# **Programming Concepts**

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https://github.com/agithasnoname/programmingConcepts

### Northwestern IT Research Computing Services

Available to any NU student, postdoc, faculty, or staff member who does research



Consultations – data and coding questions, from simple to complex: <u>bit.lv/rcsconsult</u>



Trainings – we have scheduled workshops: bit.ly/rcswinter, and we can teach workshops to your group by appointment



**Data services** – we take on a limited number of data science projects for faculty and staff each year



Mentoring – we hire Graduate Assistants and hourly graduate student data consultants (with advisor approval)

# Goals

Build familiarity with:

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

# Introductions

# **Programming languages**

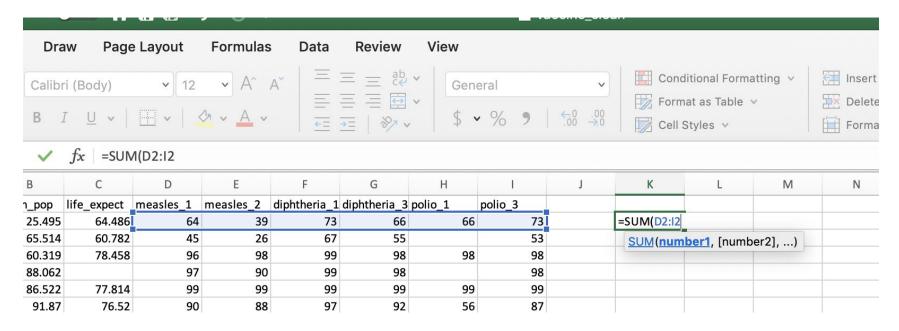
How you talk to your computer

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.

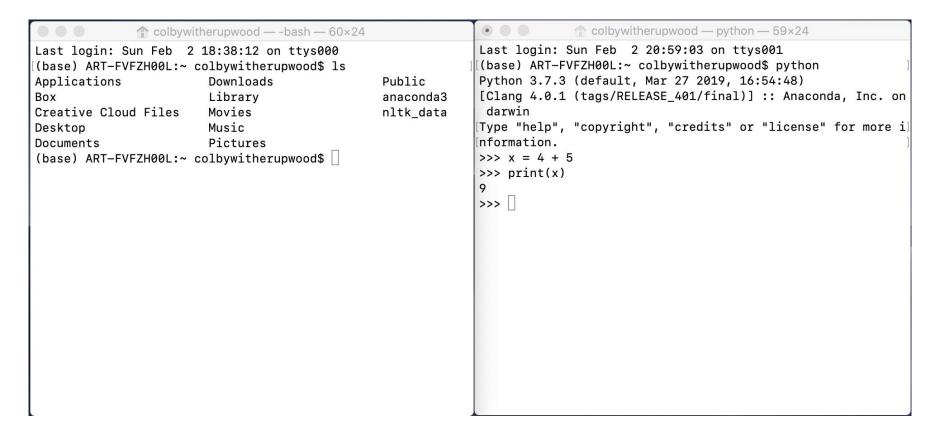
### How do we talk to our computer in Python or R?

 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**



# **Filesystems**

# **Filesystems**

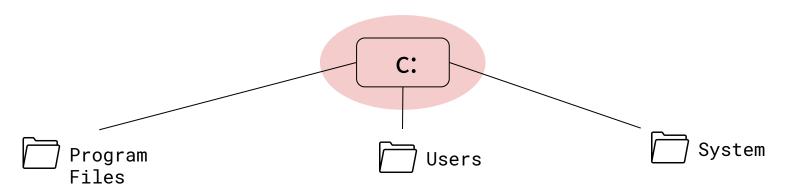
Coding requires us to move away from point and click.

