CME 193: Introduction to Scientific Python
Lecture 1: Introduction to Computing with Python

Dan Frank

Austin Benson (PAST)

Institute for Computational and Mathematical Engineering (ICME)

January 8, 2014

Course structure

- Eight 2-hour lectures, all in first four weeks
- Homework corresponding to each lecture except the last (7 total)
- Lectures:
  - 1 hour of instruction
  - 1 hour of interactive exercises
- Please bring a laptop to class!

All course materials are on `http://www.stanford.edu/~danfrank/cme193.html` and announcements/discussion will be through Piazza `https://piazza.com/class#winter2014/cme193`

Why listen to me?

- 3^{rd} year PhD in ICME
- Python for research & industry 8 years and counting
- Python at Twitter and Facebook
- Languages: R, MATLAB, Java, LISP/Clojure, HIVE & Pig, etc.

Office hours

- Immediately after class and by appointment. More arranged if there is demand.
- Please also use Piazza to ask questions.

Passing the class

The grading scheme is Satisfactory/Not Satisfactory.

To pass, you need to complete **all** homework assignments and earn at least **70%** of the points on **each** assignment. Grading is automated and you will know your score and a PASS/FAIL as you submit. You may submit as many times as you like before the deadline. Submission instructions are on the course website.

Course textbook

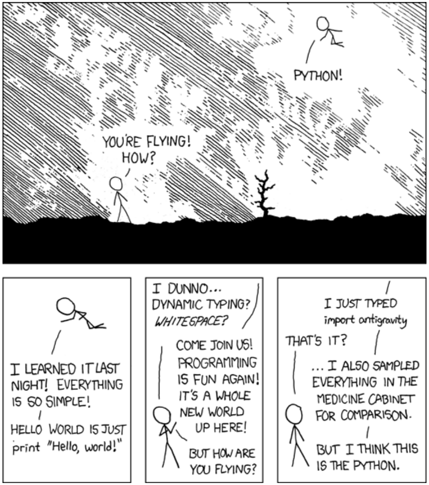
- No textbook!
- We will post online materials on the course web site

Homework 0

- Homework 0 is posted (it is not due)
- You should be comfortable with the material before starting Homework 1

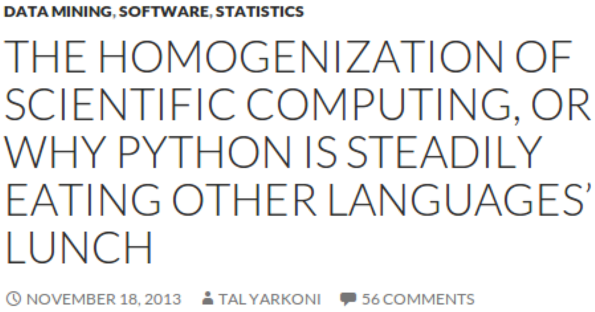
Motivation I

Why you should be excited to take this class...


PYTHON!
YOU'RE FLYING! HOW?
I LEARNED IT LAST NIGHT! EVERYTHING IS SO SIMPLE!
HELLO WORLD IS JUST print "Hello, world!"
I DUNNO... DYNAMIC TYPING? WHITESPACE?
COME JOIN US! PROGRAMMING IS FUN AGAIN! IT'S A WHOLE NEW WORLD UP HERE!
BUT HOW ARE YOU FLYING?
I JUST TYPED import antigravity
THAT'S IT?
... I ALSO SAMPLED EVERYTHING IN THE MEDICINE CABINET FOR COMPARISON.
BUT I THINK THIS IS THE PYTHON.

Motivation II

Why you should be excited to take this class...



DATA MINING, SOFTWARE, STATISTICS

THE HOMOGENIZATION OF SCIENTIFIC COMPUTING, OR WHY PYTHON IS STEADILY EATING OTHER LANGUAGES' LUNCH

NOVEMBER 18, 2013 TAL YARKONI 56 COMMENTS

Variety

One reason why we are excited to teach this class:

- Students in: Civil Engr., Mech. Engr., Chemical Engr., EE, ERE, ICME, MSE, Econ, Math, Stats, CS, Business, Biology, Medical School, Political Science, Aero/Astro, Business, Earth Systems, Undeclared
- Undergraduate: year 2, 3, 4; Graduate: year 1, 2, 3, 4+
- Problems: simulations, biology, stats/ML, web data

Course outline

1. Introduction to Computing with Python
2. Data Structures
3. File I/O, Object-oriented Python, and Introduction to NumPy
4. NumPy and SciPy
5. Data Visualization and Web Scraping
6. TBD

Python 2.x vs Python 3

- Python is currently transitioning from version 2 to 3
- Examples will be in 2.7
- Homeworks have been made compatible with both.

Basic variables

A variable holds information (1.343, 'hi', [1, 1, 2, 3, 5, 8])

In Python this is simple:

```
x = 1.343  # a number

greeting = 'hi'  # a string

arr = [1, 1, 2, 3, 5, 8]  # a list
```

# signifies the start of a comment in Python. The comment terminates at the end of the line.

Basic variables

Variables can change (they are *variable*)

```
x = 1.343

x = 2

x = 10 + 4

x = -3
```

(no more knowledge of 1.343, 2, or 14)

Types

Unlike C/C++ and Java, variables can change types. Python keeps track of the type internally.

```
x = 2

x = [3, 4, 5]

x = 'hi'
```

If you have PL theory background: Python is strongly typed but not statically typed

Arithmetic operators

```
2 + 4

3.2 * 6

(8.7 - 3.3) / 4

'hi' * 10

'hello, ' + 'world!'
```

Python supports this arithmetic on strings. (Note: Matlab does not.)

