# **Programming Concepts**

with instructor Colby Witherup Wood

will begin at 1:02 pm Central

This workshop is brought to you by

### **NUIT Research Computing Services**

Have a programming or data question about your research?

We're here to help. bit.ly/rcsconsult

This workshop was designed for anyone who is about to start learning a coding language.

Build familiarity with:

Goals:

- 1. How to give computers instructions
- 2. Common terms and concepts

### Downloading materials from GitHub

https://github.com/agithasnoname/programmingConcepts

Click on the green Clone or download button

then click on **Download ZIP** 

During this workshop, ask questions in the chat. I will answer them periodically throughout the workshop.

If my internet goes out during this workshop, that means you get a 10 minute break! You may have to log back into Zoom. Sorry!

# **Programming languages**

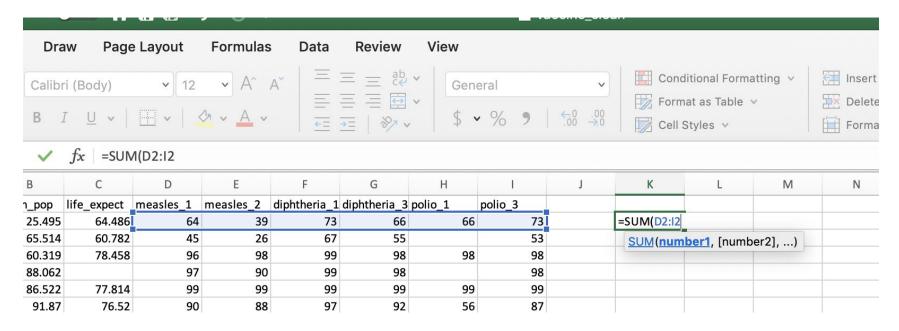
How you talk to your computer

Modern computers can interpret many different languages

GUIs (graphical user interfaces) allow you to talk to your computer without knowing any programming language

# **Programming languages**

requires you to use specific words or characters in a specific order



# **Programming languages**

The **command line** is how we can talk directly to our computer without a GUI.

Different computers have different **shells** to access the command line and different languages you use on the command line.

Mac: Terminal uses Unix Bash, PC: Windows PowerShell

These are designed for controlling your operating system and computer: installing programs, moving files, etc.

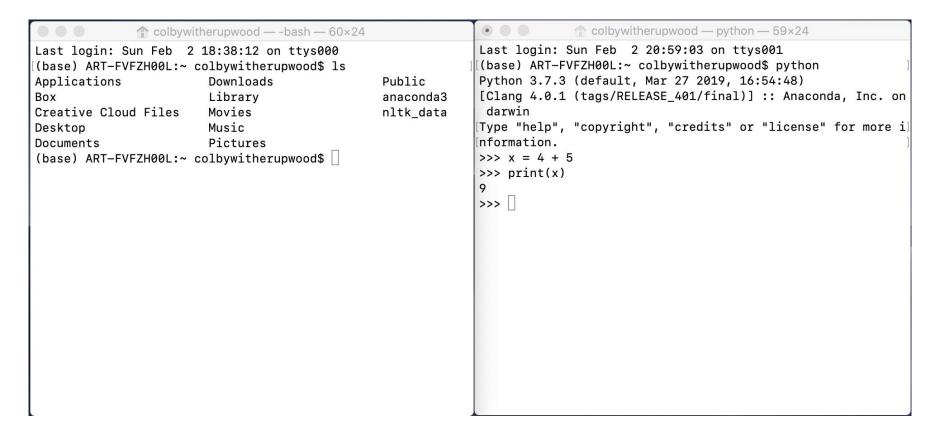
### How do we talk to our computer in Python or R?

 Interactive programming - through a shell, one line at a time

- Batch programming - running a whole script (a plain text file that contains one to many lines of code)

With the help of a GUI. GUIs for coding are called
 IDEs - Integrated Development Environments

## **Command prompts**



# Time to Review!

Open the ProgrammingConceptsReview document from the folder you downloaded.

# **Filesystems**

Reminder: If my internet goes out during this workshop, that means you get a 10 minute break! You may have to log back into Zoom. Sorry!

# **Filesystems**

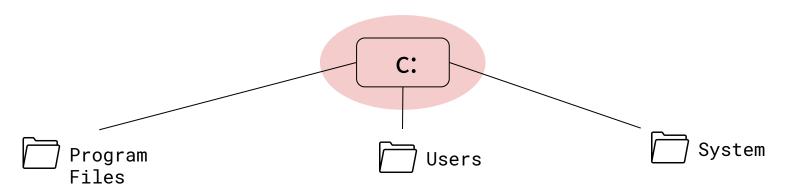
Coding requires us to move away from point and click.

We will want to work with files, so we need to know how to use words to guide the computer to the right files.

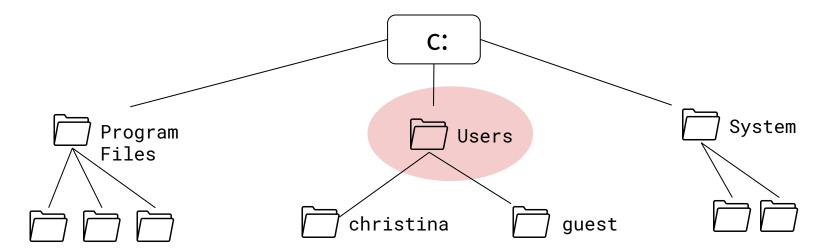
Every file has an **absolute path**, which starts with the **root**.

c:

