Programming Basics using Jupyter Notebooks

Get set up

Open your terminal, navigate to where you saved the notebook and start jupyter:

```
$ cd where/my/notebook/is
$ jupyter notebook
```

Open browser and go to http://localhost:8888/

Click on Programming basics.ipynb

Get set up / Galaxy

Go to usegalaxy.org & login Go to:

https://usegalaxy.org/u/drcris/h/immport-workshop

Import the history to your account by clicking on 'Import history', top right corner.

Click on Programming basics.ipynb Click on the graph icon Click on Jupyter



Programming syntax

Crucial for accurate interpretation

• Depends on programming language refer to your favorite language manual for specifics.

Python: pep8

Programming syntax - Comments

```
# this is a comment
green_worms = [] # this is also a comment
```

- Annotate your code (*please* do)
- Comment out line(s) for troubleshooting or development

Programming syntax - Indentation

```
green_worms = []
for worm in all_worms_on_the_plate:
   if all_worms_on_the_plate[worm]['color'] == 'green':
        green_worms.append(worm)
```

Python:

4 spaces for one indent - NOT tabs

Special characters break I

White spaces are critical, esp. in Python

```
TAB - tab key (avoid in Python)
```

SPACE - space key

NEWLINE - enter/return key

Programming syntax - End of line

End of line indicator

```
PERL
```

```
my @green_worms;
for my $i (0..$#all_worms_on_the_plate) {
    if ($worm_color[$i] eq 'green') {
        push(@green_worms, $all_worms_on_the_plate[$i]);
    }
}
```

(NOT IN PYTHON)

- Variables
- List of things
- Dictionary of things
- Functions
- Modules
- Objects

• Variables

Reserved memory location for a given construct

Variables - Declaration vs. assignment

Declaration Reserving memory slot to store value

Assignment Value of the variable is defined

```
green_worms = []
```

Python: assignment *is* declaration

Programming concepts - variables

```
worm_species = "C. remanei"
worm_dev_stage = 3
green_worms = []
all_worms_on_plate = {}
dev_stages = ("E", "L1", "L2", "L3", "L4", "A", "D")
```

Python main data types

- Variables
- List of things
- Dictionary of things
- Functions
- Modules
- Objects

- Variables
- List of things

Indexed list of constructs

Python: Lists and Tuples

Programming concepts - lists

```
empty list = []
empty tuple = ()
prime numbers = [1, 3, 5, 7, 9, 11, 13, 17]
primary colors = ("red", "green", "blue")
list of variables = [var1, var2, var3]
prime numbers[2]
>> 5
primary colors[0]
>> 'red'
```

Indexing break

Counting starts at 0 (except in R)

Programming concepts - lists

```
list of lists = [[1,2], [3,4], [5,6], [7,8]]
misc list = [1, [2,3], \{4:5, 6:7\}, (8,[9,10])]
misc tuple = (1, [2,3])
list of lists[2][0]
>> 5
misc list[2][4]
>> 5
```

- Variables
- List of things
- Dictionary of things
- Functions
- Modules
- Objects

