A beginners guide to solving biological problems in R

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Course material:
http://logic.sysbiol.cam.ac.uk/teaching/Rcourse/

Original slides by Ian Roberts and Robert Stojnić

Day 1 schedule

1. Introduction to R and its environment
2. Data structures
3. Data analysis example
4. Programming techniques
5. Statistics

Introduction to R and its environment

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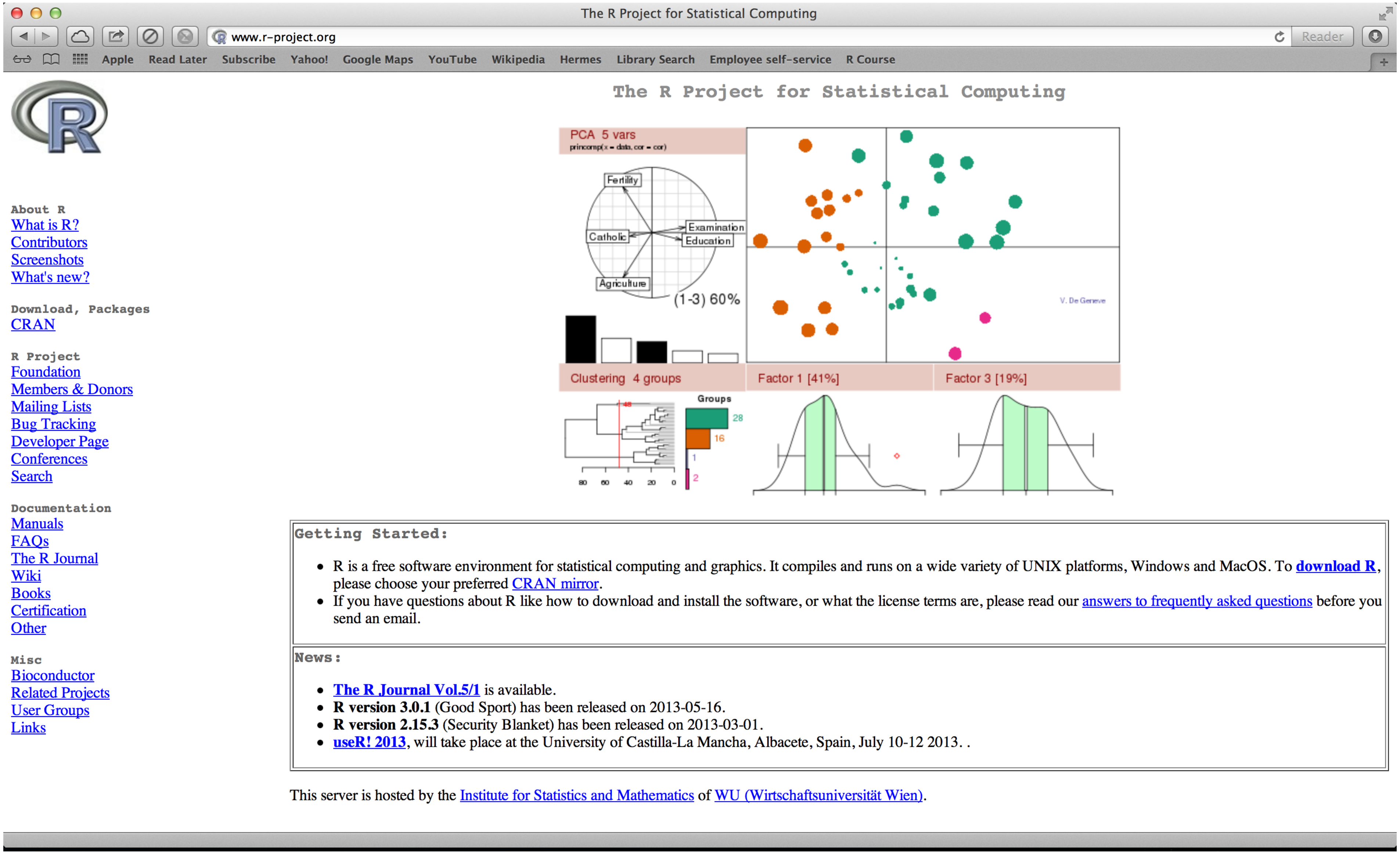
What’s R?

