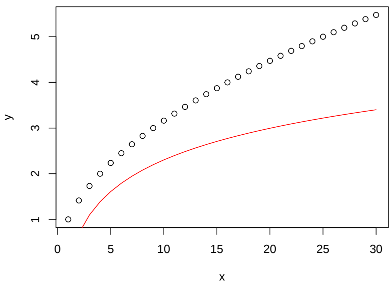
`par()` outputs the (long) list of options that control plotting behaviour.
Read `?par` for all the details!
Common options to explore:

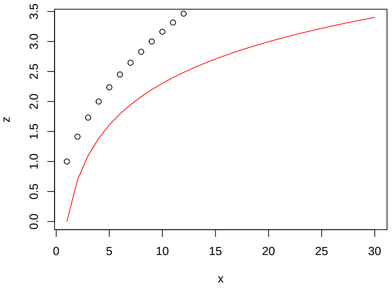
- `mfrow`, `mfcol`: multiple plots in figure
- `mar`, `oma`: margins around plot and figure.
- `ask`: whether to hit RETURN between pages of figures.

Multiple data sources on one plot

When you wish to have multiple data sources on one plot (e.g. two time-series plots), the approach is to draw the first using plot and then draw subsequent features using lines or points.
Axes are not rescaled, so draw the bigger plot first.

```
> x <- 1:30
> y <- sqrt(x); z <- log(x)
> plot(x,y); lines(x,z, col='red')
> plot(x,z, type = "l", col = "red"); points(x,y) ## some data missing
```

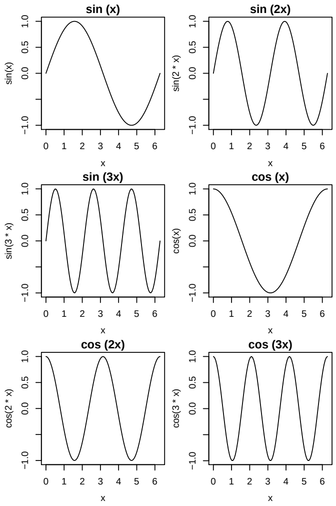




Multiple plots in one figure

`mfrow` and `mfcol` are useful parameters within `par()`, but margins often need to be changed to maximise space.

```
pdf(file = 'mfrow_eg.pdf',
    width = 4, height = 6)
par(mfrow = c(3,2))
par(mar = c(3.5, 3.5, 1.5, 0.5),
    mgp = c(2.5, 1, 0))
x <- seq(from = 0, to = 2*pi,
         len = 100)
plot(x, sin(x), main = "sin (x)",
     type = 'l')
plot(x, sin(2*x), main = "sin (2x)",
     type = 'l')
plot(x, sin(3*x), main = "sin (3x)",
     type = 'l')
plot(x, cos(x), main = "cos (x)",
     type = 'l')
plot(x, cos(2*x), main = "cos (2x)",
     type = 'l')
plot(x, cos(3*x), main = "cos (3x)",
     type = 'l')
dev.off()
```



Saving your plots

R can save plots in many formats, including PDF, postscript, PNG, JPEG. Best to use vector formats (PDF, postscript) for graphs and bitmap formats (png, jpeg) for images.
R has output devices, only one of which is active, dev.cur().

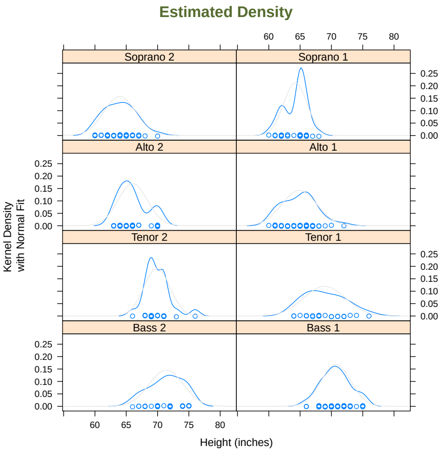
```
> dev.list()
> pdf(file='hist.pdf', width=7, height=7) ## inch
> dev.list()
> hist( rnorm(9999) )
> dev.off()                              ## close device
> png(file='hist.png', w=600, h=600) ## pixels
> hist( rnorm(9999) )
> dev.off()
```

Zoom in on text of PNG to see limitations of this format.

