Brief summary of basic Python syntax

Joakim Sundnes[1,2] Hans Petter Langtangen[1,2] Ola Skavhaug[3]

Center for Biomedical Computing, Simula Research Laboratory[1]

Dept. of Informatics, University of Oslo[2]

mCASH (formerly Dept. of Informatics, University of Oslo)[3]

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Sources for more information and documentation

- H.P. Langtangen and G. K. Sandve: Illustrating Python via Bioinformatics Examples: PDF or HTML
- `pydoc anymodule`, `pydoc anymodule.anyfunc`
- Python Library Reference (go to *index* in the upper right corner)
- Python 2.7 Quick Reference
- Python Global Module Index
- Think Python (textbook)
- Dive Into Python (texbook)
- Think Like a Computer Scientist (textbook)
- Unix Need-to-know
- Emacs Need-to-know

Video material

- A Gentle Introduction to Programming Using Python
- Introduction to Computer Science and Programming
- Learning Python Programming Language Through Video Lectures
- Python Programming Tutorials Video Lecture Course
- Python Videos, Tutorials and Screencasts

First Python encounter: a scientific hello world program

```python
#!/usr/bin/env python

from math import sin
import sys

x = float(sys.argv[1])
print "Hello world, sin({0}) = {1}".format(x, sin(x))
```

Running the script from the command line

Code in file `hw.py`.

Run with command:

```
> python hw.py 0.5
Hello world, sin(0.5) = 0.479426.
```

Linux alternative if file is executable (`chmod a+x hw.py`):

```
> ./hw.py 0.5
Hello world, sin(0.5) = 0.479426.
```

Interactive Python & IPython

- Typing `python` gives you an interactive Python shell
- IPython is better, can also run scripts:
  `In [1]: run hw.py 3.14159`
- IPython is integrated with Python's `pdb` debugger
- `pdb` can be automatically invoked when an exception occurs
- IPython supports tab completion, additional help commands, and much more, ...

Dissection of `hw.py` (1)

On Unix: find out what kind of script language (interpreter) to use:

```
#!/usr/bin/env python
```

Access library functionality like the function `sin` and the list `sys.arg` (of command-line arguments):

```
from math import sin
import sys
```

Read 1st command line argument and convert it to a floating point object:

```
x = float(sys.argv[1])
```

Dissection of `hw.py` (2)

Print out the result using a format string:

```
print "Hello world, sin({0}) = {1}".format(x, sin(x))   # v2.x
print("Hello world, sin({0}) = {1}".format(x, sin(x)))  # v3.x
```

or with complete control of the formating of floats (printf syntax):

```
print "Hello world, sin({x:g}) = {s:.3f}".format(x=x, s=sin(x))
print("Hello world, sin({x:g}) = {s:.3f}".format(x=x, s=sin(x)))
```

Python variables

Variables are not declared

Variables hold references to objects

```
a = 3          # ref to an int object containing 3
a = 3.0        # ref to a float object containing 3.0
a = '3.'       # ref to a string object containing '3.'
a = ['1', 2]   # ref to a list object containing
               # a string '1' and an integer 2
```

Test for a variable's type:

```
if isinstance(a, int): # int?
if isinstance(a, (list, tuple)): # list or tuple?
```

Common types

- Numbers: `int`, `float`, `complex`
- Sequences: `str`, `list`, `tuple`, `ndarray`
- Mappings: `dict` (dictionary/hash)
- User-defined type (via user-defined class)

Simple Assignments

```python
a = 10                # a is a variable referencing an
                      # integer object of value 10

b = True              # b is a boolean variable

a = b                 # a is now a boolean as well
                      # (referencing the same object as b)

b = increment(4)      # b is the value returned by a function

is_equal = a == b     # is_equal is True if a == b
```

Lists and tuples

```
mylist  = ['a string', 2.5, 6, 'another string']
mytuple = ('a string', 2.5, 6, 'another string')
mylist[1]  = -10
mylist.append('a third string')
mytuple[1] = -10  # illegal: cannot change a tuple
```

A tuple is a constant list (known as an *immutable* object, contrary to *mutable* objects which can change their content)