- A statistical programming environment
    - based on S
    - Suited to high level data analysis
- Open source & cross platform
- Extensive graphics capabilities
- Diverse range of add-on packages
- Active community of developers
- Thorough documentation



The R Project for Statistical Computing

About R
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Getting Started:

- R is a free software environment for statistical computing and graphics. It compiles and runs on a wide variety of UNIX platforms, Windows and MacOS. To **download R**, please choose your preferred CRAN mirror.
- If you have questions about R like how to download and install the software, or what the license terms are, please read our answers to frequently asked questions before you send an email.

News:

- **The R Journal Vol.5/1** is available.
- **R version 3.0.1** (Good Sport) has been released on 2013-05-16.
- **R version 2.15.3** (Security Blanket) has been released on 2013-03-01.
- **useR! 2013**, will take place at the University of Castilla-La Mancha, Albacete, Spain, July 10-12 2013. .

This server is hosted by the Institute for Statistics and Mathematics of WU (Wirtschaftsuniversität Wien).

www.r-project.org

Various platforms supported

- Release 3.0.1 (May 2013)
  - Base package
  - Contributed packages (general purposes extras)
  - ~4700 available packages
- Download from http://www.stats.bris.ac.uk/R/
- Windows, Mac and Linux versions available

- Executed using command line, or a graphical user interface (GUI)
- On this course, we use the RStudio GUI (www.rstudio.com)
- Everything you need is installed on the training machines
- If you are using your own machine, download both R and RStudio

Getting Started

- R is a program which, once installed on your system, can be launched and is immediately ready to take input directly from the user
- There are two ways to launch R:
  1) From the command line (particularly useful if you're quite familiar with Linux)
  2) As an application called RStudio (very good for beginners)

Prepare to launch R
From command line

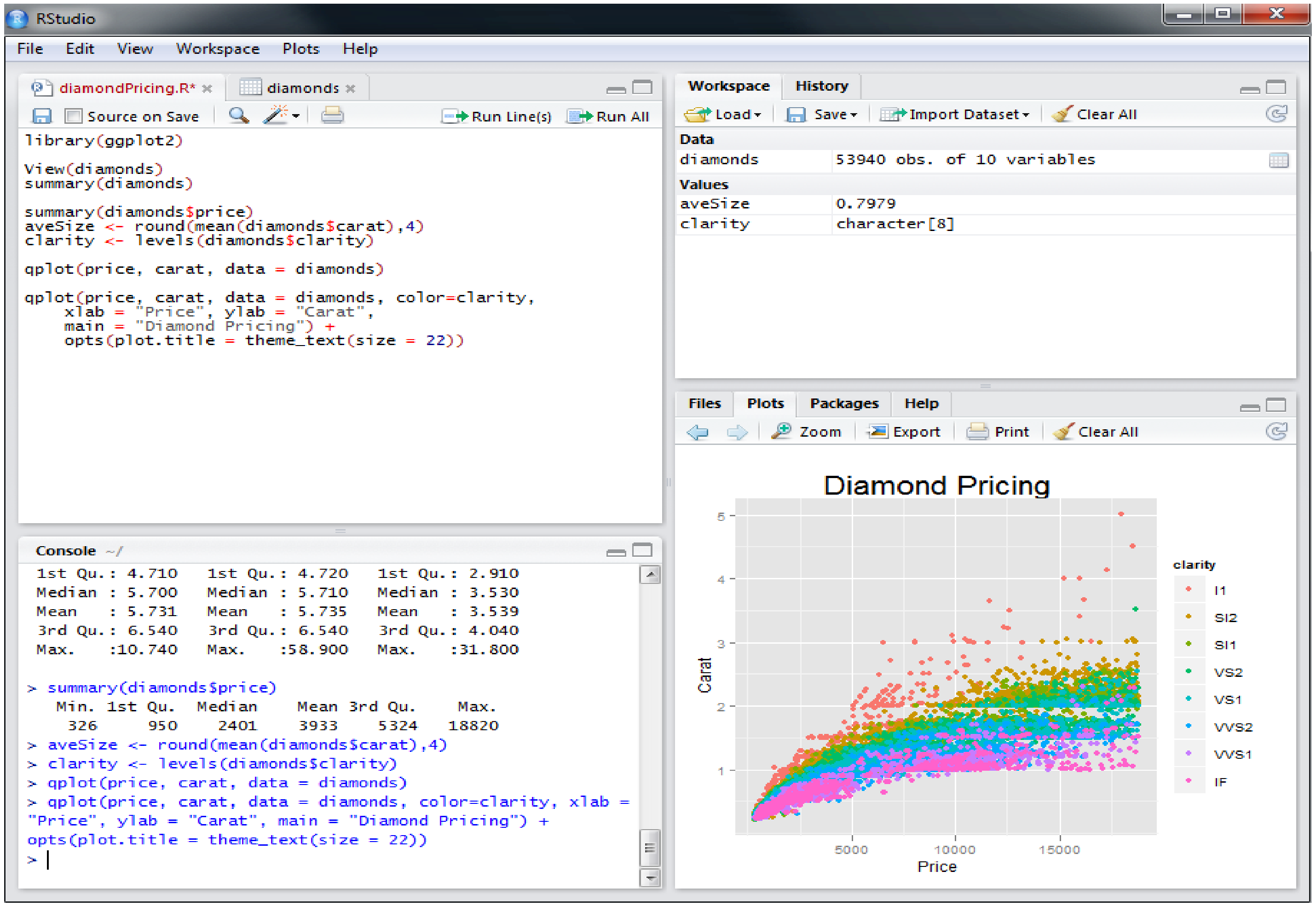
- To start R in Linux we need to enter the Linux console (also called Linux terminal and Linux shell)
- To start R, at the prompt simply type:

```
$ R
```