- Variables
- List of things
- Dictionary of things

Unordered list of key: value pairs

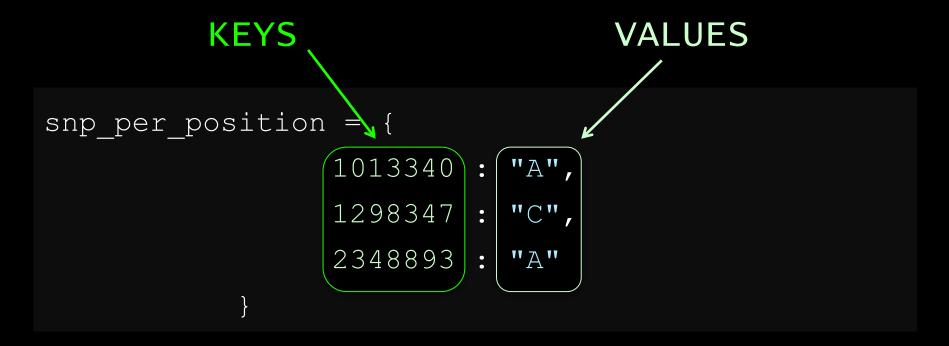
Python: Dictionaries

Programming concepts - dictionaries

SNP position	SNP
1013340	A
1298347	C
2348893	A
2458789	_
2798876	G

Semantics breaks

SNP position	SNP
1013340	А
1298347	C



Programming concepts – dictionaries

```
empty dict = {}
snp per position = {
     1013340 : "A",
                               NO index,
     1298347 : "C",
                               UNIQUE keys
     2348893 : "A"
snp per position[1298347]
>> 'C'
```

Programming concepts - dictionaries

```
dict of lists = {
     "wormA" : ["dpy", "unc", "fem"],
     "wormB" : ["gfp", "dpy"],
     "wormC" : ["dpy", "unc"]
dict of lists["wormB"][0]
>> 'gfp'
```

Programming concepts - dictionaries

Dataframes

Worm ID	Worm Sex	Developmental Stage	GFP
1	ND	L1	no
2	ND	L2	yes
3	Male	Adult	no
4	Female	L4	no
5	Female	Late L4	yes

Programming concepts – dictionaries

```
dict of dicts = {
     "worm1": {
           "sex" : "ND",
           "dev stage" : 1,
           "GFP" : False
     },
     "worm2": {
           "sex" : "ND",
           "dev stage" : 2,
           "GFP" : True
```

Programming concepts - dictionaries

```
dict of dicts = {
     "worm1": {
           "sex" : "ND",
           "dev stage" : 1,
           "GFP" : False,
           "conditions": ("20C", "OP50")
     },
     "worm2": {
           "sex" : "ND",
           "dev stage" : 2,
           "GFP" : True,
           "conditions": ("20C", "OP50")
```

Best practice break

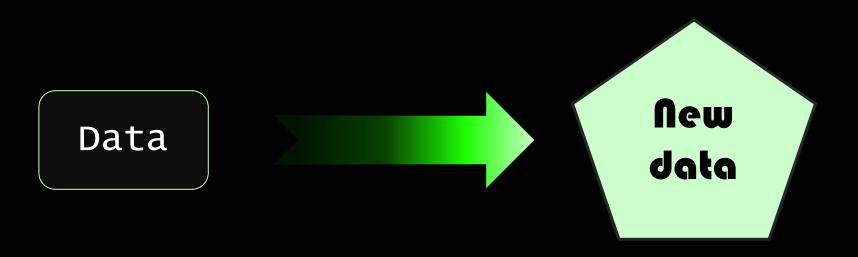
Reserved words:

Words that already mean something in programming language speak and cannot be used as variables

Don't call your list 'list' or your dictionary 'dict'

- Variables
- List of things
- Dictionary of things
- Functions
- Modules
- Objects

• Functions



Programming concepts - functions

Built-in functions

```
worm_species = "C. remanei"
print(worm_species)
>> C. remanei
```

Python list of built-in functions: https://docs.python.org/3/library/functions.html

Programming concepts - functions

User-defined functions

```
def new function(data):
     # do something to data
     # and call it new data
     new data = data + 1
     return new data
my data = 3
my new data = new function(my data)
my new data
>> 4
```

```
a = 0
def do stuff(b):
    c = b + 3
    return c
print(a)
print(b)
print(c)
```

```
a = 0
Global
                    def do stuff(b):
scope
                        c = b + 3
                        return c
                    print(a)
                    print(b)
                    print(c)
```

```
a = 0
Global
                    def do stuff(b):
scope
                        c = b + 3
             Local
                         return c
             scope
                    print(a)
                    print(b)
                    print(c)
```

```
a = 0
Global
                  def do stuff(b):
scope
                      c = p + 3
              Local
              scope return c
                  print(a)
                  print(b)
                              Error: b and c
                  print(c) not defined
```

Programming concepts

- Variables
- List of things
- Dictionary of things
- Functions
- Modules
- Objects