List functionality

Construction	Meaning
`a = []`	initialize an empty list
`a = [1, 4.4, 'run.py']`	initialize a list
`a.append(elem)`	add `elem` object to the end
`a + [1,3]`	add two lists
`a.insert(i, e)`	insert element `e` before index `i`
`a[3]`	index a list element
`a[-1]`	get last list element
`a[1:3]`	slice: copy data to sublist (here: index 1, 2)
`del a[3]`	delete an element (index 3)
`a.remove(e)`	remove an element with value `e`
`a.index('run.py')`	find index corresponding to an element's value
`'run.py' in a`	test if a value is contained in the list
`a.count(v)`	count how many elements that have the value `v`
`len(a)`	number of elements in list `a`
`min(a)`	the smallest element in `a`
`max(a)`	the largest element in `a`
`sum(a)`	add all elements in `a`
`sorted(a)`	return sorted version of list `a`
`reversed(a)`	return reversed sorted version of list `a`
`b[3][0][2]`	nested list indexing
`isinstance(a, list)`	is `True` if `a` is a list
`type(a) is list`	is `True` if `a` is a list

Dictionary functionality

Construction	Meaning
`a = {}`	initialize an empty dictionary
`a = {'point': [0,0.1], 'value': 7}`	initialize a dictionary
`a = dict(point=[2,7], value=3)`	initialize a dictionary w/string keys
`a.update(b)`	add key-value pairs from `b` in `a`
`a.update(key1=value1, key2=value2)`	add key-value pairs in `a`
`a['hide'] = True`	add new key-value pair to `a`
`a['point']`	get value corresponding to key `point`
`for key in a:`	loop over keys in unknown order
`for key in sorted(a):`	loop over keys in alphabetic order
`'value' in a`	`True` if string `value` is a key in `a`
`del a['point']`	delete a key-value pair from `a`
`list(a.keys())`	list of keys
`list(a.values())`	list of values
`len(a)`	number of key-value pairs in `a`
`isinstance(a, dict)`	is `True` if `a` is a dictionary

String operations

```
s = 'Berlin: 18.4 C at 4 pm'
s[8:17]           # extract substring
':' in s          # is ':' contained in s?
s.find(':')       # index where first ':' is found
s.split(':')      # split into substrings
s.split()         # split wrt whitespace
'Berlin' in s     # test if substring is in s
s.replace('18.4', '20')
s.lower()         # lower case letters only
s.upper()         # upper case letters only
s.split()[4].isdigit()
s.strip()         # remove leading/trailing blanks
', '.join(list_of_words)
```

Strings in Python use single or double quotes, or triple single/double quotes

Single- and double-quoted strings work in the same way: `'some string'` is equivalent to `"some string"`

Triple-quoted strings can be multi line with embedded newlines:

```
text = """large portions of a text
can be conveniently placed inside
triple-quoted strings (newlines
are preserved)"""
```

Raw strings, where backslash is backslash:

```
s3 = r'\(\s+\.\d+\)'
# in an ordinary string one must quote backslash:
s3 = '\\(\\s+\\.\\d+\\)'
```

Simple control structures

Loops:

```
while condition:
    <block of statements>
```

Here, `condition` must be a boolean expression (or have a boolean interpretation), for example: `i < 10` or `!found`

```
for element in somelist:
    <block of statements>
```

Conditionals/branching:

```
if condition:
    <block of statements>
elif condition:
    <block of statements>
else:
    <block of statements>
```

Looping over integer indices is done with `range`

```
for i in range(10):
    print(i)
```

Remark:

`range` in Pyton 3.x is equal to `xrange` in Python 2.x and generates an *iterator* over integers, while `range` in Python 2.x returns a list of integers.

Examples on loops and branching

```python
x = 0
dx = 1.0
while x < 6:
    if x < 2:
        x += dx
    elif 2 <= x < 4:
        x += 2*dx
    else:
        x += 3*dx
    print 'new x:', x
print 'loop is over'
```

(Visualize execution)

```python
mylist = [0, 0.5, 1, 2, 4, 10]
for i, x in enumerate(mylist):
    print i, x
print 'loop is over'
```

(Visualize execution)

Functions and arguments

User-defined functions:

```
def split(string, char):
    position = string.find(char)
    if  position > 0:
        return string[:position+1], string[position+1:]
    else:
        return string, ''

# function call:
message = 'Heisann'
print(split(message, 'i'))
# prints ('Hei', 'sann')
```

Positional arguments must appear before keyword arguments:

```
def split(message, char='i'):
    # ...
```

eval and exec turn strings into live code

Evaluating string expressions with `eval`:

```
>>> x = 20
>>> r = eval('x + 1.1')
>>> r
21.1
>>> type(r)
<type 'float'>
```

