BGGN 213

Data analysis with R

Lecture 4

Barry Grant

UC San Diego

http://thegrantlab.org/bggn213

Recap From Last Time:

- Substitution matrices: Where our alignment match and mis-match scores typically come from
- Comparing methods: The trade-off between *sensitivity*, *selectivity* and *performance*
- Sequence motifs and patterns: Finding functional cues from conservation patterns
- Sequence profiles and position specific scoring matrices (PSSMs), Building and searching with profiles, Their advantages and limitations
- PSI-BLAST algorithm: Application of iterative PSSM searching to improve BLAST sensitivity
- Hidden Markov models (HMMs): More versatile probabilistic model for detection of remote similarities

Feedback

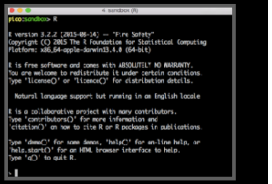
Today's Learning Goals

- 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.

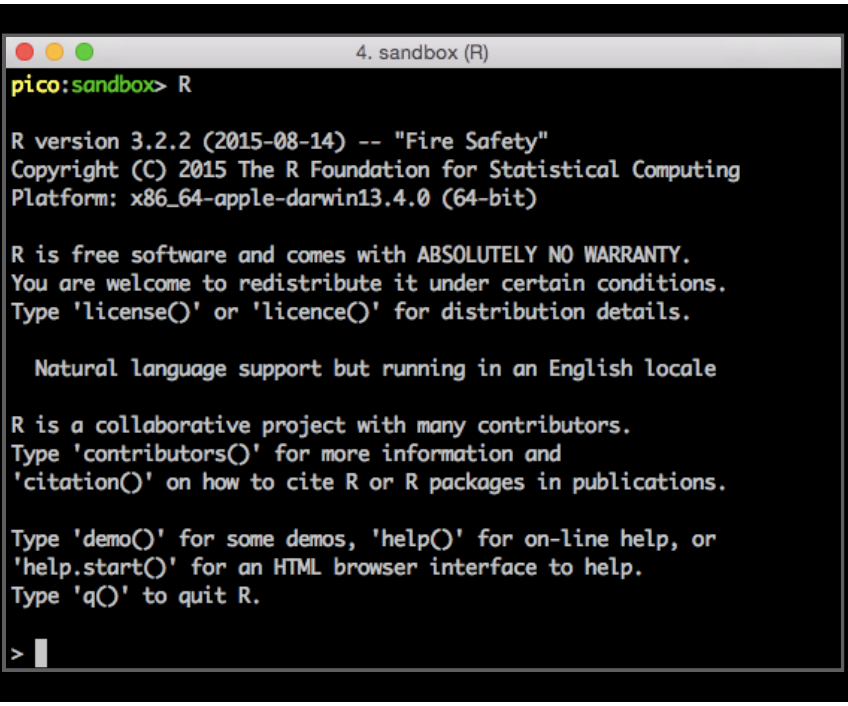
What is R?

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).



```
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)

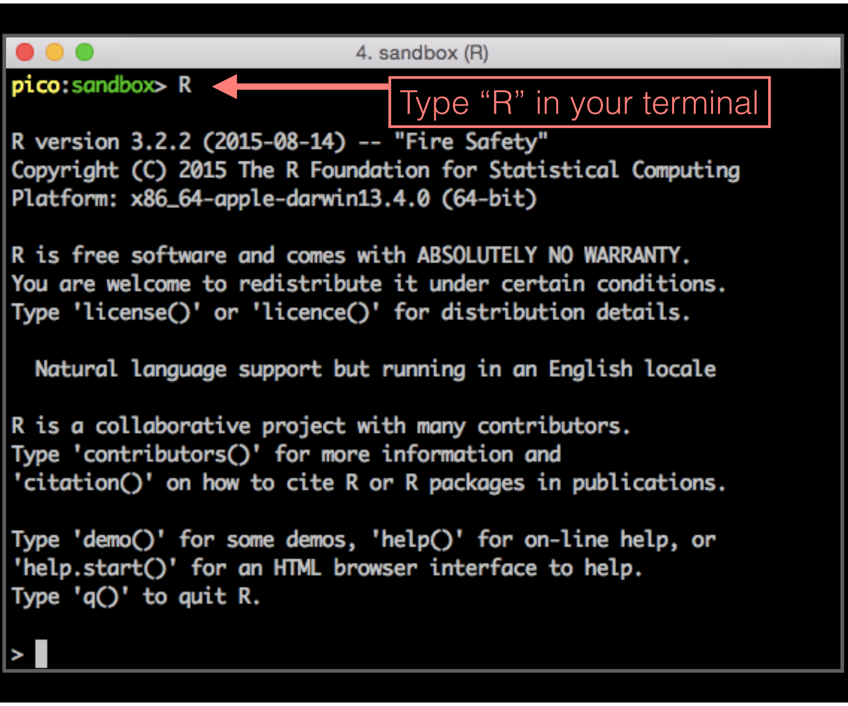
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  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.

>
```



Type “R” in your terminal

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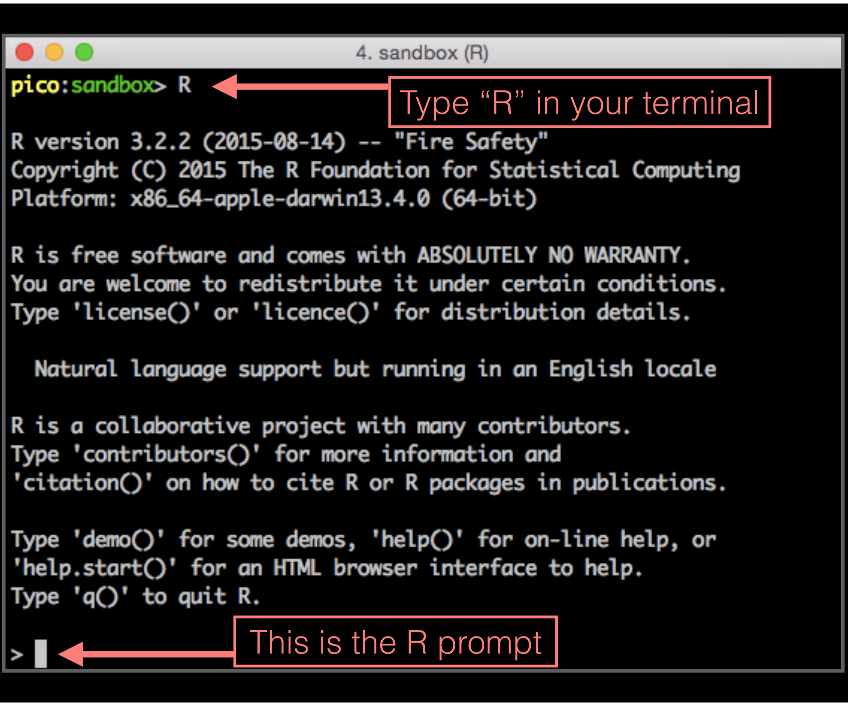

