BGGN 213

Data analysis with R

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http://thegrantlab.org/bggn213

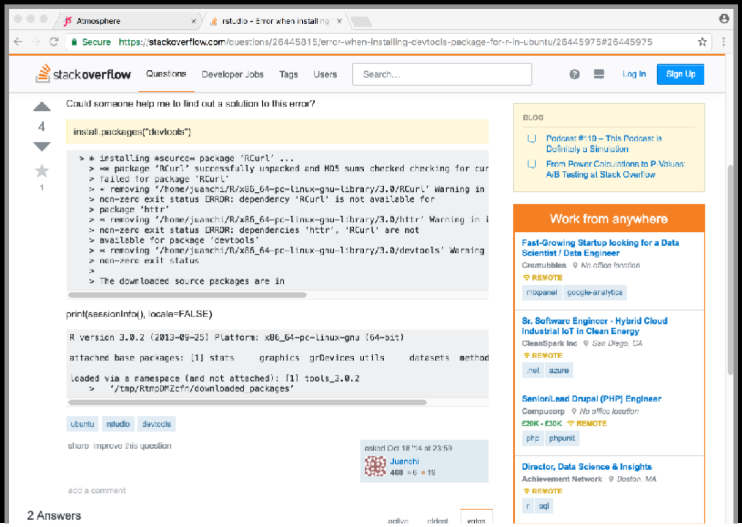
Recap From Last Time:

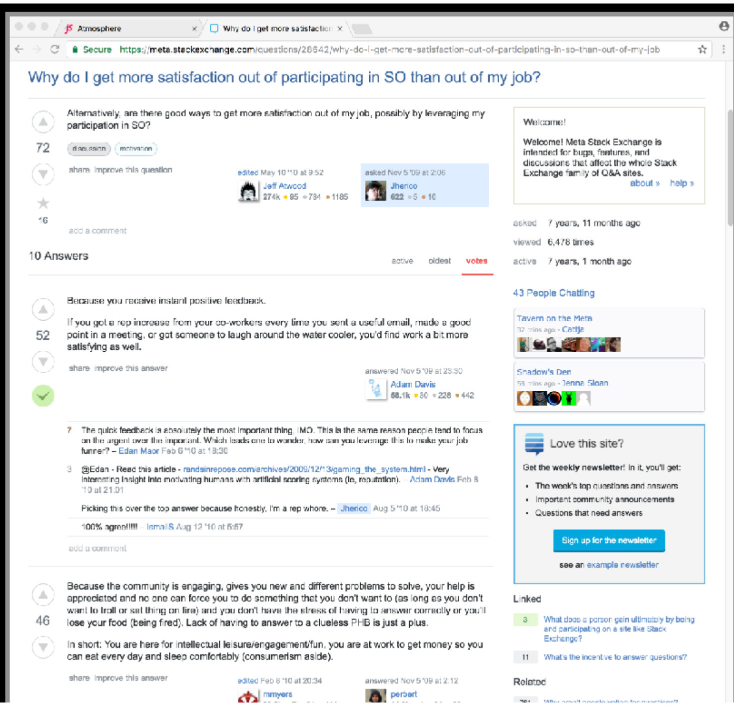
- **UNIX pipes and redirects:** How UNIX commands can be combined to generate flexible solutions to data manipulation tasks.
- **UNIX commands:** Further exploration of the 22 key UNIX commands that you will use during ~95% of your future UNIX work
- **Jetstream:** Starting up instances; ssh access from your Terminal application; *Demoed* installing and running bioinformatics software for a genome scale annotation.
- **Cloud computing:** Many bioinformatic tasks require large amounts of computing power and can't realistically be run on your own machine. These tasks are best performed using remote computers or cloud computing, which can only be accessed through a shell.

Today's Learning Goals

- Familiarity with R's basic syntax.
- Familiarity with major R data structures.
- Understand the basics of using functions.
- Be able to use R to read and parse comma-separated (.csv) formatted files ready for subsequent analysis.
- Appreciate how you can use R scripts to aid with reproducibility.

Side-Note: StackOverflow is your friend!



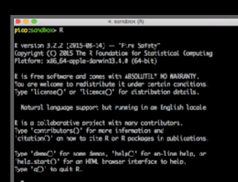


What is R?

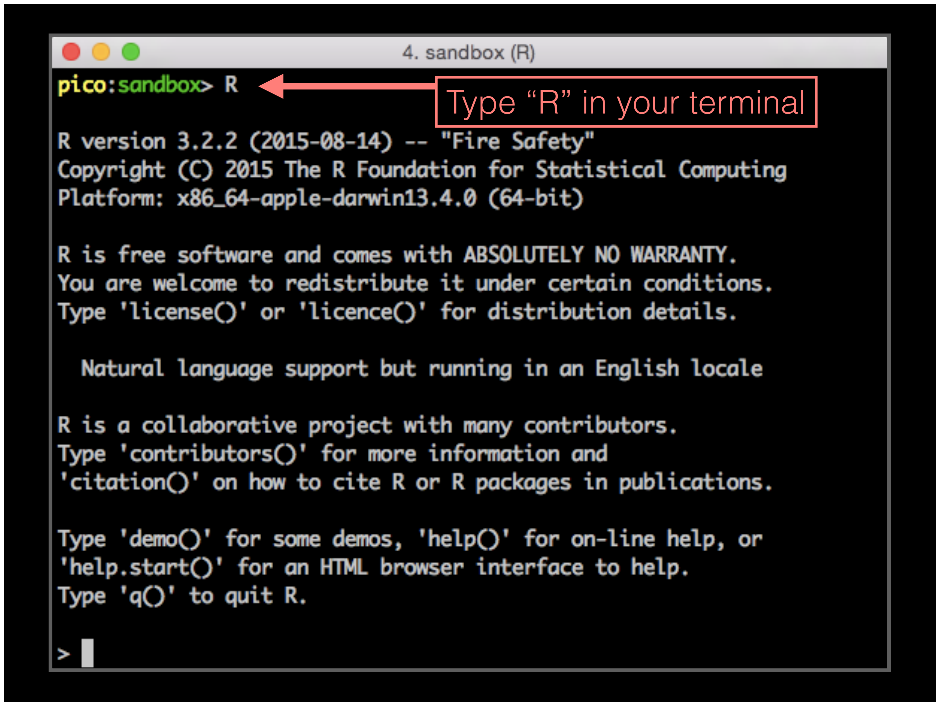
R is a freely distributed and widely used programing **language** and **environment** for statistical computing, data analysis and graphics.