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

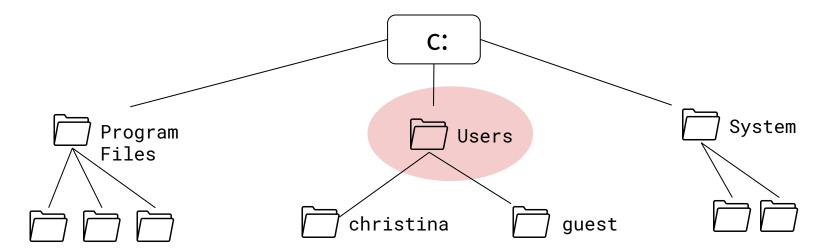
Every file has an **absolute path**, which starts with the **root**.

c:

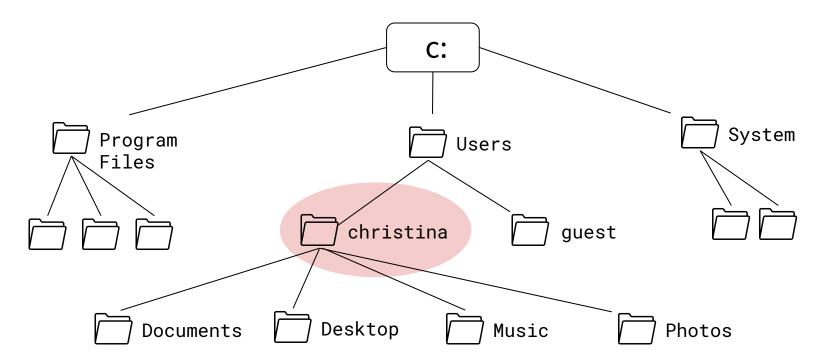
C:\



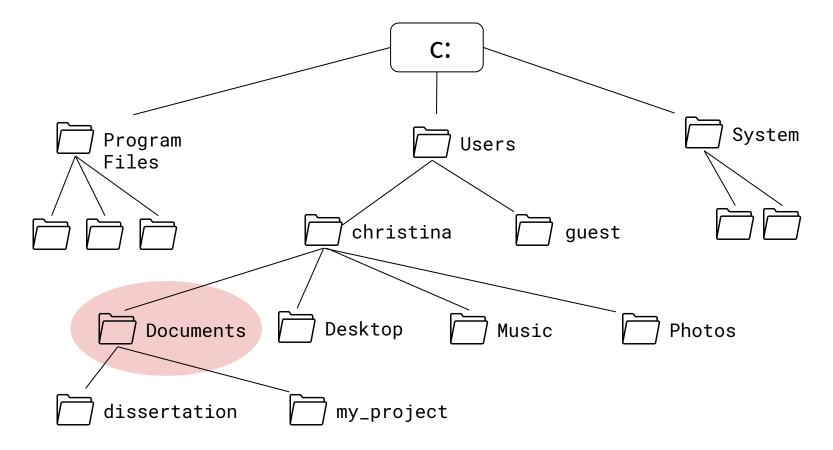
