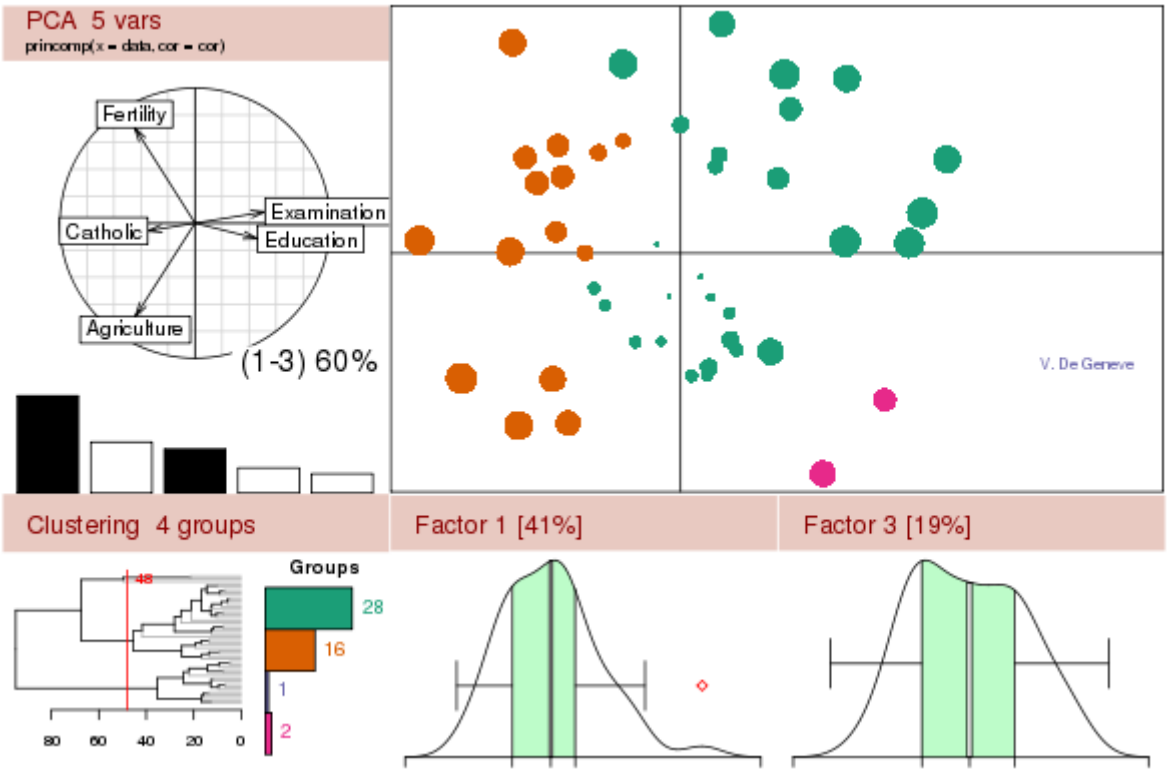
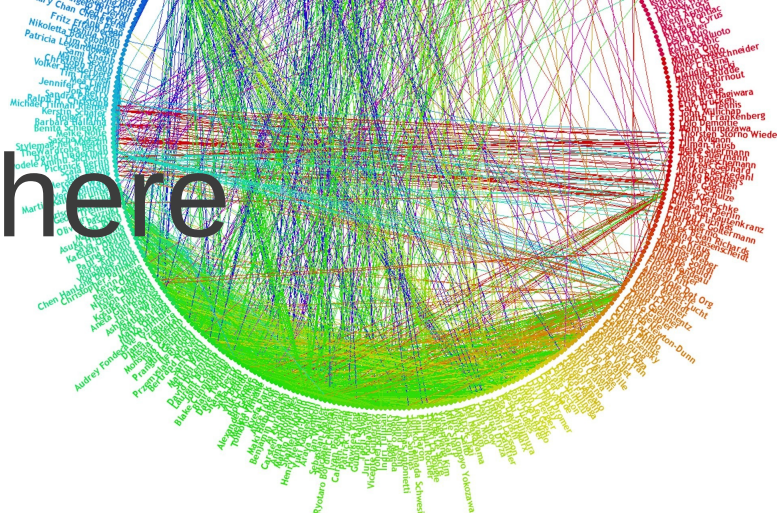
2013 Eric Pitman Summer Workshop in Computational Science