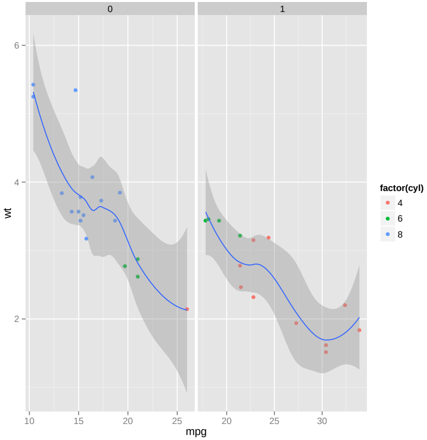
Next steps with plotting (Advanced)

R has a vast range of functions for plotting particular data types. You may read about different packages for plotting:

- base graphics (or "traditional")
- lattice/grid (lattice is built upon grid)
- ggplot2 – http://had.co.nz/ggplot2/
- Patchwork

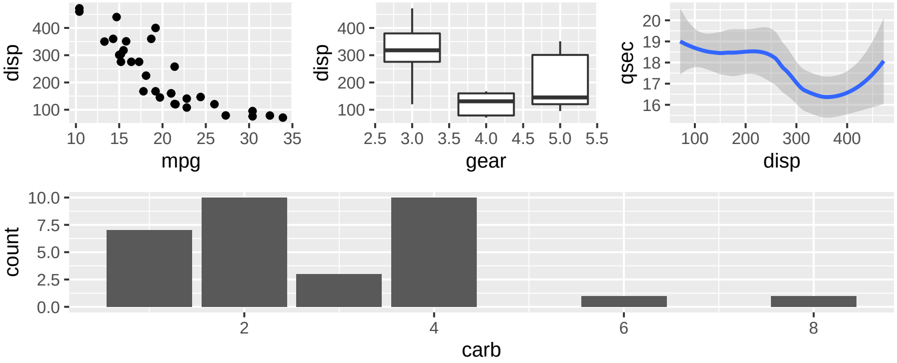


Estimated Density
Soprano 2
Soprano 1
Alto 2
Alto 1
Tenor 2
Tenor 1
Bass 2
Bass 1
Kernel Density with Normal Fit
Height (inches)
60
65
70
75
80
0.00
0.05
0.10
0.15
0.20
0.25



0
1
wt
mpg
factor(cyl)
● 4
● 6
● 8
2
4
6
10
15
20
25
30

```
> require(ggplot2); require(patchwork)
> p1 <- ggplot(mtcars) + geom_point(aes(mpg, disp))
> p2 <- ggplot(mtcars) + geom_boxplot(aes(gear, disp, group =
> p3 <- ggplot(mtcars) + geom_smooth(aes(disp, qsec))
> p4 <- ggplot(mtcars) + geom_bar(aes(carb))
> (p1 | p2 | p3) /
+       p4
```



Here are some starting points to explore:

- `demo(graphics)` to see diversity of plots.
- low-level functions: `symbols()`, `rect()`, `segments()`, `abline()`.
- `curve(x*log(x))`
- R graphics gallery
  `http://www.r-graph-gallery.com`

Outline

Reading/writing data to file system

- What's my current directory? `dir`, `getwd`, `setwd`
- `scan`, `readLines`
- `read.csv`, `read.table`, `write.table`
- `RData` files – `save` and `load`
- Further I/O functions

Interacting with the file system

- where am I currently? `getwd()`
- change me to a new directory: `setwd("/tmp")`
  (GUIs have chooser for interactively changing directory.)
- What files are in my [current] directory?

```
> dir()
> dir("/tmp")
> dir(pattern="\\.R$")  ## regexps, see later.
```

Scan, write, readLines

For basic reading/writing of data, use scan/write. Filenames are specified relative to current directory. Can even give URL as a file. Files often have a header which can be skipped over.

```
> x <- scan('files/ages.dat', skip=1)
> summary(x)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max. 
  14.00   19.25   27.25   31.58   39.25   65.00 

> s1 <- readLines('files/ages.dat')  ## treats as strings
> summary(s1)

   Length     Class      Mode 
        5 character character 

> h <- scan('http://damtp.cam.ac.uk/user/sje30/r/heights.dat') ## heights.dat
> summary(h)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max. 
  136.2   158.3   164.9   163.0   169.2   178.7 
```

Scan, write, readLines

```
> rand.vals <- round( runif(100, min=5, max=10), 2)
> tf <- tempfile()
> tf

[1] "/tmp/Rtmput9nzu/file751b5534b247d"

> write(rand.vals, tf)
> s <- scan(tf)
> all.equal(s, rand.vals)

[1] TRUE
```

read.table et al.