#### C:\Users\



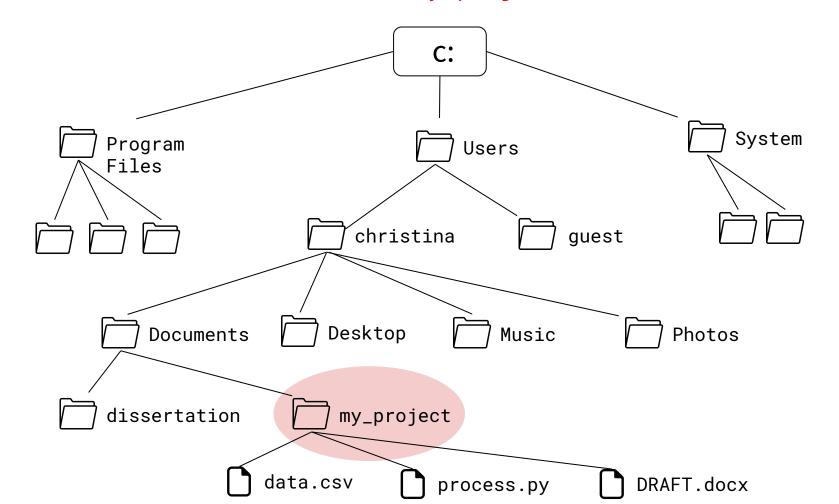
#### C:\Users\christina



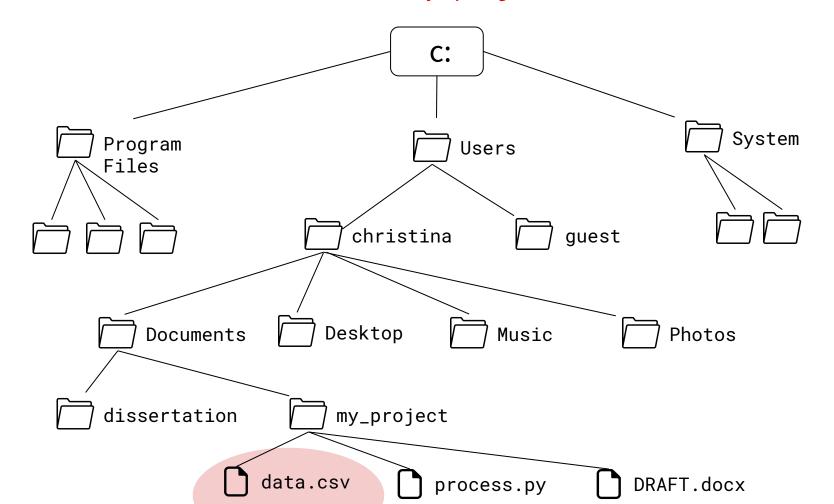
#### C:\Users\christina\Documents



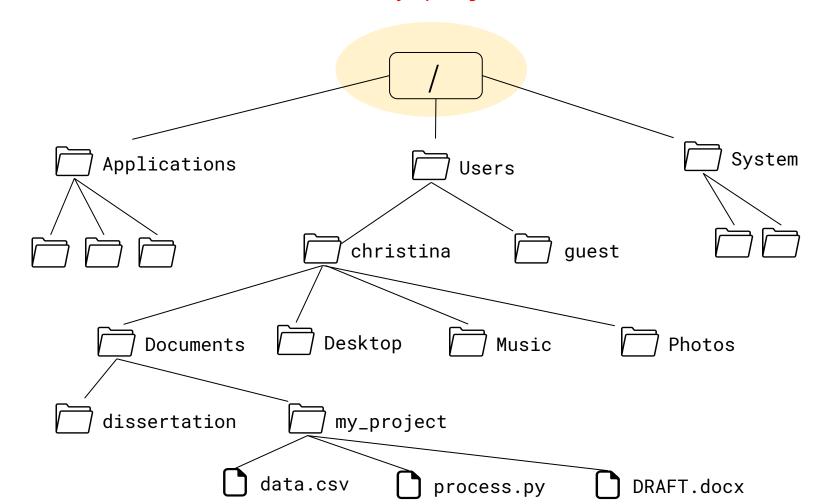
#### C:\Users\christina\Documents\my\_project