Programming concepts

• Modules / Libraries / Packages

File containing code that you can use and re-use

Programming concepts - modules



- Existing modules or packages?
- Make yours re-usable by yourself or others

Programming concepts - modules

```
# tell your computer which library you want
import package name
# use a function from the library
package name.some function()
# other valid import statements:
import package name as pn
pn.some function()
from package name import some function
some function()
```

Programming concepts - modules

Programming concepts

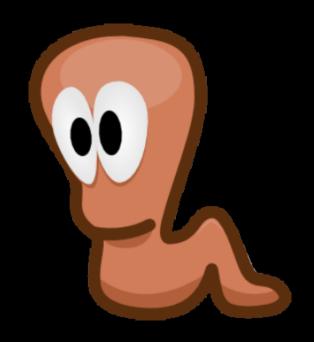
- Variables
- List of things
- Dictionary of things
- Functions
- Modules / Libraries
- Objects

Programming concepts

• Classes >> Objects

Blueprint

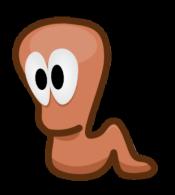
Blueprint



Blueprint -- States

Worms

- Common name: Nematodes
- Main studied species: C. elegans
- Sister species: C. remanei, C. briggsae, C.brenneri, C. japonica
- Larval stages: 4
- Mating system: Androdioceous
- Chromosomes: 5 + X



Blueprint -- Behaviors

Worms

- Common name: Nematodes
- Main studied species: C. elegans
- Sister species: C. remanei, C. briggsae, C.brenneri, C. japonica
- Larval stages: 4
- Mating system: Androdioceous
- Chromosomes: 5 + X
- Crawl around
- Eat
- Mate
- Dauer formation



Blueprint

Worms

- Common name: Nematodes
- Main studied species: C. elegans
- Sister species: C. remanei, C. briggsae,

C.brenneri, C. japonica Attributes

- Larval stages:
- Mating system: Androdioceous
- Chromosomes: 5 + X
- Crawl around
- Eat
- Mate
- Dauer formation

Methods

Programming concepts - classes & objects

An object is an instance of a class

Programming concepts - classes & objects



Every Worm:

- Common name: Nematodes
- Main studied species: C. elegans
- Sister species: C. remanei, C. briggsae,

C.brenneri, C. japonica Attributes

- Larval stages: 4
- Mating system: Androdioceous
- Chromosomes: 5 + X

Crawl around

- Eat
- Mate
- Dauer formation

Accirbaces

Methods

```
class Worm:
    def init (self, name):
        self.species name = name
        self.sister sp = []
        self.state = "hungry"
    def eat(self, food):
        if food == 'OP-50':
            self.state = "happy"
        else:
            self.state = "grumpy"
    def enter dauer(self):
        self.state = "staaaaaarving"
    def assessment(self):
        print("I'm " + self.state)
```

```
class Worm:
   def init (self, name):
       self.species name = name
                                      Attributes
       self.sister sp = []
       self.state = "hungry"
   def eat(self, food):
       if food == 'OP-50':
           self.state = "happy"
       else:
           self.state = "grumpy"
                                           Methods
   def enter dauer(self):
       self.state = "staaaaaarving"
   def assessment(self):
       print("I'm " + self.state)
```

```
harry = Worm("C. elegans")
print(harry.species name)
>> C. elegans
harry.assessment()
>> I'm hungry
harry.eat("salad")
harry.assessment()
>> I'm grumpy
harry.enter dauer()
harry.assessment()
>> I'm staaaaaarving
```

```
harry.eat("OP-50")
harry.assessment()
>> I'm happy
print(harry.sister sp)
>> []
harry.sister sp.append("C. briggsae")
print(harry.sister sp)
>> ['C. briggsae']
sally = Worm("C. elegans")
print(sally.sister sp)
>> []
```

Programming concepts - Python & objects

Everything is an object

Python main data types

Standard Data Analysis

- 1. Open File
- 2. Look at data
- 3. Curate data
- 4. Make pretty graphs
- 5. Publish cool paper
- 6. Take over the world

Standard Data Analysis

- 1. Open File
- 2. Look at data
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- 1. Double-click on file
- 2. Open in excel
- 3. Create new data in (new) file
- 4. Save file
- 5. close file

- 1. Give path to file
- 2. Read in file
- 3. Create new data in memory
- 4. Write to (new) file
- 5. Close file





- 1. Double-click on file
- 2. Open in excel
- 3. Create new data in (new) file
- 4. Save file
- 5. Close file

- 1. Give path to file
- 2. Read in file
- 3. Create new data in memory
- 4. Write to (new) file
- 5. Close file

For this tutorial, let's look at an ImmPort file.