If data are tabular, `read.table` or `read.csv` is often useful. (Useful for importing spreadsheets; just save as a comma separated value file, CSV.)

```r
x <- read.table('./files/players.dat', sep = '\t',
                header = TRUE)
names(x)
head(x)
x[2,]
x$Goals
is.data.frame(x)
tf <- tempfile()
write.csv(x, tf, row.names=FALSE)
## sort by goals scored.
x[order(x$Goals, decreasing = TRUE), ]
```

See `?read.table`.

Rdata files

Text files are useful for portably storing data, so that they can be read across applications. R has its own format for *efficiently* storing objects. Files much smaller than text files. However, this format is not universally known.

```
> n <- 99999; x <- rnorm(n)
> txt.file <- tempfile()
> rda.file <- tempfile()
> write(x, n, file = txt.file)
> save(x, n,  file = rda.file)
>
> ## Compare sizes of files with the object.
> object.size(x)
> file.info(txt.file)$size
> file.info(rda.file)$size   ## compressed
>
> rm(x,n)
> load(rda.file) ## reload data.
```

Saving your workspace with `.RData` files

When you quit `R`, you are asked:

```
> q()
Save workspace image? [y/n/c]:
```

If you answer `y`, all objects (variables and functions) in your global environment are saved for future use, using `save.image`. From ?save:

```
'save.image()' is just a short-cut for "save my current
workspace", i.e., 'save(list = ls(all=TRUE), file = ".RData")'
It is also what happens with 'q("yes")'.
```

Warning: If an `.RData` file is present in the current directory when starting `R`, it is silently loaded. I think it can be dangerous, as you may not realise what values have been silently loaded. Better to instead be explicit:

```
> save.image(file='all.Rda')    ## keep everything
> save(x, y, z, file='key.Rda') ## or just key objects
> ## ...
> load('all.Rda')                ## reload objects
```

or start R using `R --no-restore`

Further I/O functions (Advanced)

R has many facilities for I/O. See for example the following help topics.

- ?connections — interface to files, pipes, sockets, compressed files . . .
- ?sink — divert R output to a connectin
- ?dget / ?dput — read/write ASCII representation of an R object.
- Package readxl for reading Excel files.

Also: XML, DBMS, SQLite, netCDF, hdf5, . . .

Outline

Writing functions: overview

- Why bother?
- How to write (local args, return value; cannot change value)
- Example: computing std. deviation
- Local variables within functions
- Recursion.

Functions

- Functions promote code reuse.
- Black-box approach; given inputs, what output should I expect? This requires good documentation of what your function does. Can it be described without having to look at the code?
- Finding the right level of definition for a function is hard, and how to modularise comes with experience. Typically rewrite many times before getting final solution

Functions

- How to define a new function:

```
> my.fun <- function(arg1, arg2) {
+   ## Doc string here.
+   x <- arg1 * 2
+   y <- sqrt(arg2) + 5
+   z <- x * y
+   ## last value is the return value of the function.
+   ## Use a list to return several items.
+   z ## same as return(x)
+ }
```

Example of writing a new function

Compute the standard deviation of a vector of numbers:

$$std.dev = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}} \quad \text{where} \quad \bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

```
> std.dev <- function(x) {
+   ## Return std dev of X.
+   n <- length(x)
+   xbar <- sum(x)/n
+   diff <- x - xbar
+   sum.sq <- sum( diff^2)
+   var <- sum.sq / (n-1)
+   ## last value calculated is return value.
+   sqrt(var)
+ }
```

Terminology of variables within functions

- In std.dev, x is the name of a **formal argument**. In the following, y is called the **actual argument** (doesn't have to be named x – can be named however you wish).

```
> n <- 5
> y <- c(9, 2, 7, 10)
> std.dev(y)
[1] 3.559026
> print(n) ## should still be 5, not 4.
[1] 5
```

- **Local variables** within function are not available outside of function.

- Any change to formal args within a function does not change value of actual argument outside the function:

```
> sum.sq <- function(x) {
+   x <- x^2   ## change internally
+   sum(x)
+ }
> y <- c(4, 5, 6)
> sum.sq(y)
[1] 77
> y
[1] 4 5 6
```

Handling unbound variables

Variables created by assignment within a function are known as local variables (e.g. y below). If a variable is not local, or a formal argument, it is an **unbound variable**. It may be found in the enclosing environment (typically the global workspace), or an error is generated – this is **bad practice**!

```
> fn1 <- function(x) {
+   y <- x^2
+   res <- sum( (y - thresh)^2 )
+   res
+ }
> dat <- 1:5
> fn1(dat)     ## case 1

Error in fn1(dat):  object 'thresh' not found

> thresh <- 10
> fn1(dat)     ## case 2

[1] 379
```

Handling unbound variables (2)

In this case, better to define thresh as an argument of the function, and provide a default value:

```
> fn1 <- function(x, thresh=10) {
+   y <- x^2
+   res <- sum( (y - thresh)^2 )
+   res
+ }
> fn1(dat)      ## case 3

[1] 379
```

Advanced: use `codetools::checkUsage()` to find unbound vars; `codetools::findGlobals()` for globals.