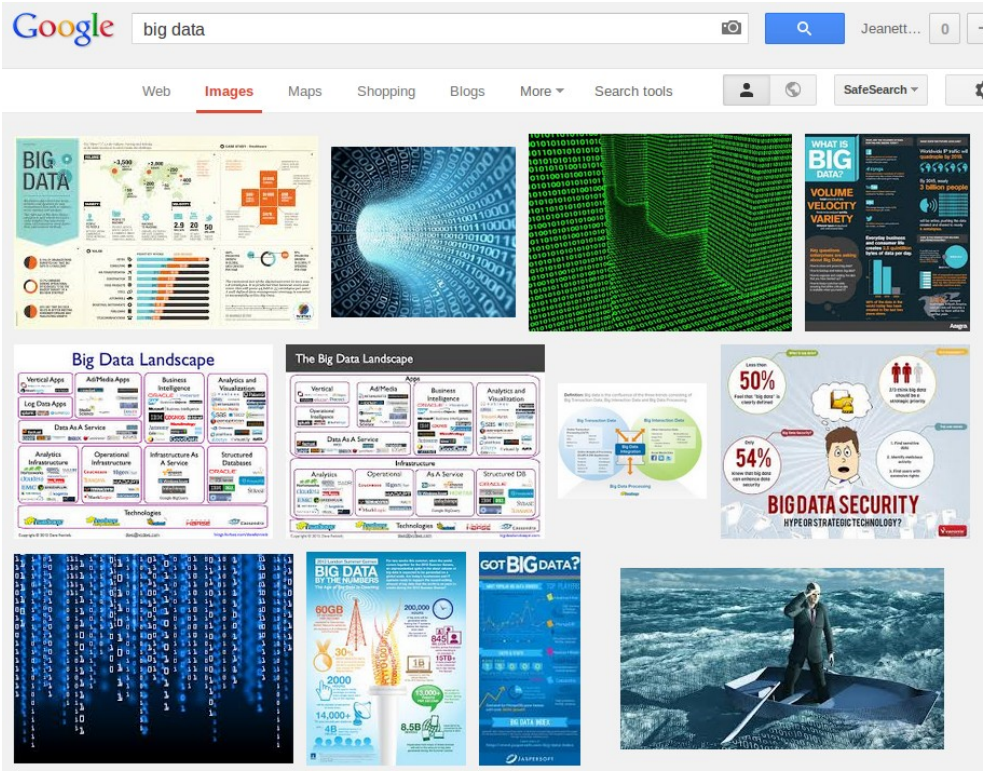
...an introduction to R, statistics, programming, and getting to know datasets

Data is Everywhere



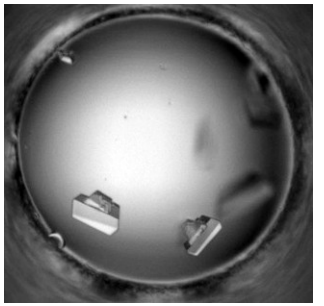
- For example:
  - Science/engineering/medicine
  - Environmental science/Social science/Law enforcement
  - Finance and marketing
  - Social media
- How do we come to an understanding of what a dataset contains?
- Can we draw conclusions from a dataset?
- Let's taste the complexities for ourselves

“Big Data” means three things



- *Volume*: lots of data
- *Velocity*: coming at you fast—Twitter, 7TB/day
- *Variety*: text, pictures, video, etc.