Locate the folder in which you saved the material for this course.

We'll use the file called *subject.txt*

```
my file = 'path/to/my/file/subject.txt'
   Or:
my file = input('File to open for analysis: ')
         Reads input and returns a string
           Pro: no hard-coding
```

Con: need to type your file path every time

Best practice break

Hard coding:

Using a value instead of a variable

Avoid this:

```
f = open('path/to/my/file/subject.txt', 'r')
```

Instead, do this:

```
my_file = 'path/to/my/file/subject.txt'
```

```
my file = 'path/to/my/file/subject.txt'
f = open(my file, 'r')
                               write
                           W
                               read (default)
                           r
     Path to file
                               read + write
                           r+
                              append
                           a
   File object
```

Assumption

```
my_file = 'path/to/my/file/subject.txt'

f = open(my_file, 'r')
```

This is a text file

```
my_file = 'path/to/my/file/subject.txt'

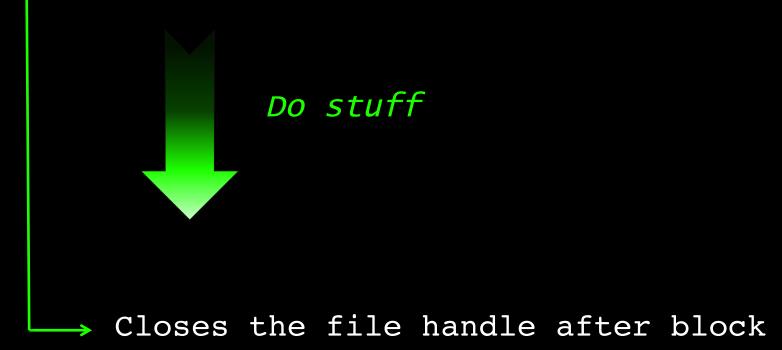
f = open(my_file, 'r')
```



```
f.close()
```

Better practice:

```
my_file = 'path/to/my/file/subject.txt'
with open(my_file, 'r') as f:
```



Standard Data Analysis

- 1. Open File
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```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline()
            Reads file up until
               first NEWLINE
            > First line in file as a string
              INCLUDING newline character
```

Useful tidbits - Strings

```
line.strip([chars])
String
```

Removes leading and trailing characters specified by *chars* in *line* (default white space)

```
my_line = " a simple example "
my_line.strip()
>> 'a simple example'
```

Special characters break II

Some non-alphanumeric characters need to be coded or 'escaped':

```
TAB - tab key - '\t'

SPACE - space key - ' '

NEWLINE - enter/return key - '\n'
```

```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
```

First line in file as a string WITHOUT newline character

Useful tidbits - Strings

```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
```

List of file's headings

```
my_file = 'path/to/my/file/subject.txt'