The ... arguments

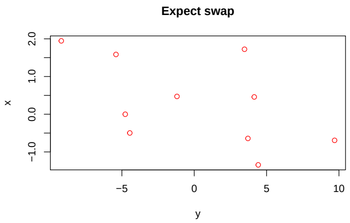
From R language definition

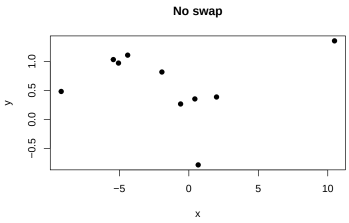
> *The ... argument is special and can contain any number of arguments. It is generally used if the number of arguments is unknown or in cases where the arguments will be passed on to another function.*

See `?cat` for an example of *number of arguments is unknown*.

The ... arguments

```
> p <- function(x, y, ...) {
+   if (diff(range(x)) > diff(range(y))) {
+     plot(x, y, ...)
+   } else {
+     plot(y, x, ...)
+   }
+ }
> p(rnorm(10, 0, 1), rnorm(10, 0, 5), main = "Expect swap",
+   col = "red")
> p(rnorm(10, 0, 5), rnorm(10, 0, 1), main = "No swap", pch = 19)
```





Writing a replacement function (Advanced)

Convention for a replacement function is that the name should end with `<-`. The last argument of the replacement function must be called `value` and is the RHS of the assignment.

```
> "threshold<-" <- function(x, value) {
+   ## X is the object to update
+   ## VALUE is the value on the RHS.
+   y <- ifelse(x > value, 1, 0)
+   return(y)
+ }
> x <- c(0.3, 0.1, 0.6, 0.7, 0.9, 0.2)
> threshold(x) <- 0.4
> x

[1] 0 0 1 1 1 0
```

In general, replacement functions are used to set variable attributes or object slots.

Tips for writing functions

- Can you think of a way to break down the problem so that a team can work on the problem, with each person assigned to a independent piece? "Divide + conquer".
- Each function should be easy to test, then you can "freeze" it. Write test cases, which can be automatically checked.

```
>  all.equal(my.fun(100,200), 300)
```

- Rule of thumb: each function should be no more than a page or two of code.
- For large projects, avoid mixing computation and plotting in the same function – separate the two jobs; this makes it easier to run in batch.

```
> res <- some.computation(par1, par2, par3)
> plot.results(res)
```

Outline

Control-flow constructs

- if
- switch
- for
- while
- Vectorization
- simple applications – numerics

if / if ... else ...

```
> x <- 8;
>
> if (x > 10) {
+   ## condition was true
+   cat("x is bigger than 10\n")
+ } else {
+   cat("x is 10 or less\n")
+ }

x is 10 or less
```

Notes:
“else ...” can be omitted if you do not need it.
if returns a value, which can be assigned, e.g. `y <- if (x <10) 40 else 20`. A better solution in this case however is the vectorized form
`y <- ifelse(x<10, 40, 20)`

Braces in conditional constructs

Curly braces not needed if there is only one expression in the if clause:

```
if ( x > 10 ) {
  y <- 1
}
```

```
if ( x > 10 )
  y <- 1
##
```

But braces are needed in multiline if/else statement:

```
if ( x > 10 ) {
  y <- 1
} else {
  y <- 0  ## OK
}
```

```
if ( x > 10 )
  y <- 1
else
  y <- 0  ## NOT OK
##
```

```
From ?Control:  Note that it is a common mistake to forget to put
braces ('{ .. }') around your statements, e.g., after 'if(..)' or
'for(....)'. In particular, you should not have a newline between
'}' and 'else' to avoid a syntax error in entering a 'if ... else'
construct at the keyboard or via 'source'. For that reason, one
(somewhat extreme) attitude of defensive programming is to always
use braces, e.g., for 'if' clauses.
```

switch (Advanced)