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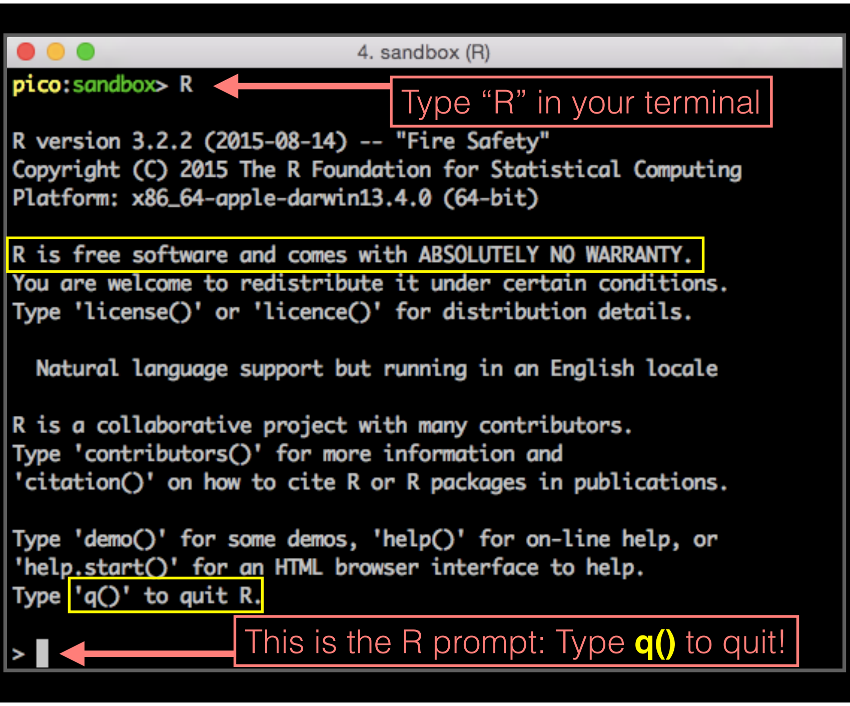
```

This is the R prompt



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> 
```

Type “R” in your terminal

This is the R prompt: Type **q()** to quit!

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.

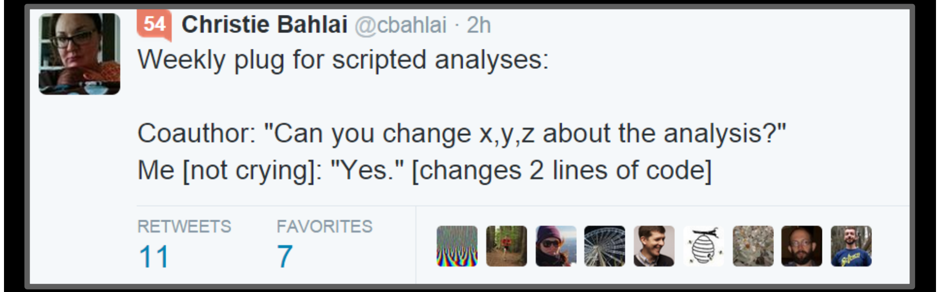
Backed by a commercial guarantee or license.

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!



Christie Bahlai @cbahlai · 2h

Weekly plug for scripted analyses:

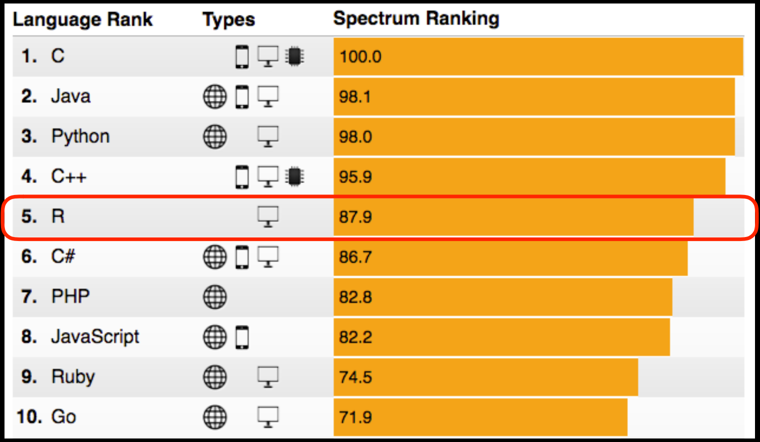
Coauthor: "Can you change x,y,z about the analysis?"
Me [not crying]: "Yes." [changes 2 lines of code]

