

APA: Advanced Programming, Algorithms and Data Structures

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Python Overview

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RESEARCH
PROGRAMME
ON BIOMEDICAL
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Python 3 Cheat Sheet

<p>integer, float, boolean, string, bytes</p> <pre> int 783 0 -192 0b010 0o642 0xF3 zero binary octal hexa float 9.23 0.0 -1.7e-6 bool True False str "One\nTwo" escaped new line 'I\m' escaped ' bytes b"toto\xfe\775" hexadecimal octal </pre> <p>Multiline string: <pre> """x\tY\tZ 1\t2\t3""" </pre> escaped tab</p> <p>Base Types</p> <p>immutables</p>	<p>Container Types</p> <p>ordered sequences, fast index access, repeatable values</p> <pre> list [1, 5, 9] ["x", 11, 8.9] ["mot"] tuple (1, 5, 9) 11, "y", 7.4 ("mot",) </pre> <p>Non modifiable values (immutables) expression with only comas → tuple</p> <p>str bytes (ordered sequences of chars / bytes)</p> <p>key containers, no a priori order, fast key access, each key is unique</p> <pre> dict {"key": "value"} dict(a=3, b=4, k="v") (key/value associations) {1: "one", 3: "three", 2: "two", 3.14: "pi"} collection set {"key1", "key2"} {1, 9, 3, 0} set() keys=hashable values (base types, immutables...) frozenset immutable set empty </pre>
<p>for variables, functions, modules, classes... names</p> <p>a...zA...Z_ followed by a...zA...Z_0...9</p> <ul style="list-style-type: none"> diacritics allowed but should be avoided language keywords forbidden lower/UPPER case discrimination <p>⊗ a toto x7 y_max BigOne ⊗ by and for</p> <p>Identifiers</p>	<p>Conversions</p> <pre> int("15") → 15 int("3f", 16) → 63 int(15.56) → 15 float("-11.24e8") → -1124000000.0 round(15.56, 1) → 15.6 bool(x) False for null x, empty container x, None or False x; True for other x str(x) → "..." representation string of x for display (cf. formatting on the back) chr(64) → '@' ord('@') → 64 repr(x) → "..." literal representation string of x bytes([72, 9, 64]) → b'H\t@' list("abc") → ['a', 'b', 'c'] dict([(3, "three"), (1, "one")]) → {1: 'one', 3: 'three'} set(["one", "two"]) → { 'one', 'two' } separator str and sequence of str → assembled str '.join(['toto', '12', 'pswd']) → 'toto:12:pswd' str splitted on whitespaces → list of str "words with spaces".split() → ['words', 'with', 'spaces'] str splitted on separator str → list of str "1,4,8,2".split(",") → ['1', '4', '8', '2'] sequence of one type → list of another type (via list comprehension) [int(x) for x in ('1', '29', '-3')] → [1, 29, -3] </pre> <p>type (expression)</p> <p>can specify integer number base in 2nd parameter</p> <p>truncate decimal part</p> <p>rounding to 1 decimal (0 decimal → integer number)</p>
<p>=</p> <p>Variables assignment</p> <p># assignment ⇔ binding of a name with a value</p> <p>1) evaluation of right side expression value</p> <p>2) assignment in order with left side names</p> <pre> x=1.2+8+sin(y) a=b=c=0 y,z,r=9.2,-7.6,0 a,b=b,a a,*b=seq *a,b=seq x+=3 x-=2 x=None del x </pre> <p>assignment to same value</p> <p>multiple assignments</p> <p>values swap</p> <p>unpacking of sequence in item and list</p> <p>increment ⇔ x=x+3</p> <p>decrement ⇔ x=x-2</p> <p>« undefined » constant value</p> <p>remove name x</p> <p>and</p> <p>*</p> <p>+=</p> <p>-=</p> <p>%</p> <p>...</p>	

negative index	-5	-4	-3	-2	-1
positive index	0	1	2	3	4
	10	20	30	40	50
positive slice	0	1	2	3	4
negative slice	-5	-4	-3	-2	-1

Items count
`len(lst) → 5`
 index from 0
 (here from 0 to 4)

Individual access to items via `lst[index]`
`lst[0] → 10` ⇒ first one `lst[1] → 20`
`lst[-1] → 50` ⇒ last one `lst[-2] → 40`
 On mutable sequences (`list`), remove with
`del lst[3]` and modify with assignment
`lst[4] = 25`

Access to sub-sequences via `lst[start slice : end slice : step]`

`lst[: -1] → [10, 20, 30, 40]` `lst[:: -1] → [50, 40, 30, 20, 10]` `lst[1: 3] → [20, 30]` `lst[: 3] → [10, 20, 30]`
`lst[1: -1] → [20, 30, 40]` `lst[:: -2] → [50, 30, 10]` `lst[-3: -1] → [30, 40]` `lst[3:] → [40, 50]`
`lst[: : 2] → [10, 30, 50]` `lst[:] → [10, 20, 30, 40, 50]` shallow copy of sequence

Missing slice indication → from start / up to end.