Nested if ... else commands can get a bit messy. Like other languages, R has a switch construct. From ?switch:

```
>       centre <- function(x, type) {
+         switch(type,
+                mean = mean(x),
+                median = median(x),
+                trimmed = mean(x, trim = .1))
+       }
>       x <- rcauchy(10)
>       centre(x, "mean")

[1] 1.963204

>       centre(x, "median")

[1] 1.940791

>       centre(x, "trimmed")

[1] 1.565386
```

Recursive functions

Here is an example of using conditionals with a divide and conquer approach; quicksort in a few lines (albeit not very efficient).

```
> qsort <- function(data) {
+   ## Sort data into ascending order.
+   n <- length(data)
+   if (n <= 1) {
+     data
+   } else {
+     pivot   <- data[floor(n/2)]
+     less    <- data[which(data <  pivot)]
+     equal   <- data[which(data == pivot)]
+     greater <- data[which(data >  pivot)]
+     c( qsort(less), equal, qsort(greater))
+   }
+ }
> all(replicate(99, {
+   data <- runif(2000, max=10)
+   all.equal(qsort(data), sort(data)) }))

[1] TRUE
```

Looping constructs

Looping constructs allow you to repeat calculations as many times as you wish. This is why computers are so useful – it is just as easy (usually) to repeat something 1000 times as 10 times.

e.g. if you want to simulate flipping a (biased) coin 100 times, and counting the number of heads, no problem. If you want to repeat this process 1000 times, no problem. (See later.)

for loops

for (var in seq) command

`seq` is a vector; `var` is set in turn to each value in the vector, and then `command` executed. Multiple commands can be given within braces. e.g.

```
> x <- 6
> for (i in 1:3) {
+   res <- x * i
+   cat(x, "*", i, "=", res, "\n")
+ }

6 * 1 = 6
6 * 2 = 12
6 * 3 = 18
```

while loops

```
while (condition) {
  command
  command
}
```

So the commands are executed until the condition is no longer true.
Typically then one of the commands will change the condition.
e.g. print all the Fibonacci numbers (`f[i] = f[i-1] + f[i-2]`) less than 100.

```
> n1 <- 0; n2 <- 1
> while (n2 < 100) {
+   print(n2)
+   old <- n2
+   n2 <- n2 + n1
+   n1 <- old
+ }
```

Breaking out of loops

`repeat expr` will repeatedly execute expr until you break out of the loop.

```
> i <- 3
> repeat {
+   if (i == 5) {
+     break
+   } else {
+     cat("i is", i, "\n")
+     i<- i+1
+   }
+ }

i is 3
i is 4
```

Breaking out of loops

`next` allows you to skip to next iteration of a loop. Both `next` and `break` can be used within other loops (`while`, `for`).

```
> for (i in 1:10) {
+   if ((i %% 2) == 0)
+     next
+   print(i)
+ }

[1] 1
[1] 3
[1] 5
[1] 7
[1] 9
```

Example: HOTPO rule

A word on indentation

Indentation helps you see the flow of the logic, rather than flattened version. (Use tab key to indent). Reformatting tools are available (e.g. within Emacs).

```r
## version 1.
i <- 3
repeat {
  if (i==10) {
    break
  } else {
    cat("i is", i, "\n")
    i<- i+1
  }
}
```

```r
## version 2.
i <- 3
repeat {
if (i==10) {
break
} else {
cat("i is", i, "\n")
i<- i+1
}
}
```

Indentation helps to show structure, and match braces.

Outline

Vectorization

When possible, operate on vectors, rather than using for loops.
Rewrite code, but beware sometimes not possible (Fibonacci).
Compute difference between times of events, `e`. Given `n` events, there will be `n-1` inter-event times. `interval[i] <- e[i+1] - e[i]`

```
> diff1 <- function(e) {
+   n <- length(e)
+   interval <- rep(0, n-1) ## good to pre-alloc!
+   for (i in 1:(n-1)) {
+     interval[i] <- e[i+1] - e[i]
+   }
+   interval
+ }
> diff2 <- function(e) {
+   n <- length(e)
+   e[-1] - e[-n]
+ }
> e <- c(2, 5, 10.2, 12, 19)
> diff2(e)

[1] 3.0 5.2 1.8 7.0

> all.equal(diff1(e), diff2(e))

[1] TRUE
```

Advantages: shorter, more readable and faster (no loops).