with open(my_file, 'r') as f:
    first_line = f.readline().strip()
    headings = first_line.split("\t")
    second_line = f.readline().strip().split("\t")
    # do something
```

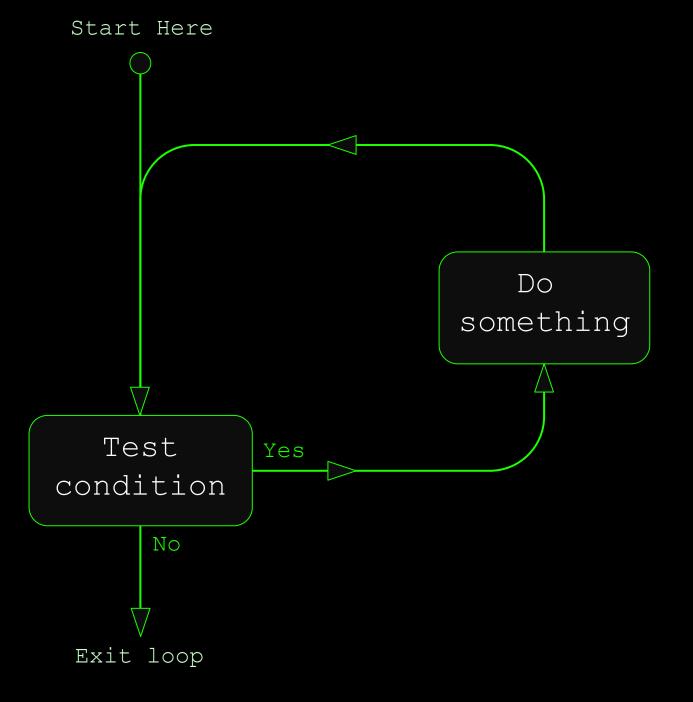
```
my_file = 'path/to/my/file/subject.txt'

with open(my_file, 'r') as f:
    first_line = f.readline().strip()
    headings = first_line.split("\t")

    second_line = f.readline().strip().split("\t")
    # do something
```

Repeat this for all lines

Loops



```
for ITEMS in LIST:
    # do something
# do something
# do something
```

```
for ITEMS in LIST:
    # do something
for i in range(0, 10):
    print(i)
for letters in 'bananas':
    print(letters)
for colors in primary colors:
    print(colors)
```

```
for i in range(0, len(some list)):
    print(i)
for index, element in enumerate (primary colors):
    print(index, element)
for words in some dictionary:
    print(words + " " + some dictionary[words])
```

```
for ITEMS in LIST:
    # do something
```

```
while condition:
    # do something
i = 0
while i < 10:
   print(i)
```

Infinite Loops Start Here Do something Condition Yes always True Exit loop

```
for ITEMS in LIST:
    # do something
```

```
while condition:
    # do something
i = 0
while i < 10:
    print(i)
    i += 1
```

```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    for line in f:
        line content = line.strip().split("\t")
```

```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, print race
```

```
if condition:
    # do something
elif condition:
    # do something
elif condition:
    # do something
else:
    # do something
```

```
if i == 0:
    print("i is null")
elif i == 1:
    print("i is 1")
elif i > 1:
    print("i is positive")
else:
    print ("i is negative. Or between 0 and 1")
```

```
if carrots:
    print("let's make a salad")
else:
    print("where is the rabbit?")
```

Useful tidbits - Boolean

Will evaluate as:

true	false
True	False
	None
1, 1.3, 4J	0, 0.0, Oj
'hi', [1,2], (2,3)	'', [], ()
{fr: "non", en: "no"}	{ }

```
color = "red"
if color in primary_color:
    print(color + " is a primary color")

if color not in primary_color:
    print(color + " is not a primary color")
```

```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, print race:
        if line content[4] == 'Male':
            print(line content[5])
```

String matching

