

Python Lab: Fundamentals

Proteomics Informatics, Spring 2014

Week 3

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Programs

- perform computations
 - on some **input data** to generate some **output**
- according to a well-defined series of steps (**algorithm**)
- implemented using some programming language
- which follows a **syntax**

Data – Types & Values

Object Type	Example Creation
Numbers (integers or floating-point/real-numbers)	10, 1234.5, 22.7
Strings	“Are you kidding?”, ‘This Python class rocks’
Boolean	True, False
...	...
...	...

- Fundamental “things” that programs work with (Data)
- Every data object has a type
 - Try in ipython shell:
 - `type(1)`, `type('PEPTIDE')`
- Creation
 - from keyboard, files, remote server, through data processing

Variables

- Store for later use
- Assign data to variables
 - $x = 2$
 - $y = \text{'abc'}$ or "abc"
 - $\text{name} = \text{'Roger Federer'}$
 - $\text{aa_sequence} = \text{"GAMRPODSTK"}$
- Use meaningful names

Operations

- Numbers:
 - Operators (Ex. *, /, +, -, ** etc.)
 - Mathematical funcs (Ex. math.pow, math.sqrt)
 - import math
 - math.pow?, math.pow(10, 2)
- Strings (aa_seq = "GAMRPODSTK")
 - Access:
 - Indexing (forward and backward): x[2], x[-1]; index starts at 0
 - Slicing: aa_seq[0:3], aa_seq[1:], aa_seq[1:5:2], aa_seq[::2], x[::-1]
 - Concatenation: aa_seq + aa_seq, aa_seq + "MDP"
 - aa_seq.<tab> (in ipython shell)
 - Repetition: aa_seq*8
 - Membership: 'G' in aa_seq
 - aa_seq.find('E'), aa_seq.replace("MR", "NT"), aa_seq.lower(); len(x)
- Built-in vs. user-defined

Data Structures

- Containers for build composite/complex data objects
- Stored in a specific format, depending on data access and processing needs

Lists

- Most general sequence object
- Positionally ordered collection of arbitrarily typed objects: `x = [1, 'a', [1,2,3]]`
 - Heterogeneous
 - Arbitrarily nest-able
- Various operations:
 - Ex. `x = [1,2,3,4,5]`
 - Indexing, slicing etc. same as strings
 - Slice assignment: `x[1:3] = ["replacement", "string"]`
 - **Generic functions:** `len(x)`, `type(x)`
 - **Type-specific functions:** `x.append('b')`, `x.pop(2)`, `x.reverse()`, `x+y`, `x*3`, `x.extend([5,6,7])`, `x.sort()`... `x` to check the entire list

Dictionaries

- Unordered collection of mappings (key-value pairs)
 - Ex. `y = {'a': 1, 'b': 2}`
 - Ex. `codon → AminoAcid`
 - Ex. `geneID → nucleotide sequence`; `protID → AminoAcid seq`
- Keys must be unique
- Objects are accessed by 'keys' and not by relative position
 - `y['a'] = 1`
- Heterogeneous, can be arbitrarily nested:

```
rec = {'name': {'first': 'Bob', 'last': 'Smith'},  
      'job': ['dev', 'mgr'],  
      'age': 30}
```
- Various operations:
 - **Generic:** `len(y)`, `type(y)`
 - **Type-specific:** `y.has_key('a')` or `'a' in y`, `y.update(<another dict>)`, `y.keys()`, `y.values()`, `y.items()`



Statements

- **Assignment:**
thisIs = "Python Lecture 2"
- **Function calls:**
x.reverse() where x is a list obj
- **Print:** print x, "\t", y
- **Select action:**
If <condition 1>:
 action 1
elif <condition 2>:
 action 2
else:
 action 3
- **Sequence Iteration (loops):**
for x in myList:
 action
while X > Y:
 action/pass
- **Building Functions:**
def add(x, y):
 return x+y
- **Module access:**
import numpy
from numpy import ndarray
from matplotlib import pyplot as plt
- **Exception Handling, OOP, global, del, exec, assert, documentation strings/comments etc.**
- **Indentation for compound statements**

Getting help: Documentation

- IPython shell
 - `x = [1,2,3,4]`
 - `x.<tab>`
 - `help(x)`, `help(x.<function name>)`, `x.<function name>?`
 - Ex. `x.append?`
 - `L.append(object)` -- append object to end
 - Similar to $f(x)$ notation in math. But more general...

Interactive vs. Script Mode

Practice some!!

- Create some data objects (list, dictionary string) in IPython shell
- Check their “types”, and explore documentation for some of the their operations/functions
- Run some functions to see what happens

Next Class

- Compound statements:
 - for/while loops
- Real examples