Introduction to Python

BIO334

Dean Sumner & Maria Heimlicher
Christian von Mering's group
courtesy of Tackmann, Dmitrijeva & Gable

dean.sumner@uzh.ch
maria.heimlicher@uzh.ch

https://github.com/meringlab/Bio334.git

Schedule

What is Python?

1. Dynamic, interpreted **programming language**
2. **Simple syntax** with fast learning curve

Most Loved, Dreaded, and Wanted Languages

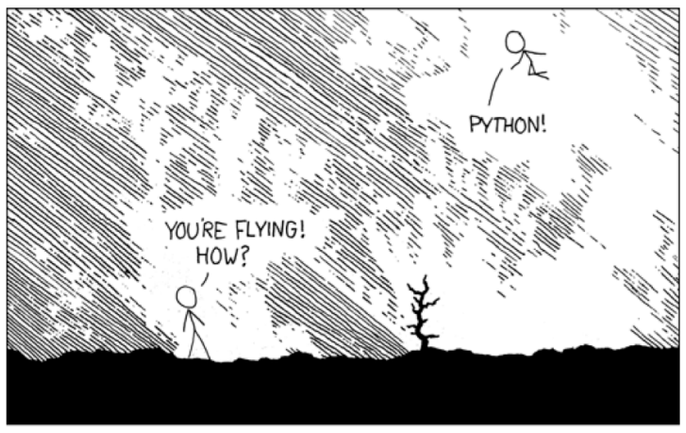
Loved | Dreaded | Wanted

Rust	83.5%	
Python	73.1%	
TypeScript	73.1%	
Kotlin	72.6%	
WebAssembly	69.5%	

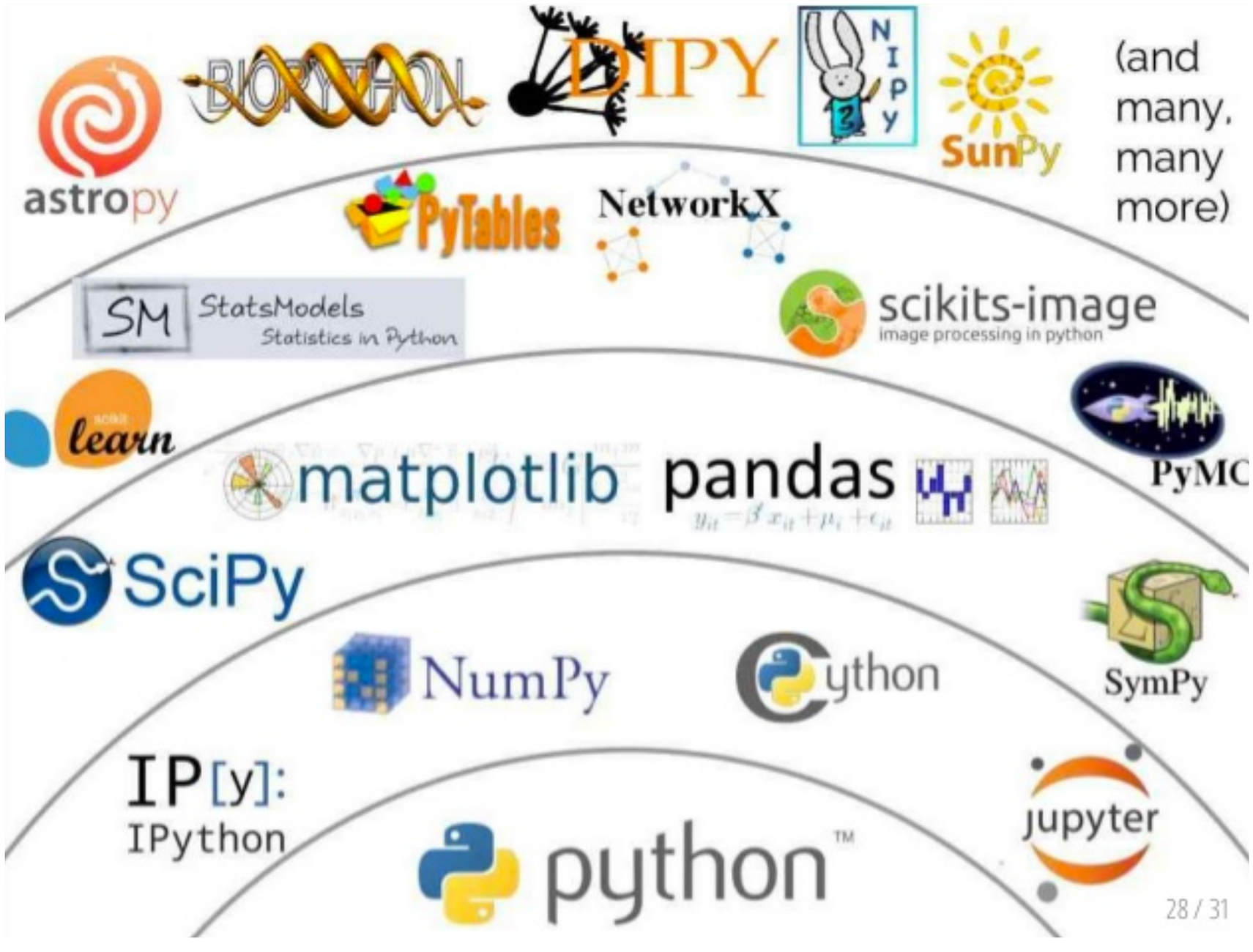
Most Loved, Dreaded, and Wanted Languages