Our Plan for the Workshop

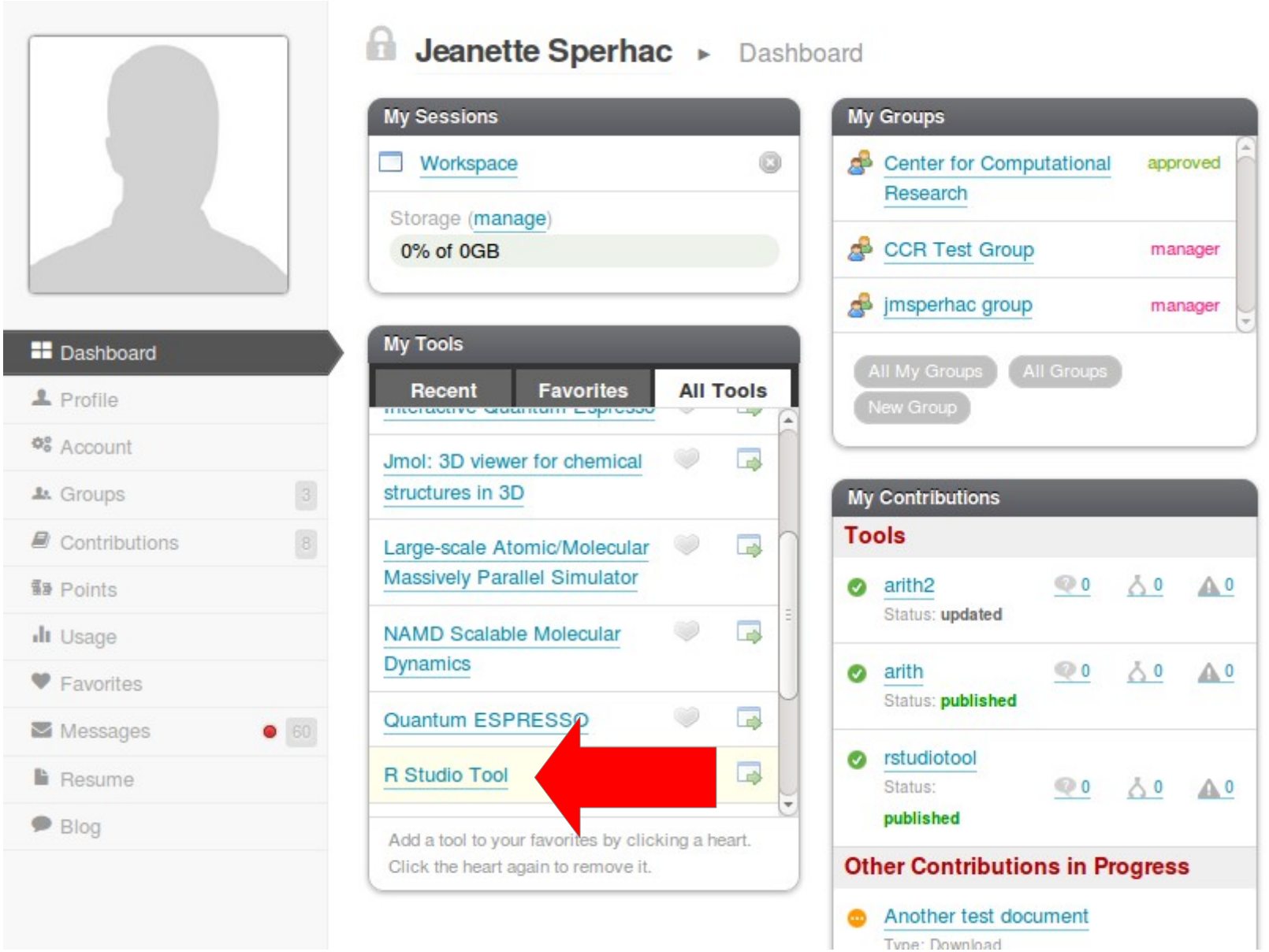


- Introduce the R language
- Do some programming
- Examine, model, and visualize datasets
- Project: explore and characterize protein crystallization data from HWI

Intro to 

1. Using the command line;
variables;
and a test flight

hpc2 My Tools: R Studio Tool



R Practical Matters

- R is case sensitive (R != r)
- Command line prompt is >
- To run R code: use command line, or save script and
  source("script_name")
- To separate commands, use ; or a newline
- The # character marks a non-executed *comment*
- To display help files:

  ?<command-name> or ??<command-name>

R as a calculator

```
> 2 + 3 * 5       # Order of operations.
> (2 + 3) * 5

> 2+3*5           # Equivalent to the above!
                  # Spaces are optional.
> (2+3)*5
```

On the command line...

R output

```
> 2 + 3 * 5      # In the console
[1] 17
```

Q: What's that [1] about?