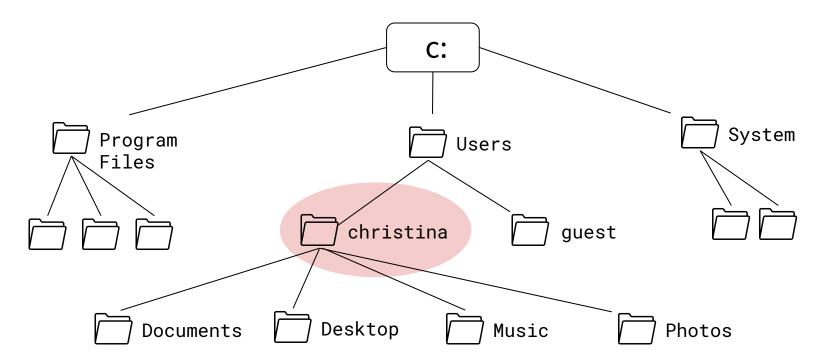
C:\



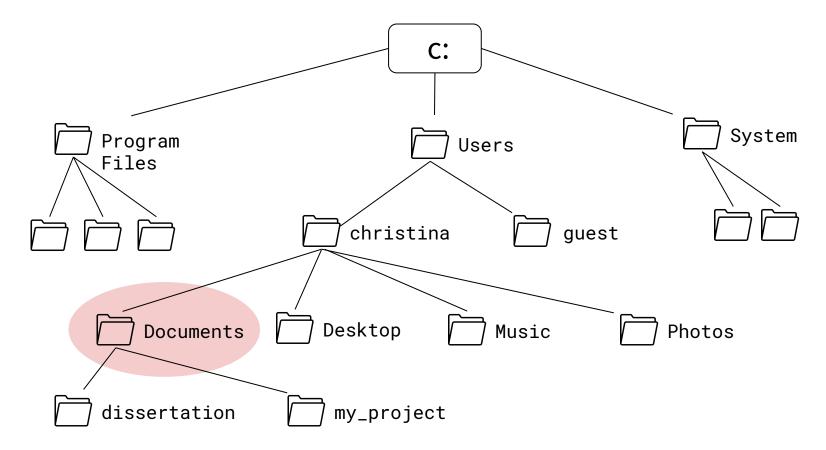
#### C:\Users\



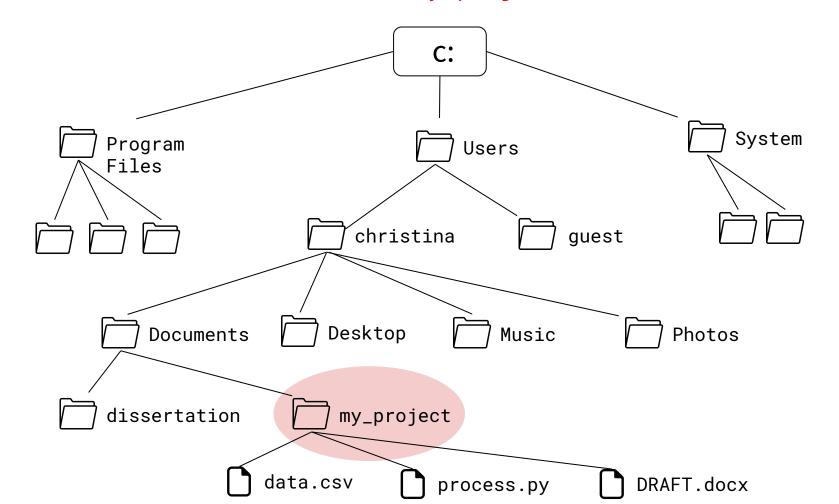
#### C:\Users\christina



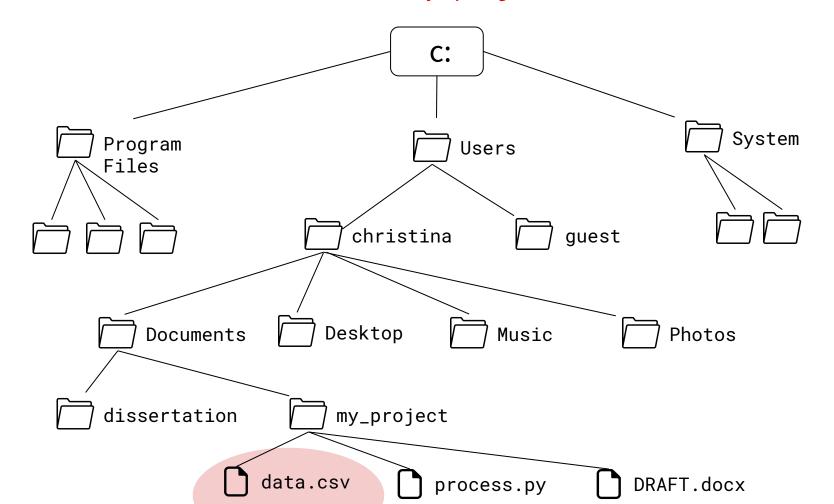
#### C:\Users\christina\Documents



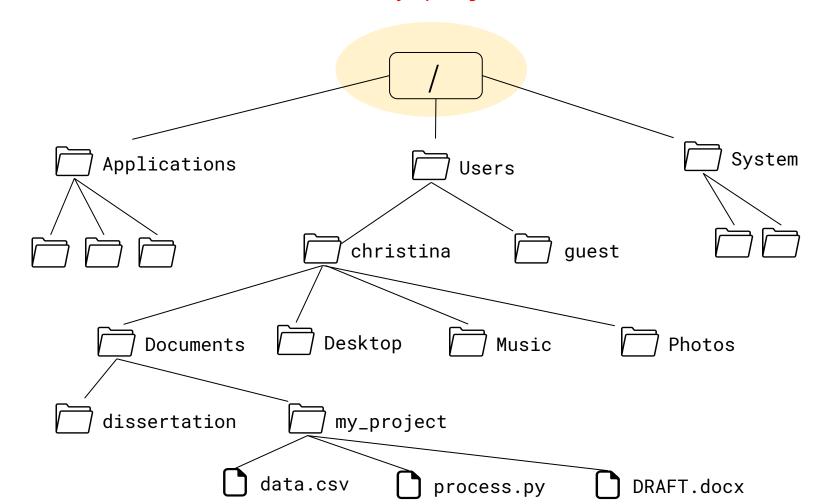
#### C:\Users\christina\Documents\my\_project



#### C:\Users\christina\Documents\my\_project\data.csv



#### /Users/christina/Documents/my\_project/data.csv



#### **Absolute Paths**

C:\Users\christina\Documents\my\_project\data.csv

/Users/christina/Documents/my\_project/data.csv

# **Home directory**

In addition to a root directory, computers have a **home directory**. As a shortcut, you can refer to the home directory as ~