Loved | Dreaded | Wanted

Python	25.7%	
JavaScript	17.8%	
Go	15.0%	
TypeScript	14.6%	
Kotlin	11.1%	



Scientific Python stack



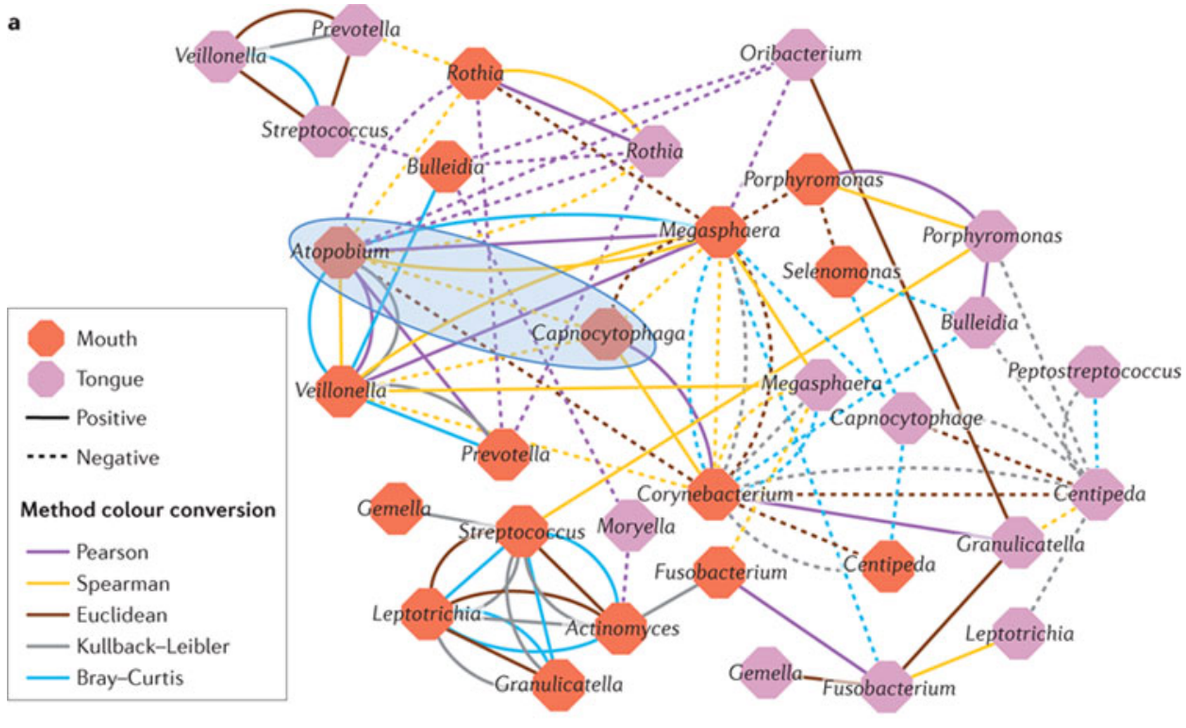
Today's goals

1. get your hands dirty with the basics
   - simple statements, for loops, control flow
2. learn how to read a sequence file, extract useful information

You already know Python?

Jump to (optional) exercise #3:

create a pipeline to infer simple ecological relationships in the Human Microbiome



You already know Python?

Jump to (optional) exercise #4:

Learn the basics of **Pandas**, a powerful python module for data analysis, including reading, writing, filtering, merging, arithmetic operations on and sorting of tabular data

```
age animal  priority    visits
b   3.0 cat yes 3
d   NaN dog yes 3
f   2.0 cat no  3
```

	age	animal	priority	visits
b	3.0	cat	yes	3
d	NaN	dog	yes	3
f	2.0	cat	no	3

Today's program

1. Introduction to programming

   basic concepts with small hands-on sessions in JupyterLab using iPython

2. Break

3. Writing Python code

4. Go through solutions of exercise 1 and 2

   (~30min before the end)

Part 1:

Programming basics

Variables

- Store a piece of data and give it a specific name with the “=“ (equal) operator

```
a = 4
pi = 3.14159
```

```
my_string = "hello"
# single and double ticks are equal
# (just stick to one) ‘hello’ or “hello”

my_protein_sequence  = 'MRHIAHTQRCLSRLTSLVALLLIVLP'
```

- Basic rules for variable names:
  - don’t include spaces, don’t start with numbers, use descriptive names

Operators

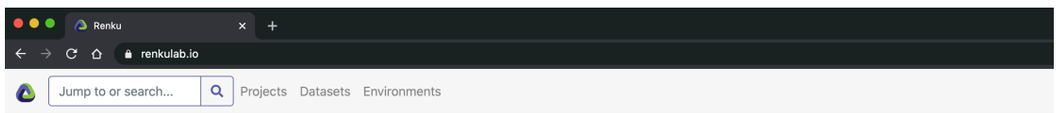
1. Arithmetic operations
    1. addition + , subtraction –
    2. division / , multiplication *
    3. exponent **
    4. parenthesis ( )
2. Boolean operations
    1. return `True` or `False`
    2. == , > , < ,
    3. & (AND) , | (OR)

