Introduction to Python

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Overview

- Development Environments
- Global and Local Variables
- Data Types/Structures
- Control Flow
- File I/O
- Functions

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Development Environments

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)

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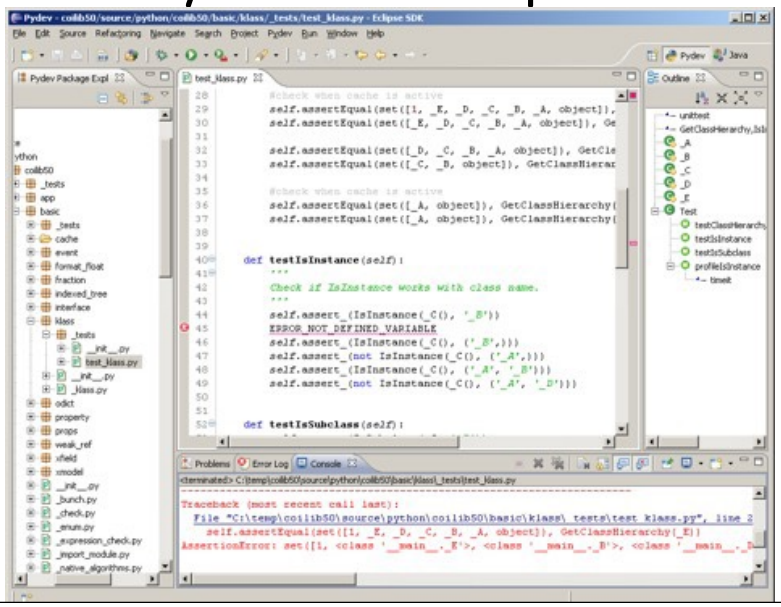
Pydev with Eclipse



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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.
>>>
```

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Python Interactive Shell

You can type things directly into a running Python session

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

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Global and Local Variables [2]

- An example

```
def f():
    print(s)
s = "I hate spam"
f()
```

- s is a global variable
- What is the output?

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Global and Local Variables

- Another example

```
def f():
    s = "Me too."        s is a local variable.
    print(s)
s = "I hate spam."       s is a global variable.
f()
print(s)
```

- What is the output?

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Global and Local Variables

- A third example

```
def f():
    print(s)
    s = "Me too."
    print(s)
s = "I hate spam."
f()
print(s)
```

- What is the output?

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Global and Local Variables

- UnboundLocalError: local variable 's' referenced before assignment
- Python assumes that we want a local variable due to the assignment to s in f()
- How can we tell Python that we want to use the global variable?

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Global and Local Variables

- Correction

```
def f():
    global s
    print(s)
    s = "Me too."
    print(s)
s = "I hate spam."
f()
print(s)
```

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Data Types/Structures

- List
- String
- Tuple
- Dictionary
- Set

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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
```

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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
```

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

Out of range values raise an exception

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Use [ ] to index items in the list

```
>>> names[-1]
'Yaqin'
>>> names[-2]
'Chen'
>>> names[-3]
'Ben'
```

Negative values go backwards from the last element.

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Strings share many features with lists

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

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Strings share many features with lists

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

Use "slice" notation to get a substring

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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.

Split the string into parts with "." as the delimiter

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String operators: in, not in

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

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

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Lists are mutable

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

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Lists are mutable

```
>>> del ids[0]
>>> ids
['2plv', '1crn', '1alm']
>>> ids.sort()
>>> ids
['1alm', '1crn', '2plv']
>>> ids.reverse()
>>> ids
['2plv', '1crn', '1alm']
```

remove an element

sort by default order

reverse the elements in a list

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Lists are mutable

```
>>> ids.insert(0, "9pti")
>>> ids
['9pti', '2plv', '1crn', '1alm']
```

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

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Zipping Lists Together

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

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

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

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Tuple: Like Immutable List

```
>>> yellow = (255, 255, 0) # r, g, b
>>> one    = (1,)
>>> yellow[0]
>>> 255
>>> 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
```

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Tuple: Like Immutable List

Very common in string interpolation:

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

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Dictionary

- 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"
}
```

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Dictionary

- Duplicate keys are not allowed
- Duplicate values are just fine
- Keys can be any immutable value numbers, strings, tuples, **not list, dictionary, set**, …

```
>>> symbol_to_name["C"]
'carbon'
>>> "O" in symbol_to_name, "U" in
  symbol_to_name
(True, False)
```

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Set

- Sets are lists with no duplicate entries

```
>>> a = set(["Jake", "John", "Eric"])
>>> b = set(["John", "Jill"])
>>> a.intersection(b)
set(['John'])
>>> a.difference(b)
set(['Jake', 'Eric'])
>>> a.symmetric_difference(b)
set(['Jill', 'Jake', 'Eric'])
```

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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().

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Control Flow

Things that are True

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

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Examples

```
>>> smiles = "BrC1=CC=C(C=C1)NN.Cl"
>>> bool(smiles)
True
>>> not bool(smiles)
False
```

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If-statement

```
>>> if not smiles:
...     print "The SMILES string is empty"
...
```

- Indentation is important to indicate program structure
- The “else” case is always optional

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"elif" is used 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
```

"raise" is the Python way to raise exceptions

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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"
```

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For-statement

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

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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)
```

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Tuple Assignment in For Loops

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

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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
...
```

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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).

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Range()

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

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Reading Files

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

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Read Lines in a Loop

```
>>> 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']
```

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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"

Functions

- Python provides many built-in functions like print(), etc.
- But you can also create your own functions—*user-defined functions*

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def

```
#!/usr/bin/python

# Function definition is here
def printme( str ):
    print str
    return;
```

- # Now you can call printme function
- printme("I'm first call to user defined function!")
- printme("Again second call to the same function")

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Nested Functions

```
def outer(num1):
    def inner_increment(num1):
        return num1 + 1
    num2 = inner_increment(num1)
    print(num1, num2)
```

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Program Assignment 1

- An Evaluator for Logical Expressions Written in Postfix Notation
  - Write a Python program that computes the value of logic expressions provided in postfix notation.
  - E.g., given the string "0!1&" (infix: "!0&1"), where "0" means "False" and "1" means "True". Your calculator will compute "1" as the answer
  - All strings provided will be valid

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Program Assignment 1

- The logic manipulation operators are:

"!" logical NOT	**RIGHT** associative
"&" logical AND	**LEFT** associative
"/" logical NOT EQUAL	**LEFT** associative
"=" logical EQUAL	**LEFT** associative
"|" logical OR	**LEFT** associative

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Program Assignment 1

- Your calculator will use stack to compute/store all intermediate computations
- You will implement your own push and pop stack operations
- The ONLY library or built-in method that you can use is len()
- Download python 3.5.2 from www.python.org

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Program Assignment 1

- Write your program following the structure and specs given in the assignment descriptions
  - Define your own stack structure
  - Use the specified variables in the template
  - Define nested functions
  - …
- Due date: 10/6/16, 12:30pm
- Submit both an electronic copy via canvas, and a hard copy in-class

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Reference

[1] Chen Lin, Python Tutorial, www.cs.brandeis.edu/~cs134/Python_tutorial.ppt

[2] Global and Local Variables, http://www.python-course.eu/global_vs_local_variables.php

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