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

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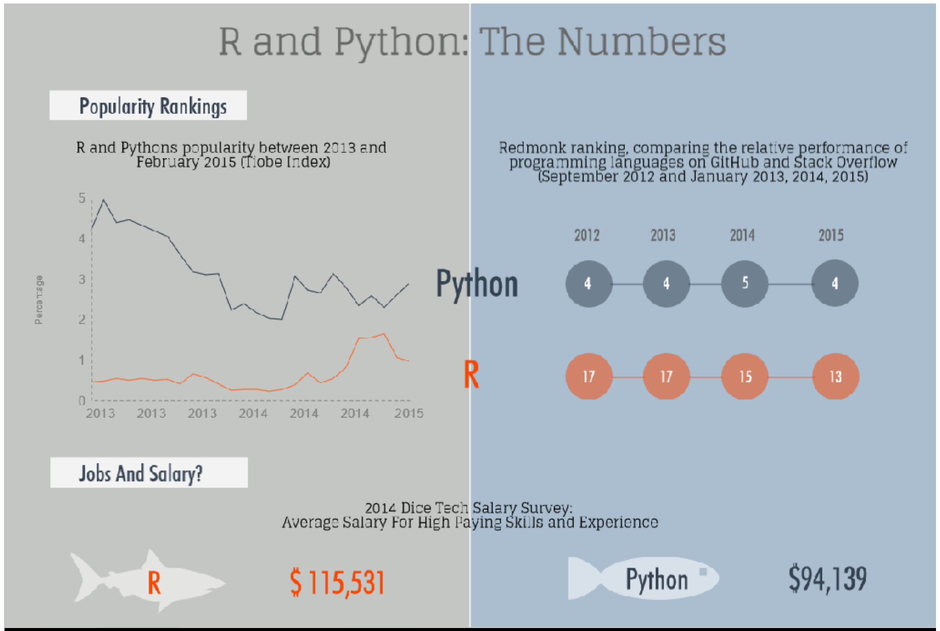

http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html?utm_medium=email&utm_source=flipboard

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- R is the “lingua franca” of data science in industry and academia.
- Large user and developer community.
  - As of April 13th 2018 there are 12,481 add on **R packages** on **CRAN** and 1,473 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

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Modularity

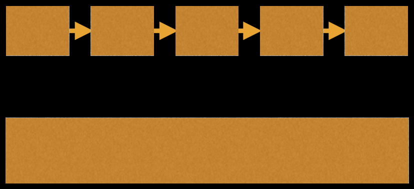
R was designed to allow users to interactively build complex workflows by interfacing smaller ‘**modular’ functions** together.

get.seq() → **hmmer()** → **pdbaln()** → **pdbfit()** → **pca()** → **plot()**

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.

All-in-one custom ‘Monster’ program

Which would you prefer and why?



Modular

vs

Custom

Advantages/Disadvantages

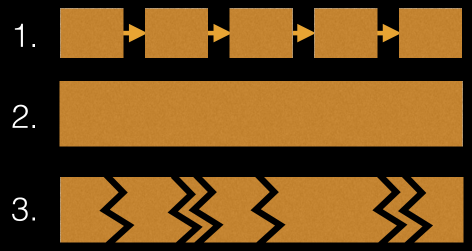
The ‘monster approach’ is customized to a particular project but results in massive, fragile and difficult to modify (therefore inflexible, untransferable, and error prone) code.

With **modular workflows**, it’s easier to:

- Spot errors and figure out where they’re occurring by inspecting intermediate results.
- Experiment with alternative methods by swapping out components.
- Tackle novel problems by remixing existing modular tools.

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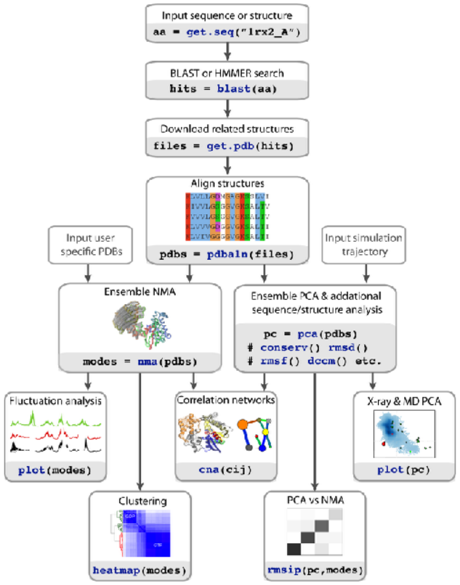
Bioinformatics data is intrinsically **high dimensional** and frequently ‘messy’ requiring **exploratory data analysis** to find patterns - both those that indicate interesting biological signals or suggest potential problems.



Input sequence or structure
`aa = get.seq("1rx2_A")`

BLAST or HMMER search
`hits = blast(aa)`

Download related structures
`files = get.pdb(hits)`

Align structures
`pdbs = pdbaln(files)`

Input user specific PDBs

Input simulation trajectory

Ensemble NMA
`modes = nma(pdbs)`

Ensemble PCA & addational sequence/structure analysis
```
pc = pca(pdbs)
# conserv() rmsd()
# rmsf() dccm() etc.
```

Fluctuation analysis
`plot(modes)`

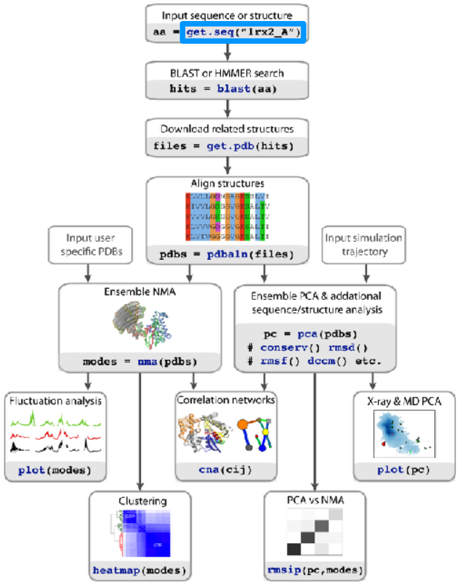
Correlation networks
`cna(cij)`

X-ray & MD PCA
`plot(pc)`

Clustering
`heatmap(modes)`

PCA vs NMA
`rmsip(pc,modes)`

R Features = **functions()**



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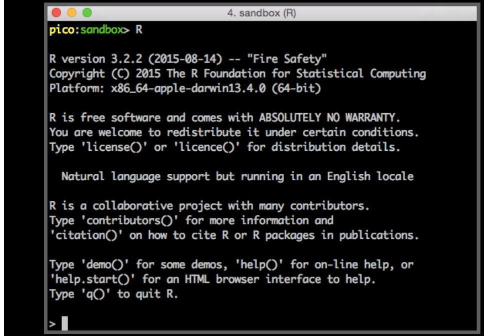
How do we use R?