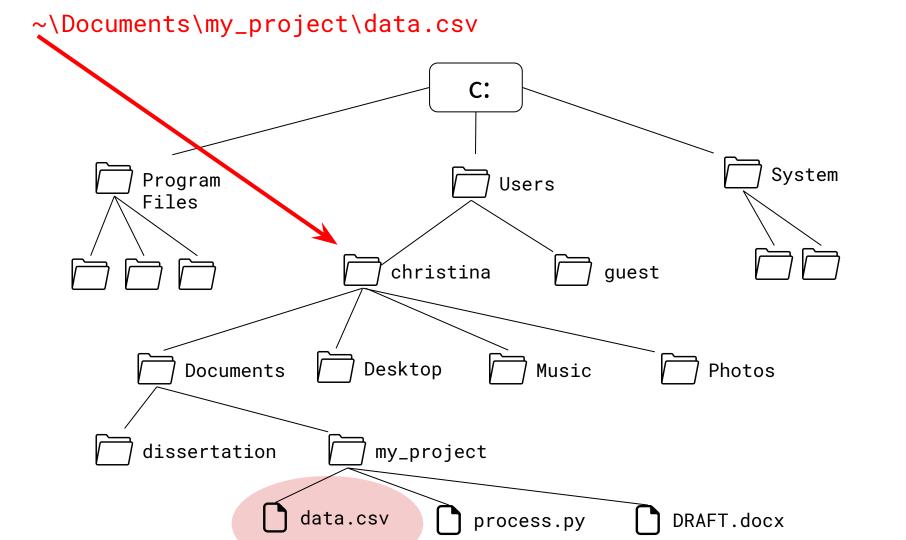
### Home Directory: C:\Users\christina C: System Program Users Files christina guest Documents Desktop Music **Photos**

my\_project

data.csv

dissertation





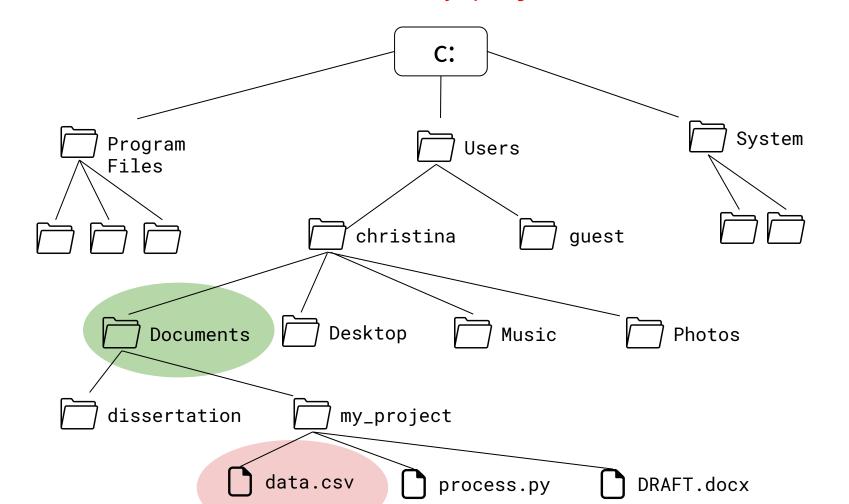
# **Working Directory**

A working directory is the directory associated with a running process or program

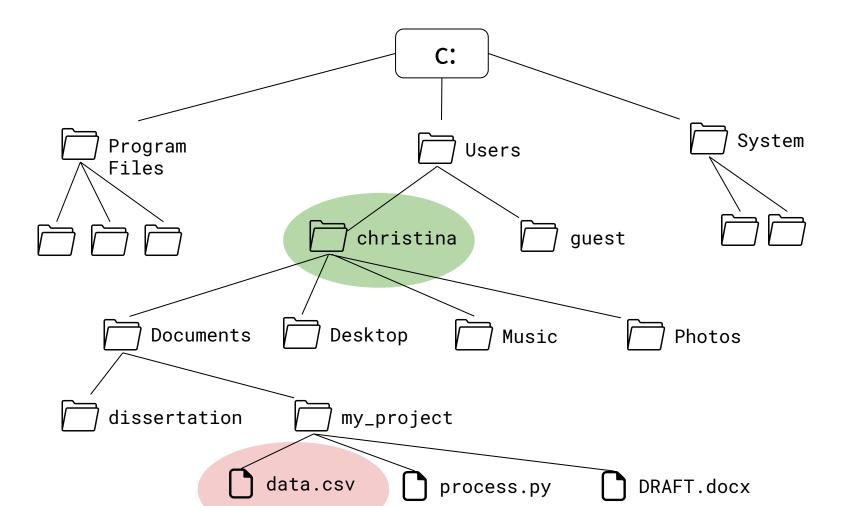
This is where the computer starts when looking for files

You can use **relative file paths** from your working directory

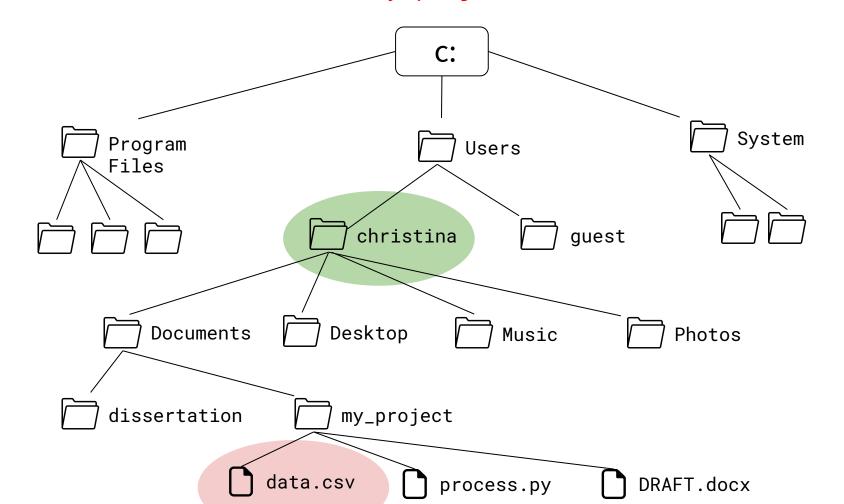
#### Relative Path from Documents: my\_project/data.csv