#### 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 ~

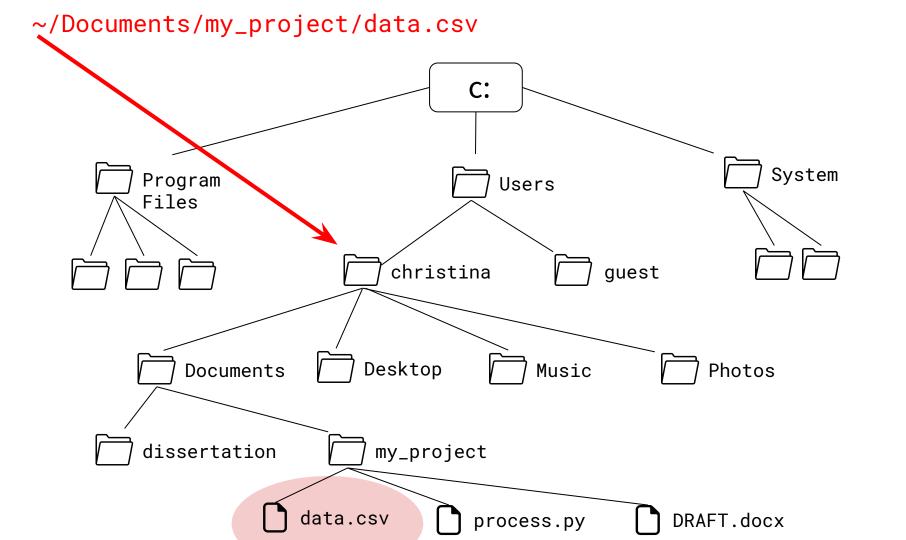
### Home Directory: C:\Users\christina C: System Program Users Files christina guest Documents Desktop Music Photos

my\_project

data.csv

dissertation

process.py DRAFT.docx



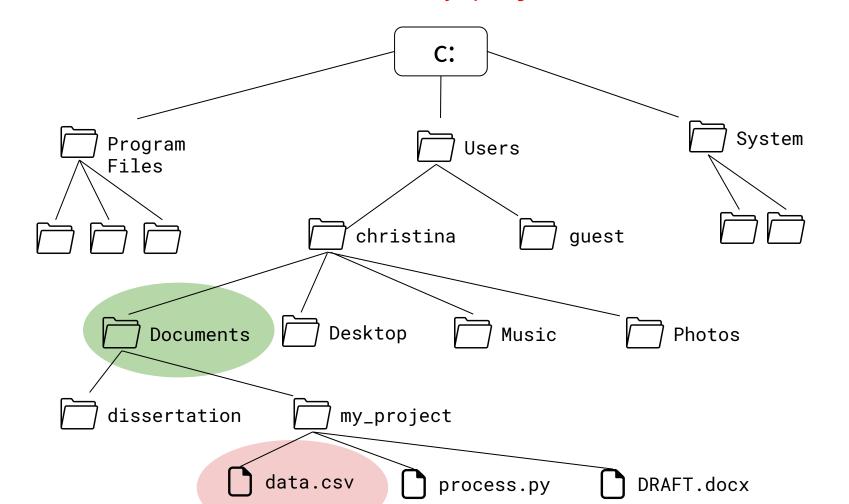
# **Working Directory**

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

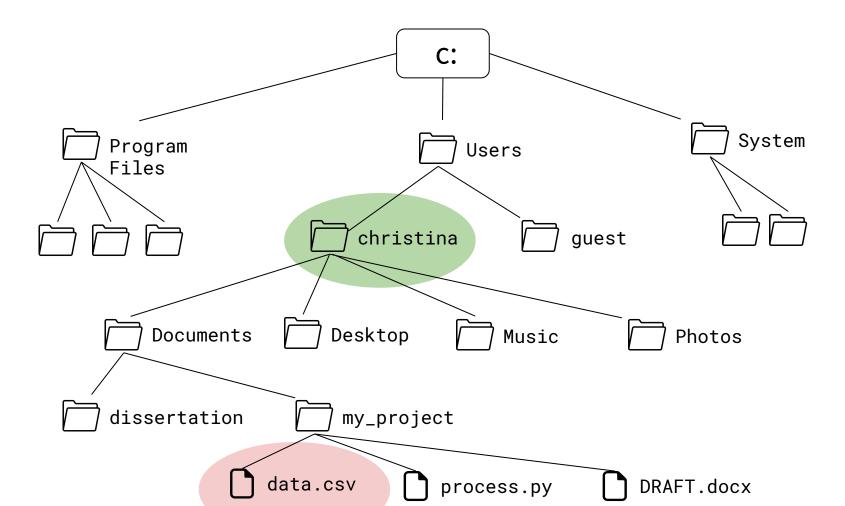
This is where the computer starts when looking for files