```
str.startswith(prefix)
str.endswith(suffix)
True/False
```

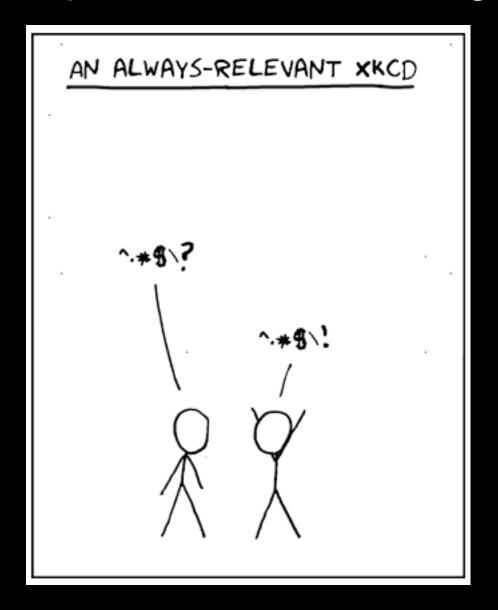
Checks if str starts or ends with prefix/suffix

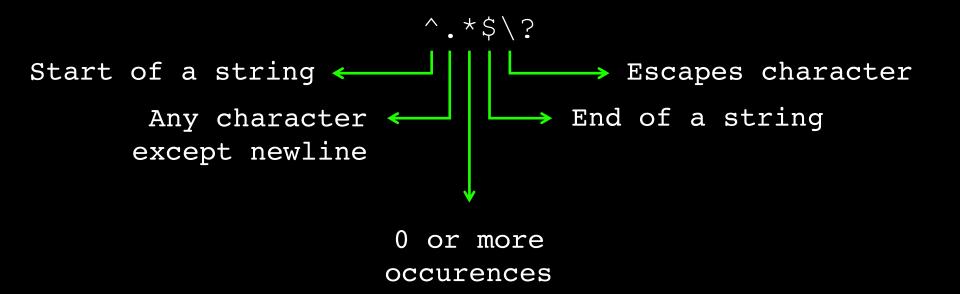
```
new_line1 = 'a simple example'
if new_line1.startswith('a'):
    print('yay!')
>> yay!
```

For more complex string matching:

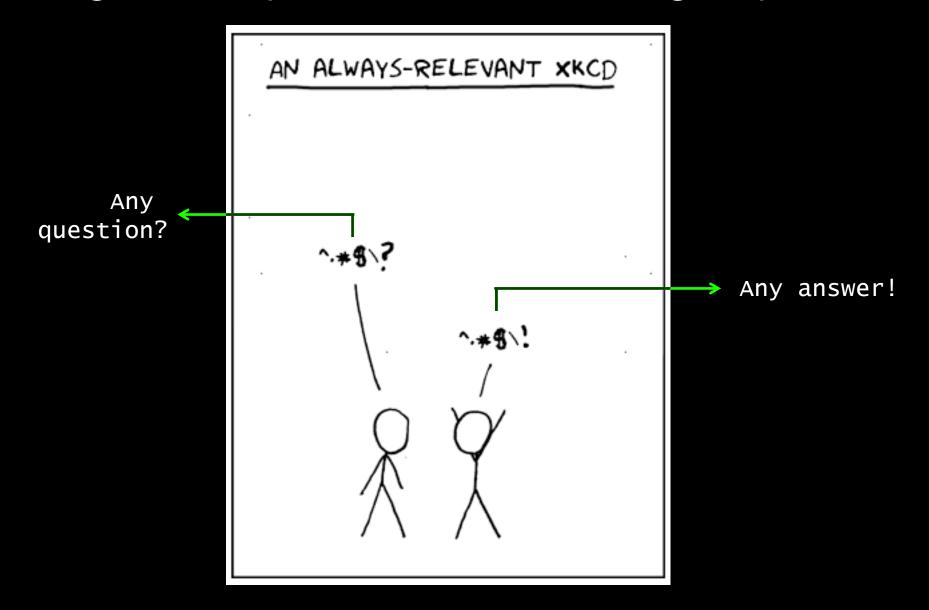
```
re module:
   https://docs.python.org/3/library/re.html
```

Sequence of characters that defines a pattern





https://www.debuggex.com/cheatsheet/regex/python http://www.pyregex.com/



```
my file = 'path/to/my/file/subject.txt'
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, print race:
        if line content[4].startswith('M'):
            print(line content[5])
```

```
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    male div = []
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, remember race:
        if line content[4].startswith('M'):
            male div.append(line content[5])
```

ightharpoonup Add element to list

```
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    male div = []
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, remember race:
        if line content[4].startswith('M'):
            male div.append(line content[5])
```

```
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    male div = []
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, remember race:
        if line content[4].startswith('M'):
          male div.append(line content[5])
```

```
with open (my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    male div = []
    sex ratio = {'M':0, 'F':0}
    for line in f:
        line content = line.strip().split("\t")
        # if subject is male, remember race:
        if line content[4].startswith('M'):
            male div.append(line content[5])
          \Rightarrow sex ratio['M'] += 1
```

```
with open(my file, 'r') as f:
    first line = f.readline().strip()
    headings = first line.split("\t")
    male div = []
    sex ratio = {'M':0, 'F':0}
    for line in f:
```

Get data back?