Executing strings with Python code, using `exec`:

```
import sys
user_expression = sys.argv[1]

# Wrap user_expression in a Python function
# (assuming the expression involves x)

exec("""
def f(x):
    return %s
""" % user_expression

# or

f = eval('lambda x: %s' % user_expression)
```

File reading

Reading a file:

```
infile = open(filename, 'r')
for line in infile:
    # process line

lines = infile.readlines()
for line in lines:
    # process line

for i in xrange(len(lines)):
    # process lines[i] and perhaps next line lines[i+1]

fstr = infile.read()  # fstr contains the entire file
fstr = fstr.replace('some string', 'another string')
for piece in fstr.split(';'):
    # process piece (separated by ;)

infile.close()
```

File writing

```
outfile = open(filename, 'w')   # new file or overwrite
outfile = open(filename, 'a')   # append to existing file

outfile.write("""Some string
....
""")
outfile.writelines(list_of_lines)

outfile.close()
```

Using modules

Import module:

```
import sys
x = float(sys.argv[1])
```

Import module member argv into current namespace:

```
from sys import argv
x = float(argv[1])
```

Import everything from sys (not recommended)

```
from sys import *
x = float(argv[1])

flags = ''
# Ooops, flags was also imported from sys, this new flags
# name overwrites sys.flags!
```

Import argv under an alias:

```
from sys import argv as a
x = float(a[1])
```

Making your own Python modules

- Reuse scripts by wrapping them in classes or functions
- Collect classes and functions in library modules
- How? just put classes and functions in a file `MyMod.py`
- Put `MyMod.py` in one of the directories where Python can find it (see next slide)

Examples:

```
import MyMod
# or
import MyMod as M    # M is a short form
# or
from MyMod import *
# or
from MyMod import myspecialfunction, myotherspecialfunction
```

How Python can find your modules?

Python has some "official" module directories, typically

```
/usr/lib/python2.7
/usr/lib/python2.7/site-packages
/usr/lib/python3.4
/usr/lib/python3.4/site-packages
```

+ current working directory

The environment variable `PYTHONPATH` may contain additional directories with modules

```
> echo $PYTHONPATH
/home/me/python/mymodules:/usr/lib/python3.4:/home/you/yourlibs
```

Python's `sys.path` list contains the directories where Python searches for modules, and `sys.path` contains "official" directories, plus those in `PYTHONPATH`

Packages

- A class of modules can be collected in a *package*
- Normally, a package is organized as module files in a directory tree
- Each subdirectory has a file `__init__` (can be empty)

Can import modules in the tree like this:

```
from MyMod.numerics.pde.grids import fdm_grids

grid = fdm_grids()
grid.domain(xmin=0, xmax=1, ymin=0, ymax=1)
...
```

Here, class `fdm_grids` is in module `grids` (file `grids.py` in the directory `MyMod/numerics/pde`

Test block in a module

Module files can have a test/demo section at the end:

```
if __name__ == '__main__':
    infile = sys.argv[1]; outfile = sys.argv[2]
    for i in sys.argv[3:]:
        create(infile, outfile, i)
```

- The block is executed *only if* the module file is run as a program
- The tests at the end of a module often serve as good examples on the usage of the module

Installing modules

- Python has its own tool, Distutils, for distributing and installing modules
- Installation is based on the script `setup.py`

Standard command:

```
> sudo python setup.py install
```

Writing your own setup.py script

Suppose you have a module in `mymod.py` that you want to distribute to others such that they can easily install it by `setup.py install`.

```
from distutils.core import setup
name='mymod'

setup(name=name,
      version='0.1',
      py_modules=[name],          # modules to be installed
      scripts=[name + '.py'],     # programs to be installed
      )
```

Now, `setup.py` will be installed both as a module and as an executable script (if it has a test block for sensible code).

Can easily be extended to install a package of modules, see the introduction to Distutils

Use doc strings in functions, classes, and modules!

Doc strings = first string in a function, class, or file (module)

```
def ignorecase_sort(a, b):
    """Compare strings a and b, ignoring case."""
    return cmp(a.lower(), b.lower())
```

Doc strings in modules are a (often long multi-line) string starting in the top of the file

```
"""
This module is a fake module
for exemplifying multi-line
doc strings.
"""
import sys
import collections

def somefunc():
    ...
```

Doc strings serve many purposes

- Documentation in the source code
- Online documentation
  (Sphinx can automatically produce manuals with doc strings)
- Balloon help in sophisticated GUIs (e.g., IDLE)
- Automatic testing with the `doctest` module