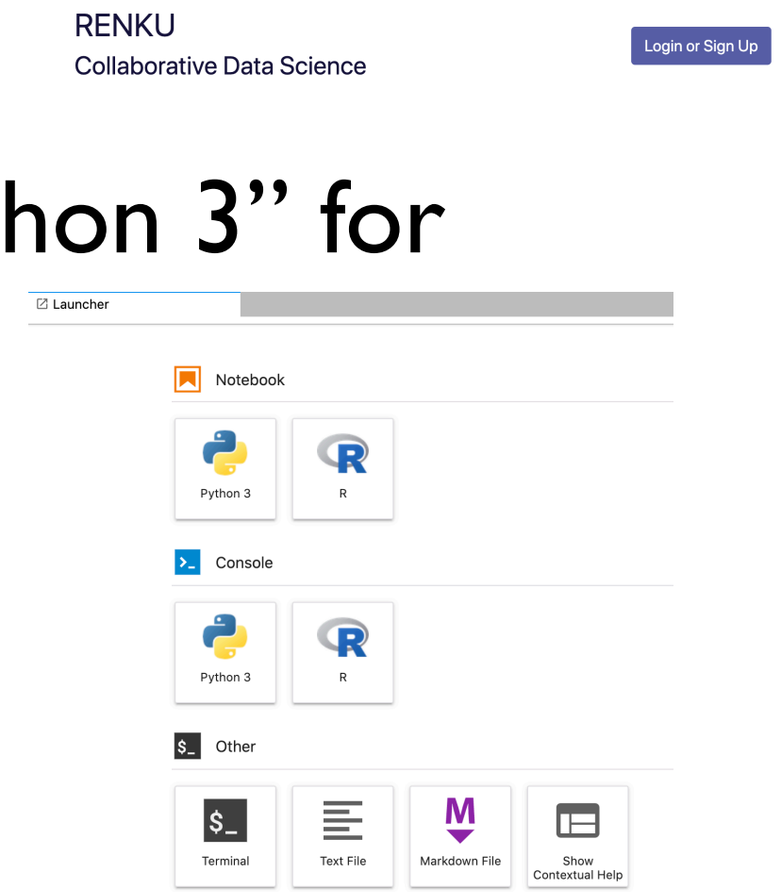
```
>>> 2 + 3
5
>>> 23 - 3
20
>>> 22.0 / 12
1.8333333333333333
>>> (1 + 2) * 3
```

```
>>> 1 < 2
True
>>> 3 > 34
False
>>> 23 == 45
False
>>> 34 != 323
True
```

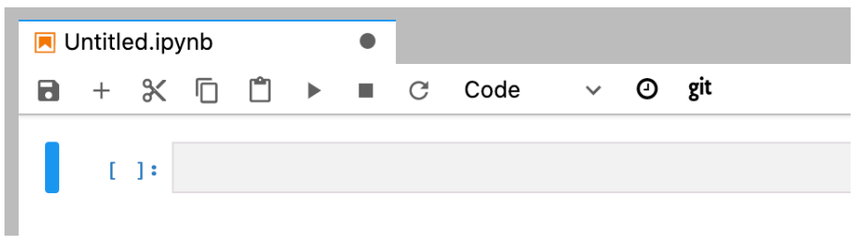
First live session

- Start by opening https://renkulab.io/ in your browser





- Launch Jupyter Notebook "Python 3" for an interactive session



Show how to use **JupyterLab** and checkout **Cheat Sheets**

To access the files you need enter the following command in a terminal window

`git clone` https://github.com/meringlab/Bio334.git

Session 1: Type a command and hit `shift + enter`

```
welcome_message = 'hello world!' # hit [shift + enter] after every line
welcome_message

# Use python as your advanced calculator
a = 4
b = a + 3
(a + b) * 4

a / 8

a**2

# Let's try with strings
welcome_message + welcome_message

a = '4'
a + 3 # anything strange?

# whats the difference?
a + str(3)
int(a) + 3
```

Arithmetics

```
>>> welcome_message = 'hello world!' # hit [shift + enter]
>>> welcome_message
'hello world!'

# Use python as your advanced calculator
>>> a = 4
>>> b = a + 3
>>> (a + b) * 4
44

# float division (caveat: Python 2 would return 0!)
>>> a / 8
0.5

>>> a**2
16
```

Concatenation

```
# Let's try with strings

# use + to add two strings
>>> welcome_message + welcome_message
'hello world!hello world!'

>>> a = '4'

# We need to have the same type to add elements
>>> a + 3      # anything strange?
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: cannot concatenate 'str' and 'int' objects

# whats the difference?
>>> a + str(3)
'43'
>>> int(a) + 3
7
```