Two main ways to use R



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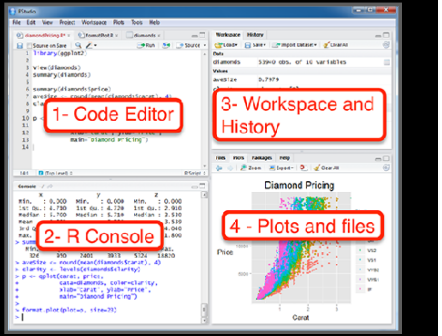
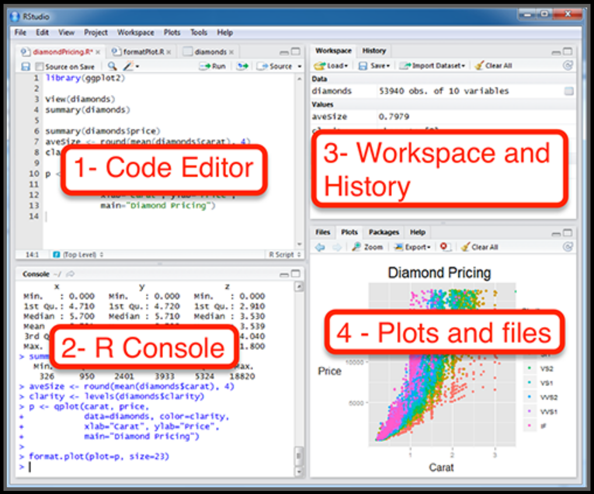


1. Terminal

2. RStudio

We will use **RStudio** today



```
library(ggplot2)

view(diamonds)
summary(diamonds)

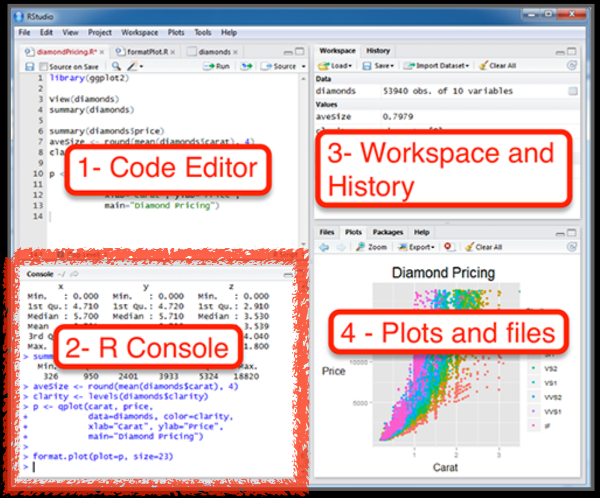
summary(diamonds$price)
aveSize <- round(mean(diamonds$carat), 4)
```

```
Data
diamonds      53940 obs. of 10 variables
Values
aveSize       0.7979
```

```
         x                  y                  z
Min.   : 0.000     Min.   : 0.000     Min.   : 0.000
1st Qu.: 4.710     1st Qu.: 4.720     1st Qu.: 2.910
Median : 5.700     Median : 5.710     Median : 3.530
   326      950     2401     3933     5324    18820
> aveSize <- round(mean(diamonds$carat), 4)
> clarity <- levels(diamonds$clarity)
> p <- qplot(carat, price,
+            data=diamonds, color=clarity,
+            xlab="Carat", ylab="Price",
+            main="Diamond Pricing")
>
> format.plot(plot=p, size=23)
>
```