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

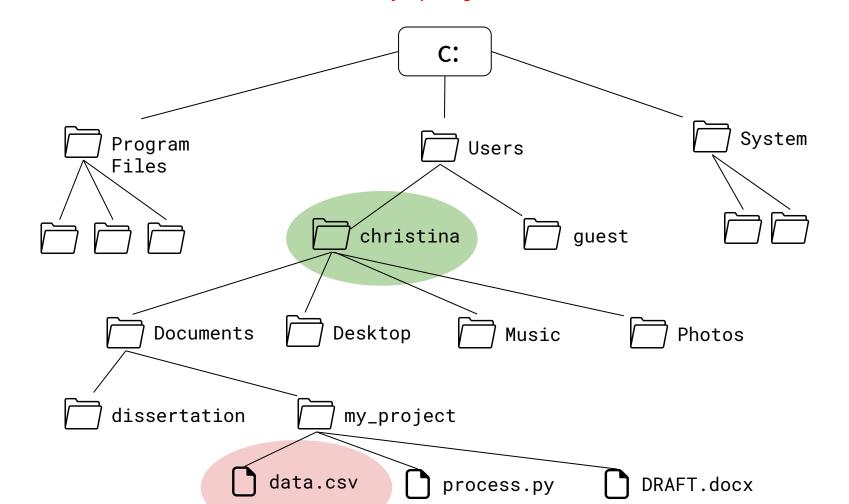
#### Relative Path from Documents: my\_project/data.csv



#### From christina:



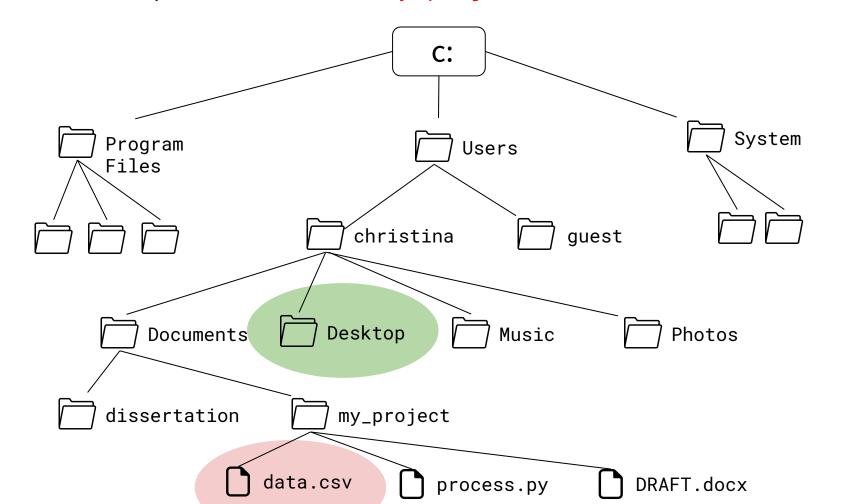
#### From christina: Documents/my\_project/data.csv



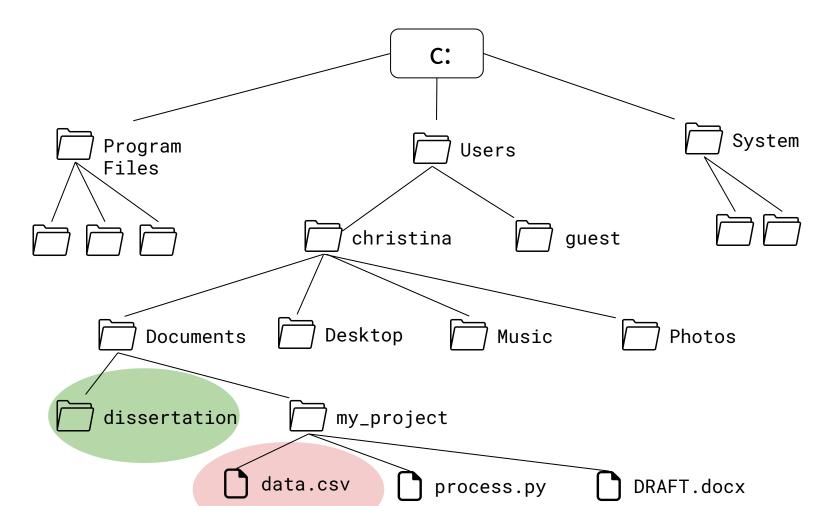
Another shortcut is .. which goes up one