Functions

1. function: stores instructions (not values)
2. basic use:
    1. `function_name(arguments)`
3. functions loaded by default in python, e.g.
    1. `str()` - convert an object into a string
    2. `int()` - convert an object into an integer
    3. `float()` - convert a object into a floating point number
    4. `type()` - tells you the type of an object
4. see many other in the cheat-sheet and find them on
    1. https://docs.python.org/3/library/functions.html

Functions

```
# Let's create a function using “def” (for define)
```

[ ]:
```
def add_things(a, b):
    result = a + b
    return result
```

```
# We need to have the same type to add elements
```

```
add_things(3, 5)
```

```
8
```

```
add_things("Hello ", "there")
```

```
'Hello there'
```

```
add_things("3", 5)
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-14-df373cddff49> in <module>
----> 1 add_things("3", 5)

<ipython-input-12-eb66cd937434> in add_things(a, b)
      1 def add_things(a, b):
----> 2     result = a + b
      3     return result

TypeError: can only concatenate str (not "int") to str
```

List data structure

1. like a shopping list we have an object that can store multiple objects at once.

```
my_list = ['butter','milk','oranges']
```

3. it can hold different objects as well

```
my_list = ['butter',1,1.5,'milk']
```

5. Every element has an index, starting from 0 which you can access with the square brackets [ ]

    1. e.g.

```
>>> my_list[0]
'butter'
```

List data structure

1. get subsets of a list (“slicing”)

```
>>> my_list[0:2]
['butter','milk']
```

3. assign new values to list elements

```
my_list[0] = 'bananas'
```

5. powerful list operations
    1. e.g. sort, reverse, insert, search

Session 11: Work with lists

```
# create your first list and try accessing it with indices

my_list = [1,2,3,4,5]
my_list[1]
my_list[5]
my_list[0:3]
my_list[-1]

len(my_list)

# mixed lists, put different variable types in your list

my_mixed_list = ['UZH','founded in',1833]
my_mixed_list[2] = 1833
del my_mixed_list[1]
my_mixed_list.append('A.D.')

my_mixed_list

my_mixed_tuple[2] = 1833

# apply the arithmetic operators on lists

[1,2,3] + [3,4,6]

['Hello'] * 4
```

Accessing list elements

```
# create your first list and try accessing it with indices
>>> my_list = [1,2,3,4,5]
>>> my_list[1]
2
>>> my_list[5]
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
IndexError: list index out of range
```

```
# slice your list with index ranges
>>> my_list[0:3]
[1, 2, 3]
>>> my_list[-1]
5

# Check how many elements your list contains
>>> len(my_list)
5
```

List modifications

```
# mixed lists, put different variable types in your list
>>> my_mixed_list = ['UZH','founded in',1834]
>>> my_mixed_list[2] = 1834

>>> my_mixed_list
['UZH', 'founded in',1834]

# delete an element at a specified index
>>> del my_mixed_list[1]

>>> my_mixed_list
['UZH', 1834]

# add another element to the list with the append command
>>> my_mixed_list.append('A.D.')

>>> my_mixed_list
['UZH', 1834, 'A.D.']
```

List concatenation

```
# apply the arithmetic operators on lists

# use + to make a longer list out of two small ones

>>> [1,2,3] + [3,4,6]
[1, 2, 3, 3, 4, 6]

# Use * to form a new list by repeating the content of a list

>>> ['Hello'] * 4
['Hello', 'Hello', 'Hello', 'Hello']
```

Strings & Lists

1. Strings can also be considered lists of characters and can be accessed by index
2. To convert them to an actual list (and make them mutable) use `list`

```
>>> my_sequence = 'MRHIAHTQRCLSRL'
>>> list(my_sequence)
['M', 'R', 'H', 'I', 'A', 'H', 'T', 'Q', 'R', 'C', 'L', 'S', 'R', 'L']
```

5. While this opens many possibilities, check the cheat-sheet for convenient built-in string operations
    1. e.g. split, join, replace

Dictionaries

1. Similar to lists but elements are accessed through a user defined ‘key’

```
my_proteins_seqs = {}
my_proteins_seqs = dict() # same as above
my_proteins_seqs['DROME_HH_Q02936'] = 'MRHIAHTQRCLSRLTSLVA'
my_proteins_seqs['DROME_PATC_P18502'] = 'MDRDSLPRVPDTHGDVVD'
```

4. retrieve their **value** by using the **key**

```
>>> my_proteins_seqs['DROME_HH_Q02936']
'MRHIAHTQRCLSRLTSLVA'
```

Dictionary definition

```
# create your first dictionary

>>> dna_to_rna = {}
>>> dna_to_rna['A'] = 'A'
>>> dna_to_rna['T'] = 'U'
>>> dna_to_rna['C'] = 'C'
>>> dna_to_rna['G'] = 'G'

>>> dna_to_rna
{'A': 'A', 'C': 'C', 'T': 'U', 'G': 'G'}

#or in one line

>>> dna_to_rna = {'A':'A','T':'U','C':'C','G':'G'}
>>> dna_to_rna
{'A': 'A', 'C': 'C', 'T': 'U', 'G': ‘G'}
```

