

BIMM 143 R Functions Lecture 6 Barry Grant UCSan Diego http://thegrantlab.org/bimm143

Recap From Last Time:

- Why it is important to visualize data during exploratory data analysis.
- Discussed data visualization best practices and how good visualizations optimize for the human visual system.
- Introduced the extensive graphical capabilities of base R with a focus on generating and customizing scatterplots, histograms, bar graphs, boxplots, (dendrograms and heatmaps).
- Use the par() function to control fine grained details of the afore mentioned plot types.
- Used (and SAVED!) an R script with all our work!

[MPA Link]

Today's Learning Goals

- · Last days R visualization hands-on exercise revisited...
 - Make our work error free and produce a nice report!
- More on data import
 - File pre-check recommendations
 - Using read.table() and friends for flat files
- · Writing your own functions
 - What, Why, When and How
- · Hands-on session
 - Practice, tips, techniques for troubleshooting, and best practice guidelines for writing and debugging your functions

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Class 5 Revisited

- Open your previous class05 RStudio project (and your saved R script)
- Can you source this class05.R file to re-generate all your plots without error?

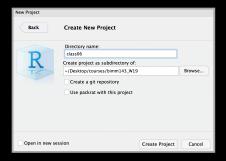


 If so you can now generate a nice HTML report of your work to date...

[Take 2-3 minutes]

Pre-check recommendations

- Get organized!
 - Start a new 'project' in your class directory (e.g. a folder on your Desktop where you are storing all your class material)
 - In RStudio File > New Project > New Directory > ... class06



Pre-check recommendations

- Get organized!
 - Start a new 'project' in your class directory (e.g. a folder on your Desktop where you are storing all your class material)
 - In RStudio File > New Project > New Directory > ... class06
- Inspect the file
 - Move the input file into your project directory
- Open it from the RStudio Files tab.
- Does it have a header line or comments to be included, ignored or removed?
- Avoid file (or field names) with spaces or special characters such as ?, \$,%, ^, &, *, } etc.
- Short names are preferred over longer names.
- Does the file end with a blank line or a RTN?

Do ji You

read.table() and friends for flat files

- · The read.table() function is the base of all flat file import functions
 - read.delim("filename.txt", sep="\t")

TAB

• read.csv("filename.txt", sep=",")

COMMA SEMI-COLON

read.csv2("filename.txt", sep=";")
 read.table("filename.txt", sep="")

WHITE SPACE

- · What other differences are there between these functions?
- MS EXCEL file import options include:
 - Export (i.e. "Save As...") your excel data to plain text CSV format.
 - Or if you must, use readxl::read_excel() to read specified parts of your sheets.
- · For fast and convenient reading of very large flat files files
 - Try data.table::fread() use is similar to read.table() but it automatically finds field separators and header rows. It is also much faster!
- · Saving and loading .RData files...
 - Use the functions save() and load() for saving and loading multiple objects to space efficient binary format files.

https://bioboot.github.io/bimm143 W19/class-material/test3.txt

https://bioboot.github.io/bimm143 W19/class-material/test1.txt

https://bioboot.github.io/bimm143 W19/class-material/test2.txt

Your turn!

- Start a new RStudio Project in your class directory
- Open a new **Rmarkdown document** and give it a name and descriptive text.
- Download each of the above files and move them into your *Project*
- Experiment with **read.table()** to get their data successfully input into your R session.

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What is a function

```
name.of.function <- function(arg1, arg2) {
    statements
    return (something)
}</pre>
```

- 1 Name (can be almost anything you want)
- **2 Arguments** (i.e. input to your function)
- **3 Body** (where the work gets done)

What is a function

- 1 Name (in this case "add")
- 2 Arguments (here "x" and "y")
- **3 Body** (will return the result of the last statement)

Why would you write a function

When you find yourself doing the same thing 3 or more times it is time to write a function.

```
## What does this code do?

df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))

df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))

df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))

df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))
```

Your function is treated just like any other function...

```
add <- function(x, y=1) {
    # Sum the input x and y
    x + y
}

add(x=1, y=4)
add(1, 4)
add(1)

add(c(1, 2, 3) )
add(c(1, 2, 3), 4 )

add(1, 2, 2)
add(x=1, y="b")</pre>
```

Why would you write a function

When you find yourself doing the same thing 3 or more times it is time to write a function.

```
## Consider copy and paste errors:

df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))

df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))

df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))

df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))</pre>
```

Why would you write a function

Consider the advantages:

```
## Here the intent is far more clear
df$a <- rescale(df$a)</pre>
```

- Makes the purpose of the code more clear
- Reduce mistakes from copy/paste
- Makes updating your code easer
- Reduce duplication and facilitate re-use.