#### From christina:



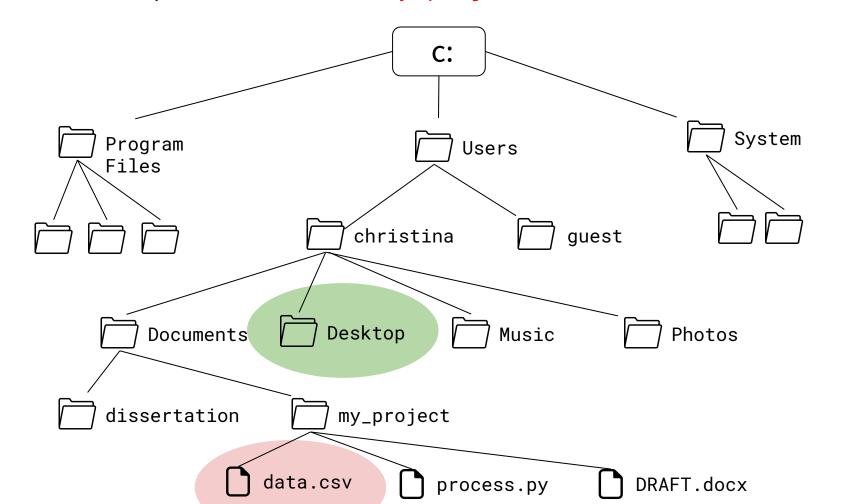
#### From christina: Documents/my\_project/data.csv



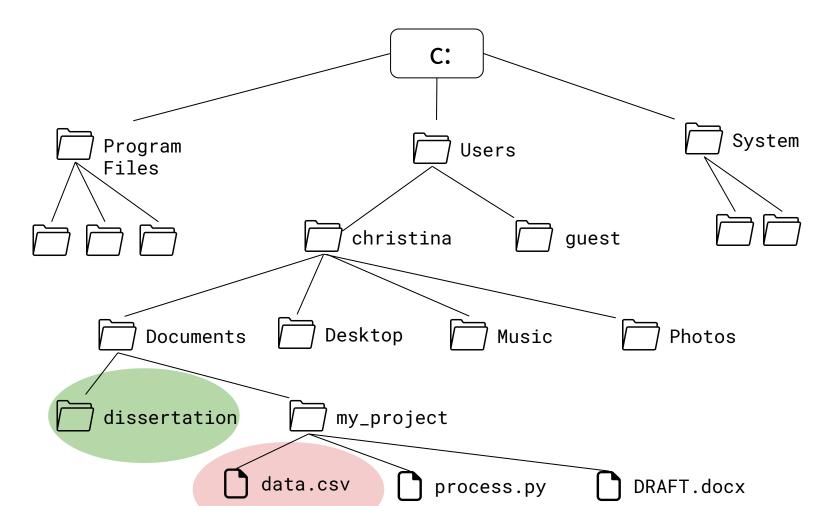
Another shortcut is .. which goes up one

directory.

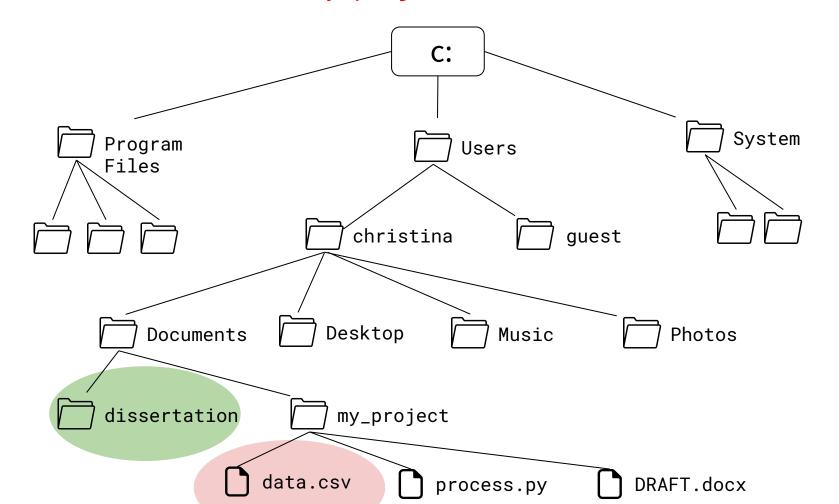
From Desktop: ../Documents/my\_project/data.csv



#### From dissertation:



From dissertation: ../my\_project/data.csv



# But what is the default Working Directory?

#### Python:

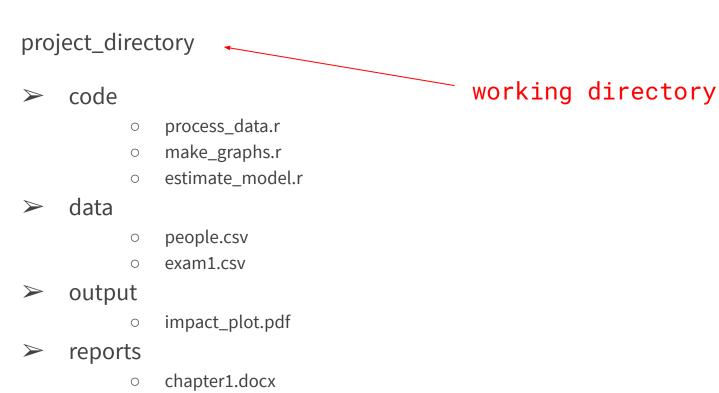
- Where you start Python from
- Where you call a Python script from

