Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 3

Imperial College
London

Today: *Getting started with Python*
Command-line basics; numbers; modules; lists, tuples, and strings. Programming basics: if statements, loops

Python overview

- Python ‘core’: General-purpose programming language
- Python is an *interpreted* language: code does not need to be compiled as in c or fortran

Python overview

- Python ‘core’: General-purpose programming language
- Python is an *interpreted* language: code does not need to be compiled as in c or fortran
- Matlab-style scientific computing via add-on modules:
  - numpy: basic linear algebra
  - matplotlib: 2d plotting
  - scipy: large range of capabilities
    - Differential equations
    - Signal processing
    - Optimization
    - Statistics
- Will often see code like:

```
In [3]: import numpy as np

In [4]: import scipy.optimize as sco
```

Python overview

Can use Python is several ways:

- **At the terminal (like the Matlab command window)**
- **Writing scripts in a text editor**
- **Creating notebooks (like Mathematica)**
- **Canopy Python distribution provides a nice interface for each of these approaches**

Getting started at the terminal

- **The basic python terminal is… basic**
- **So, we use *interactive* python or *ipython* along with *qtconsole:***

```
$ ipython qtconsole
```

- **Nice help features, user-friendly, used by Canopy by default**
- **Depending on how/when you installed software, may have option of using jupyter:**

```
$ jupyter qtconsole
```

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```

- Will almost always want *numpy* and *matplotlib*
- Can be easily imported with: `In [1]: %pylab`

Getting started at the terminal

Can use terminal as a calculator:

```
In [13]: x=2

In [14]: y=3

In [15]: x+y
Out[15]: 5

In [16]: sin(x)
Out[16]: 0.9092974268256817 1

In [17]: sqrt(2.)
Out[17]: 1.4142135623730951
```

Getting help

A few different approaches:

- **Using “?”**
- **<tab> completion**
- **lookfor(“something”)**
- **google**

Getting help

At the terminal, try: `sin?`

or: `numpy?`

<tab> completion:

Try sin **<tab>:**

```
In [93]: sin
sin          sinc         single       singlecomplex  sinh
```

or numpy. **<tab>**

Getting help

Can use these approaches for user-defined variables as well:

```
In [112]: x=4+2j

In [113]: x?
Type:       complex
String form: (4+2j)
Docstring:
complex(real[, imag]) -> complex number

Create a complex number from a real part
and an optional imaginary part.
This is equivalent to (real + imag*1j) where
imag defaults to 0.

In [114]: x. <tab>
x.conjugate  x.imag       x.real
```

Number types

We have integers, floating-point (real) numbers, Booleans, (and we have seen complex numbers)

```
In [130]: type(3)
Out[130]: int

In [131]: type(3.)
Out[131]: float

In [132]: 1<2
Out[132]: True

In [133]: type(1<2)
Out[133]: bool
```

Number types

Booleans are only useful if we know Python's relational operators:

```
x == y      # Produce True if ... x is equal to y
x != y      # ... x is not equal to y
x > y       # ... x is greater than y
x < y       # ... x is less than y
x >= y      # ... x is greater than or equal to y
x <= y      # ... x is less than or equal to y
```

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x == y      # Produce True if ... x is equal to y
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x > y       # ... x is greater than y
x < y       # ... x is less than y
x >= y      # ... x is greater than or equal to y
x <= y      # ... x is less than or equal to y
```

…which can also be combined:

```
In [141]: x=pi

In [142]: y=3

In [143]: (x>y) and (y>0)
Out[143]: True

In [144]: (x>y) or (y<0)
Out[144]: True
```

Containers

Containers: ‘collections’ of data – strings, tuples, lists, dictionaries

```
In [185]: type("this is a string")
Out[185]: str

In [186]: type(("this","is","a","tuple"))
Out[186]: tuple

In [187]: type(["this","is","a","list"])
Out[187]: list

In [188]: type({"num1":12.3,"num2":24.0})
Out[188]: dict
```

Strings

Useful for processing input, producing nicely-formatted output

Use <tab> completion to see built-in Python capabilities:

```
In [212]: name="first last"

In [213]: name. <tab>
```

For example:

```
In [2]: name="first last"

In [3]: name
Out[3]: 'first last'

In [4]: name.center(20)
Out[4]: '     first last     '
```

Tuples

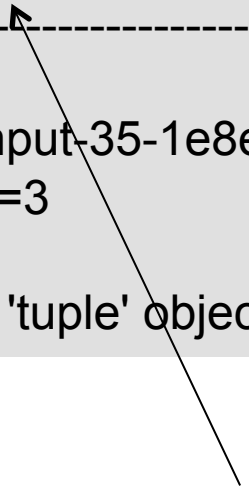
Immutable collection of items

```
In [33]: a=(1,2,"three","four")

In [34]: a[2]
Out[34]: 'three'

In [35]: a[2]=3
---------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-35-1e8e286566a0> in <module>()
----> 1 a[2]=3

TypeError: 'tuple' object does not support item assignmentme="first last”
```



Can’t change 3rd element

Tuples

Often used as input/output for functions

Useful for “switching” values of variables:

```
In [47]: x,y=2,3

In [48]: x,y
Out[48]: (2, 3)

In [49]: x,y=y,x

In [50]: x,y
Out[50]: (3, 2)
```

Lists

Mutable collection of items

```
In [52]: a=[1,2,"three","four"]

In [53]: a[2]
Out[53]: 'three'

In [54]: a[2]=3

In [55]: a
Out[55]: [1, 2, 3, 'four']
```

Lists

Python has a lot of nice features for working with lists…

```
In [61]: a
Out[61]: [1, 2, 3, 'four']