Vectorization example

Q: Flip a biased coin [p=0.6 of heads] 100 times; how many heads do you get? Repeat this for 1000 trials.

```
> n <- 100    ## number of coin flips in trial
> p <- 0.6    ## prob of getting heads
> ntrials <- 1000
```

```
> trial1 <- function(n, p.heads) {
+   count <- 0
+   for (i in 1:n) {
+     if (runif(1) < p.heads)
+       count <- count +1
+   }
+   count
+ }
>
> res <- rep(0, ntrials)
> for (j in 1:ntrials) {
+   res[j] <- trial1(n, p)
+ }
> hist(res)
```

Vectorization example

Q: Flip a biased coin [p=0.6 of heads] 100 times; how many heads do you get? Repeat this for 1000 trials.

```
> n <- 100    ## number of coin flips in trial
> p <- 0.6    ## prob of getting heads
> ntrials <- 1000
```

```
> trial1 <- function(n, p.heads) {
+   count <- 0
+   for (i in 1:n) {
+     if (runif(1) < p.heads)
+       count <- count +1
+   }
+   count
+ }
>
> res <- rep(0, ntrials)
> for (j in 1:ntrials) {
+   res[j] <- trial1(n, p)
+ }
> hist(res)
```

```
> trial2 <- function(n, p.heads) {
+   rand.vals <- runif(n)
+   sum( rand.vals < p.heads)
+ }
>
> res <- replicate(ntrials,
+                  trial2(n, p))
> hist(res)
```

Vectorization example

Q: Flip a biased coin [p=0.6 of heads] 100 times; how many heads do you get? Repeat this for 1000 trials.

```
> n <- 100    ## number of coin flips in trial
> p <- 0.6    ## prob of getting heads
> ntrials <- 1000
```

```
> trial1 <- function(n, p.heads) {
+   count <- 0
+   for (i in 1:n) {
+     if (runif(1) < p.heads)
+       count <- count +1
+   }
+   count
+ }
>
> res <- rep(0, ntrials)
> for (j in 1:ntrials) {
+   res[j] <- trial1(n, p)
+ }
> hist(res)
```

```
> trial2 <- function(n, p.heads) {
+   rand.vals <- runif(n)
+   sum( rand.vals < p.heads)
+ }
>
> res <- replicate(ntrials,
+                  trial2(n, p))
> hist(res)
```

In this case, `hist( rbinom(1000, 100, 0.6))` would also work!

apply family

e.g. how to compute sum of each row of a matrix? `sum(A)` will normally return the sum of all elements of `A`.

```
apply(X, MARGIN, FUN, ...)
MARGIN = 1 for row, 2 for cols.
FUN = function to apply
... = extra args to function.
```

```
> A <- matrix(1:6, 2,3)
> sum(A)                                    #sum of entire arr

[1] 21

> col.sums  <- apply(A, 2, sum, na.rm=TRUE) ## colSums
> row.means <- apply(A, 1, mean) ## or rowMeans
```

apply family

Other functions: `lapply` (apply to list), `sapply` (simplify), `replicate`, . . .

```
> lapply(ls(), object.size)
> sapply(ls(), object.size)
> tapply(1:20, factor(rep(letters[1:5], each = 4)), sum)
> ## see also ?by
> mapply(sum, 1:5, 1:5, 1:5)
> hist( replicate(200, mean(rnorm(100)) ))
```

How to `*apply` – `http://stackoverflow.com/questions/3505701`

Exercise: Why is this better than writing a for loop?
(Eglen, 2009); parallel package: `mclapply()`, `parLapply()`, ...

Anonymous functions (Advanced)

Sometimes you don't want to pollute name space by defining a new function, so just use an "anonymous function", i.e. a function without a name. Particularly useful e.g. in an `apply` call.

```
> my.mat <- matrix(1:10, ncol=5)
> apply(my.mat, 2, function(x) { sum(x^2) + 10 })
```

Since functions are just objects, anonymous functions are just objects without names, similar to 'anonymous numbers' like a+b in an expression a+b+c.

Fibonacci sequence

$$0, 1, 1, 2, 3, 5, 8, 13, 21, \ldots$$

$$f[n] = f[n-1] + f[n-2]$$

How to vectorize?
Exercise: write a function, `fibonnaci(n)` that returns the n^{th} element of the sequence. Assume that `fibonnaci(1) == 0`, `fibonacci(2) == 1`.
Exercise: use `fibonacci()` to estimate the golden ratio.

Efficiency

“premature optimization is the root of all evil” (Knuth, 1974).