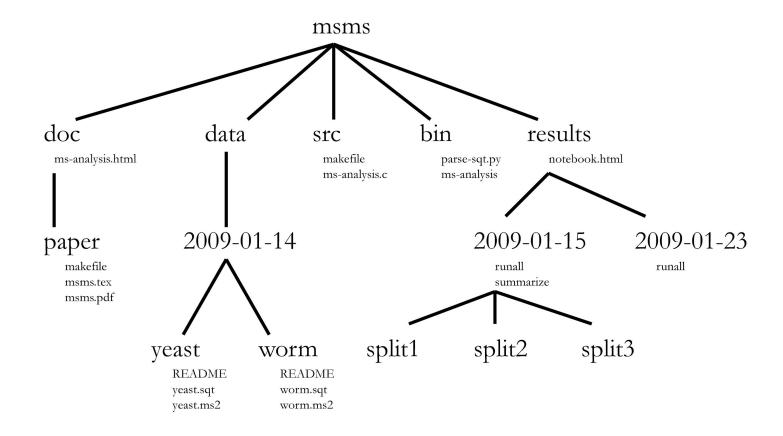
R

- Default: home directory
- RStudio Projects: the folder you associate with the project

You can always set or change the working directory

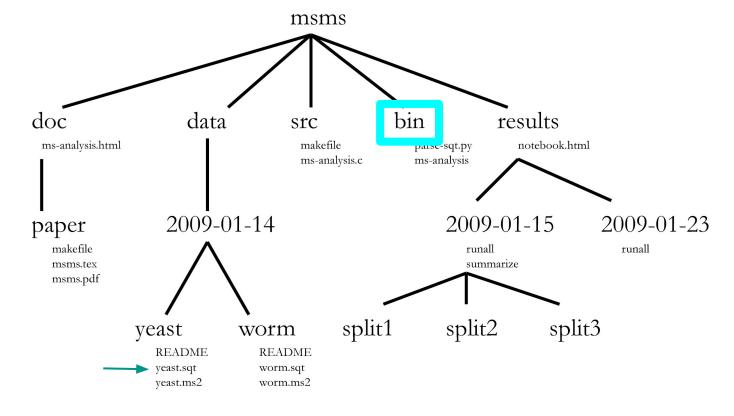
# **Store Project Files Together**





#### A Quick Guide to Organizing Computational Biology Projects

William Stafford Noble, Published: July 31, 2009, <a href="https://doi.org/10.1371/journal.pcbi.1000424">https://doi.org/10.1371/journal.pcbi.1000424</a>



A) data/2009-01-14/yeast/yeast.sqt
B) ../data/2009-01-14/yeast/yeast.sqt
C) ~/data/2009-01-14/yeast/yeast.sqt

# **Files**

Reminder: If my internet goes out during this workshop, that means you get a 10 minute break! You may have to log back into Zoom. Sorry!

# Reading and Writing

Read: Open a file to get the contents

Write: Open a file to put information in

## Modes

Read: get information, can't change it

Write: empties the file! then allows writing

Append: add to the bottom of the file

# File Types

Text: Restricted set of characters

>> Data can be opened and viewed directly

Binary: Custom data

>> Needs a program to interpret and
display the data

# NO FORMATTING NO IMAGES

# **Plain Text Files**

```
Common extensions: .txt, .tab, .csv
Also plain text:
  Data files: XML, JSON
  Markup: HTML, Markdown (.md), LaTeX (.tex)
  Code: R scripts (.r), Python scripts (.py)
```

```
# R Workshops
  This repository is a clearing house for resources for individual R workshops from [Resear
  # Workshops
  ## Current Workshops
  [Intro to R](https://github.com/nuitrcs/r intro june2018)
  [`ggplot2`](https://github.com/nuitrcs/r ggplot july2018)
  [Databases](https://github.com/nuitrcs/databases workshop/tree/master/r): Information on
  useful reference, but you'll need a database connection to run it. See that repository 1
  [R Markdown](https://github.com/nuitrcs/rmarkdown workshop)
  [R Shiny](https://github.com/nuitrcs/rshiny)
  # Software
  For workshops, it's best to install R and RStudio on your own laptop (both are free).
  [Install R](https://cran.rstudio.com/)
  [Install PStudio Deskton]/https://www.retudio.com/products/retudio/download/)
https://raw.githubusercontent.com/nuitrcs/rworkshops/master/README.md
```

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4	ATOM	2	Н	1	0.257	0.727	0.000
5	ATOM	3	Н	1	0.771	-0.727	0.890
5	ATOM	4	Н	1	0.771	-0.727	-0.890
7	TER	5		1			
8	END						