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
```

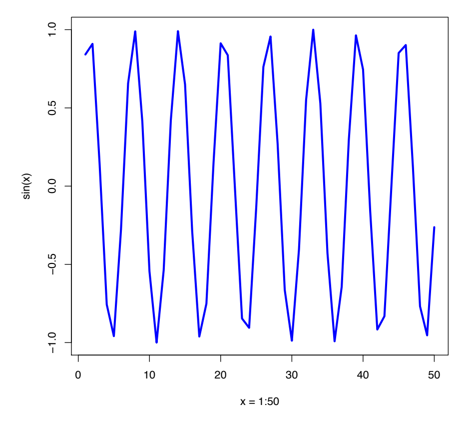
7
```
> log(2.718282)
[1] 1
```

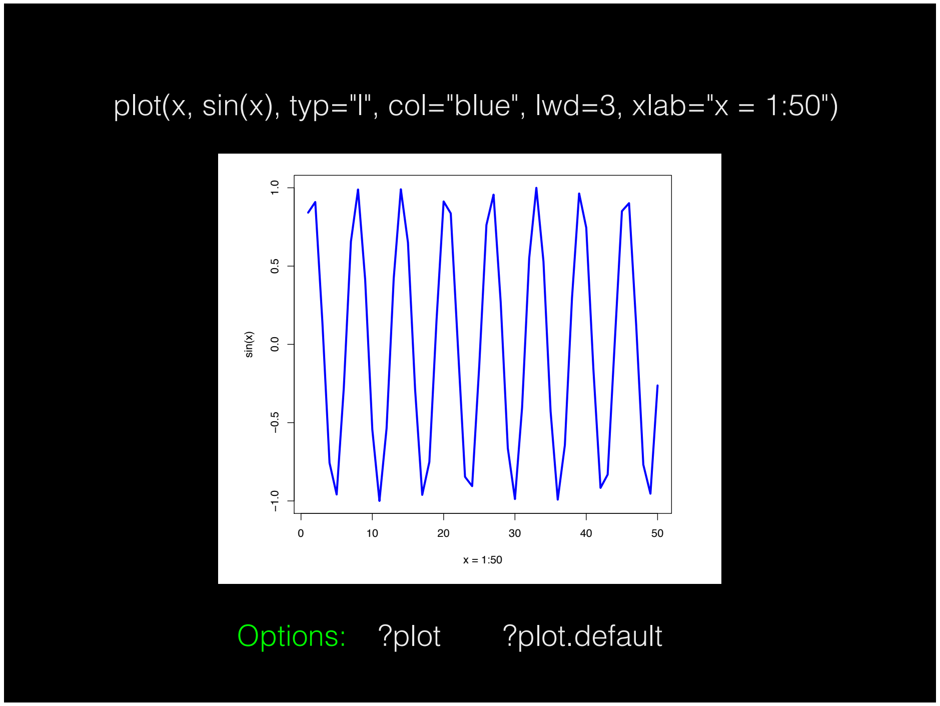
8
```
> log(10, base=10)
[1] 1
```
Optional argument

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

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

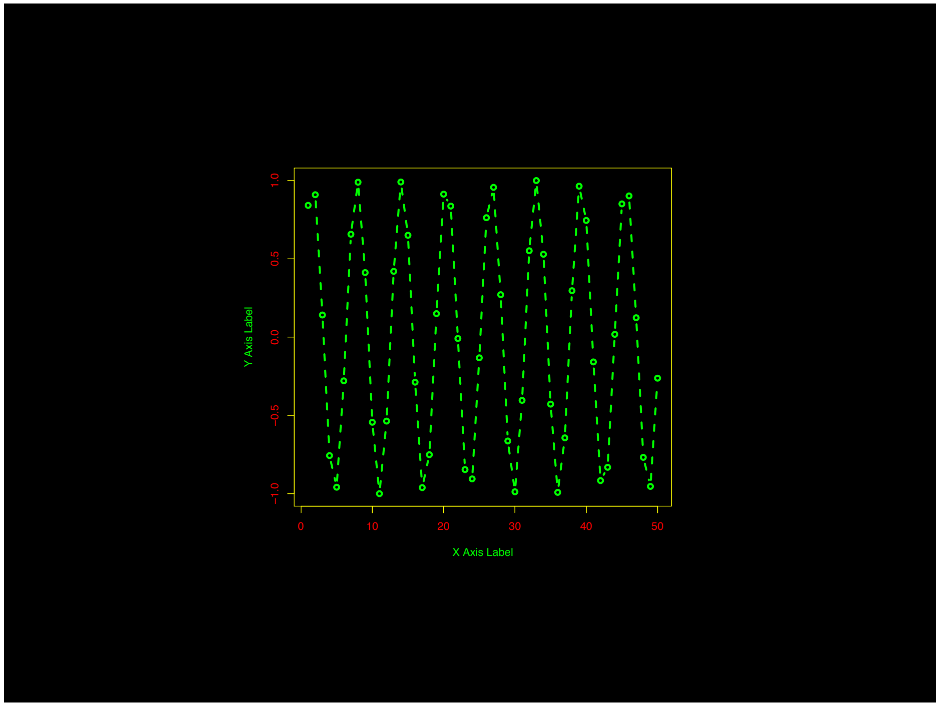
Does your plot look like this?

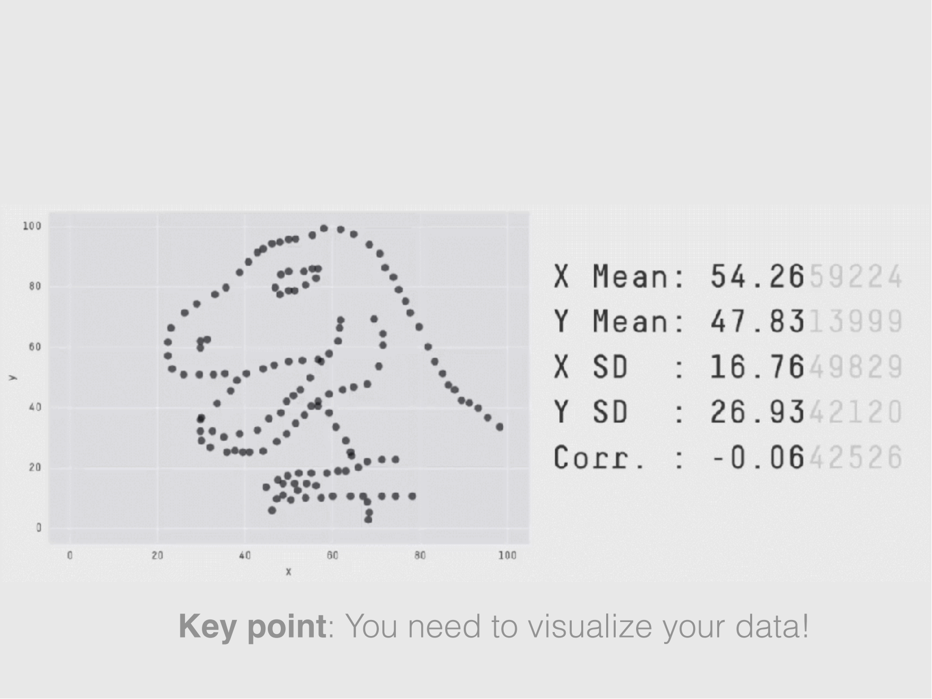




```
plot(x, sin(x), typ="l", col="blue", lwd=3, xlab="x = 1:50")
```

Options: `?plot` `?plot.default`





```
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!

https://bioboot.github.io/bggn213_S18/class-material/04_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

Topics Covered:

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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 include:

- **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

Topics Covered:

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

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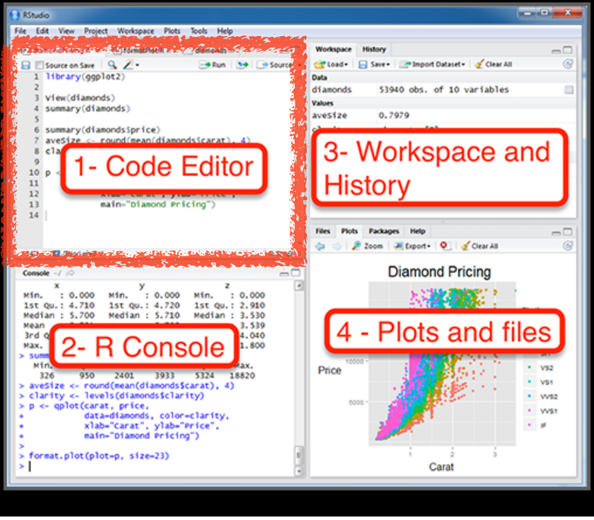
RStudio **projects**

Side-note: Use the code editor for R scripts



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```
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Values
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>
> format.plot(plot=p, size=23)
> |
```

1- Code Editor

2- R Console

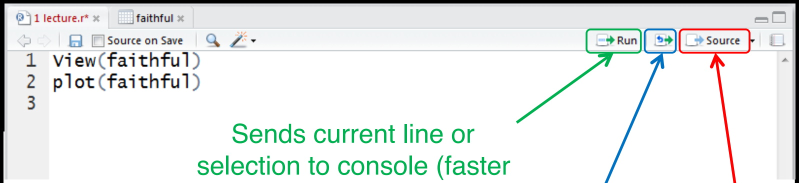
3- Workspace and History

4 - Plots and files

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