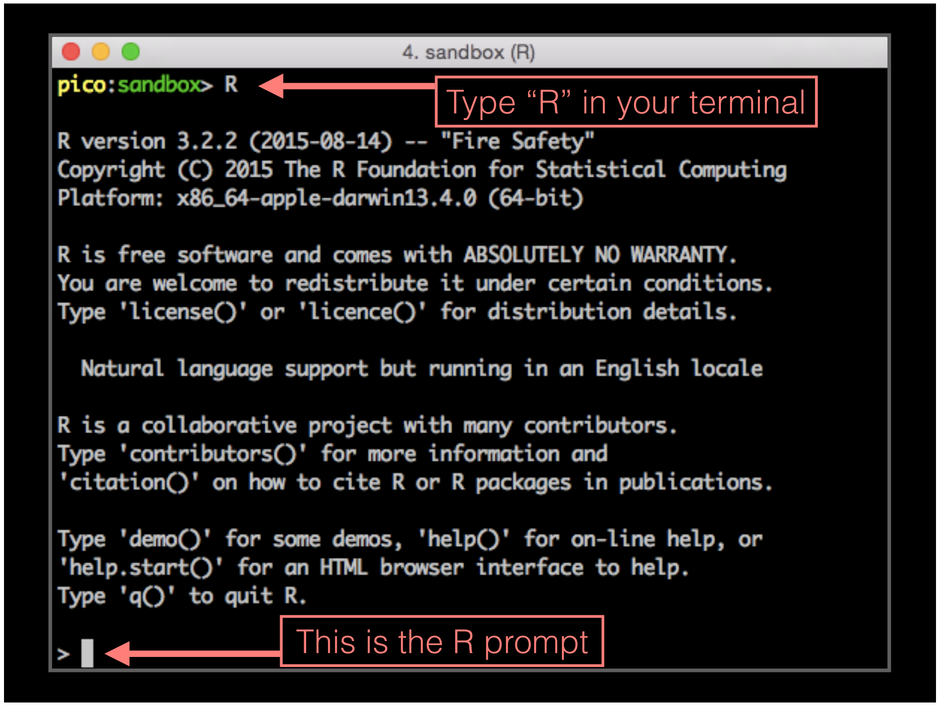
R provides an unparalleled interactive environment for data analysis.

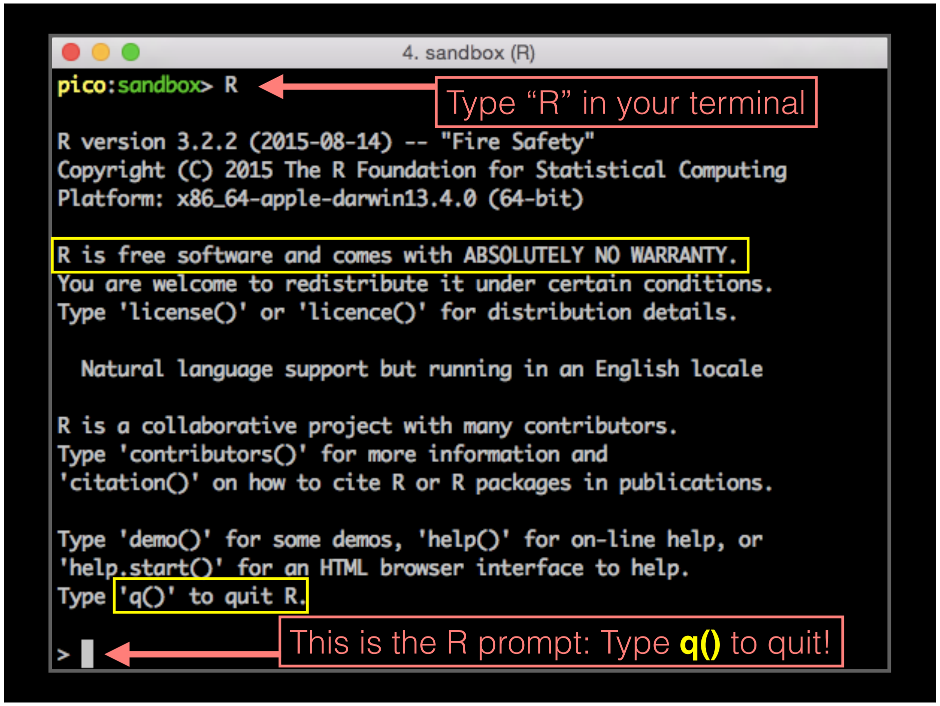
It is script-based (*i.e.* driven by computer code) and not GUI-based (point and click with menus).



```
4. sandbox (R)
pico:sandbox> R

R version 3.2.2 (2015-08-14) -- "Fire Safety"
Copyright (C) 2015 The R Foundation for Statistical Computing
Platform: x86_64-apple-darwin13.4.0 (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.

>
```







What R is **NOT**

A performance optimized software library for incorporation into your own C/C++ etc. programs.

A molecular graphics program with a slick GUI.

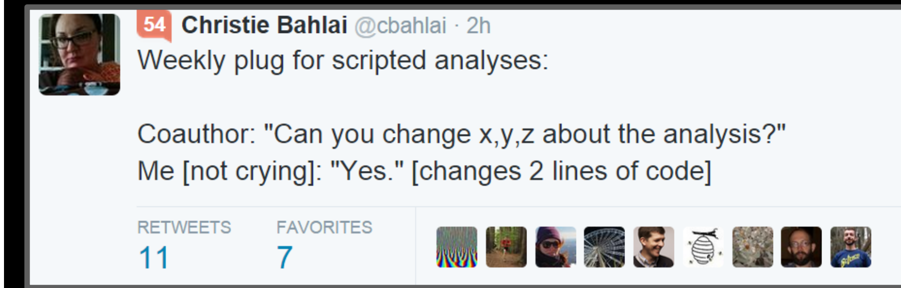
Backed by a commercial guarantee or license.

Microsoft Excel!

What about Excel?

- Data manipulation is easy
- Can see what is happening
- **But**: graphics are poor
- Looping is hard
- Limited statistical capabilities
- Inflexible and irreproducible
- There are many many things Excel just cannot do!

Use the right tool!