In [62]: b
Out[62]: [5.0, 6, 7]

In [63]: a+b
Out[63]: [1, 2, 3, 'four', 5.0, 6, 7]

In [64]: a*2
Out[64]: [1, 2, 3, 'four', 1, 2, 3, 'four']

In [65]: a. <tab>
a.append  a.count  a.extend  a.index  a.insert  a.pop  a.remove  a.reverse  a.sort
```

List indexing

- **List indices run from zero to N-1 (*where N=len(list)*)**
- **Can also use negative indices as shown in example:**

```
In [7]: a=[1,2,'three','four']

In [8]: [a[0],a[1],a[2],a[len(a)-1]]
Out[8]: [1, 2, 'three', 'four']

In [9]: [a[-1],a[-2],a[-3],a[-4]]
Out[9]: ['four', 'three', 2, 1]
```

List slices

- List slices take the form list[*start*:*end*:*step*]
- This gives the values from *start* to *end-1* with stepsize given by *step*
- The default value of *step*=1 is used if step is omitted
- The default values *start*=0 and *end*=len(list) are used if *start* and *end* are omitted

```
In [1]: a=[1,2,'three','four']

In [2]: a[1:3]
Out[2]: [2, 'three']

In [3]: a[1:4:2]
Out[3]: [2, 'four']

In [4]: a[1::2]
Out[4]: [2, 'four']
```

Other containers

- *dictionaries* and *classes* are also important container types
- We will (probably) not cover them in this class
- See supplementary material section on course webpage

Loops and if statements

- **Loops and if statements are building blocks of most codes**
- **Python requires colon, ":" to indicate start of block**
- **Indentation sets the size of the block**

```
if < Boolean expression 1>:
        <block 1>
elif < Boolean expression 2> :
        <block 2>
else:
        <block 3>
```

Loops and if statements

- **Loops and if statements are building blocks of most codes**
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```
if < Boolean expression 1>:
        <block 1>
elif < Boolean expression 2> :
        <block 2>
else:
        <block 3>
```

```
x=rand(1)[0]
if x<0.5:
    print "left: x=%s" %(x)
elif x>=0.5:
    print "right: x=%s" %(x)
else:
    print "error, x is not numeric"

right: x=[ 0.97813575]
```

if block

Code generates random variable between zero and one and determines if it is greater than or less than 0.5

while loops

- **Structure of while loop is similar to if statement**

```
while < Boolean expression 1>:
        <block 1>
```

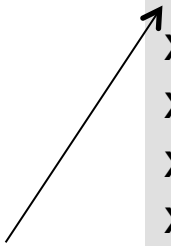
While loops

- **Structure of while loops is similar to if statements**

```
while < Boolean expression 1>:
        <block 1>
```

```
x = rand(1)
while x<1:
    print "x=%s" %(x)
    x=x+0.1
```

```
x=[ 0.17099121]
x=[ 0.27099121]
x=[ 0.37099121]
x=[ 0.47099121]
x=[ 0.57099121]
x=[ 0.67099121]
x=[ 0.77099121]
x=[ 0.87099121]
x=[ 0.97099121]
```



Generate random variable, x, and add increments of 0.1 until x>1

for loops

- **for loops iterate through items in a list:**

```
for x in list:
        <block>
```

for loops

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```
for x in list:
        <block>
```

```
In [37]: y=0

In [38]: for x in [1,2,3]:
    ....:     y = y + x #can also write y += x
    ....:     print "y = %s" %(y)
    ....:
y = 1
y = 3
y = 6
```

for loops

- **for loops iterate through items in a list:**

```
for x in list:
        <block>
```

```
In [37]: y=0

In [38]: for x in [1,2,3]:
    ....:     y = y + x #can also write y += x
    ....:     print "y = %s" %(y)
    ....:
y = 1
y = 3
y = 6
```

- **Can also iterate through:**
  - **Items in a tuple**
  - **Characters in a string**

for loops

range function is useful for generating lists:

```
In [23]: range(4)
Out[23]: [0, 1, 2, 3]

In [24]: range(2,6)
Out[24]: [2, 3, 4, 5]

In [25]: range(2,6,2)
Out[25]: [2, 4]
```

for loops

range function is useful for generating lists:

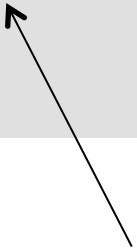
```
In [23]: range(4)
Out[23]: [0, 1, 2, 3]

In [24]: range(2,6)
Out[24]: [2, 3, 4, 5]

In [25]: range(2,6,2)
Out[25]: [2, 4]
```

```
In [45]: L = ["a","few","words"]

In [46]: for i in range(3):
    ....:     print i,L[i]
    ....:
0 a
1 few
2 words
```

Block controls: *break* and *continue*

***continue* allows you to skip remaining steps in block**

```
In [65]: words = ["yes","yes","no","yes"]

In [66]: for w in words:
    ....:     if w == "yes":
    ....:         continue
    ....:     print w
    ....:
    no
```



print statement is only executed if w is not equal to “yes”

Block controls: *break* and *continue*

***break* statement allows premature ending of loop:**

```
In [54]: words = ["yes","yes","no","yes"]

In [55]: for w in words:
    ....:     if w == "no":
    ....:         print "breaking for loop"
    ....:         break
    ....:     else:
    ....:         print w
    ....:
yes
yes
breaking for loop
```

Overview of Lab 2

- Practice with git/bitbucket
  - Using git to keep up-to-date with course material
- Practice with python: working with lists and loops
- Wednesday: You will need a working installation of ipython notebook (comes with Canopy) or jupyter notebook.
  - If using Windows, will also need to have installed git in your virtual machine.