- If R doesn't print the welcome message, call us to help!

Prepare to launch R
Using RStudio

- To launch RStudio, find the RStudio icon in the menu bar on the left of the screen and double-click


RStudio
File Edit View Workspace Plots Help
diamondPricing.R* diamonds
Source on Save Run Line(s) Run All
Workspace History
Load Save Import Dataset Clear All
Files Plots Packages Help
Zoom Export Print Clear All
Console ~/
Diamond Pricing
Carat
Price
clarity
I1
SI2
SI1
VS2
VS1
VVS2
VVS1
IF

```
library(ggplot2)

View(diamonds)
summary(diamonds)

summary(diamonds$price)
aveSize <- round(mean(diamonds$carat),4)
clarity <- levels(diamonds$clarity)

qplot(price, carat, data = diamonds)

qplot(price, carat, data = diamonds, color=clarity,
    xlab = "Price", ylab = "Carat",
    main = "Diamond Pricing") +
    opts(plot.title = theme_text(size = 22))
```

Data	
diamonds	53940 obs. of 10 variables
Values	
aveSize	0.7979
clarity	character[8]

```
 1st Qu.: 4.710   1st Qu.: 4.720   1st Qu.: 2.910
 Median : 5.700   Median : 5.710   Median : 3.530
 Mean   : 5.731   Mean   : 5.735   Mean   : 3.539
 3rd Qu.: 6.540   3rd Qu.: 6.540   3rd Qu.: 4.040
 Max.   :10.740   Max.   :58.900   Max.   :31.800

> summary(diamonds$price)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
    326     950    2401    3933    5324   18820
> aveSize <- round(mean(diamonds$carat),4)
> clarity <- levels(diamonds$clarity)
> qplot(price, carat, data = diamonds)
> qplot(price, carat, data = diamonds, color=clarity, xlab =
"Price", ylab = "Carat", main = "Diamond Pricing") +
opts(plot.title = theme_text(size = 22))
> |
```

The Working Directory (wd)

- Like many programs R has a concept of a working directory (wd)
- It is the place where R will look for files to execute and where it will save files, by default
- For this course we need to set the working directory to the location of the course scripts
- At the command prompt in the terminal or in RStudio console type:

```
> setwd("R_course/Day_1_scripts")
```

- Alternatively in RStudio use the mouse and browse to the directory location
- Tools → Set Working Directory → Choose Directory...