On mutable sequences (`list`), remove with `del lst[3: 5]` and modify with assignment `lst[1: 4] = [15, 25]`

Boolean Logic

Comparisons: `<` `>` `<=` `>=` `==` `!=`
 (boolean results) `<=` `>=` `==` `!=`

`a and b` logical and both simultaneously

`a or b` logical or one or other or both

⚠ pitfall: `and` or `or` return value of `a` or of `b` (under shortcut evaluation).

⇒ ensure that `a` and `b` are booleans.

`not a` logical not

`True`
`False` } True and False constants

⚠ floating numbers... approximated values

Operators: `+` `-` `*` `/` `//` `%` `**`
 Priority (...) `x ÷ ÷` `↑` `ab`
 integer ÷ ÷ remainder

@ → matrix × python 3.5 + numpy

`(1+5.3)*2 → 12.6`
`abs(-3.2) → 3.2`
`round(3.57, 1) → 3.6`
`pow(4, 3) → 64.0`

⚠ usual order of operations

Statements Blocks

parent statement:
 statement block 1...
 :
 parent statement:
 statement block2...
 :
 next statement after block 1

⚠ configure editor to insert 4 spaces in place of an indentation tab.

Maths

angles in radians
`from math import sin, pi...`
`sin(pi/4) → 0.707...`
`cos(2*pi/3) → -0.4999...`
`sqrt(81) → 9.0` ✓
`log(e**2) → 2.0`
`ceil(12.5) → 13`
`floor(12.5) → 12`
 modules `math`, `statistics`, `random`,
`decimal`, `fractions`, `numpy`, etc. (cf. doc)

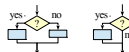
Modules/Names Imports

module `truc` ⇔ file `truc.py`
`from monmod import nom1, nom2 as fct`
 → direct access to names, renaming with `as`
`import monmod` → access via `monmod.nom1...`
 ⚠ modules and packages searched in python path (cf `sys.path`)

statement block executed only
 if a condition is true

`if logical condition:`
 → statements block

Conditional Statement



Can go with several `elif`, `elif...` and only one final `else`. Only the block of first true condition is executed.

⚠ with a var `x`:
`if bool(x) == True: ⇔ if x:`
`if bool(x) == False: ⇔ if not x:`

`if age <= 18:`
 `state = "Kid"`
`elif age > 65:`
 `state = "Retired"`
`else:`
 `state = "Active"`

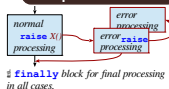
Signaling an error:

`raise ExcClass(...)`

Errors processing:

`try:`
 → normal processing block
`except Exception as e:`
 → error processing block

Exceptions on Errors



modify original list

```
lst.append(val)    add item at end
lst.extend(seq)    add sequence of items at end
lst.insert(idx, val) insert item at index
lst.remove(val)    remove first item with value val
lst.pop([idx]) → value remove & return item at index idx (default last)
lst.sort() lst.reverse() sort / reverse list in place
```

Operations on Lists

Operations on Dictionaries

```
d[key]=value      d.clear()
d[key] → value    del d[key]
d.update(d2)      { update/add
                  { associations
d.keys()          { iterable views on
d.values()        { keys/values/associations
d.items()         {
d.pop(key,[default]) → value
d.popitem() → (key,value)
d.get(key,[default]) → value
d.setdefault(key,[default]) → value
```

Operations on Sets

Operators:

- | → union (vertical bar char)
- & → intersection
- ^ → difference/symmetric diff.
- < <= > >= → inclusion relations

Operators also exist as methods.

```
s.update(s2) s.copy()
s.add(key) s.remove(key)
s.discard(key) s.clear()
s.pop()
```

storing data on disk, and reading it back

```
f = open("file.txt", "w", encoding="utf8")
```

file variable for operations name of file on disk (+path...)

opening mode

- 'r' read
- 'w' write
- 'a' append

encoding of chars for text files:

- utf8
- ascii
- latin1 ...