Examples adopted from `www.mathworks.com/res/code_segments`
`f1` is bad; should pre-allocate vector, rather than rely on `R` to allocate memory repeatedly[3].

```
> f1 <- function() {
+   n <- 1e4; decay <- 0.9995

+   out <- 1.0
+   for (i in 2:n)
+     out[i] <- out[i-1] * decay
+   out
+ }
> system.time(o1 <- f1())

   user  system elapsed
  0.008   0.000   0.008
```

```
> f2 <- function() {
+   n <- 1e4; decay <- 0.99995
+   out <- rep(0, n)   ##pre-alloc
+   out[1] <- 1.0
+   for (i in 2:n)
+     out[i] <- out[i-1] * decay
+   out
+ }
> system.time(o2 <- f2())

   user  system elapsed
  0.007   0.000   0.007
```

[3]This is not optimisation, but rather good coding practice.

A final word on efficiency

- Rule 1 of optimization: don't bother (Kernighan).
- For loops are not always a bad thing. See last example in Help Desk article (May 2008).
  http://cran.r-project.org/doc/Rnews/Rnews_2008-1.pdf

Numerics issues

Although integer arithmic is reliable, floating-point arithmetic is to be treated with care! (All R 's calculations are in what C programmers call "double precision".) Compare:

```
> 1.0 + 2.0 == 3.0

[1] TRUE

> 0.1 + 0.2 == 0.3

[1] FALSE
```

From FAQ (7.31?)

```
> a <- sqrt(2)
> a * a == 2

[1] FALSE

> a * a  - 2

[1] 4.440892e-16
```

Numerics issues

Solution - testing *near equality*

```
> all.equal( 0.1 + 0.2, 0.3)

[1] TRUE
```

If there is a difference, you get a summary of differences. Within a function, you might prefer just to test whether result is TRUE or not:

```
> x = 1:4
> y = rnorm(4,sd=0.2)
> all.equal(x,y)

[1] "Mean relative difference: 0.9932982"

> isTRUE(all.equal(x,y))

[1] FALSE
```

How big is infinity?

Use while loop to estimate it:

```
> x <- 1
> while ( is.finite(x*2) ) {
+   x <- x*2
+ }
>
> x ## 8.988466e+307

[1] 8.988466e+307

> x*2 ## Inf

[1] Inf

> (x*2)/2 ## Inf

[1] Inf

> .Machine$double.xmax

[1] 1.797693e+308
```

How small is epsilon?

How big can ϵ be such that $1 + \epsilon = 1$? (Taken from Goldberg (1991) ACM article, p220).

```
> eps <- 1
> while (eps + 1 > 1) {
+   eps <- eps * 0.5
+ }
> eps ##1.110223e-16

[1] 1.110223e-16

> 1 + eps ## 1

[1] 1

> (1 + eps == 1) ## TRUE

[1] TRUE

> 1 + (2*eps) ##1

[1] 1

> (1 + (2*eps) == 1) ## FALSE

[1] FALSE
```

Outline

Random number generation

Computers usaully generate “pseudo-random numbers”. They are generated based on some iterative formula:

$$x_{new} = f(x_{old}) \mod N$$

where modulo operation provides the “remainder” division.
To generate the first random number, you need a **seed**.
Setting the seed allows you to reliably generate the same sequence of numbers, which can be useful when debugging programs.
`R` has many routines for generating random samples from various distributions, but for now we will just use runif(), (and maybe rnorm()).
Exercise: write a random number generator. See: “Randu: a bad random number generator”. `http://physics.ucsc.edu/~peter/115/randu.pdf`
Exercise: Apply the central limit theorem to generate samples from a normal distribution by adding together samples from a uniform distribution.

Outline

Debugging (Advanced)

See **An introduction to the Interactive Debugging Tools in** `R` **, Roger D Peng** for detailed usage.
http://www.biostat.jhsph.edu/~rpeng/docs/R-debug-tools.pdf
For a more modern approach https://www.rstudio.com/products/rstudio/release-notes/debugging-with-rstudio/

- warnings vs errors; converting warnings to errors; `stopifnot()`.
- what to do when I get an error: `traceback()`
- simple `print` statements are often useful.
- Use of `browser()` at key points in code.
- `debug(fn)`, `undebug(fn)`
- Using `recover()` rather than `browser()`

Warnings and errors

- A warning is softer than an error; if a warning is generated your program will still continue, whereas an error will stop the program.

```
> log(c(2, 1, 0, -1, 2))
Warning in log(c(2, 1, 0, -1, 2)):  NaNs produced
[1] 0.6931472 0.0000000      -Inf       NaN 0.6931472
> xor( c(TRUE, FALSE))
Error in xor(c(TRUE, FALSE)): argument "y" is missing,
with no default
```