```
View(faithful)
plot(faithful)
```

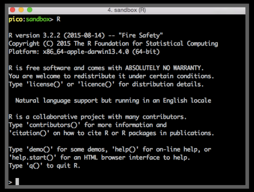
Sends current line or selection to console (faster to type: **command/ctrl+enter**)

Re-send the lines of code you last ran to the console (useful after edits)

Sends entire file to console

Other RStudio shortcuts!
Up/Down arrows (recall cmds)
Ctrl + 2 (move cursor to console)
Ctrl +1 (move cursor to editor)

Rscript: Third way to use 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)

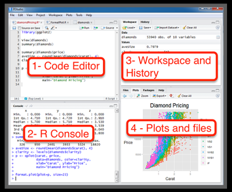
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  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.

>
```



\> Rscript --vanilla my_analysis.R

1. Terminal

2. RStudio

3. Rscript

From the command line!

\> Rscript --vanilla **my_analysis.R**

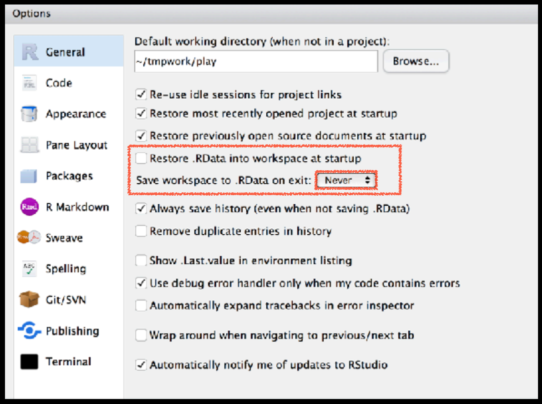
\# or within R: source(**my_analysis.R**)

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!

R workspaces

- Set **Tools** > **Global Options**



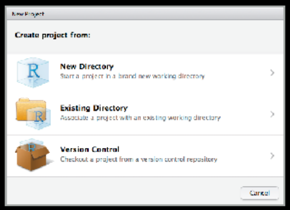
Default working directory (when not in a project):
~/tmpwork/play

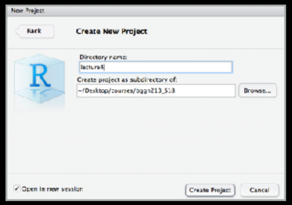
☑ Re-use idle sessions for project links
☑ Restore most recently opened project at startup
☑ Restore previously open source documents at startup
☐ Restore .RData into workspace at startup
Save workspace to .RData on exit: Never
☑ Always save history (even when not saving .RData)
☐ Remove duplicate entries in history
☐ Show .Last.value in environment listing
☑ Use debug error handler only when my code contains errors
☐ Automatically expand tracebacks in error inspector
☐ Wrap around when navigating to previous/next tab
☑ Automatically notify me of updates to RStudio

RStudio Projects

- We will use a new RStudio **project** for each new class going forward.

  File > **New Project** > **New Directory** > **New Project**…





Directory name: lecture4

Create project as subdirectory of: ~/Desktop/courses/bggn213_S18 Browse...

☑ Open in new session

- These projects will help keep us **organized** and divide our work into multiple contexts, each with their own working directory, workspace, history, and source documents.

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/ >

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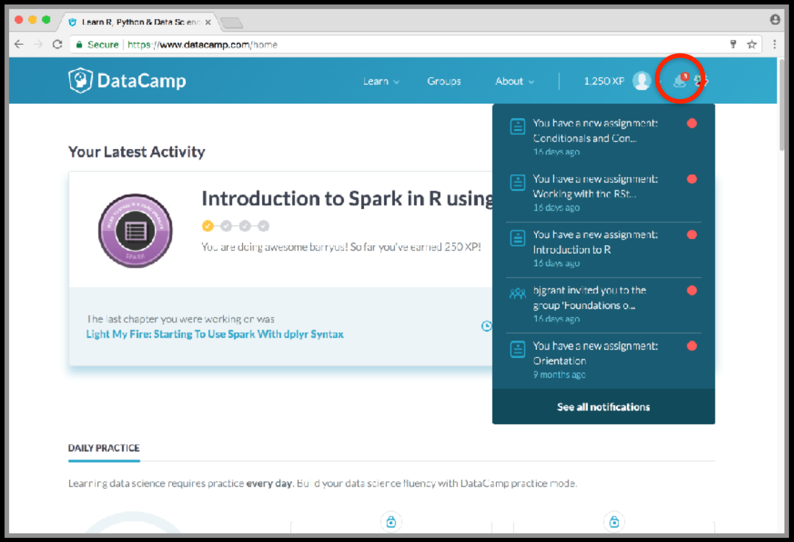
< https://www.datacamp.com/ >



Your Latest Activity

Introduction to Spark in R using

You are doing awesome barryus! So far you've earned 250 XP!

The last chapter you were working on was
Light My Fire: Starting To Use Spark With dplyr Syntax

You have a new assignment: Conditionals and Con...
16 days ago

You have a new assignment: Working with the RSt...
16 days ago

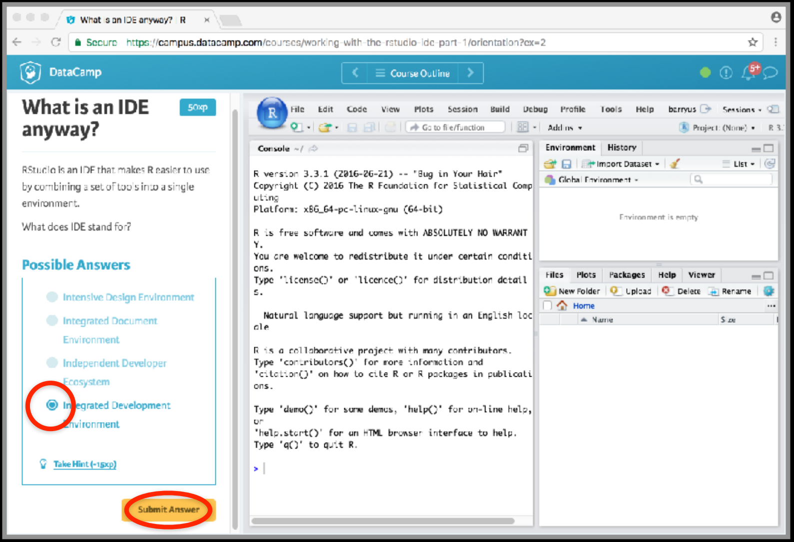
You have a new assignment: Introduction to R
16 days ago

bjgrant invited you to the group 'Foundations o...
16 days ago

You have a new assignment: Orientation
9 months ago

Learning data science requires practice **every day**. Build your data science fluency with DataCamp practice mode.

