Introduction to Python

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For More Information?

http://python.org/

- documentation, tutorials, beginners guide, core distribution, ...

Books include:

- *Learning Python* by Mark Lutz
- *Python Essential Reference* by David Beazley
- *Python Cookbook*, ed. by Martelli, Ravenscroft and Ascher
- (online at http://code.activestate.com/recipes/langs/python/)
- http://wiki.python.org/moin/PythonBooks

Python Videos

http://showmedo.com/videotutorials/python

- “5 Minute Overview (What Does Python Look Like?)”
- “Introducing the PyDev IDE for Eclipse”
- “Linear Algebra with Numpy”
- And many more

4 Major Versions of Python

- “Python” or “CPython” is written in C/C++
  - Version 2.7 came out in mid-2010
  - Version 3.1.2 came out in early 2010

- “Jython” is written in Java for the JVM
- “IronPython” is written in C# for the .Net environment

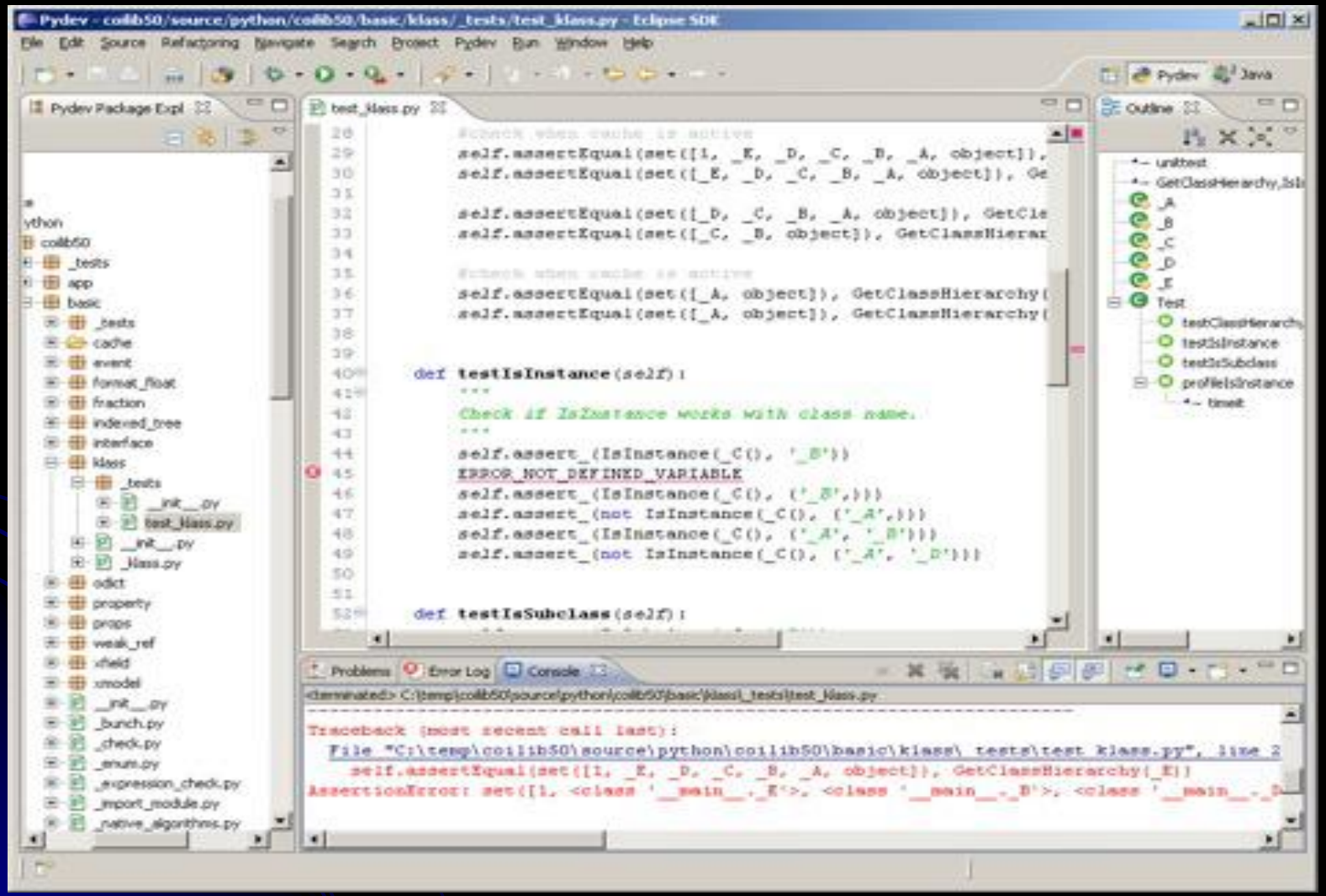
Go To Website

Development Environments

what IDE to use? http://stackoverflow.com/questions/81584

1. PyDev with Eclipse
2. Komodo
3. Emacs
4. Vim
5. TextMate
6. Gedit
7. Idle
8. PIDA (Linux)(VIM Based)
9. NotePad++ (Windows)
10. BlueFish (Linux)

Pydev with Eclipse



Python Interactive Shell

```
% python
Python 2.6.1 (r261:67515, Feb 11 2010, 00:51:29)
[GCC 4.2.1 (Apple Inc. build 5646)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

You can type things directly into a running Python session

```
>>> 2+3*4
14
>>> name = "Andrew"
>>> name
'Andrew'
>>> print "Hello", name
Hello Andrew
>>>
```

- Background
- Data Types/Structure
- Control flow
- File I/O
- Modules
- Class
- NLTK

List

A compound data type:

[0]

[2.3, 4.5]

[5, "Hello", "there", 9.8]

[]

Use len() to get the length of a list

```
>>> names = [“Ben", “Chen", “Yaqin"]
>>> len(names)
3
```

Use [ ] to index items in the list

```
>>> names[0]
'Ben'
>>> names[1]
'Chen'
>>> names[2]
'Yaqin'
>>> names[3]