54 **Christie Bahlai** @cbahlai · 2h

Weekly plug for scripted analyses:

Coauthor: "Can you change x,y,z about the analysis?"
Me [not crying]: "Yes." [changes 2 lines of code]

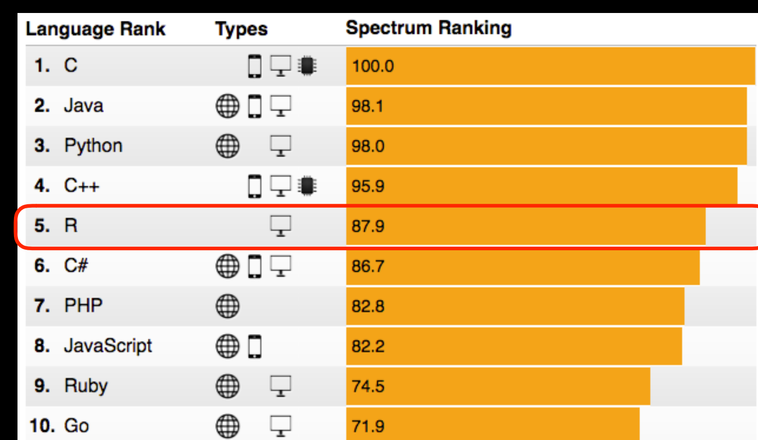
RETWEETS 11 FAVORITES 7

Rule of thumb: Every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly!

Why use R?

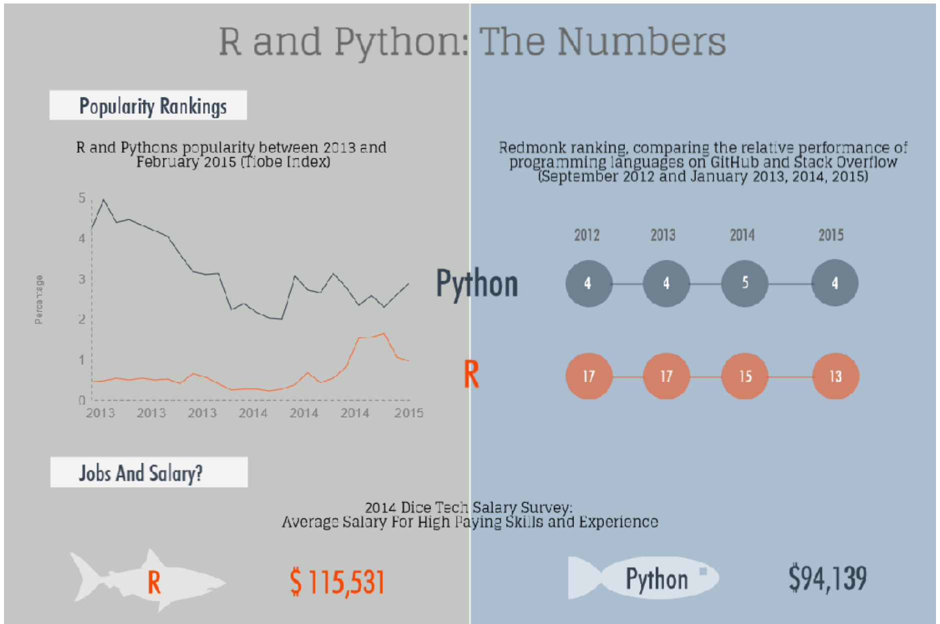
Productivity
Flexibility
Designed for data analysis

IEEE 2016 Top Programming Languages



Language Rank	Types	Spectrum Ranking
1. C		100.0
2. Java		98.1
3. Python		98.0
4. C++		95.9
5. R		87.9
6. C#		86.7
7. PHP		82.8
8. JavaScript		82.2
9. Ruby		74.5
10. Go		71.9

http://spectrum.ieee.org/computing/software/the-2016-top-programming-languages



http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html?utm_medium=email&utm_source=flipboard

- R is the “lingua franca” of data science in industry and academia.
- Large user and developer community.
  - As of Aug 1st 2016 there are 8811 add on **R packages** on **CRAN** and 1211 on **Bioconductor** - more on these later!
- Virtually every statistical technique is either already built into R, or available as a free package.
- Unparalleled exploratory data analysis environment.

Modularity	Core R functions are modular and work well with others
Interactivity	R offers an unparalleled exploratory data analysis environment
Infrastructure	Access to existing tools and cutting-edge statistical and graphical methods
Support	Extensive documentation and tutorials available online for R
R Philosophy	Encourages open standards and reproducibility

Modularity	Core R functions are modular and work well with others
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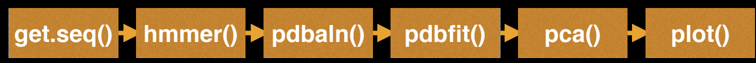
Modularity

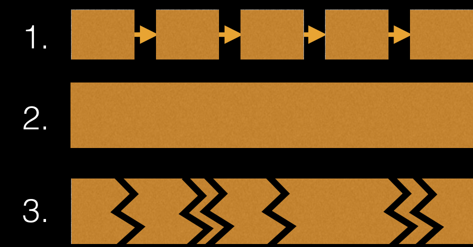
R was designed to allow users to interactively build complex workflows by interfacing smaller ‘**modular’ functions** together.



An alternative approach is to write a **single complex program** that takes raw data as input, and after hours of data processing, outputs publication figures and a final table of results.

‘Scripting’ approach

Another common approach to bioinformatics data analysis is to write individual scripts in Perl/ Python/Awk/C etc. to carry out each subsequent step of an analysis



This can offer many advantages but can be challenging to make robustly modular and interactive.

Interactivity & exploratory data analysis

Learning R will give you the freedom to explore and experiment with your data.

“*Data analysis, like experimentation, must be considered as a highly interactive, iterative process, whose actual steps are selected segments of a stubbily branching, tree-like pattern of possible actions*”. [**J. W. Tukey**]

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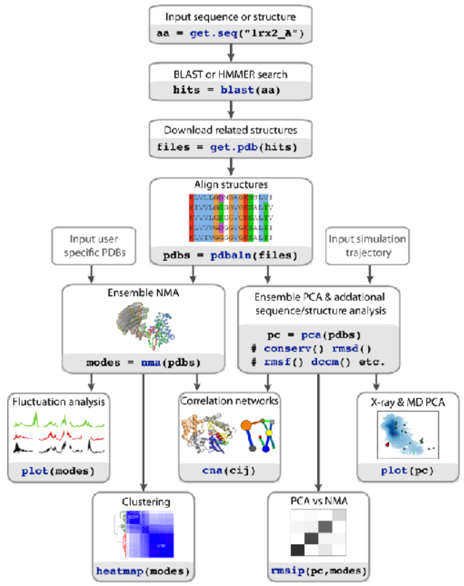
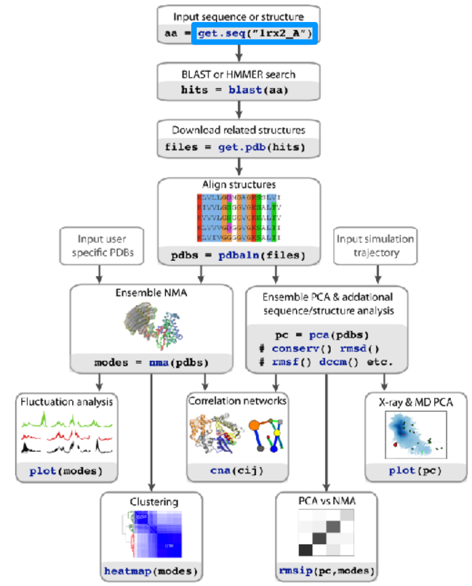
Bioinformatics data is intrinsically **high dimensional** and frequently ‘messy’ requiring **exploratory data analysis** to find patterns - both those that indicate interesting biological signals or suggest potential problems.