A: R numbers outputs with [*n*]

Try this in the command line:
> 1:500

About Comments

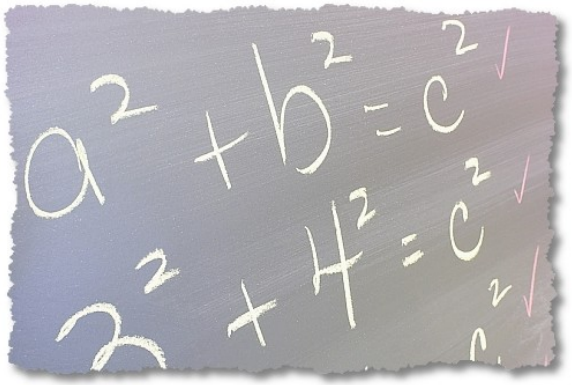
```
> 2 + 3 * 5       # Order of operations.

#  A comment is:
#  Text useful to humans, ignored by computer
#  Helps you understand what code does, or why
#  Denoted by a pound sign in R
```

Use them!!

R as a calculator

Try these in your RStudio console:

```
> 4^2          # 4 raised to the second power
> 3/2          # Division
> sqrt(16)     # Square root
> 3 - 7        # Subtraction
> log(10)      # Natural logarithm
               #         with base e=2.718282
```



Variables: save it

How do we keep a value for later use?

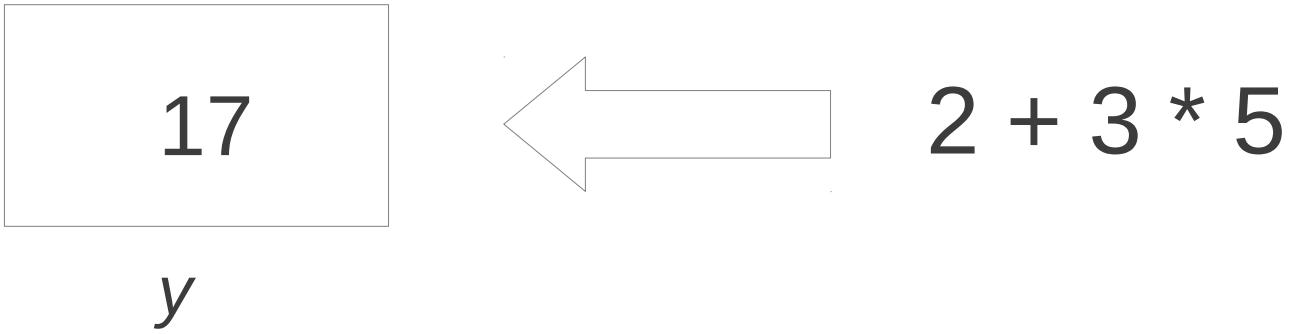
Variable assignment!

```
> y = 2 + 3 * 5      # Do some arithmetic
> y                  # R stores this value as y
[1] 17
```

y can be found under Values in the Workspace window

Variable Assignment

```
> y = 2 + 3 * 5   # R stores this value as y
```



y can be found under Values in the Workspace window

Naming Variables in R

A variable name may consist of letters, numbers and the dot or underline characters. It should start with a letter.

Good:

> y = 2

> try.this = 33.3

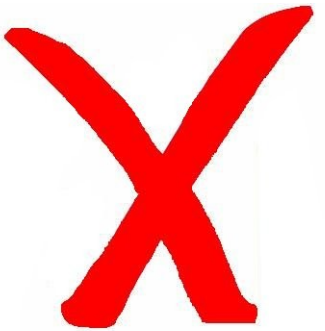
> oneMoreTime = “woohoo”

Bad:

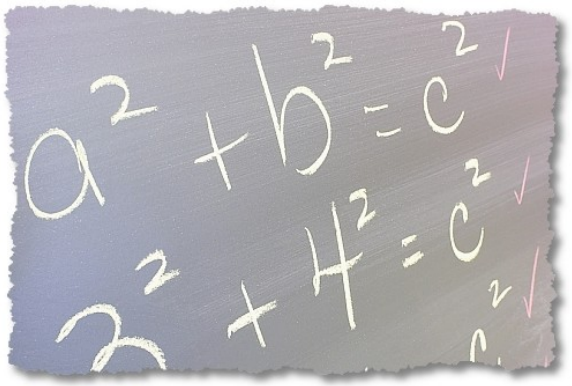
> 2y = 2

> _z = 33.3

> function = “woohoo”