Basic concepts in R
command line calculation

- The command line can be used as a calculator. Type:

```
> 2 + 2
[1] 4


> 20/5 - sqrt(25) + 3^2
[1] 8


> sin(pi/2)
[1] 1
```

- Note: The number in the square brackets is an indicator of the position in the output. In this case the output is a 'vector' of length 1 (i.e. a single number). More on vectors coming up...

Basic concepts in R
variables

- A variable is a letter or word which takes (or contains) a value. We use the assignment 'operator', **<-**

```
> x <- 10
> x
[1] 10
> myNumber <- 25
> myNumber
[1] 25
```

- We can perform arithmetic on variables:

```
> sqrt(myNumber)
[1] 5
```

- We can add variables together:

```
> x + myNumber
[1] 35
```

Basic concepts in R
variables

- We can change the value of an existing variable:

```
> x <- 21
> x
[1] 21
```

- We can set one variable to equal the value of another variable:

```
> x <- myNumber
> x
[1] 25
```

- We can modify the contents of a variable:

```
> myNumber <- myNumber + sqrt(16)
[1] 29
```

Basic concepts in R
functions

- **Functions** in R perform operations on **arguments** (the input(s) to the function). We have already used **sin(x)** which returns the sine of **x**. In this case the function has one argument, **x**. Arguments are *always* contained in parentheses, i.e. curved brackets **()**, separated by commas.
- Try these:

```
> sum(3, 4, 5, 6)
[1] 18
> max(3, 4, 5, 6)
[1] 6
> min(3, 4, 5, 6)
[1] 3
```

- Arguments can be named or unnamed, but if they are unnamed they must be ordered (we will see later how to find the right order).

```
> seq(from=2, to=10, by=2)
[1] 2 4 6 8 10
> seq(2, 10, 2)
[1] 2 4 6 8 10
```

Basic concepts in R
vectors

- The basic data structure in R is a **vector** – an ordered collection of values. R even treats single values as 1-element vectors. The function **c()** *combines* its arguments into a vector:

```
> x <- c(3, 4, 5, 6)
> x
[1] 3 4 5 6
```

- As mentioned, the square brackets **[]** indicate position within the vector (the **index**). We can extract individual elements by using the **[]** notation:

```
> x[1]
[1] 3
> x[4]
[1] 6
```

- We can even put a vector inside the square brackets (vector indexing):

```
> y <- c(2, 3)
> x[y]
[1] 4 5
```

Basic concepts in R
vectors

- There are a number of shortcuts to create a vector. Instead of:

```
> x <- c(3, 4, 5, 6, 7, 8, 9, 10, 11, 12)
```

- we can write:

```
> x <- 3:12
```

- or we can use the **seq()** function, which returns a vector:

```
> x <- seq(2, 10, 2)
> x
 [1] 2 4 6 8 10
> x <- seq(2, 10, length.out = 7)
```

-
```
> x
 [1] 2.00000 3.33333 4.66667 6.00000 7.33333 8.66667 10.00000
```

- or the **rep()** function:

```
> y <- rep(3, 5)
```

-
```
> y
[1] 3 3 3 3 3
> y <- rep(1:3, 5)
> y
[1] 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3
```

Basic concepts in R

vectors

- We have seen some ways of extracting elements of a vector. We can use these shortcuts to make things easier (or more complex!)

```
> x <- 3:12
> x[3:7]
[1] 5 6 7 8 9
> x[seq(2, 6, 2)]
[1] 4 6 8
> x[rep(3, 2)]
[1] 5 5
```

- We can add an element to a vector

```
> y <- c(x, 1)
> y
[1] 3 4 5 6 7 8 9 10 11 12 1
```