- If you try to isolate warnings, you can change warnings to errors: `options(warn=2)`. See `?options` for further details.
- Add warnings and errors to your code using `warning()`, `stop()`.
- Can add “assertions” into your code to check that certain values hold.

```
> stopifnot(x>0)
```

- Other useful safety checks: `all(x>0)`, `any(x>0)`

Traceback

When your program generates an error, use `traceback()` to find out where it went wrong:

```
> start <- function() { go( sqrt(10)) }
> go <- function(x) { inner(x, '-13')}
> inner <- function(a, b) {
+   c <- sqrt(b)
+   a * log(c)
+ }
> start() ## error
> traceback() ## postmortem debugging
```

Single-stepping through your code

Use `browser()` to single-step through your code. Place it within your function at the point you want to examine (e.g.) local variables.

Can use `debug(function.name)` to step through entire function. `undebug()` will remove that debug call.
Within the browser, you can enter expressions as normal, or you can give a few debug commands:

- n: single-step
- c: exit browser and continue
- Q: exit browser and abort, return to top-level.
- where: show stack trace.

Debug on `stddev.R`

Safety-checks: browser

Here's a possible usage of browser() that I have in my code:

```
find.high <- function(x, t) {
  ## Return samples in x bigger than t.
  ## (Better to use x[x>t] in real-life!)
  max.length <- 100  ## should be upper limit...
  results <- rep(0, max.length)
  counter <- 0
  for (i in x) {
    if (i > t) {
      counter <- counter + 1
      if (counter > max.length) {
        browser()
      } else {
        results[counter] <- i
      }
    }
  }
  results[1:counter]
}
x <- rnorm(100)
find.high(x, 0.7)

x <- rnorm(1000)
(1- pnorm(0.7)) * length(x) ## expected.
find.high(x, 0.7)
```

recover

recover() is like browser(), except you can choose which level to inspect, rather than the level at which browser was called.
Following allows recover() to be launched when you hit an error:

```
options(error=recover)
```

Here we simply tell R that when an error is generated, we call the function "recover". The default is NULL, in which case stop is called.

From ?options:

> *Note that these need to specified as e.g. 'options(error=utils::recover)' in startup files such as '.Rprofile'.*

Packages

- `R` has a packaging system for external code.
- A **package** is loaded from a **library** using `library("pkg.name")`.
- Beware: don't call a package a library! A library is a group of folders where packages are stored . . .

```
> library()                      ## view available packages
> library(help="cluster")        ## what's in this?
> library("cluster")             ## load package
> example(pam)                   ## can use pam and friends.
> detach("package:cluster")      ## remove pkg.
```

CRAN: Comprehensive R Archive Network

CRAN: Site(s) for downloading `R` , and also its many contributed *packages*.
Mac/Win have a GUI for installing packages, or it can be done on the command line:

```
install.packages(c("splancs", "sp"))
```

Or, from the shell, you can do: `R CMD INSTALL mypackage.tar.gz`.
If asked to selected a CRAN mirror, in UK use:
https://www.stats.bris.ac.uk/R.

For Bioconductor

```
> source("http://www.bioconductor.org/biocLite.R")
> library("BiocInstaller")
> biocLite("Biobase")
```

Managing libraries

If you do not have write access to the default library, R will create a local one in your home directory. Multiple libraries are supported:

```
> .libPaths()

[1] "/home/stephen/NOBACKUP/RLIB"
[2] "/usr/lib/R/library"
```

You can also set R libraries as a global shell environment in your .bashrc file (e.g. linux)

```
export R_LIBS=$HOME/NOBACKUP/RLIB
```

(Be careful! Check that you are not overwriting an existing R_LIBS setting.)

Bioconductor

A success story of `R` . Started 2001 with aims to:

- provide access to stat/graphical methods for analysis of *genomic* data.
- link seamlessly to on-line databases (PubMed/GenBank).
- allow rapid development of extensible software.
- provide training in methods (short courses).
- promote software with high quality docs and reproducible research (vignettes) . . .
- Gentleman et al. (2004) Genome Biology 5:R80. `http://genomebiology.com/2004/5/10/R80`

Other topics of interest (Advanced)

- `S3`, `S4` and `S4 Reference classes` for OOP.
- Building your own packages. Useful for packaging up your code, data sets and documentation. You may wish to do this for large projects that you wish to share with others. Read *Writing* `R` *Extensions* manual and see `package.skeleton` to get started.
- Access to databases. Computational Biology datasets are often quite large, and you might wish to access data via databases. `R` package DBI provides common interface to SQLite, MySQL, Oracle. See Gentleman (2008), Chapter 8.