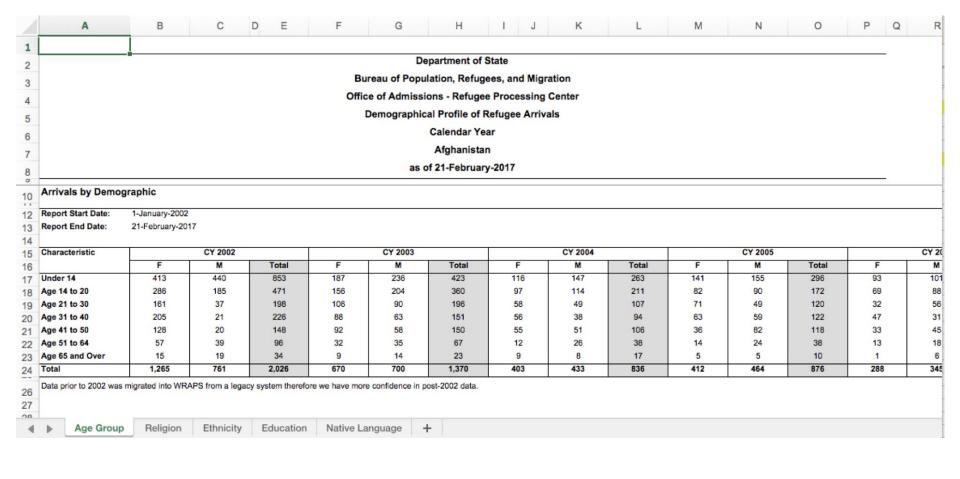
File: ammonia.pdb

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Characteristic, CY 2002, ,,, CY 2003, ,, CY 2004, ,,, CY 2005, ,, CY 2006, ,,, CY 2007, ,, CY 2008, ,, CY 2009, ,, CY 2010, ,, CY
2011,,,CY 2012,,,CY 2013,,,CY 2014,,,CY 2015,,,CY 2016,,,CY 2017,,,Cumulative Total,%
.F .M .Total..F .M .Total.F ..M .Total.F ..M .Total.F ..M .Total.F .M .Total.F .M .Total.F .M .Total.F .M .Total.F
,M ,Total,F ,M ,Total,F ,M ,Total,F ,M ,Total,F ,M ,Total,F ,M ,Total,F ,M ,Total,,Total
Under
14.413.440.853.187.236.423.116..147.263.141.155.296.93..101.194.65.55.120.78.85.163.55.51.106.75.78.153.44.61.105
.83.96.179.84.106.190.102.100.202.145.190.335.464.447.911.54.76.130."4.623".31.96%
Age 14 to
20.286.185.471..156.204.360.97..114.211.82.90.172.69..88.157.34.55.89.63.66.129.29.43.72.48.68.116.47.38.85.56.79.
135,63,92,155,97,87,184,120,197,317,311,385,696,36,58,94,"3,443",23.80%
Age 21 to
30, 161, 37, 198, 106, 90, 196, 58, 49, 107, 71, 49, 120, 32, 56, 88, 39, 24, 63, 50, 42, 92, 24, 32, 56, 45, 67, 112, 46, 37, 83, 41, 48, 89, 66
.64.130.82.52.134.119.91.210.303.277.580.39.25.64."2.322".16.05%
Age 31 to
40, 205, 21, 226, 88, 63, 151, 56, 38, 94, 63, 59, 122, 47, 31, 78, 34, 26, 60, 47, 42, 89, 31, 26, 57, 35, 38, 73, 30, 32, 62, 50, 43, 93, 57, 37
.94.51.27.78.82.61.143.225.138.363.29.23.52."1.835".12.69%
Age 41 to
50, 128, 20, 148, 92, 58, 150, 55, 51, 106, 36, 82, 118, 33, 45, 78, 20, 23, 43, 38, 53, 91, 15, 22, 37, 24, 17, 41, 23, 12, 35, 31, 21, 52, 35, 2
```

#### **Plain Text Editors**

Integrated Development Environments (IDEs) for R and Python let you write plain text files.

Stand alone options:

https://workshops.rcs.northwestern.edu/install/texteditor/

# Time to Review!

# **Data Types**

#### **Numbers**

Integers

Decimal/Float

-38291423

3.0

-432.2343253

4.938e-10

#### Character

AKA: text, string

Enclosed in single or double quotation marks.

```
"This is a string"
```

'This is a string 2'

```
" " (empty string)
```

" (this is NOT an empty string)

#### **Special Characters**

\n New Line
| "whitespace"
| Tab | T

"This is line 1.\nThis is line 2."

#### Case and type matter

```
"A" is not equal to "a"
"3" (string) is not the same as integer 3
```

## Sorting Strings: Alphabetical Order

"Mushroom"

"110 cats"	"110 cats"	"110 cats"
"3 cats"	"3 cats"	"3 cats"
"apple"	"Apple"	"apple"
"mushroom"	"Mushroom"	"Apple"
"Apple"	"apple"	"mushroom"

"mushroom"

"Mushroom"

#### String Indexing (aka string slicing)

"String indexing is fun"

	S	t	r	i	n	g		i	n	d	е	X	i	n	g		i	s
Python	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
R	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

## produces substrings

## **Joining Strings: Concatenate**

```
"Red" + "bull" = "Redbull"

"Red" + " " + "bull" = "Red bull"
```

```
paste("Red", "bull", sep=" ") = "Red bull"
paste("Red", "bull", sep="") = "Redbull"
```

**Boolean** 

# TRUE

# FALSE

TRUE FALSE T F True False

## **Boolean Operators**

NOT: ! not AND: & and OR: | or

#### **Boolean Operators: AND**

TRUF and TRUE = TRUETRUE and FALSE = FALSEFALSE and TRUE = FALSEFALSE and FALSE = FALSE

## **Boolean Operators: OR**

TRUE or TRUE = TRUETRUE or FALSE = TRUEFALSE or TRUE = TRUE FALSE or FALSE = FALSE

## **Boolean Operators: NOT**

not TRUE = FALSE not FALSE = TRUE TRUE and not TRUE = FALSETRUE and not FALSE = TRUE

## **Boolean Operators: Grouping**

```
(TRUE and FALSE) or
not (FALSE and TRUE) =
```

#### **Converting Between Data Types**

```
TRUE as integer = 1

FALSE as integer = 0

3.5 as string = "3.5"
```

## **Special Types**

NULL

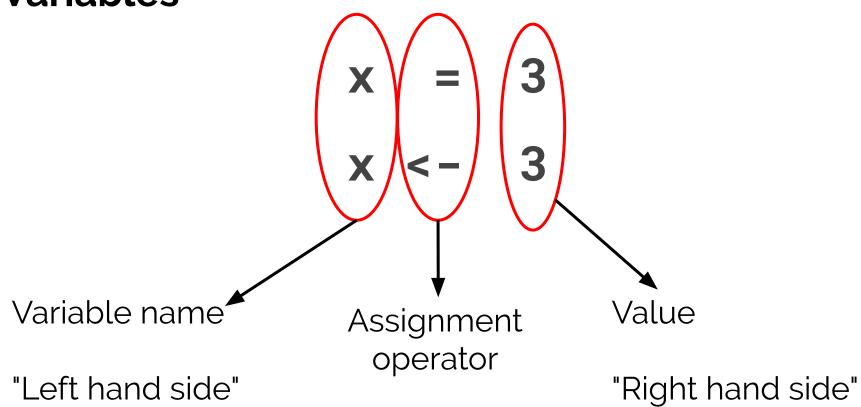
None

Missing Data: NA

# Time to Review!

Variables let us refer to a value with a name. We can use the same name, but change the value.

Variables can be used to name integers, floats, strings, lists, arrays, equations, dictionaries, dataframes, the text in files, and more.



$$x = 3 + 5$$

$$x$$

$$x = 3$$

$$x + 5$$

X

$$x = 3$$

$$x = x + 5$$

$$x$$

$$x = 3$$

$$y = 5$$

$$x = x + y$$

$$x$$

# **Variables**