How would you write this function

Start with a **working code snippet**, simplify, reduce calculation duplication,...

```
## First consider the original code:

df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))

df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))

df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))

df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))</pre>
```

How would you write this function

Start with a working code snippet, **simplify**, reduce calculation duplication,...

```
## Simplify to work with a generic vector named "x"  x <- (x - \min(x)) / (\max(x) - \min(x))
```

How would you write this function

Start with a working code snippet, simplify, **reduce** calculation duplication,...

```
## Note that we call the min() function twice... x <- (x - min(x)) / (max(x) - min(x))
```

How would you write this function

Start with a working code snippet, simplify, **reduce** calculation duplication,...

How would you write this function

Start with a working code snippet, simplify, **reduce** calculation duplication,...

```
## Further optimization to use the range() function...
rng <- range(x)
x <- (x - rng[1]) / (rng[2] - rng[1])</pre>
```

How would you write this function

Start with a working code snippet, simplify, reduce calculation duplication, finally turn it into a function

```
## You need a "name", "arguments" and "body"...

rescale <- function(x) {
   rng <-range(x)
   (x - rng[1]) / (rng[2] - rng[1])
}

# Test on a small example where you know the answer rescale(1:10)</pre>
```

How would you write this function

Test, Fail, Change, Test again,...

```
# Test on a small example where you know the answer
rescale(1:10)

# How would you get your function to work here...
rescale( c(1,2,NA,3,10) )

# What should your function do here?
recale( c(1,10,"string") )
```

Side-Note: Seeing and using your function in RStudio

- An easy way to visualize the code of a function is to type its name without the parentheses ().
- If you have your new function saved to a separate file then you can load and execute it using the source() function. E.g. source("MyUtils.R")
- The return() statement is not required in a function but it is advisable to use it when the function performs several computations. It has the effect of ending the function execution and returning control to the code which called it.

```
rescale <- function(x, na.rm=TRUE, plot=FALSE) {
   if(na.rm) {
      rng <-range(x, na.rm=TRUE)
   } else {
      rng <-range(x)
   }
   print("Hello")

   answer <- (x - rng[1]) / (rng[2] - rng[1])
   return(answer)
   print("is it me you are looking for?")

   if(plot) {
      plot(answer, typ="b", lwd=4)
   }
   print("I can see it in ...")
}</pre>
```

```
rescale <- function(x, na.rm=TRUE, plot=FALSE) {
    rng <-range(x, na.rm=na.rm)
    print("Hello")

answer <- (x - rng[1]) / (rng[2] - rng[1])

print("is it me you are looking for?")

if(plot) {
    plot(answer, typ="b", lwd=4)
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print("I can see it in ...")
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O it Yourself

Your turn!

https://bioboot.github.io/bimm143 W19/lectures/#6

Concentrate on **Section 1B** and questions 1 to 6. Other sections are there for your benefit.

[Also aim to generate a HTML report from your R script]

Homework!

New **DataCamp** Assignments

- Introduction to R Markdown
- Functions
- Loops
- Your lecture6 function homework

Muddy Point Assessment Form Link

```
#Can you improve this analysis code?

library(bio3d)

s1 <- read.pdb("4AKE")  # kinase with drug

s2 <- read.pdb("1AKE")  # kinase no drug

s3 <- read.pdb("1E4Y")  # kinase with drug

s1.chainA <- trim.pdb(s1, chain="A", elety="CA")

s2.chainA <- trim.pdb(s2, chain="A", elety="CA")

s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

s1.b <- s1.chainA$atom$b

s2.b <- s2.chainA$atom$b

s3.b <- s3.chainA$atom$b

plotb3(s1.b, sse=s1.chainA, typ="1", ylab="Bfactor")

plotb3(s2.b, sse=s2.chainA, typ="1", ylab="Bfactor")

plotb3(s3.b, sse=s3.chainA, typ="1", ylab="Bfactor")

plotb3(s3.b, sse=s3.chainA, typ="1", ylab="Bfactor")
```

HOW TO ENCOURAGE STUDENTS

Growth Mindset What to say:

What not to say:

"When you learn how to do a new kind of problem, it grows your math brain!"

"Not everybody is good at math. Just do your best."

Fixed Mindset

"If you catch yourself saying, "I'm not a math person," just add the word 'yet' to the end of the sentence." "That's OK, maybe math is not one of your strengths."

"That feeling of math being hard is the feeling of your brain growing." if you keep trying."*

*If students are using the wrong strategies, their efforts might not work. Plus they may feel particularly inept if their efforts are fruitless.

"Don't worry, you'll get it

"The point isn't to get it all right away. The point is to grow your understanding step by step. What can you try next?"

"Great effort!
You tried your best"*
*Don't accept less than optimal



Side-Note:

Replace "math" with "R programing" to help reframe your self criticism when learning...