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



What is an IDE anyway?

50xp

RStudio is an IDE that makes R easier to use by combining a set of tools into a single environment.

What does IDE stand for?

Possible Answers

- ○ Intensive Design Environment
- ○ Integrated Document Environment
- ○ Independent Developer Ecosystem
- ● Integrated Development Environment

Take Hint (-15xp)

Submit Answer

Environment is empty

```
R version 3.3.1 (2016-26-21) -- "Bug in Your Hair"
Copyright (C) 2016 The R Foundation for Statistical Comp
uting
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANT
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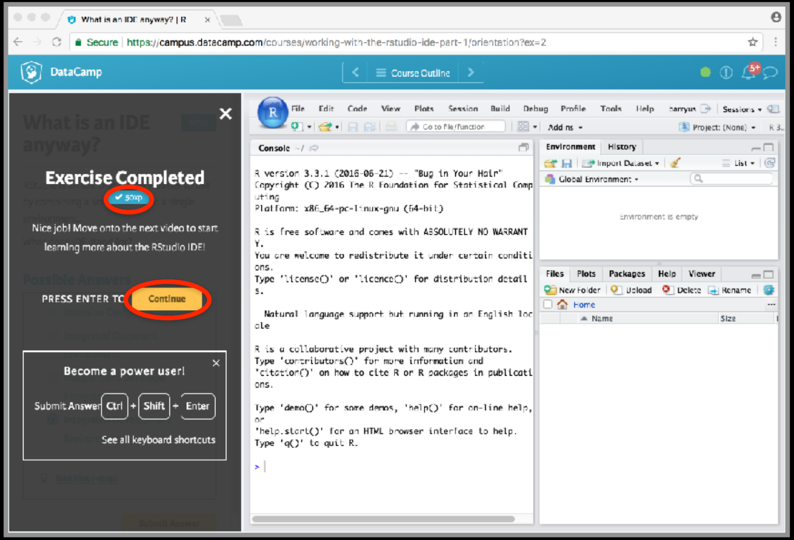
or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> |
```

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



Exercise Completed

✔ 50xp

Nice job! Move onto the next video to start learning more about the RStudio IDE!

PRESS ENTER TO Continue

Become a power user!

Submit Answer Ctrl + Shift + Enter

See all keyboard shortcuts

Environment is empty

```
R version 3.3.1 (2016-06-21) -- "Bug in Your Hair"
Copyright (C) 2016 The R Foundation for Statistical Comp
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Platform: x86_64-pc-linux-gnu (64-bit)

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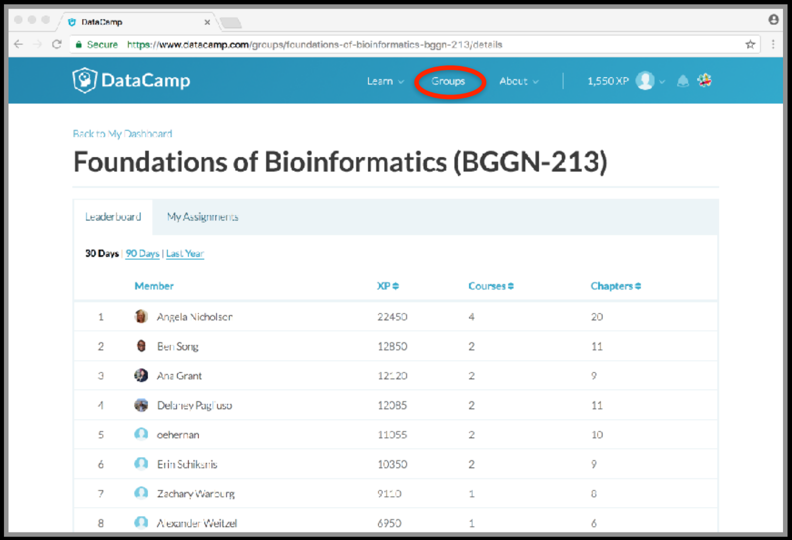
< https://www.datacamp.com/ >



Back to My Dashboard

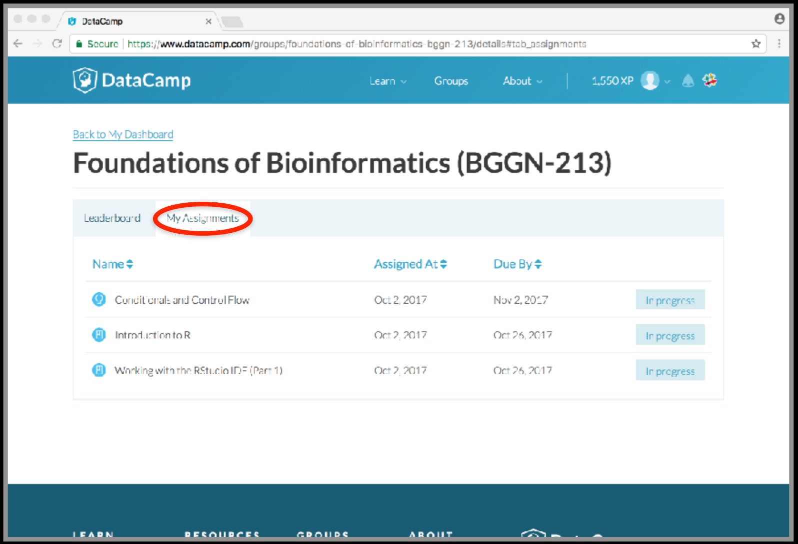
Foundations of Bioinformatics (BGGN-213)

Leaderboard | My Assignments

30 Days | 90 Days | Last Year

	Member	XP	Courses	Chapters
1	Angela Nicholson	22450	4	20
2	Ben Song	12850	2	11
3	Ana Grant	12120	2	9
4	Delaney Pagliuso	12085	2	11
5	oehernan	11055	2	10
6	Erin Schiksnis	10350	2	9
7	Zachary Warburg	9110	1	8
8	Alexander Weitzel	6950	1	6

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



Back to My Dashboard

Foundations of Bioinformatics (BGGN-213)

Leaderboard | My Assignments

Name	Assigned At	Due By	
Conditionals and Control Flow	Oct 2, 2017	Nov 2, 2017	In progress
Introduction to R	Oct 2, 2017	Oct 26, 2017	In progress
Working with the RStudio IDE (Part 1)	Oct 2, 2017	Oct 26, 2017	In progress

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**.
- **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.

Link: Muddy point assessment

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
```