directory.

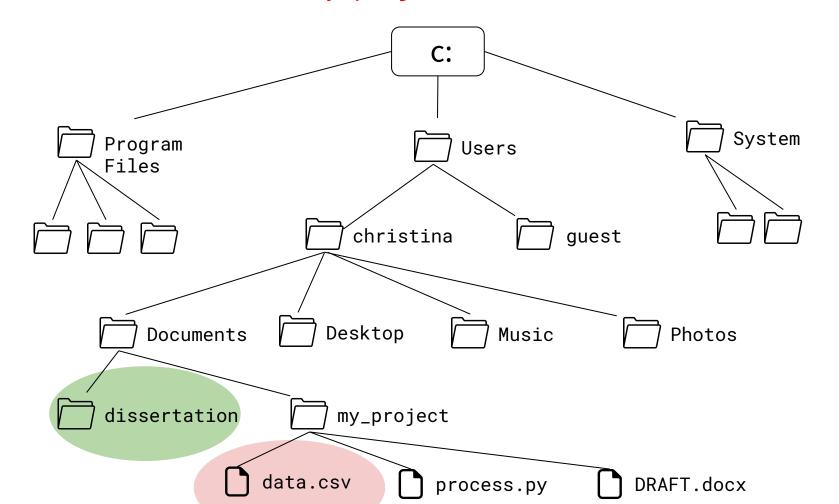
From Desktop: ../Documents/my\_project/data.csv



#### From dissertation:



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



# But what is the default Working Directory?

R

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

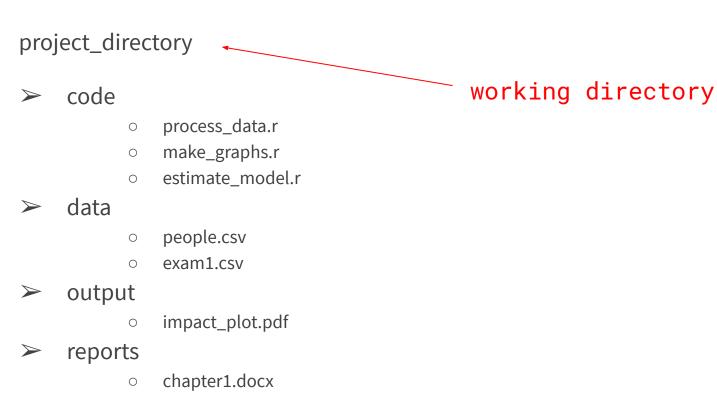
#### Python:

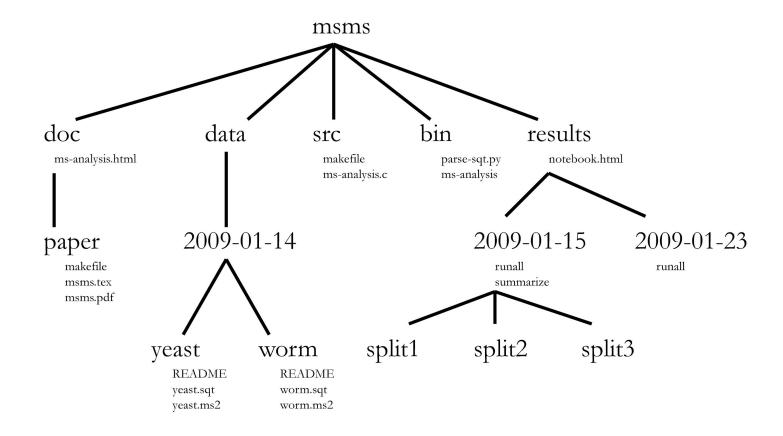
- Where you start Python from
- Where you call a Python script from

You can always set or change the working directory

Why not just use absolute paths?