Dictionary usage

```
#access an element with its key
>>> dna_to_rna['U']
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
KeyError: 'U'

# Test if a key is in the dictionary
>>> 'U' in dna_to_rna
False

# See all keys in the dictionary
>>> list(dna_to_rna.keys())
['A', 'C', 'T', 'G']

# Dictionaries don't support concatenation
>>> dna_to_rna + dna_to_rna
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for +: 'dict' and 'dict'
```

Session 11: Strings and dictionaries

```
# Try accessing a string like a list

my_string = 'hello world!'

my_string[6]
my_string[-1] = '?'

my_list = list(my_string)
my_list[-1] = '?'
my_modified_string = ''.join(my_list)

# create your first dictionary

dna_to_rna = {}
dna_to_rna['A'] = 'A'
dna_to_rna['T'] = 'U'
dna_to_rna['C'] = 'C'
dna_to_rna['G'] = 'G'

#or in one line

dna_to_rna = {'A':'A','T':'U','C':'C','G':'G'}

#dictionary operations

dna_to_rna['U']
'U' in dna_to_rna
dna_to_rna.keys()
dna_to_rna + dna_to_rna
```

String lists

```
# accessing a character by index

>>> my_string = 'hello world!'
>>> my_string[6]
'w'

# Changes are not allowed

>>> my_string[-1] = '?'
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: 'str' object does not support item assignment

# Convert your string to a list to do that

>>> my_list = list(my_string)
>>> my_list[-1] = '?'

# Combine your list into a string with the join method
>>> my_modified_string = ''.join(my_list)
>>> my_modified_string
'hello world?'
```

Methods

1. functions of a specific object class
2. access by <variable_name>.<method>(*arguments*)

```
>>> s = 'The quick brown fox jumps over the lazy dog'
>>> s.split()
['The', 'quick', 'brown', 'fox', 'jumps', 'over', 'the', 'lazy', ‘dog']
>>> s.split('fox')
[‘The quick brown ‘, ‘ jumps over the lazy dog']
```

6. in `ipython`: write . after a variable name and press <tab> to get an overview about available methods
7. alternatively: `dir(object)`
8. use `?` / `??` (in `ipython`) or help() to get information about a method and its arguments e.g. `?str.split` or `help(str.split)`

Break

Part 2:

Writing Python code

Why write a script?

1. Organize your commands in a text file and build more complicated workflows that can be executed at once.
2. save typing, make your work reproducible
3. Use comments (#) to describe your code
4. Run it at any point by executing your script

Scripting ingredients

1. Use the **`print`** function to print the output

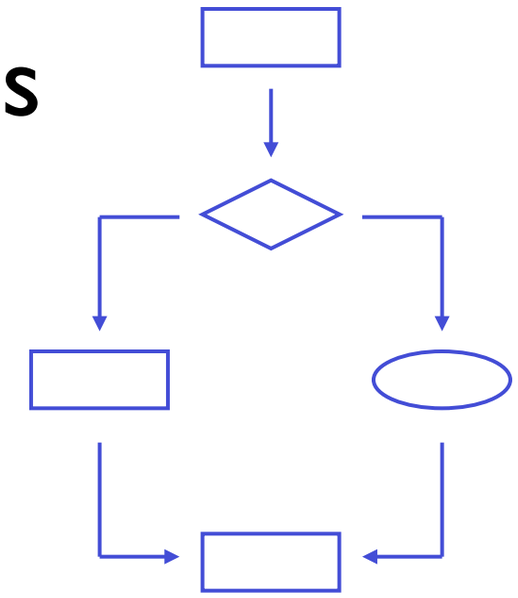
```
>>> print(“Hello”,”Python!”)
Hello Python!
```

```
print(“Hello”,”Python!”) # use this (for Python 3)
print 'hello world!'  # not this (for Python 2)
```

Conditional statements

1. Use if/else clauses to make decisions

```
if boolean_expression:
    print(“The statement is True”)
else:
    print(“The statement is False”)
```



4. Remember the indentation!

    1. While other programming languages use brackets or end statements, Python uses whitespace to structure code. Simply use tabulator to indent.

Loops

1. Loops are essential for repeating an action several times
2. The `for` loop executes the nested statements as many times as there are elements in the input list.

```
>>> input_list = [1,2,3,4,5]
>>> for my_number in input_list:
...     print(my_number)
...
1 2 3 4 5
```

- Note: Don't forget the colon (:) at the end.

`for` loop for reading

[1]:
```
1 for line in open("my_file.txt", "r"):
2     print(line)
```

```
1st line

2nd line

3rd line
```

File:
my_file.txt

```
1st line
2nd line
3rd line
EOF
```

Conditional loop

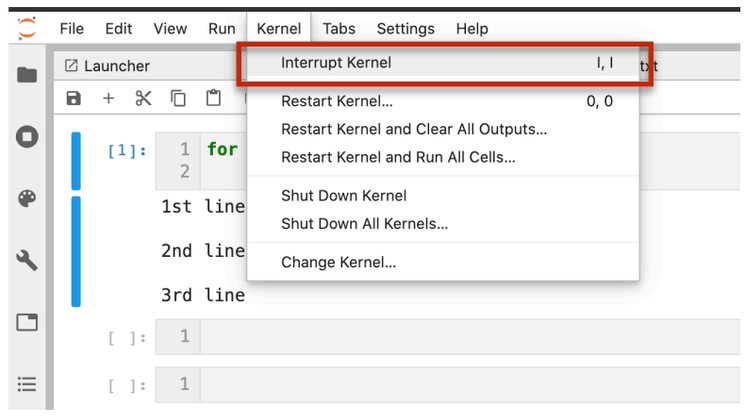
1. Use the **`while`** loop to continue an action until a condition is not satisfied anymore

```
>>> number_apples = 3
>>> while number_apples > 0:
...     number_apples -= 1
...     print(“Ate an apple,”,number_apples,'left')
...
Ate an apple,  2 left
Ate an apple,  1 left
Ate an apple,  0 left
```