```
x = 3
  y = 5
x = x + y
  y = 7
```

x is 8

### **Variable Names**

```
Case matters
Start with a letter
Make names meaningful
Style conventions
  camelCase
  separate_with_underscores
```

Lists, vectors, arrays

### Multiple Related Values

Ages of students: 42, 30, 24, 24, 27, 35, 39, 22

### Lists, Vectors, Arrays

```
Python List - enclosed in square brackets
ages = [42, 30, 24, 24, 27, 35, 39, 22]
        0 1 2 3 4 5 6 7
R vector
ages \leftarrow c(42, 30, 24, 24, 27, 35, 39, 22)
```

### Lists, Vectors, Arrays

```
students = ["Michael", "Chen", "Yishu", "June", "Amy"]
evanston_resident = [True, False, True, False, True]
sample_vals = [3.544, 10.0, 18.32]
```

### **Nested Lists**

```
[ [1, 2, 3], ["a", "b", "c", "d"] ]
```

### Lists, Vectors, Arrays

```
Length = number of elements
length([42, 30, 24, 24, 27, 35, 39, 22]) = 8
```

```
Empty list or vector
[]
c()
```

# **List Indexing (Python)**

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
ages[1]
```

30

# **List Indexing (Python)**

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
ages[1:4]
```

[30, 24, 24] Python indexing is exclusive of the end position

# **Vector Indexing (R)**

```
ages <- c(42, 30, 24, 24, 27, 35, 39, 22) ages[1:4]
```

[42, 30, 24, 24] R indexing is *inclusive* of the end position

### **List Variables**

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
ages[1] = 54
ages
```

[42, 54, 24, 24, 27, 35, 39, 22]

### **List Variables**

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
ages = 54
ages
```

**54** 

# **Appending and Prepending**

[42, 30, 24, 24, 27, 35, 39, 22]

Append: [42, 30, 24, 24, 27, 35, 39, 22, **50**]

Prepend (R): [50, 42, 30, 24, 24, 27, 35, 39, 22]



















# Time to Review!

# **Conditions**

### **Conditions**

Expressions that produce a boolean value:

True or False

# Comparisons

# **Comparisons**

age = 
$$13$$

Assignment

age < 21

age == 14

Comparisons

### **Compound Conditions**

```
first_age = 13
second_age = 15
```

first\_age < 21 or second\_age < 21

# **Compound Conditions**

$$first_age = 13$$

first\_age <= 19 and first\_age > 13

```
evanston_resident = True
nu_staff = True
```

evanston\_resident == True and nu\_staff == True

```
evanston_resident = True
nu_staff = True
```

```
evanston_resident -- True and nu_staff -- True
```

evanston\_resident and nu\_staff

evanston\_resident & nu\_staff

```
evanston_resident = True
nu_staff = True
```

not evanston\_resident and nu\_staff

!evanston\_resident & nu\_staff

```
evanston_resident = False
nu_staff = False
```

not evanston\_resident and not nu\_staff

!evanston\_resident & nu\_staff

### **Exercise: Two Truths and a Lie**

Open the exercise from the folder you downloaded.

Complete the top of the page first, and then write your three statements. (6 minutes)

Then, I will assign you to breakout rooms to share your Two Truths and a Lie with other participants. Share your screens one at a time and try to guess which of their statements are the lies. (7 minutes)

# Control Flow: if/then/else

if condition
 do something

if condition

do something

Evaluates to a single TRUE or FALSE value

```
if age >= 18
  print "Go Vote!"
```

if condition do something else do something different

```
if age >= 18
  print "Go Vote!"
else
  print "Too young!"
```

### **Chained If Statements**

```
if condition
  do something
else if condition2
  do something different
else
  do a third thing
```

## **Chained If Statements**

```
if age >= 18
                             18, 19, 20, 21...
  print "Go Vote!"
else if age >= 16
                             16, 17
  print "Learn to drive"
                             15, 14, 13, 12,
else
                             11, 10...
  print "Too young!"
```

## If Statements: Multiple Actions

```
if age >= 18
   print "Go Vote!"
else if age >= 16
   print "Learn to drive"
   print "Stay in school"
else
   print "Too young!"
```

## **If Statements: Syntax**

```
if age >= 18:
                                  if (age >= 18) {
                                      print("Go Vote!")
   print("Go Vote!")
                                  } else if (age >= 16) {
elif age >= 16:
   print("Learn to drive")
                                      print("Learn to drive")
                                      print("Stay in school")
   print("Stay in school")
                                  } else {
else:
                                      print("Too young!")
   print("Too young!")
```

## **Writing Pseudocode**

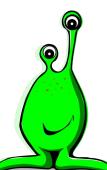
if color is green and has eye stalks

send to Mars

else

send to Earth







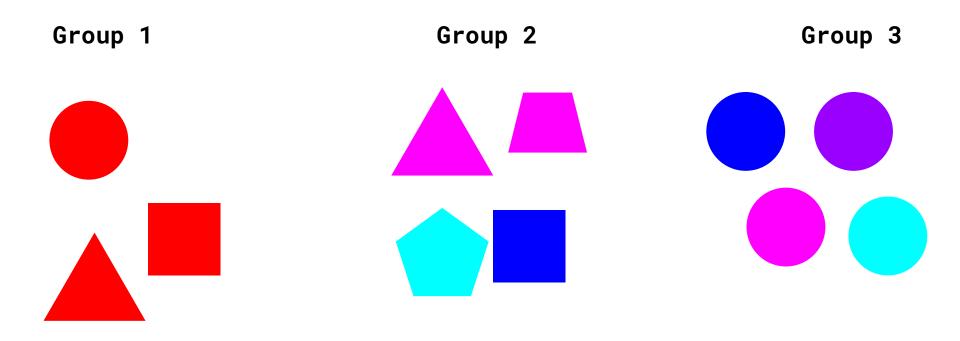






#### **Exercise**

Write an if/else statement that would sort the shapes below into the correct groups



#### **Exercise**

```
if shape is red
  Put in group 1
else if shape is circle
  Put in group 3
else
  Put in group 2
```

#### If Statements and Lists/Vectors

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
```

```
if ages > 18
  Do something
```

## Time to Review!

## Loops

### For Loop

Loops are how we repeat the same action many times

for variable in list/vector of values
 do something

### For Loop

```
ages = [42, 30, 24, 24, 27, 35, 39, 22]
                  Variable called age
for (age) in ages
  print(age)
                              for i in ages
                                 print(i)
```



Ruff!