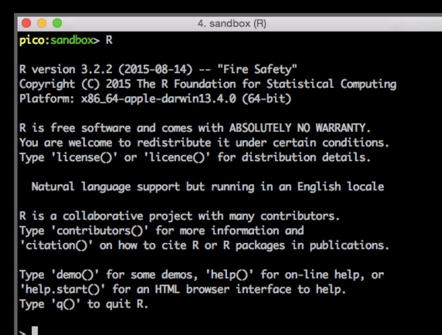


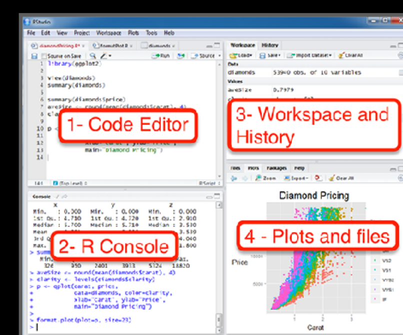
R Features = **functions()**



How do we use R?

Two main ways to use R

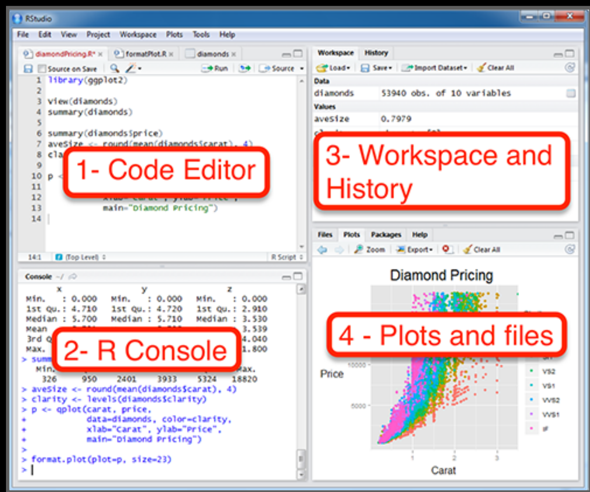




1. Terminal

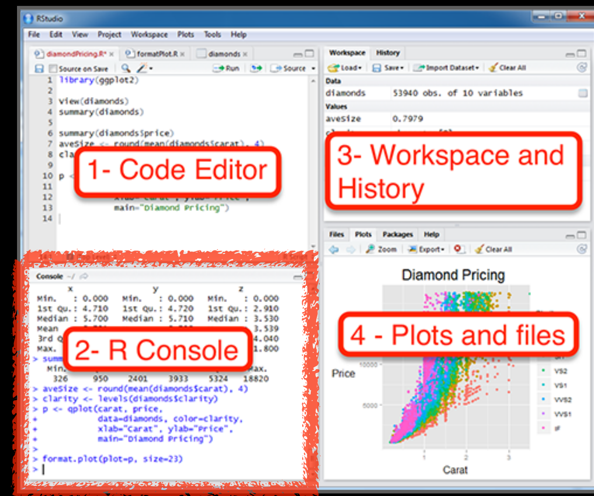
2. RStudio

We will use RStudio today



Lets get started…

Do it Yourself!



Some simple R commands

Do it Yourself!

R prompt!

1.
```
> 2+2
[1] 4
```
Result of the command

2.
```
> 3^2
[1] 9
```

3.
```
> sqrt(25)
[1] 5
```

4.
```
> 2*(1+1)
[1] 4
```

5.
```
> 2*1+1
[1] 3
```
Order of precedence

6.
```
> exp(1)
[1] 2.718282
```

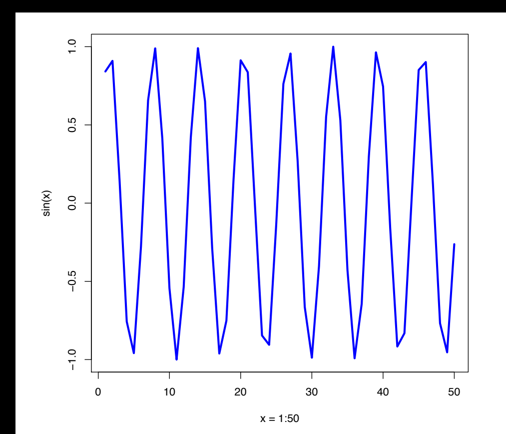
7.
```
> log(2.718282)
[1] 1
```

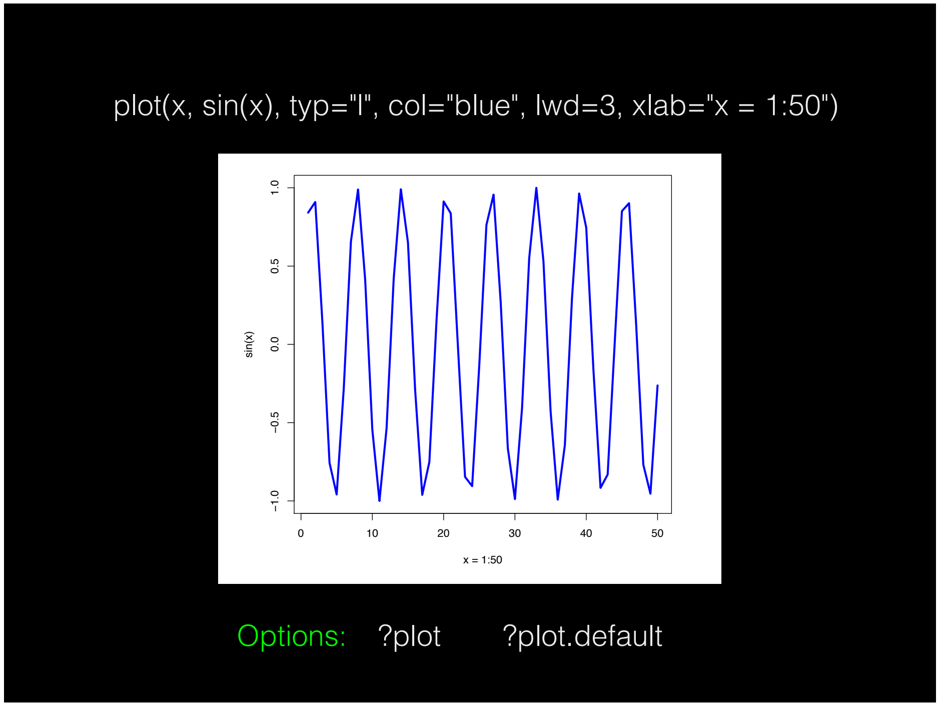
8.
```
> log(10, base=10)
[1] 1
```
Optional argument