* *function* is a reserved word in R

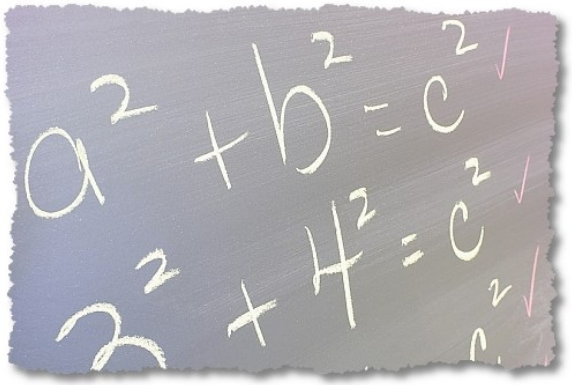


Assign Variables

Try these in your RStudio console:

```
# make variable assignments
> abc = 3
> Abc = log(2.8) * pi
> ABC = "fiddle"
```

Now, check Workspace: Values



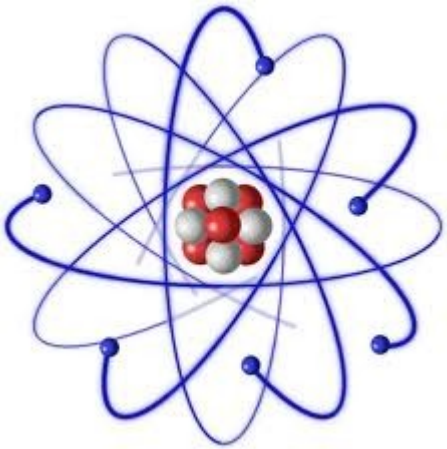
Variables: save it

Alternate R syntax for assignment

```
> y =  2 + 3 * 5
> z <- 2 + 3 * 5        # Same thing as y
```

Variable assignment: Use = or <-

R's atomic data types



Let's take a look at some available data types:

- Numeric (includes integer)
  3.14, 1, 2600

- Character (string)
  “hey, I'm a string”

- Logical
  TRUE or FALSE

- NA
  No value known

Numeric data

Find the type of a variable using class()

```
> class(8)                    # numeric type
[1] "numeric"

> class(6.02e+24)             # numeric type
[1] "numeric"

> class(pi)                   # numeric type (predefined in R)
[1] "numeric"
```

Character and Logical data

Find the type of a variable using class()


```
> class("phooey")  # character type:
[1] "character"    # notice the quotes

> class(TRUE)      # logical type: no quotes
[1] "logical"

> class(NA)        # NA (no quotes) means “no value known”
[1] "logical"
```

RStudio test flight

To whet your appetite for RStudio, let's try:

- Using the editor
- Entering data
- Making a plot in R
- Sourcing a file

The M&M Exercise

On your workstation:

- Sign in to hpc2.org
- Start the RStudio tool
- Create/Access Project from GitHub

  git://github.com/jsperhac/workshop-dev.git

- Files pane: click *examples*, then

  mm-single-example.R

The M&M Exercise

Inside mm-single-example.R:

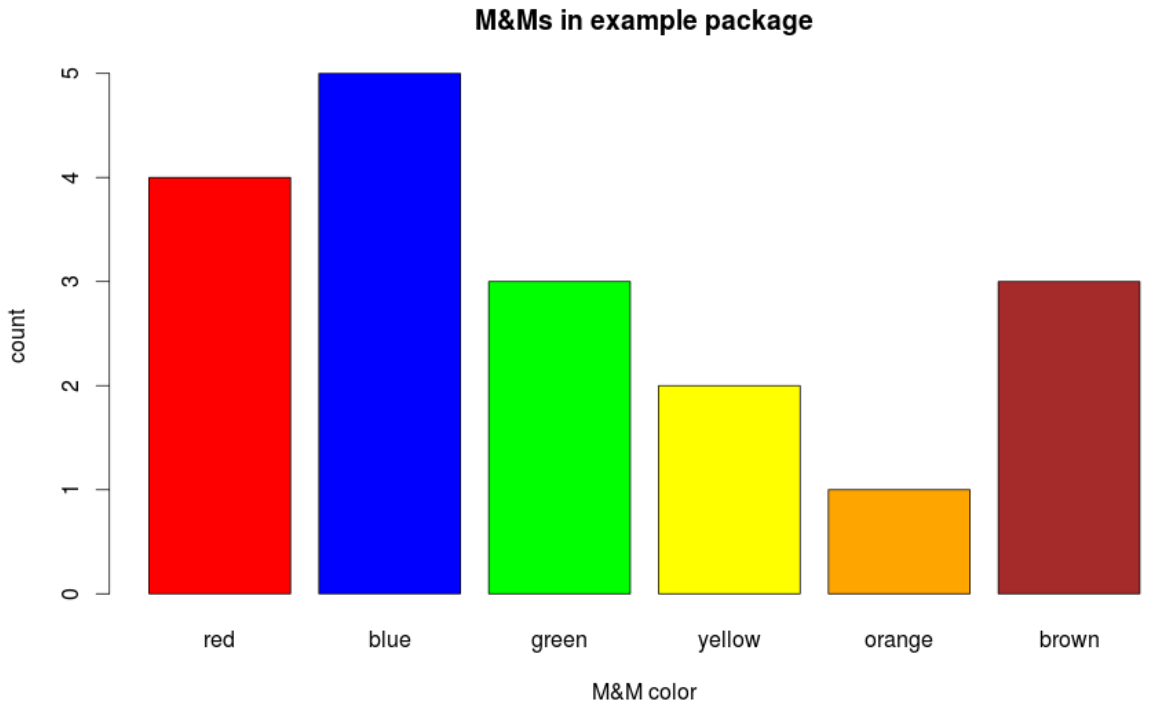
- Change the M&M color counts in the mv variable
- Edit ptitle, if you want

```
# EDIT HERE: ...
mvl = c("red", "blue", "green", "yellow", "orange", "brown")
mv = c(   4,      5,      3,       2,       1,       3)
ptitle = "M&Ms in example package"
```

The M&M Exercise

Inside mm-single-example.R:

- Save the file (File:Save)
- Source the file (Source button)



The M&M Exercise

Questions:

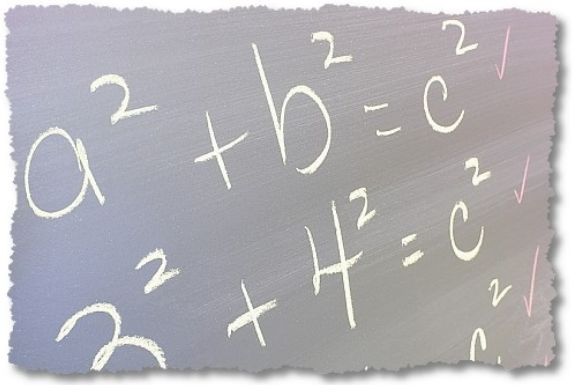
- What have you plotted?
- What outputs does R provide in the console?
- What variables were created?
- What else happens inside this source file?

OK, now you can eat...

Using Logical Operators


```
1==2          # equivalence test: double equals
9 != 19       # “not equal” test
3 < 204       # less-than test
18 > 44       # greater-than test
“tree”==89    # comparing mixed data types
```

What should the results of these tests be?



A logical test

Compare R syntax for assignment

```
> y =  2 + 3 * 5
> z <- 2 + 3 * 5      # Same thing as y

> y==z                # Here's the test...
[1] TRUE
```

Logical data

A logical value is often created from a comparison between variables.

```
u & v       # Are u AND v both true?
u | v       # Is at least one of u OR v true?
!u          # “NOT u” flips the logical value of
            #         variable u
```

Learning about Object x

R stores everything, variables included, in Objects.

Object x


```
> x <- 2.71
> print(x)          # print the value of the object
[1] 2.71

> class(x)          # what data type or object type?
[1] "numeric"

> is.na(x)          # is.na() tests whether a value has a
                    # known value
[1] FALSE
```

Interlude

Complete variable/atomic datatype exercises.

Open in the RStudio source editor:

<workshop>/exercises/exercises-variables-atomic-datatypes.R