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
IndexError: list index out of range
>>> names[-1]
'Yaqin'
>>> names[-2]
'Chen'
>>> names[-3]
'Ben'
```

[0] is the first item.
[1] is the second item
...

Out of range values
raise an exception

Negative values
go backwards from
the last element.

Strings share many features with lists

```
>>> smiles = "C(=N)(N)N.C(=O)(O)O"
>>> smiles[0]
'C'
>>> smiles[1]
'('
>>> smiles[-1]
'O'
>>> smiles[1:5]
'(=N)'
>>> smiles[10:-4]
'C(=O)'
```

Use “slice” notation to get a substring

String Methods: find, split

```
smiles = "C(=N)(N)N.C(=O)(O)O"
>>> smiles.find("(O)")
15
>>> smiles.find(".")
9
>>> smiles.find(".", 10)
-1
>>> smiles.split(".")
['C(=N)(N)N', 'C(=O)(O)O']
>>>
```

Use “find” to find the start of a substring.

Start looking at position 10.

Find returns -1 if it couldn’t find a match.

Split the string into parts with “.” as the delimiter

String operators: in, not in

```
if "Br" in “Brother”:
   print "contains brother“

email_address = “clin”
if "@" not in email_address:
   email_address += "@brandeis.edu“
```

String Method: “strip”, “rstrip”, “lstrip” are ways to remove whitespace or selected characters

```
>>> line = '' # This is a comment line \n''
>>> line.strip()
'# This is a comment line'
>>> line.rstrip()
' # This is a comment line'
>>> line.rstrip("\n")
' # This is a comment line '
>>>
```

More String methods

email.startswith(“c") endswith(“u”)
True/False

>>> "%s@brandeis.edu" % "clin"
'clin@brandeis.edu'

>>> names = [“Ben", “Chen", “Yaqin"]
>>> ", ".join(names)
‘Ben, Chen, Yaqin‘

>>> “chen".upper()
‘CHEN'

Unexpected things about strings

```
>>> s = "andrew"
>>> s[0] = "A"
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
TypeError: 'str' object does not support item
   assignment
>>> s = "A" + s[1:]
>>> s
'Andrew‘
```

Strings are read only

“\” is for special characters

\n -> newline

\t -> tab

\\ -> backslash

...

But Windows uses backslash for directories!