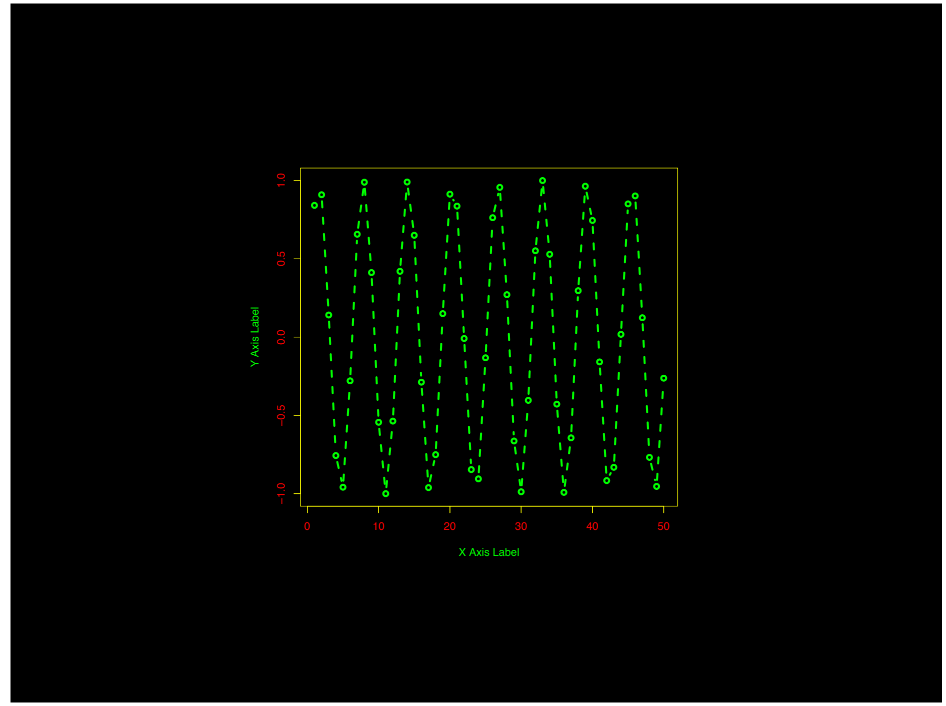
9.
```
> log(10
+        , base = 10)
[1] 1
```
Incomplete command

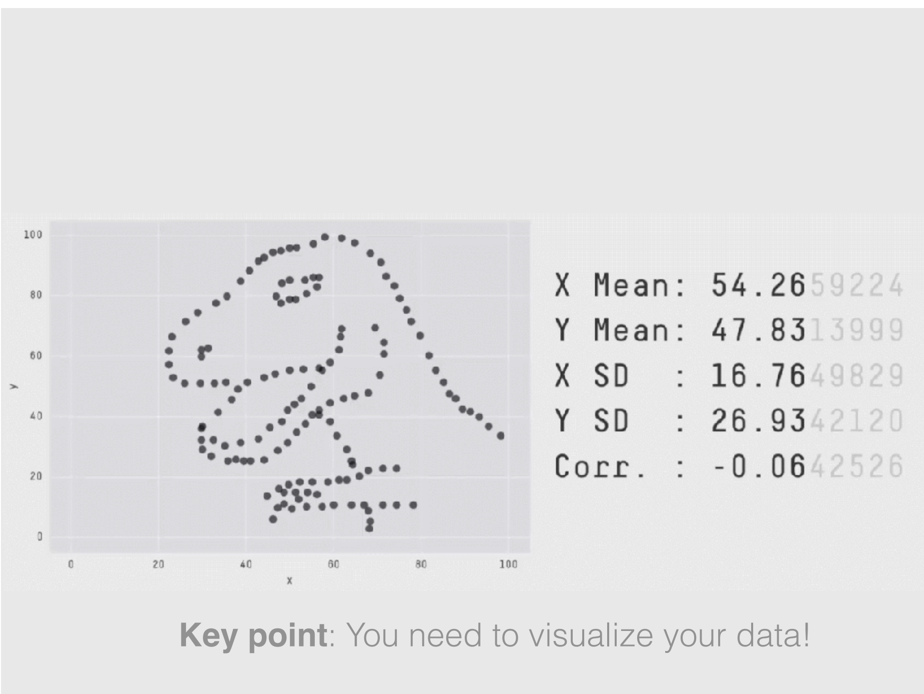
10.
```
> x=1:50
> plot(x, sin(x))
```

Does your plot look like this?




plot(x, sin(x), typ="l", col="blue", lwd=3, xlab="x = 1:50")
sin(x)
x = 1:50
Options: ?plot ?plot.default


Y Axis Label
X Axis Label


X Mean: 54.2659224
Y Mean: 47.8313999
X SD : 16.7649829
Y SD : 26.9342120
Corr. : -0.0642526
Key point: You need to visualize your data!


Learning a new
language is hard!

Error Messages

Sometimes the commands you enter will generate errors.
Common beginner examples include:

- Incomplete brackets or quotes *e.g.*
  ((4+8)*20 <enter>
  +
  This eturns a + here, which means you need to enter the remaining bracket - R is waiting for you to finish your input.
  Press <ESC> to abandon this line if you don't want to fix it.
- Not separating arguments by commas *e.g.*
  plot(1:10 col="red")
- Typos including miss-spelling functions and using wrong type of brackets *e.g.*
  exp{4}

Do it Yourself!