- We can glue vectors together

```
> z <- c(x, y)
> z
[1] 3 4 5 6 7 8 9 10 11 12 3 4 5 6 7 8 9 10 11 12 1
```

Basic concepts in R
vectors

- We can remove element(s) from a vector

```
> x <- 3:12
> x[-3]
 [1]  3  4  6  7  8  9 10 11 12
> x[-(5:7)]
[1]  3  4  5  6 10 11 12
> x[-seq(2, 6, 2)]
[1]  3  5  7  9 10 11 12
```

- Finally, we can modify the contents of a vector

```
> x[6] <- 4
> x
[1]  3  4  5  6  7  4  9 10 11 12
> x[3:5] <- 1
> x
[1]  3  4  1  1  1  4  9 10 11 12
```

- Remember! **Square** brackets for indexing **[]**, **parentheses** for function arguments **()**.

Basic concepts in R
vector arithmetic

- When applying all standard arithmetic operations to vectors, application is element-wise

```
> x <- 1:10
> y <- x*2
> y
[1] 2 4 6 8 10 12 14 16 18 20
> z <- x^2
> z
[1] 1 4 9 16 25 36 49 64 81 100
```

- Adding two vectors

```
> y + z
[1] 3 8 15 24 35 48 63 80 99 120
```

- If vectors are not the same length, the shorter one will be recycled:

```
> x + 1:2
[1] 2 4 4 6 6 8 8 10 10 12
```

- But be careful if the vector lengths aren't factors of each other:

```
> x + 1:3
```

Exercise: genes and genomes

- Let's try some vector arithmetic. Here are the genome lengths and number of protein coding genes for several model organisms:

Species	Genome size (Mb)	Protein coding genes
Homo sapiens	3,102	20,774
Mus musculus	2,731	23,139
Drosophila melanogaster	169	13,937
Caenorhabditis elegans	100	20,532
Saccharomyces cerevisiae	12	6,692

- Create **genome.size** and **coding.genes** vectors to hold the data in each column using the **c** function.

Exercise: genes and genomes

- Let's assume a coding gene has an average length of 1.5 kilobases. On average, how many base pairs of each genome is made of coding genes? Create a new vector to record this called **coding.bases**.
- What percentage of each genome is made up of protein coding genes? Use your **coding.bases** and **genome.size** vectors to calculate this. (See earlier slides for how to do division in R.)
- How many times more bases are used for coding in the human genome compared to the yeast genome? How many times more bases are in the human genome in total compared to the yeast genome? Look up indices of your vectors to find out.

Answers to genome exercise

- Creating vectors:

```
> genome.size<-c(3102,2731,169,100,12)
> coding.genes<-c(20774,23139,13937,20532,6692)
```

- To calculate the number of coding bases, we need to use the same scale as we used for genome size: 1.5 kilobases is 0.0015 Megabases.

```
> coding.bases<-coding.genes*0.0015
> coding.bases
[1] 31.1610 34.7085 20.9055 30.7980 10.0380
```

- To calculate the percentage of coding bases in each genome:

```
> coding.pc<-coding.bases/genome.size*100
> coding.pc
[1]  1.004545  1.270908 12.370118 30.798000 83.650000
```

- To compare human to yeast:

```
> coding.bases[1]/coding.bases[5]
[1] 3.104304
> genome.size[1]/genome.size[5]
[1] 258.5
```