```
filename = "M:\nickel_project\reactive.smi" # DANGER!
filename = "M:\\nickel_project\\reactive.smi" # Better!
filename = "M:/nickel_project/reactive.smi" # Usually works
```

Lists are mutable - some useful methods

```
>>> ids = ["9pti", "2plv", "1crn"]
>>> ids.append("1alm")
>>> ids
['9pti', '2plv', '1crn', '1alm']
>>>ids.extend(L)
    Extend the list by appending all the items in the given list; equivalent to a[len(a):] = L.
>>> del ids[0]
>>> ids
['2plv', '1crn', '1alm']
>>> ids.sort()
>>> ids
['1alm', '1crn', '2plv']
>>> ids.reverse()
>>> ids
['2plv', '1crn', '1alm']
>>> ids.insert(0, "9pti")
>>> ids
['9pti', '2plv', '1crn', '1alm']
```

append an element

remove an element

sort by default order

reverse the elements in a list

insert an element at some specified position. (Slower than .append())

Tuples: sort of an immutable list

```
>>> yellow = (255, 255, 0) # r, g, b
>>> one    = (1,)
>>> yellow[0]
>>> yellow[1:]
(255, 0)
>>> yellow[0] = 0
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
TypeError: 'tuple' object does not support item assignment
```

Very common in string interpolation:

```
>>> "%s lives in %s at latitude %.1f" % ("Andrew", "Sweden", 57.7056)
'Andrew lives in Sweden at latitude 57.7'
```

zipping lists together

```
>>> names
['ben', 'chen', 'yaqin']

>>> gender = [0, 0, 1]

>>> zip(names, gender)
[('ben', 0), ('chen', 0), ('yaqin', 1)]
```

Dictionaries

- Dictionaries are lookup tables.
- They map from a “key” to a “value”.

```
symbol_to_name = {
        "H": "hydrogen",
        "He": "helium",
        "Li": "lithium",
        "C": "carbon",
        "O": "oxygen",
        "N": "nitrogen"
}
```

- Duplicate keys are not allowed
- Duplicate values are just fine

Keys can be any immutable value
numbers, strings, tuples, frozenset,
not list, dictionary, set, ...

```
atomic_number_to_name = {
1: "hydrogen"
6: "carbon",
7: "nitrogen"
8: "oxygen",
}
nobel_prize_winners = {
(1979, "physics"): ["Glashow", "Salam", "Weinberg"],
(1962, "chemistry"): ["Hodgkin"],
(1984, "biology"): ["McClintock"],
}
```

A set is an unordered collection with no duplicate elements.

Dictionary

```
>>> symbol_to_name["C"]
'carbon'
>>> "O" in symbol_to_name, "U" in symbol_to_name
(True, False)
>>> "oxygen" in symbol_to_name
False
>>> symbol_to_name["P"]
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
KeyError: 'P'
>>> symbol_to_name.get("P", "unknown")
'unknown'
>>> symbol_to_name.get("C", "unknown")
'carbon'
```

Get the value for a given key

Test if the key exists
("in" only checks the keys,
not the values.)

[] lookup failures raise an exception
Use ".get()" if you want
to return a default value.

Some useful dictionary methods

```
>>> symbol_to_name.keys()
['C', 'H', 'O', 'N', 'Li', 'He']

>>> symbol_to_name.values()
['carbon', 'hydrogen', 'oxygen', 'nitrogen', 'lithium', 'helium']

>>> symbol_to_name.update( {"P": "phosphorous", "S": "sulfur"} )
>>> symbol_to_name.items()
[('C', 'carbon'), ('H', 'hydrogen'), ('O', 'oxygen'), ('N', 'nitrogen'), ('P',
    'phosphorous'), ('S', 'sulfur'), ('Li', 'lithium'), ('He', 'helium')]

>>> del symbol_to_name['C']
>>> symbol_to_name
{'H': 'hydrogen', 'O': 'oxygen', 'N': 'nitrogen', 'Li': 'lithium', 'He': 'helium'}
```

- Background
- Data Types/Structure

  list, string, tuple, dictionary
- Control flow
- File I/O
- Modules
- Class
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Control Flow

Things that are False

- The boolean value False
- The numbers 0 (integer), 0.0 (float) and 0j (complex).
- The empty string "".
- The empty list [], empty dictionary {} and empty set set().

Things that are True

- The boolean value True
- All non-zero numbers.
- Any string containing at least one character.
- A non-empty data structure.

If

```
>>> smiles = "BrC1=CC=C(C=C1)NN.Cl"
>>> bool(smiles)
True
>>> not bool(smiles)
False
>>> if not smiles:
...     print "The SMILES string is empty"
...
```

- The “else” case is always optional

Use “elif” to chain subsequent tests