Your turn!

http://tinyurl.com/bggn213-rintro

If you have done the introductory DataCamp course then feel free to jump to section #3 *Object Assignment*

Topics Covered:

Calling Functions
Getting help in R
Vectors and vectorization
Workspace and working directory
RStudio projects

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Calling Functions
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Workspace and working directory
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Vectors

- Vectors are the most basic data structure in R
- All elements of a vector must be the same type

```
dbl_var <- c(1, 2.5, 4.5)
log_var <- c(TRUE, FALSE, T, F)
chr_var <- c("these are", "some", "strings")
```

- When you attempt to combine different types they will be coerced to the most flexible type.

```
var <- c(1, "G", "4", 0.05, TRUE)
```

Names

- You can name a vector in several ways:
  - When creating it: `x <- c(a = 1, b = 2, c = 3)`
  - By modifying an existing vector in place:

```
x <- 1:3; names(x) <- c("a", "b", "c")
```

- You can then use the names to access (subset) vector elements:

```
x [ c("b", "a") ]
```

Why is this useful?

- Because if you know the name (i.e. your label) then you don't have to remember which element of a vector the data you are after was stored in. Consider this *fictional* example:

```
> grades <- c(alice=80, barry=99, chandra=60, chris=100)
> grades["barry"]
barry
  99
> which.max(grades)
chris
   4
> sort(grades)
chandra   alice   barry   chris
     60      80      99     100
```

What would happen?

1. `> x <- 1:3; names(x) <- c("a", "b", “c”, “d”)`
2. `> x <-1:3; names(x) <- 3:1;  x[3]`
3. `> x["3"]`

R has many data structures

These included:

- **vector**
- **data frame**
- list
- matrix
- factors

data.frame

- **data.frame** is the *de facto* data structure for most **tabular data** and what we use for statistics and plotting with **ggplot2** - more on this later!
- Arguably the most important R data structure
- Data frames can have additional attributes such as **rownames()** and **colnames()**, which can be useful for annotating data, with things like subject_id or sample_id

data.frame continued…

Do it Yourself!

- Created with the function **data.frame()**

```
dat <- data.frame(id = letters[1:10], x = 1:10, y = 11:20)
```

- Or more commonly when reading delimited files (*i.e.* **importing data**) with the functions **read.csv()**, **read.table()**, **read_xlsx()** *etc…*

```
dep <- read.csv2("http://bio3d.uib.no/data/pdb_deposition2.csv")
```

- R Studio can do this for you via:
  File > Import Dataset > From CSV…

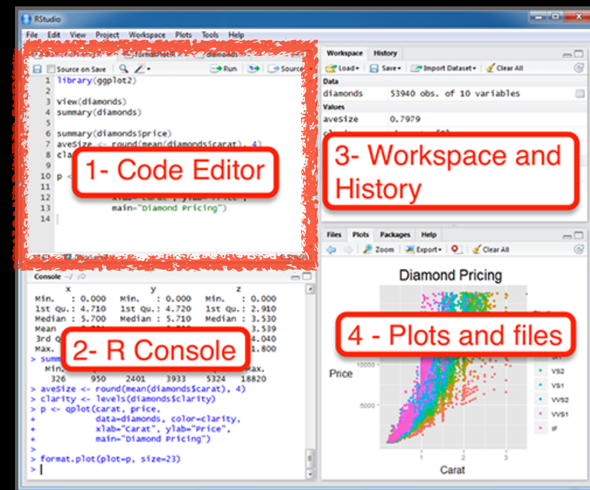
Useful **data.frame** Functions

- **head()** -and **tail()** shows first 6 rows and last 6 rows respectively
- **dim()** - returns the dimensions (i.e. number of rows and columns)
- **nrow()** and **ncol()** returns the number of rows and columns separately.
- **rownames()** and **colnames()**- shows the names attribute for rows and columns
- **str()** - returns the structure including name, type and preview of data in each column

Key Points

- R's basic data types are **logical**, **character**, **numeric**, integer and complex.
- R's basic data structures include **vectors**, lists, **data frames**, matrices and factors.
- Objects may have attributes, such as **name**, **dim**ension, and **class**.

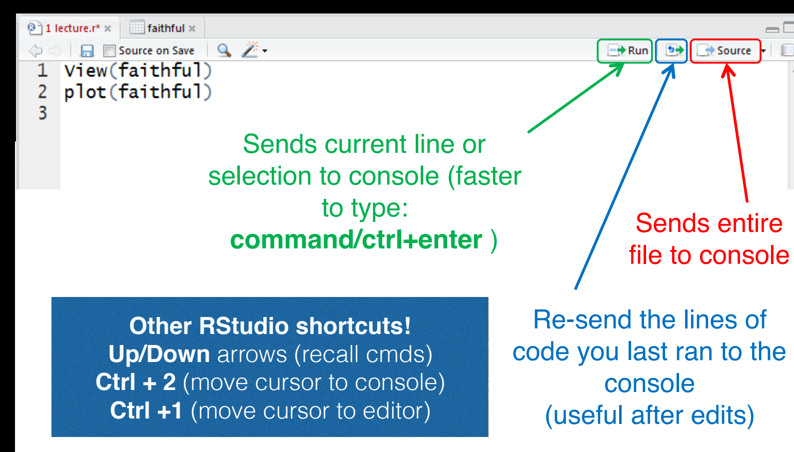
Side-note: Use the code editor for R scripts



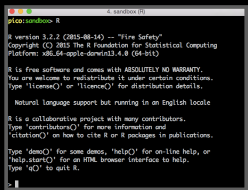
R scripts

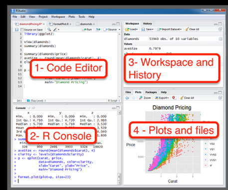
- A simple text file with your R commands (*e.g.* lecture7.r) that contains your R code for one complete analysis
- **Scientific method**: complete record of your analysis
- **Reproducible**: rerunning your code is easy for you or someone else
- In RStudio, select code and type <ctrl+enter> to run the code in the R console
- **Key point**: Save your R script!