Session IV: Loops and friends

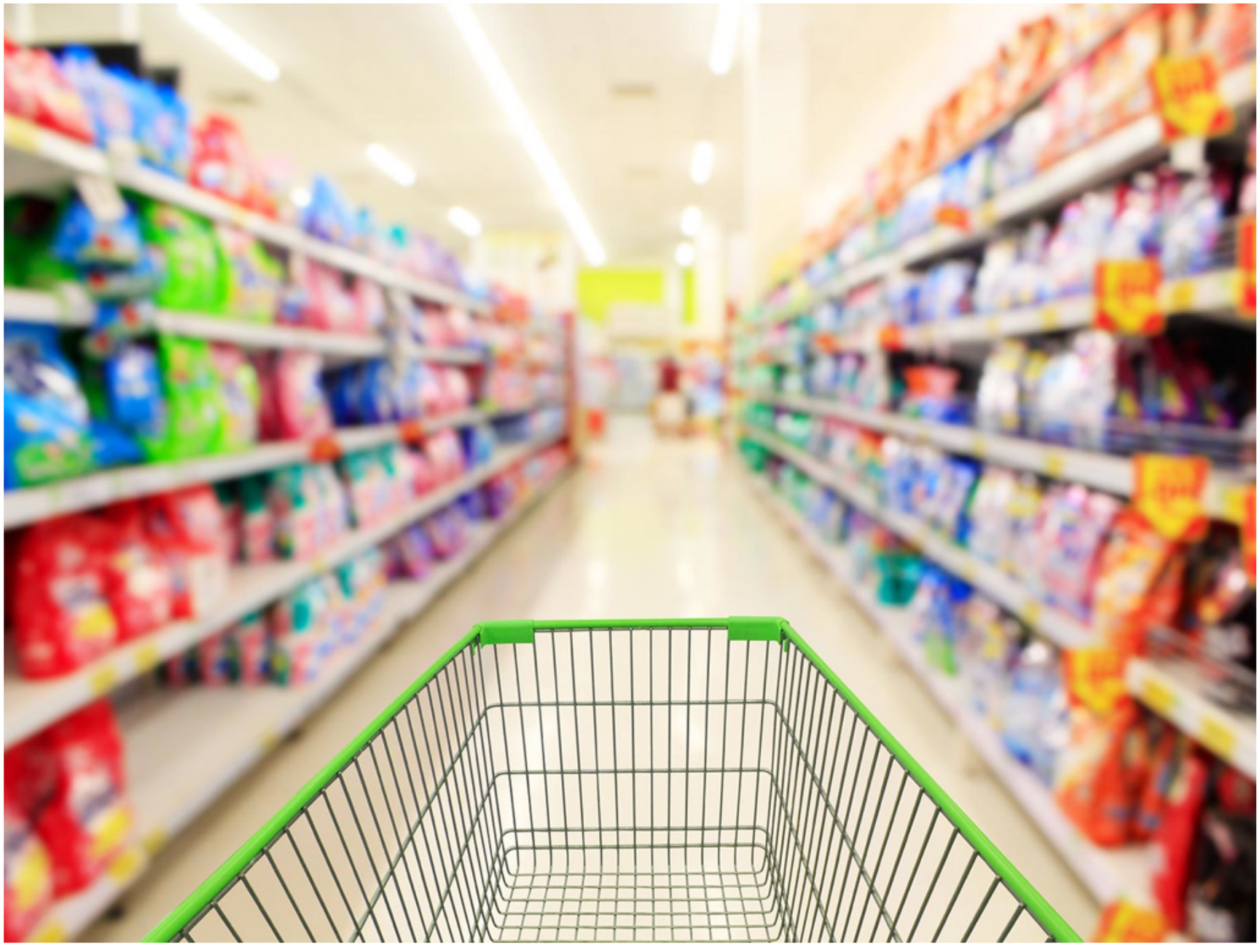
```
# 1. try out this for loop

for my_number in range(6):
     print(my_number)

# 2. A new loop key-word: continue

for my_number in range(6):
    if my_number == 5:
         continue
    print(my_number)
```

```
# 3. try using break instead of continue

# 4. when will this while loop finish?

my_number = 1
from time import sleep
while my_number < 5:
     print("hurray! my number is increasing:",
my_number)
     sleep(1)
```