```
>>> mode = "absolute"
>>> if mode == "canonical":
...         smiles = "canonical"
...     elif mode == "isomeric":
...         smiles = "isomeric”
...     elif mode == "absolute":
...         smiles = "absolute"
...     else:
...         raise TypeError("unknown mode")
...
>>> smiles
' absolute '
>>>
```

“raise” is the Python way to raise exceptions

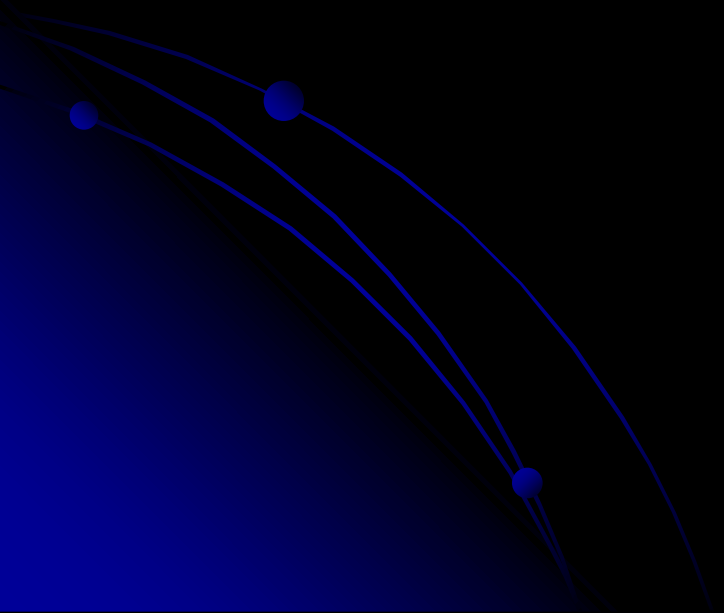
Boolean logic

Python expressions can have “and”s and “or”s:

```
if (ben <= 5 and chen >= 10 or
chen == 500 and ben != 5):
    print “Ben and Chen“
```

Range Test

```
if (3 <= Time <= 5):
    print “Office Hour"
```



For

```
>>> names = [“Ben", “Chen", “Yaqin"]
>>> for name in names:
...     print smiles
...
Ben
Chen
Yaqin
```

Tuple assignment in for loops

```
data = [ ("C20H20O3", 308.371),
    ("C22H20O2", 316.393),
    ("C24H40N4O2", 416.6),
    ("C14H25N5O3", 311.38),
    ("C15H20O2", 232.3181)]

for (formula, mw) in data:
    print "The molecular weight of %s is %s" % (formula, mw)
```

```
The molecular weight of C20H20O3 is 308.371
The molecular weight of C22H20O2 is 316.393
The molecular weight of C24H40N4O2 is 416.6
The molecular weight of C14H25N5O3 is 311.38
The molecular weight of C15H20O2 is 232.3181
```

Break, continue

```
>>> for value in [3, 1, 4, 1, 5, 9, 2]:
...         print "Checking", value
...         if value > 8:
...                 print "Exiting for loop"
...                 break
...         elif value < 3:
...                 print "Ignoring"
...                 continue
...         print "The square is", value**2
...
```

Use “break” to stop the for loop

Use “continue” to stop processing the current item

```
Checking 3
The square is 9
Checking 1
Ignoring
Checking 4
The square is 16
Checking 1
Ignoring
Checking 5
The square is 25
Checking 9
Exiting for loop
>>>
```

Range()

- “range” creates a list of numbers in a specified range
- range([start,] stop[, step]) -> list of integers
- When step is given, it specifies the increment (or decrement).

```
>>> range(5)
[0, 1, 2, 3, 4]
>>> range(5, 10)
[5, 6, 7, 8, 9]
>>> range(0, 10, 2)
[0, 2, 4, 6, 8]
```

How to get every second element in a list?