## For Loop

```
total = 0

for i in 1:10

total = total + i

print total
```

# For Loop total = 0

for i in 1:8

total = total + i

print total

total

10

21 28

6

15

36

#### For Loop total total = 0ages = [42,30,24,24,27,35,39,22]for i in ages total = total + iprint total

## For Loop with if/else statements

```
shapes = [
```

```
for shape in shapes
if shape is red
Put in group 1
else if shape is circle
Put in group 3
else
Put in group 2
```







for dog in row if dog ears up bark(dog) Mung!



## **Functions**

#### **Functions**

- Take input values
- Can return an output value
- Python and R functions usually don't alter their input values (but they sometimes do!)

#### **Functions**

The *len()* function in Python takes a list as input and returns the length of that list:

The *length()* function in R takes a vector as input and returns the length of that vector:

length(
$$c(1, 2, 3, 4)$$
) 4

#### **Function Definitions**

open(file, mode='r', buffering=-1, encoding=None, errors=None, newline=None, closefd=True, opener=None)

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

#### **Function Definitions: Function Name**

open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True,
opener=None)

#### **Function Definitions: Parameters**

```
open(file, mode='r', buffering=-1, encoding=None, errors=None, newline=None, closefd=True, opener=None)
```

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

#### **Function Definitions: Parameter Names**

```
open(file, mode='r', buffering=-1, encoding=None, errors=None, newline=None, closefd=True, opener=None)
```

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

#### **Function Definitions: Default Values**

open(file, mode='r', buffering=-1, encoding=None, errors=None, newline=None, closefd=True, opener=None)

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

#### **Function Definitions: Required Parameters**

open(file, mode='r', buffering=-1, encoding=None, errors=None, newline=None, closefd=True, opener=None)

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

## **Calling Functions: Python**

```
open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True, opener=None)
```

```
open("results.txt", mode='w')
```

#### **Calling Functions: Arguments**

open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True, opener=None)

```
open("results.txt", mode='w')
```

#### Calling Functions: Keyword Arguments

```
open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True, opener=None)
```

```
open("results.txt", mode='w')
```

### Calling Functions: Non-Keyword Arguments

```
open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True, opener=None)
```

```
open("results.txt", mode='w')
open("results.txt", 'w')
```

#### **Calling Functions: Order Matters**

```
open(file, mode='r', buffering=-1, encoding=None,
errors=None, newline=None, closefd=True, opener=None)
open(file="results.txt", 'w')
open(mode='w', "results.txt")
open(mode='w', file="results.txt")
open("results.txt", 'w')
```

#### **Calling Functions: R**

```
read.csv(file, header = TRUE, sep = ",", quote = "\"",
    dec = ".", fill = TRUE, comment.char = "", ...)
read.csv("results.txt", sep="\t")
read.csv("results.txt", "\t")
read.csv("results.txt", TRUE, "\t")
```

#### Calling Functions: R: Positional and Named

```
read.csv(file, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

```
read.csv(file="results.txt", TRUE, "\t")
```

#### Calling Functions: R: Positional and Named

#### Calling Functions: R: Positional and Named

```
read.csv(file, <u>header = TRUE</u>, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

```
read.csv(header=TRUE, "results.txt", "\t")
```

#### **Calling Functions: Return Values**

Some functions return a value:

```
abs(-3)
```

Returns 3

The return value can be assigned to a variable:

```
x = abs(-3)
```

x is 3

#### Calling Functions: No Return Value

Other functions do not return a value, but are called to do something:

```
print("Hello World!")
```

They cannot be assigned to a variable:

```
x = print("Hello World!")
```

### Calling Functions: Variable Arguments

# Arguments can be variables: x = "Hello World!" print(x) file = "results.csv" open(file)

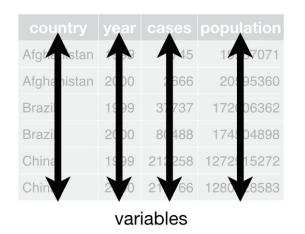
### Packages/Libraries/Modules

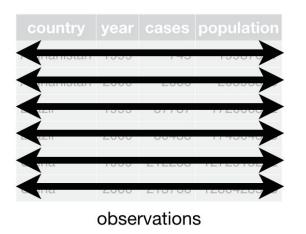
- Collections of functions, data, and other code
- Some must be installed, others are standard
- installed it has been downloaded to the computer
- **imported** it has been loaded into the current script or interactive instance (must happen before you can use it)
- Using packages/libraries/modules is expected!
- Look for pre-existing code/solutions
  - O How do you know it's good/correct?

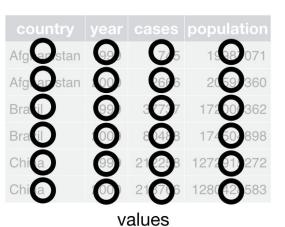
# Time to Review!

# **Data**

# Rectangles of Data







# **Rows: Observations**

```
Person (or mouse, worm, etc.)
Country
Year
Run/trial of an experiment
Chemical
```

Sample

# Columns: Variables

Measurements

Grouping/identification variables:

- > trial/sample
- > condition
- > label for the observation (country name)

Each ID variable in its own column

## **Exercise - reshape this data**

	1 min				5 min			
strain	normal		mutant		normal		mutant	
Α	111	170	375	384	277	234	207	466
В	336	169	491	233	392	341	213	472



strain	genotype	minute	trial	response
А	normal	1	1	111
А	normal	1	2	170
А	mutant	1	1	375
А	mutant	1	2	384
А	normal	5	1	277
А	normal	5	2	234
А	mutant	5	1	207
А	mutant	5	2	466
В	normal	1	1	336
В	normal	1	2	169
В	mutant	1	1	491
В	mutant	1	2	233
В	normal	5	1	392
В	normal	5	2	341
В	mutant	5	1	213
В	mutant	5	2	472