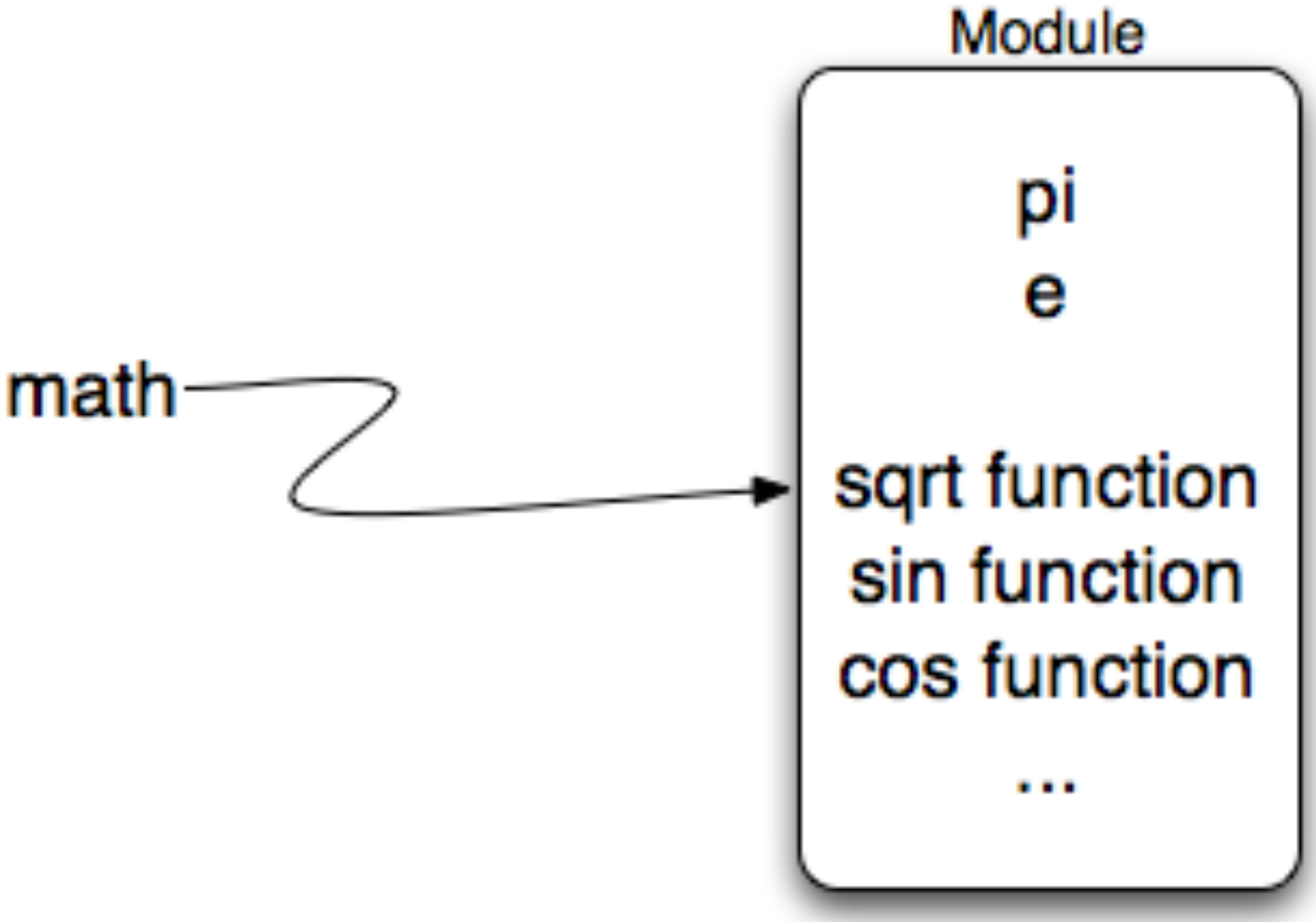


HINT: use Kernel —> Interrupt Kernel to stop the running program

python modules



`math` module



Import statement

1. Use `import` to load additional modules for more functionalities
2. For example the `math` module:

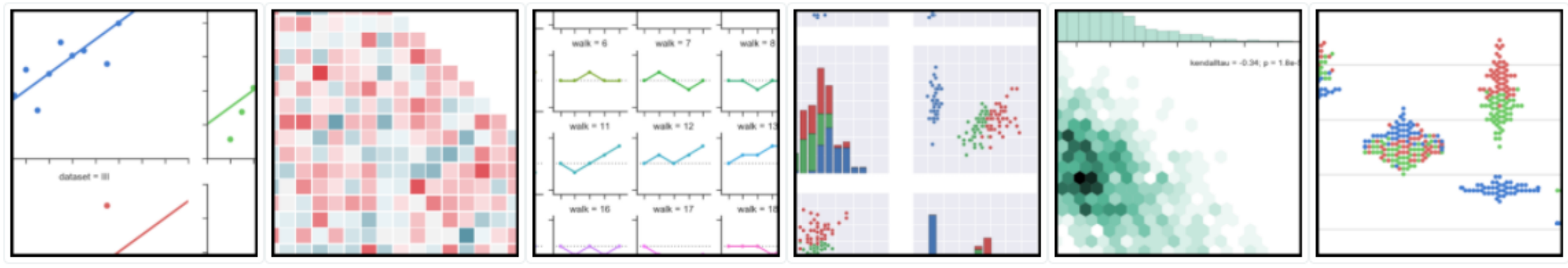
```
Script: print_pi.py

import math
print('Pi is equal to', math.pi)
print('or in degrees', math.degrees(math.pi))
```

```
davide$ python print_pi.py
Pi is equal to 3.141592653589793 or in degrees 180.0
```

more details at: https://docs.python.org/3/library/math.html

Much more to discover

1. `ipython` magics make your life a lot easier
    1. time your code, debug it, call other languages
2. make python lightning fast using `numpy`, `scipy`, and `cython/pypy/numba`
3. visualize your data with `seaborn`, `bokeh` and `matplotlib`