```
for i in range(0, len(data), 2):
    print data[i]
```

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Reading files

```
>>> f = open(“names.txt")
>>> f.readline()
'Yaqin\n'
```

Quick Way

```
>>> lst= [ x for x in open("text.txt","r").readlines() ]
>>> lst
['Chen Lin\n', 'clin@brandeis.edu\n', 'Volen 110\n', 'Office
    Hour: Thurs. 3-5\n', '\n', 'Yaqin Yang\n',
    'yaqin@brandeis.edu\n', 'Volen 110\n', 'Offiche Hour:
    Tues. 3-5\n']
```

- **Ignore the header?**

```
for (i,line) in enumerate(open('text.txt',"r").readlines()):
        if i == 0: continue
        print line
```

Using dictionaries to count occurrences

```
>>> for line in open('names.txt'):
...         name = line.strip()
...         name_count[name] = name_count.get(name,0)+ 1
...
>>> for (name, count) in name_count.items():
...         print name, count
...
Chen 3
Ben 3
Yaqin 3
```

File Output

```
input_file = open(“in.txt")
output_file = open(“out.txt", "w")
for line in input_file:
        output_file.write(line)
```

“w” = “write mode”
“a” = “append mode”
“wb” = “write in binary”
“r” = “read mode” (default)
“rb” = “read in binary”
“U” = “read files with Unix or Windows line endings”

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Modules

- When a Python program starts it only has access to a basic functions and classes.
  ("int", "dict", "len", "sum", "range", ...)
- "Modules" contain additional functionality.
- Use "import" to tell Python to load a module.

```
>>> import math
>>> import nltk
```

import the math module

```
>>> import math
>>> math.pi
3.1415926535897931
>>> math.cos(0)
1.0
>>> math.cos(math.pi)
-1.0
>>> dir(math)
['__doc__', '__file__', '__name__', '__package__', 'acos', 'acosh',
'asin', 'asinh', 'atan', 'atan2', 'atanh', 'ceil', 'copysign', 'cos',
'cosh', 'degrees', 'e', 'exp', 'fabs', 'factorial', 'floor', 'fmod',
'frexp', 'fsum', 'hypot', 'isinf', 'isnan', 'ldexp', 'log', 'log10',
'log1p', 'modf', 'pi', 'pow', 'radians', 'sin', 'sinh', 'sqrt', 'tan',
'tanh', 'trunc']
>>> help(math)
>>> help(math.cos)
```

“import” and “from … import …”

```
>>> import math
math.cos
>>> from math import cos, pi
cos
>>> from math import *
```

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Classes

```
class ClassName(object):
        <statement-1>
        . . .
        <statement-N>

class MyClass(object):
        """A simple example class"""
        i = 12345
        def f(self):
            return self.i

class DerivedClassName(BaseClassName):
        <statement-1>
        . . .
        <statement-N>
```

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http://www.nltk.org/book
NLTK is on berry patch machines!

```
>>>from nltk.book import *
>>> text1
<Text: Moby Dick by Herman Melville 1851>
>>> text1.name
'Moby Dick by Herman Melville 1851'
>>> text1.concordance("monstrous")
>>> dir(text1)
>>> text1.tokens
>>> text1.index("my")
4647
>>> sent2
['The', 'family', 'of', 'Dashwood', 'had', 'long', 'been', 'settled', 'in',
    'Sussex', '.']
```

Classify Text

```
>>> def gender_features(word):
...             return {'last_letter': word[-1]}
>>> gender_features('Shrek')
{'last_letter': 'k'}
>>> from nltk.corpus import names
>>> import random
>>> names = ([(name, 'male') for name in names.words('male.txt')] +
...          [(name, 'female') for name in names.words('female.txt')])
>>> random.shuffle(names)
```

Featurize, train, test, predict

```
>>> featuresets = [(gender_features(n), g) for (n,g) in names]

>>> train_set, test_set = featuresets[500:], featuresets[:500]

>>> classifier = nltk.NaiveBayesClassifier.train(train_set)

>>> print nltk.classify.accuracy(classifier, test_set)
0.726
>>> classifier.classify(gender_features('Neo'))

'male'
```

from nltk.corpus import reuters

- Reuters Corpus:10,788 news
  1.3 million words.
- Been classified into 90 topics
- Grouped into 2 sets, "training" and "test“
- Categories overlap with each other

http://nltk.googlecode.com/svn/trunk/doc/book/ch02.html

Reuters

```
>>> from nltk.corpus import reuters
>>> reuters.fileids()
['test/14826', 'test/14828', 'test/14829', 'test/14832', ...]
>>> reuters.categories()
['acq', 'alum', 'barley', 'bop', 'carcass', 'castor-oil', 'cocoa', 'coconut',
    'coconut-oil', 'coffee', 'copper', 'copra-cake', 'corn', 'cotton', 'cotton-
    oil', 'cpi', 'cpu', 'crude', 'dfl', 'dlr', ...]
```