```
with open (output file, 'w') as outf:
   outf.write('stuff')
           Opens file for writing.
           If the file already
            exists, erases it
           Writes to file
```

Special characters break III

White space are not included automagically.

```
TAB - tab key - '\t'

SPACE - space key - ' '

NEWLINE - enter/return key - '\n'
```

```
with open(output_file, 'w') as outf:
   outf.write('stuff\n')
```

Adds a newline character

```
with open(output_file, 'w') as outf:
   outf.write('GENDER\tDIVERSITY\tCOUNT\n')
```

Useful tidbits - Strings

```
sep.join(list)
String
```

Creates a single string from *list* elements joined by *sep*

```
new_line2 = ['a', 'simple', 'example']
"-".join(new_line2)
>> 'a-simple-example'
```

I/O operations

```
with open (output file, 'w') as outf:
    outf.write('GENDER\tDIVERSITY\tCOUNT\n')
    for gender in sex ratio:
        line to write = "\t".join([
                               gender,
                               div[gender],
                               sex ratio[gender]
                          ])
```

Useful tidbits - Unique set

```
set(list) List
```

Gets unique set of elements in *list*

```
rep_list = ['a', 'b', 'c', 'a', 'c', 'b']
unique_list = set(rep_list)
print(unique_list)
>> ['a', 'b', 'c']
```

I/O operations

```
with open (output file, 'w') as outf:
    outf.write('GENDER\tDIVERSITY\tCOUNT\n')
    for gender in sex ratio:
        diversity = set(div[gender])
        line to write = "\t".join([
                               gender,
                               diversity,
                               sex ratio[gender]
                          ])
```

Useful tidbits - Type casting

```
str(object)

Changes object to string
```

```
not_a_string = 3
str(not_a_string)
>> '3'
```

Useful tidbits - Type casting

```
an integer = 2
a float = 2.0
int(3.8)
>> 3
float(5)
>> 5.0
```

Pro-tip: be aware that with Python 2.x, 1/2 = 0

I/O operations

```
with open (output file, 'w') as outf:
    outf.write('GENDER\tDIVERSITY\tCOUNT\n')
    for gender in sex ratio:
        diversity = set(div[gender])
        line to write = "\t".join([
                               gender,
                               str(diversity),
                               str(sex ratio[gender])
                          ])
        outf.write(line to write + "\n")
```

Reality check break

There are many many valid ways to do things

Standard Data Analysis

- 1. Open File
- 2. Look at data the easier way
- 3. Curate data
- 4. Make pretty graphs
- 5. Publish cool paper
- Take over the world

Exploratory Data Analysis

```
import pandas as pd
my file = 'path/to/my/file/subject.txt'
df = pd.read table(my file)
            Reads in a general delimited file
    DataFrame object (eq. to R's dataframes)
```

Standard Data Analysis

- 1. Open File
- 2. Look at data
- 3. Curate data
- 4. Make pretty graphs
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Pre-analysis Data Curation

- Familiarize yourself with the file structure:

 How many columns, how are they separated, headings or not, strings or numbers...
- Expect inconsistent data:
 Empty columns / Nas / Os, inconsistent data types,
 missing columns, 'hi' vs. 'Hi', Excel misconception of dates...
- Strategize your code to minimize I/O operations

Standard Data Analysis

- 1. Open File
- 2. Look at data
- 3. Curate data
- 4. Make pretty graphs
- 5. Publish cool paper
- 6. Take over the world

EDA - Resources

Coursera class R. Peng, J. Leek and B. Caffo (in R) https://www.coursera.org/learn/exploratory-data-analysis

Analyzing and Manipulating Data with Pandas by J. Rocher

https://www.youtube.com/watch?v=0CFFTJUZ2dc

Awesome Data Science. 2.0 Introduction to Pandas and Exploratory Data Analysis

https://www.youtube.com/watch?v=ZrRpN_IrcBA

More advanced Jupyter / Pandas tutorial by J. Vanderplas

https://www.youtube.com/playlist?list=PLYCpMb24Gp0C704u09svUrihl-HY1tTJJ

Going back to functions

If you are going to be using this snippet of code you just wrote a lot, make it into a function.

Modules / libraries

If this code you just wrote would be useful to more than just you, make it into a library.

Consider sharing it with the community.

Consider making it a Galaxy tool.

Troubleshooting