Arithmetic operators

Shorthand to combine assignment and addition statements:

```
x = 4
x += 2  # x = x + 2

y = 'hi'
y *= 4   # y = y * 4
```

`x` is now 6 and `y` is now `'hihihihi'`

Comparison operators

```
x == 1 # check for equality
y != 'hello' # check for inequality
2 > 2  # False
2 >= 2 # True
2.1 < z < 5.4 # chained inequalities
```

Boolean operations

```
x = 1
y = 'hello'

x == 1 or y == 'hi'
x > 0 and y != 'hi'

y = 0
x or y
x and y
not y
```

Python conveniently uses the keywords and, or, not instead of the symbols &&, ||, !

if

The `if` statement is the most basic way to control the direction and flow of a program

```
if x:
    print 'hello1'

if not x:
    print 'hello2'

if not x and y:
    print 'hello3'
```

if/else

`if` is often accompanied by `else` to specify a second path for the code if the `if` statement is false

```
if x:
    print 'hello'
else:
    print 'hi!'
```

Evaluating numerical values

As boolean values, the numerical value 0 is False and all other numerical values are True (1, 4.33, -12, ...).

```
x = -5
y = 5
z = 0

if x and y and z:
    print 'hello1' # will not print

if (x and y) or z:
    print 'hello2' # will print
```

while

The `while` loop repeatedly executes a task while a condition is true

```
i = 1
s = 0
while i < 10:
    s += i
    i = i + 1




# next lecture
s = sum(range(10))
```

while

```
x = 7.0
lower = 0.0
upper = x
guess = (upper + lower) / 2
while (abs(x - guess * guess) > 0.1):
    if guess * guess > x:
        upper = guess
    else:
        lower = guess
    guess = (upper + lower) / 2
```

What is this code doing?

for

The `for` loop also repeatedly executes a task

Typically, `for` provides more structure:

$$\text{for } (i = 0;\ i < n;\ i = i + 1)$$

Python for

- Python uses `for` differently than Matlab, C++, ...
- `for` is used to iterate over elements in an “object”
- This is one reason why Python is easy and powerful
- More next lecture on how you can iterate over a “object”

Python for

```
arr = [1, 2, 3, 4, 5, 6, 7, 8, 9]
for number in arr:
    print number * 2
```

more next lecture...

Functions

Functions are used to organize programs into coherent pieces

In other words, functions are used to generalize or “abstract” components of a program

Root finding

What is a limitation of this code?

```
x = 7.0
lower = 0.0
upper = x
guess = (upper + lower) / 2
while (abs(x - guess * guess) > 0.1):
    if guess * guess > x:
        upper = guess
    else:
        lower = guess
    guess = (upper + lower) / 2
```

Root finding

We do not want a $\sqrt{7}$ method, we want a $\sqrt{x}$ method

We still have the same capabilities (just let $x = 7$), but now our "abstracted" root finder can be used for more cases

Root finding

With this function, we can call `root(7)`

```
def root(x):
    lower = 0.0
    upper = x
    guess = (upper + lower) / 2
    while (abs(x - guess * guess) > 0.1):
        if guess * guess > x:
            upper = guess
        else:
            lower = guess
        guess = (upper + lower) / 2
    return guess
```

Root finding

More general, we can call `root(7, 0.1)`:

```
def root(x, tol):
    lower = 0.0
    upper = x
    guess = (upper + lower) / 2
    while (abs(x - guess * guess) > tol):
        if guess * guess > x:
            upper = guess
        else:
            lower = guess
        guess = (upper + lower) / 2
    return guess
```

Root finding

Python makes it easy to provide default argument values:

```
def root(x, tol=0.1):
    lower = 0.0
    upper = x
    guess = (upper + lower) / 2
    while (abs(x - guess * guess) > tol):
        if guess * guess > x:
            upper = guess
        else:
            lower = guess
        guess = (upper + lower) / 2
    return guess
```

Can call `root(3)`, `root(113, 0.01)`

Root finding

A few things to think about:

- Are there cases where `root()` will have an error?
- Are there cases where `root()` will run forever? (fail to converge)
- How else can we generalize the function?

Basic functions

What will happen when this code runs?

```
x = 5

def printer(y):
    print x + y

printer(5)
```

Basic functions

What about this code?

```
x = 5

def printer(x, y):
    print x + y

printer(4, 5)
```

More function examples

```
def polyval(p, x):
    val = 0
    i = 0
    for coeff in p:
        val += coeff * (x ** i)  # ** is ^
        i = i + 1
    return val

print polyval([1, 2, 0, 1], 4)  # prints '73'
```

More function examples

```
def polyval(p, x):
    val = 0
    for i, coeff in enumerate(p):
        val += coeff * (x ** i)
    return val

print polyval([1, 2, 0, 1], 4)  # prints '73'
```

Indentation / white space

Python uses indentation ("white space") to group statements

Each code block is indented the same amount (for loop, while loop, function definition, etc.)

Python will complain if your indentation is incorrect

Indentation

```
a = 10
b = 2
while a > 1:
  print a + b
    a = a - 1  # wrong indentation --> error!
```

2-space or 4-space indentation is standard.

Identation

```
def func_incorrect1(x, y, z):
if x < y:    # wrong indentation --> error!
  return z
return 0

def func_incorrect2(x, y, z):
  if x < y:
  return z  # wrong indentation --> error!
  return 0

def func_correct(x, y, z):
  if x < y:
    return z
  return 0
```

White space

Some people like this indentation structure and some people do not.

... Python isn't going to stop using it

End

- Assignment 1 is posted on the course web site (due Tuesday 1/14)
- In-class exercises, python codes from slides, and readings also posted

Next time:

1. More on Python functions
2. Strings
3. Lists
4. Dictionaries
5. Tuples