Side-note: RStudio shortcuts



Rscript: Third way to use R





> Rscript --vanilla my_analysis.R

1. Terminal **2. RStudio** **3. Rscript**

From the command line!
> Rscript --vanilla **my_analysis.R**
or within R: source(**my_analysis.R**)

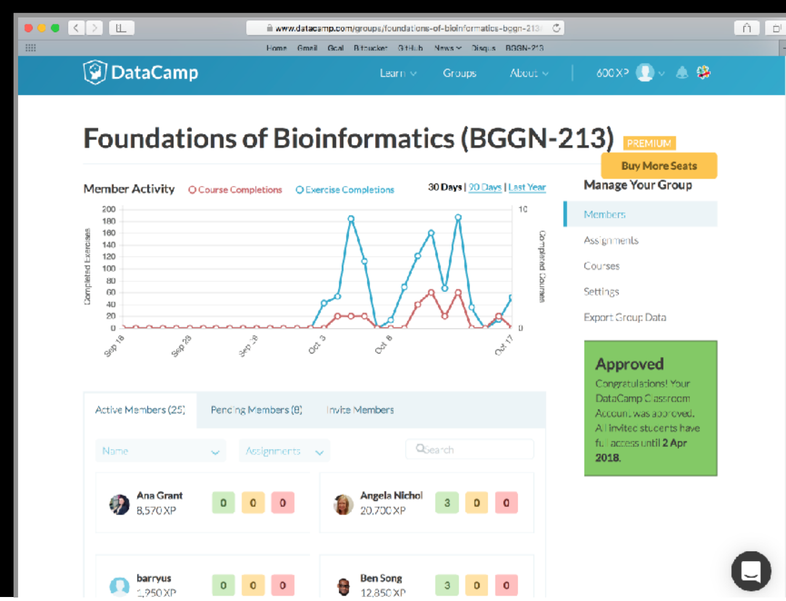
Side-Note: R workspaces

- When you close RStudio, SAVE YOUR .R SCRIPT
- You can also save data and variables in an R workspace, but this is generally not recommended
- Exception: working with an enormous dataset
- Better to start with a clean, empty workspace so that past analyses don't interfere with current analyses
- rm(list = ls()) clears out your workspace
- You should be able to reproduce everything from your R script, so save your R script, don't save your workspace!

Learning Resources

- **TryR**. An excellent interactive online R tutorial for beginners.
  < http://tryr.codeschool.com/ >
- **RStudio**. A well designed reference card for RStudio.
  < https://help.github.com/categories/bootcamp/ >
- **DataCamp**. Online tutorials using R in your browser.
  < https://www.datacamp.com/ >
- **R for Data Science**. A new O'Reilly book that will teach you how to do data science with R, by Garrett Grolemund and Hadley Wickham.
  < http://r4ds.had.co.nz/ >

< https://www.datacamp.com/ >



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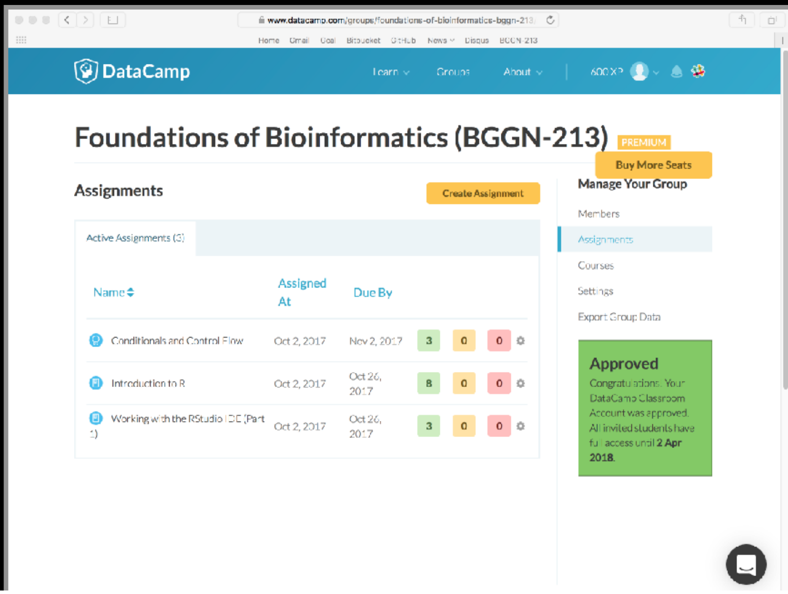

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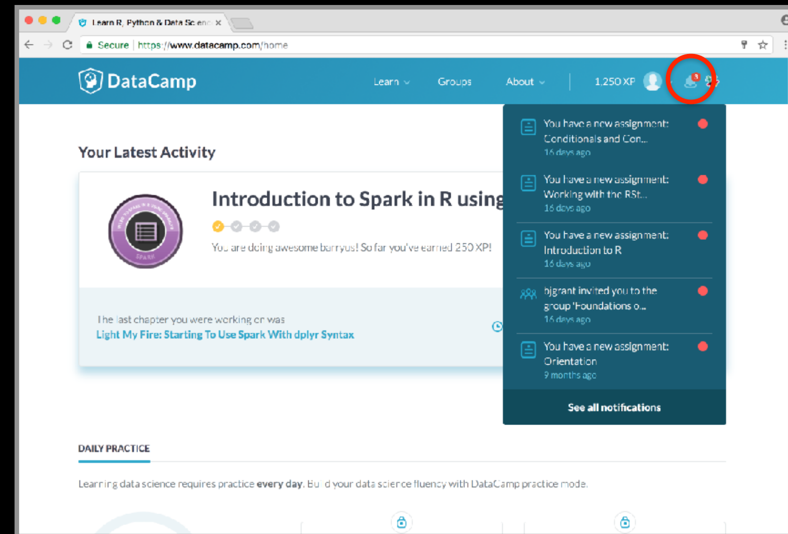

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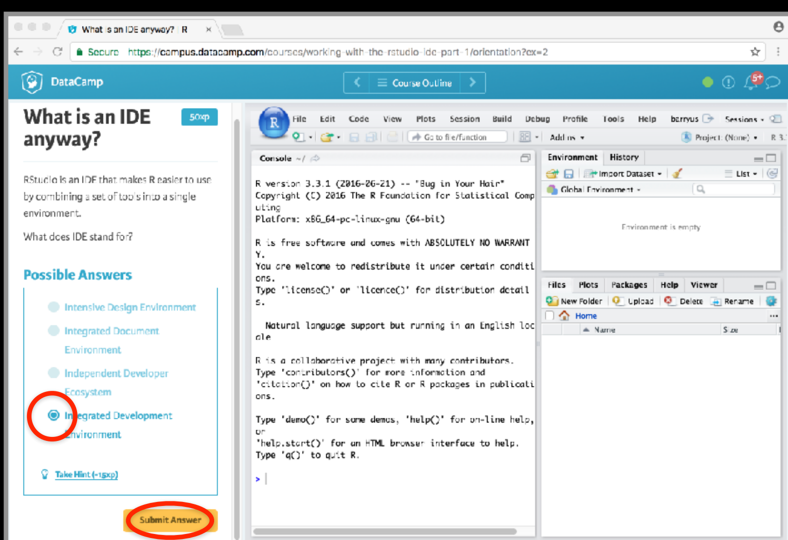