```
print p[k]
  File "<ipython-input-31-25a740847cb6>", line 1
    print p[k]
SyntaxError: Missing parentheses in call to 'print'
```

Troubleshooting

```
print(p[k])
NameError
<ipython-input-32-cfed065d0920> in <module>()
---> 1 print(p[k])
NameError: name 'p' is not defined
```

```
FileNotFoundError
                                          Traceback (most recent call last)
<ipython-input-3-d47 19b41a5f7> in <module>()
      ________.read table("./Data/SDY212/Tab/subject.txt",sep="\t")
      2 arm 2 subject = pd.read table("./Data/SDY212/Tab/arm 2 subject.txt", sep="\t")
      3 arm_or_cohort = pd.read_table("./Data/SDY212/Tab/arm_or_cohort.txt",sep="\t")
/Users/thomascg/miniconda3/lib/python3.6/site-packages/pandas/io/parsers.py in parser f(filepath or buffer, sep, deli
miter, header, names, index col, usecols, squeeze, prefix, mangle dupe cols, dtype, engine, converters, true values,
 false values, skipinitialspace, skiprows, nrows, na values, keep default na, na filter, verbose, skip blank lines, p
arse dates, infer datetime format, keep date col, date parser, dayfirst, iterator, chunksize, compression, thousands,
 decimal, lineterminator, quotechar, quoting, escapechar, comment, encoding, dialect, tupleize cols, error bad lines,
 warn bad lines, skipfooter, skip footer, doublequote, delim whitespace, as recarray, compact ints, use unsigned, low
memory, buffer_lines, memory_map, float_precision)
    644
                            skip blank lines=skip blank lines)
    645
--> 646
                return read(filepath or buffer, kwds)
    647
            parser_f.__name__ = name
    648
/Users/thomascg/miniconda3/lib/python3.6/site-packages/pandas/io/parsers.py in read(filepath or buffer, kwds)
    387
    388
            # Create the parser.
--> 389
            parser = TextFileReader(filepath or buffer, **kwds)
    390
    391
            if (nrows is not None) and (chunksize is not None):
/Users/thomascg/miniconda3/lib/python3.6/site-packages/pandas/io/parsers.py in init (self, f, engine, **kwds)
    728
                    self.options['has index names'] = kwds['has index names']
    729
--> 730
                self. make engine(self.engine)
    731
    732
            def close(self):
/Users/thomascg/miniconda3/lib/python3.6/site-packages/pandas/io/parsers.py in make engine(self, engine)
    921
            def make engine(self, engine='c'):
    922
                if engine == 'c':
--> 923
                    self. engine = CParserWrapper(self.f, **self.options)
    924
                else:
    925
                    if engine == 'python':
/Users/thomascg/miniconda3/lib/python3.6/site-packages/pandas/io/parsers.py in __init__(self, src, **kwds)
   1388
                kwds['allow_leading_cols'] = self.index_col is not False
   1389
-> 1390
                self. reader = parser.TextReader(src, **kwds)
   1391
   1392
                # XXX
pandas/parser.pyx in pandas.parser.TextReader. cinit (pandas/parser.c:4184)()
pandas/parser_pay in pandas_parser_TextReader_ setup parser_source_(pandas/parser_c:8449)()
FileNotFoundError: File b'./Data/SDY212/Tab/subject.txt' does not exist
```

Troubleshooting

Read the traceback to see where the error comes from

• Google

Stack overflow

Any more questions?

Immport.org
Material and more tutorials:
immport.org/resources/tutorials

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