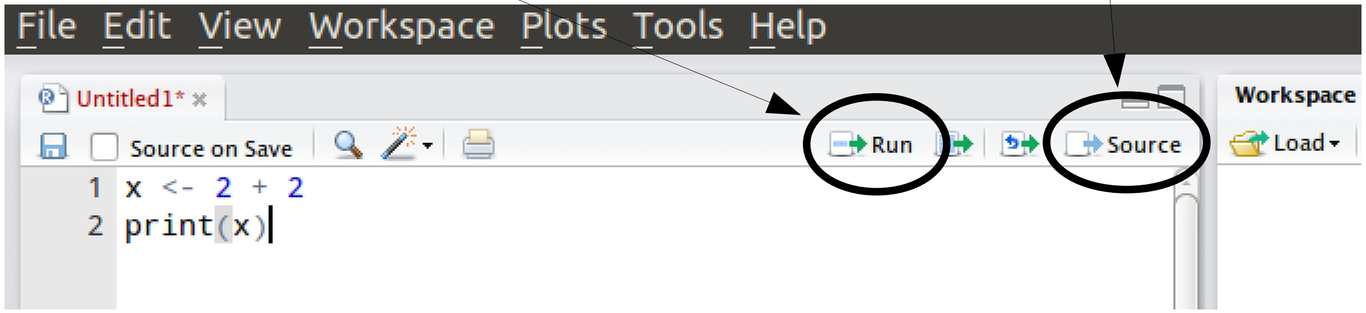
Writing scripts with Rstudio

Typing lots of commands directly to R can be tedious. A better way is to write the commands to a file and then load it into R.

- Click on **File -> New** in Rstudio
- Type in some R code, e.g.

```
x <- 2 + 2
print(x)
```

- Click on **Run** to execute the **current line**, and **Source** to execute the **whole script**



```
x <- 2 + 2
print(x)
```

Sourcing can also be performed manually with `source("myScript.R")`

Getting Help

- To get help on any R function, type `?` followed by the function name. For example:

```
> ?seq
```

- This retrieves the syntax and arguments for the function. You can see the default order of arguments here. The help page also tells you which **package** it belongs to.
- There will typically be example usage, which you can test using the **example** function:

```
> example(seq)
```

- If you can't remember the exact name type `??` followed by your guess. R will return a list of possibles

```
> ??rint
```

Interacting with the R console

- R console symbols
    - ; end of line
        - Enables multiple commands to be placed on one line of text
    - # comment
        - indicates text is a comment and not executed
    - + command line wrap
        - R is waiting for you to complete an expression
- Ctrl-c or escape to clear input line and try again
- Ctrl-l to clear window
- Press q to leave help (using R from the terminal)
- Use the TAB key for command auto completion
- Use up and down arrows to scroll through the command history

R packages

- R comes ready loaded with various libraries of functions called **packages**. e.g. the function **sum()** is in the **base** package and **sd()**, which calculates the standard deviation of a vector, is in the **stats** package
- There are 1000s of additional packages provided by third parties, and the packages can be found in numerous server locations on the web called **repositories**
- The two repositories you will come across the most are
    - **The Comprehensive R Archive Network (CRAN)**
    - **Bioconductor**
- CRAN is mirrored in many locations. Set your local mirror in RStudio using Tools → Options, and choose a CRAN mirror
- Set the Bioconductor package download tool by typing:

```
> source("http://bioconductor.org/biocLite.R")
```

- Bioconductor packages are then loaded with the biocLite() function:

```
> biocLite("PackageName")
```

R packages

- 4700+ packages on CRAN:
  - Use CRAN search to find functionality you need:

    http://cran.r-project.org/search.html
  - Or, look for packages by theme:

    http://cran.r-project.org/web/views/
- 670+ packages in Bioconductor:
  - Specialised in genomics:

    http://www.bioconductor.org/packages/release/bioc/
- **Other repositiories:**
- 1600+ projects on R-forge:
  - http://r-forge.r-project.org/
- R graphical manual:
  - http://rgm3.lab.nig.ac.jp/RGM

Bottomline: **always** first look if there is already an R package that does what you want before trying to implement it yourself

Exercise: Install Packages Matrix and aCGH

- Matrix is a CRAN extras package
  - Use **`install.packages()`** function...

    `install.packages("Matrix")`
  - or in RStudio goto Tools → Install Packages... and type the package name
- aCGH is a BioConductor package (www.bioconductor.org)
  - Use **`biocLite()`** function

  `biocLite("aCGH")`

- R needs to be told to use the new functions from the installed packages
  - Use **`library(…)`** function to load the newly installed features

    ```
    library("Matrix") # loads matrix functions
    library("aCGH") # loads aCGH functions
    ```
  - **`library()`**
    - Lists all the packages you've got installed locally