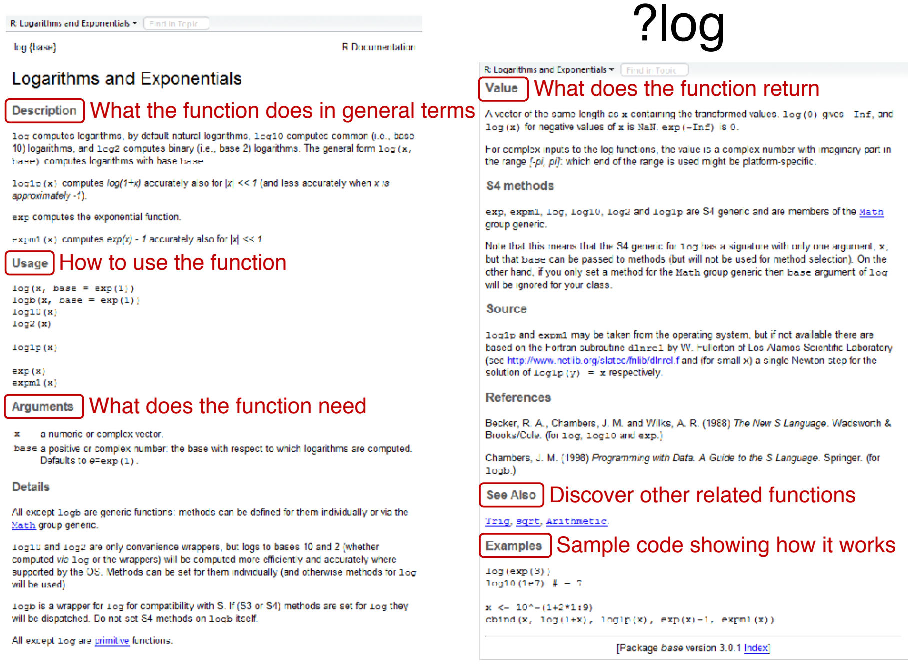
- Searching across packages

```
> 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



R: Logarithms and Exponentials ▾ Find in Topic

log {base} R Documentation

Logarithms and Exponentials

Description What the function does in general terms

`log` computes logarithms, by default natural logarithms, `log10` computes common (i.e., base 10) logarithms, and `log2` computes binary (i.e., base 2) logarithms. The general form `log(x, base)` computes logarithms with base `base`.

`log1p(x)` computes *log(1+x)* accurately also for |*x*| << *1* (and less accurately when *x* is *approximately -1*).

`exp` computes the exponential function.

`expm1(x)` computes *exp(x) - 1* accurately also for |*x*| << 1

Usage How to use the function

```
log(x, base = exp(1))
logb(x, base = exp(1))
log10(x)
log2(x)

log1p(x)

exp(x)
expm1(x)
```

Arguments What does the function need

`x` a numeric or complex vector.

`base` a positive or complex number: the base with respect to which logarithms are computed. Defaults to `e=exp(1)`.

Details

All except `logb` are generic functions: methods can be defined for them individually or via the `Math` group generic.

`log10` and `log2` are only convenience wrappers, but logs to bases 10 and 2 (whether computed *via* `log` or the wrappers) will be computed more efficiently and accurately where supported by the OS. Methods can be set for them individually (and otherwise methods for `log` will be used).

`logb` is a wrapper for `log` for compatibility with S. If (S3 or S4) methods are set for `log` they will be dispatched. Do not set S4 methods on `logb` itself.

All except `log` are primitive functions.

R: Logarithms and Exponentials ▾ Find in Topic

Value What does the function return

A vector of the same length as `x` containing the transformed values. `log(0)` gives `-Inf`, and `log(x)` for negative values of `x` is `NaN`. `exp(-Inf)` is `0`.

For complex inputs to the log functions, the value is a complex number with imaginary part in the range *[-pi, pi]*: which end of the range is used might be platform-specific.

S4 methods

`exp`, `expm1`, `log`, `log10`, `log2` and `log1p` are S4 generic and are members of the `Math` group generic.

Note that this means that the S4 generic for `log` has a signature with only one argument, `x`, but that `base` can be passed to methods (but will not be used for method selection). On the other hand, if you only set a method for the `Math` group generic then `base` argument of `log` will be ignored for your class.

Source

`log1p` and `expm1` may be taken from the operating system, but if not available there are based on the Fortran subroutine `dlnrel` by W. Fullerton of Los Alamos Scientific Laboratory (see http://www.netlib.org/slatec/fnlib/dlnrel.f and (for small x) a single Newton step for the solution of `log1p(y) = x` respectively.

References

Becker, R. A., Chambers, J. M. and Wilks, A. R. (1988) *The New S Language*. Wadsworth & Brooks/Cole. (for `log`, `log10` and `exp`.)

Chambers, J. M. (1998) *Programming with Data. A Guide to the S Language*. Springer. (for `logb`.)

See Also Discover other related functions

`Trig`, `sqrt`, `Arithmetic`.

Examples Sample code showing how it works

```
log(exp(3))
log10(1e7) # = 7

x <- 10^-(1+2*1:9)
cbind(x, log(1+x), log1p(x), exp(x)-1, expm1(x))
```

[Package *base* version 3.0.1 Index]

Optional Exercise

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

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

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

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

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