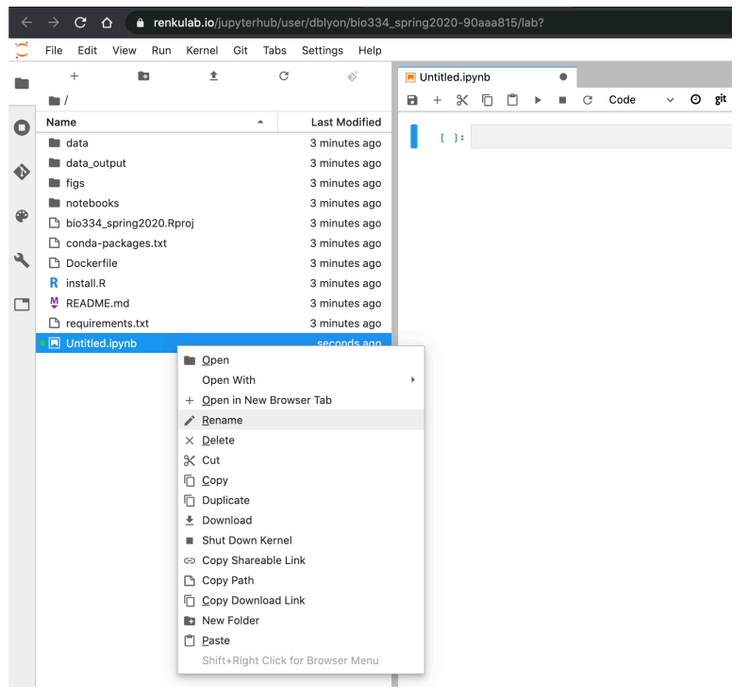
Further reading

1. https://snakify.org/ (interactive tutorial)
2. http://www.diveintopython.net/(comprehensive, general purpose)
3. http://swcarpentry.github.io/python-novice-inflammation/ (scientific python by example)
4. http://www.scipy-lectures.org/intro/intro.html (intro by the scientific python consortium)
5. https://github.com/dblyon/pandasintro (extensive introduction to pandas)
6. https://cs50.harvard.edu/college/2021/spring/weeks/0/

Exercise session

1. Within https://renkulab.io/projects/mark.robinson/bio334-spring2021 create a new Python3 Jupyter Notebook and start exploring

2. Change the name of your newly created file by right clicking on `Untitled.ipynb`



3. To execute a cell press `Shift + Enter`

4. To access the files you need enter the following command in a terminal window

`git clone` https://github.com/meringlab/Bio334.git

DON'T FORGET TO DOWNLOAD YOUR OWN .IPYNB SCRIPTS AT THE END OF THE DAY

optional exercise slides follow

Optional exercise session

1. Create a new text document and rename it, giving it a ".py" ending
2. To execute you launch a terminal tab within Renku and enter

```
ipython <script_name>.py
```

3. Files can be found within Renku (if you've git cloned them)

```
/Bio334
```

5. Good luck!

`os` module

1. Another built-in module that contains miscellaneous operating system interfaces
2. For example we can use it to obtain the name of the user currently logged in:

Script: check_directory.py

```
1  import os
2
3  dir_ = "Bio334"
4  if not os.path.exists(dir_):
5      print("It seems you haven't cloned the git repository yet. \
6            Please enter the following command in a terminal window.")
7      print("git clone https://github.com/meringlab/Bio334.git")
8  else:
9      print("Great! The 'Bio334' directory exists. You are good to go.")
```

Run the script in a terminal window

```
base  work ❯ bio334_spring2020_dbl  master  3?  $  python check_directory.py
Great! The 'Bio334' directory exists. You are good to go._
```

`sys` module

1. A built-in module that contains system-specific parameters and functions
2. For example we can use it to read arguments from the command line:

```
Script: say_hello.py
import sys
print('Hello there', sys.argv[1])
    # Command line arguments are in sys.argv[1], sys.argv[2]...
    # sys.argv[0] is the script name itself
```

```
davide$ python say_hello.py bio334_Students
Hello there bio334_Students
```

Alternatively

To accept user input from the command line within a python script using the argparse module

```
Script: say_hello.py
import argpase

parser = argparse.ArgumentParser(description="Bio334 Exercise.")
parser.add_argument('--name', help="Name, dtype: String")
args = parser.parse_args()

# Reference the command line args by specifying args.[argument_name]
print('Hello there ', args.name)
```

```
dean$ python say_hello.py --name Dean
Hello there Dean
```