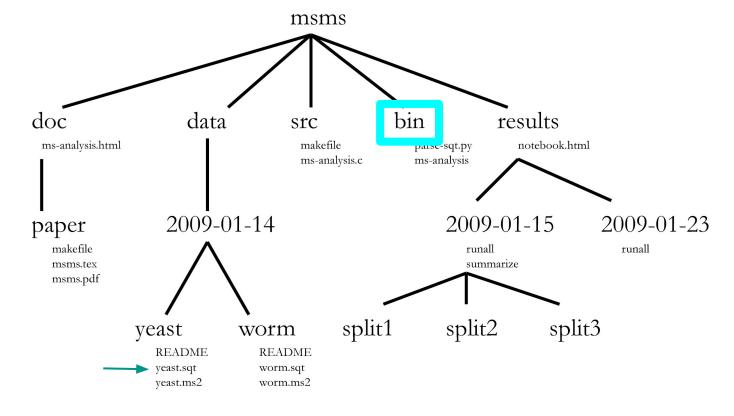
# **Store Project Files Together**





#### 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**

# 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						

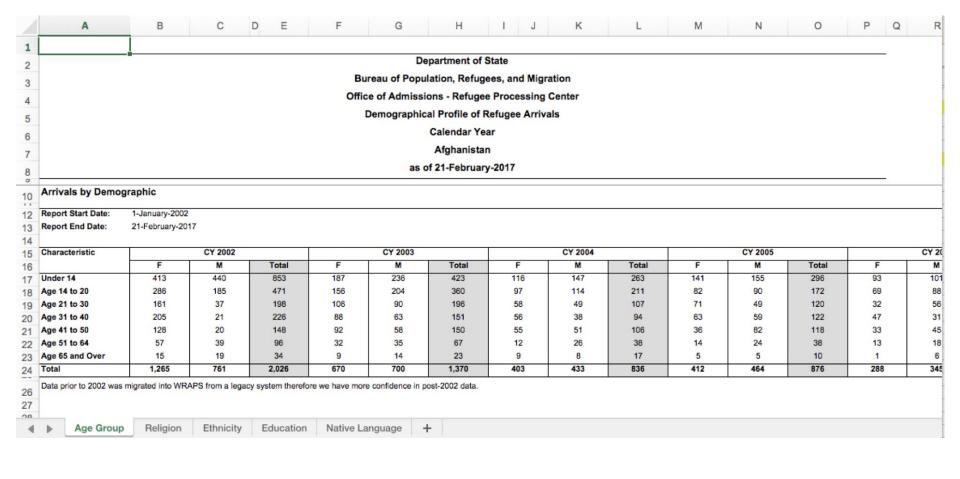
File: ammonia.pdb

```
3
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4
      <<
 5
      /Length 1063
      /Filter /FlateDecode
 6
      >>
8
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```

?#?z?a



```
............
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

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

"Apple" "apple" "mushroom"