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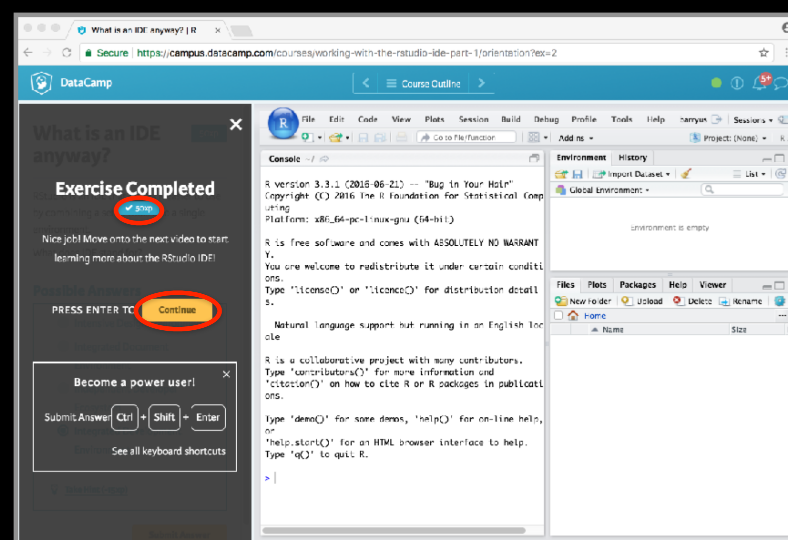

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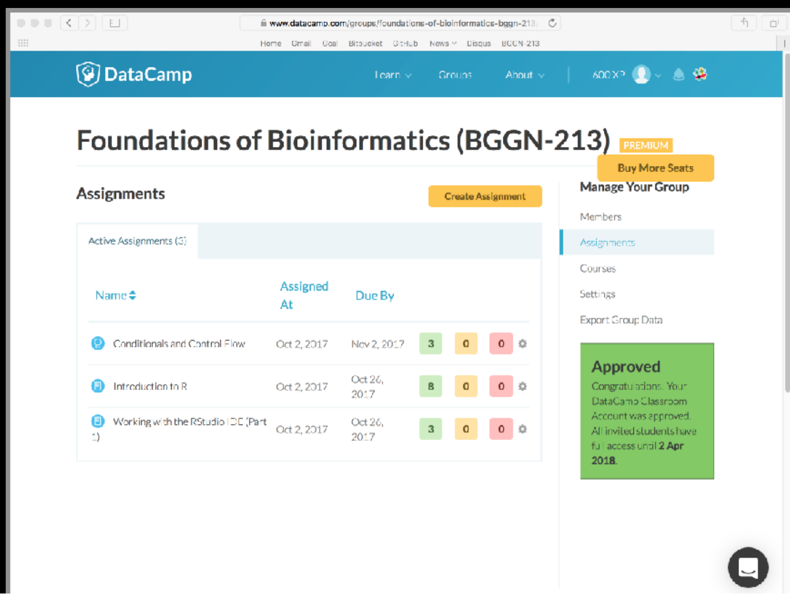

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- Objects may have attributes, such as **name**, **dim**ension, and **class**.
- **DataCamp**, StackOverflow and **help()** are your friends.

Final Knowledge Check!

- What is R and why should we use it?
- Familiarity with R's basic syntax.
- Familiarity with major R data structures namely *vectors* and *data.frames* (with more on *lists* and *matrices* next day).
- Understand the basics of using functions (arguments, vectorizion and re-cycling).
- Be able to use R to read and parse comma-separated (.csv) formatted files ready for subsequent analysis.
- Appreciate how you can use R scripts to aid with reproducibility.

Optional!

http://swcarpentry.github.io/r-novice-inflammation/

Sections: 1, 11 & 12 only!

Help from within R

- Getting help for a function

```
> help("log")
> ?log
```

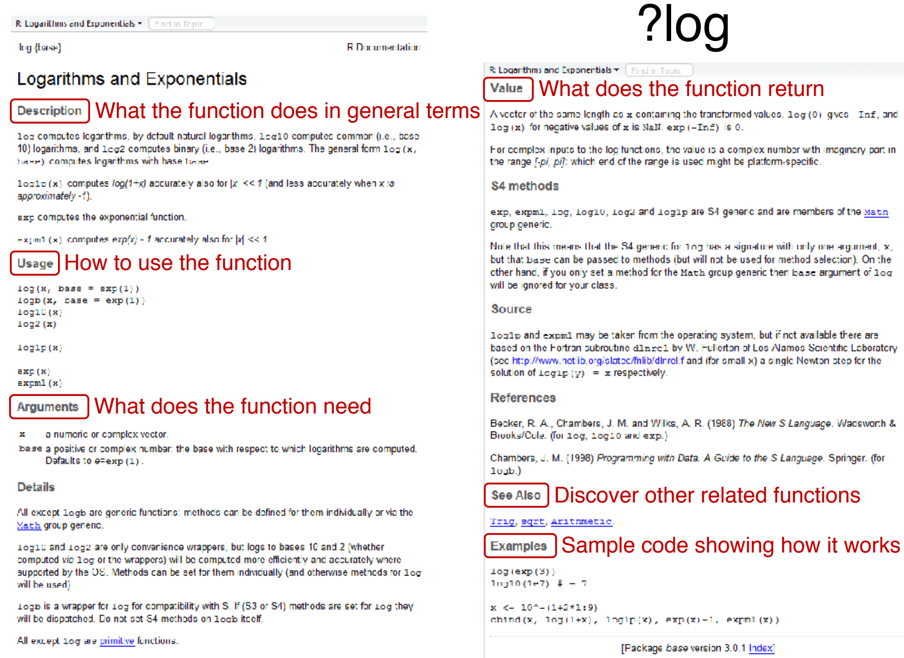
- Searching across packages

```
> help.search("logarithm")
```

- Finding all functions of a particular type

```
> apropos("log")
[7] "SSlogis" "as.data.frame.logical" "as.logical"
  "as.logical.factor" "dlogis" "is.logical"
[13] "log" "log10" "log1p" "log2" "logLik" "logb"
[19] "logical" "loglin" "plogis" "print.logLik" "qlogis"
  "rlogis"
```

?log



Optional Exercise

Use R to do the following. Create a new script to save your work and code up the following four equations:

$$1 + 2(3 + 4)$$

$$\ln(4^3+3^{2+1})$$

$$\sqrt{(4+3)(2+1)}$$

$$\left(\frac{1+2}{3+4}\right)^2$$