"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

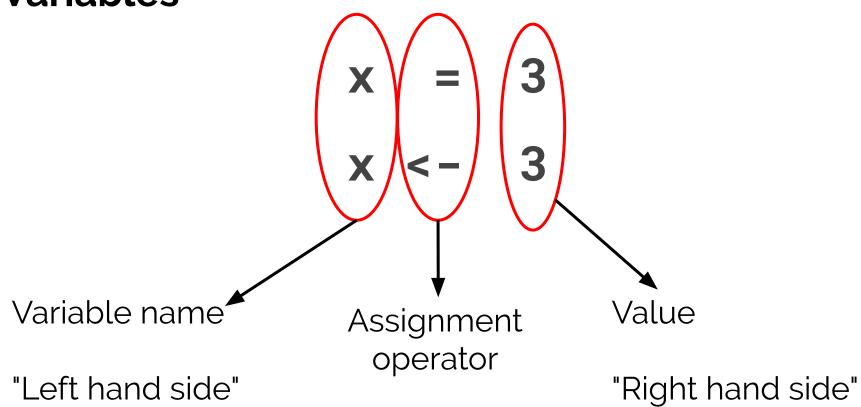
None

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 is 8

$$x = 3$$

$$x + 5$$

X

x is 3

$$x = 3$$

$$x = x + 5$$

$$x$$

x is 8

### **Variables**

$$x = 3$$

$$y = 5$$

$$x = x + y$$

$$x$$

x is 8

## **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]

#### **Vector Variables (R)**

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

[42, 30, 24, 24]

#### **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: [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**

## 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**

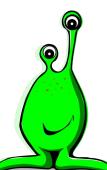
if color is green and has eye stalks

send to Mars

else

send to Earth







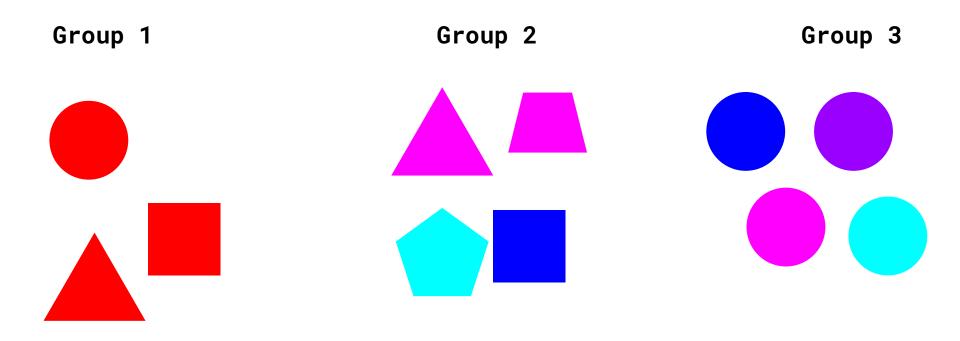






#### **Exercise**

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

Loops are how we repeat the same action many times

for variable in list/vector of values
 do something

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

```
for current_person in workshop_participants
  raise_hand(current_person)
  say_name(current_person)
```

```
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

6

10 15

21 28

36

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

```
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 current_person in workshop_participants
  if first_initial(current_person) < "J"
    raise_hand(current_person)
    say_name(current_person)</pre>
```

## **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!)

#### **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, header = TRUE, sep = ",", quote = "\"", dec = ".", fill = TRUE, comment.char = "", ...)
```

```
read.csv(<del>header=TRUE,</del> "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)

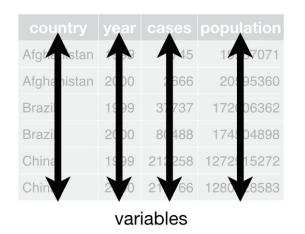
### Packages/Libraries/Modules

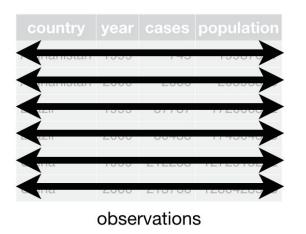
- Collections of functions, data, and other code
- Some must be installed, others are standard
- installed it has been downloaded to the computer
- **imported** it has been loaded into the current script or interactive instance (must happen before you can use it)
- Using packages/libraries/modules is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

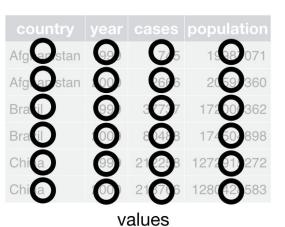
## Time to Review!

## **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**

	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