cf. modules **os**, **os.path** and **pathlib**

Files

writing

```
f.write("coucou")
f.writelines(list of lines)
```

reading

```
f.read([n]) → next chars
if n not specified, read up to end !
f.readlines([n]) → list of next lines
f.readline() → next line
```

text mode **t** by default (read/write **str**), possible binary mode **b** (read/write **bytes**). Convert from/to required type !

```
f.close()    # dont forget to close the file after use !
```

```
f.flush() write cache
f.truncate([size]) resize
reading/writing progress sequentially in the file, modifiable with:
f.tell() → position
f.seek(position[,origin])
```

Very common: opening with a guarded block (automatic closing) and reading loop on lines of a text file:

```
with open(...) as f:
    for line in f:
        # processing of line
```

Function Definition

function name (identifier)

named parameters

```
def fct(x,y,z):
```

documentation

```
"""documentation"""
```

statements block, res computation, etc.

```
return res
```

result value of the call, if no computed result to return: **return None**

parameters and all variables of this block exist only in the block and during the function call (think of a "black box")

Advanced: **def fct(x,y,z,*args,a=3,b=5,**kwargs):**

- *args variable positional arguments (→ tuple), default values,
- **kwargs variable named arguments (→ dict)

fct

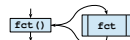
Function Call

```
r = fct(3,i+2,2*i)
```

storage/use of returned value one argument per parameter

this is the use of function name with parentheses which does the call

Advanced: *sequence **dict



Operations on Strings

```
s.startswith(prefix,[start,end])
s.endswith(suffix,[start,end]) s.strip([chars])
s.count(sub,[start,end]) s.partition(sep) → (before,sep,after)
s.index(sub,[start,end]) s.find(sub,[start,end])
s.is...() tests on chars categories (ex. s.isalpha())
s.upper() s.lower() s.title() s.swapcase()
s.casefold() s.capitalize() s.center([width,fill])
s.ljust([width,fill]) s.rjust([width,fill]) s.zfill([width])
s.encode(encoding) s.split([sep]) s.join(sep)
```

Formatting

formatting directives values to format

```
"model{ } { } { }".format(x,y,r) → str
"{selection:formatting!conversion}"
```

Selection:

```
2
nom
0.nom
4[key]
0[2]
```

Examples:

```
"{:+2.3f}".format(45.72793)
→ '+45.728'
"{1:>10s}".format(8,"toto")
→ 'toto'
"{x!r}".format(x="I'm")
→ "'I' 'm'"
```

Formatting:

```
fill char alignment sign mini width . precision-maxwidth type
```

<> ^ = + - space 0 at start for filling with 0

integer: **b** binary, **c** char, **d** decimal (default), **o** octal, **x** or **X** hexa...

float: **e** or **E** exponential, **f** or **F** fixed point, **g** or **G** appropriate (default), **s** ... percent

Conversion: **s** (readable text) or **r** (literal representation)

High-level, dynamically typed, easily readable

```
def quicksort(arr):  
    """ An example (not necessarily most efficient) implementation of quicksort algorithm """  
  
    if len(arr) <= 1:  
        return arr  
  
    pivot = arr[len(arr) // 2]  
  
    left = [x for x in arr if x < pivot]  
    middle = [x for x in arr if x == pivot]  
    right = [x for x in arr if x > pivot]  
  
    return quicksort(left) + middle + quicksort(right)  
  
print(quicksort([3,6,8,10,1,2,1]))  
# Output: [1, 1, 2, 3, 6, 8, 10]
```

Source: Justin Johnson (accessed on Nov 2019)

Understanding Reference Semantics

- **Assignment manipulates references**

- `x = y` **does not make a copy** of the object `y` references

- `x = y` makes `x` **reference** the object `y` references

- **Very useful; but beware!**

- **Example:**

```
>>> a = [1, 2, 3] # a now references the list [1, 2, 3]
>>> b = a        # b now references what a references
>>> a.append(4)   # this changes the list a references
>>> print b      # if we print what b references,
[1, 2, 3, 4]      # SURPRISE! It has changed...
```

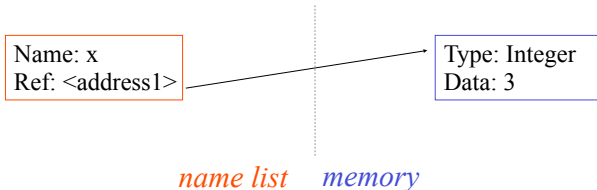
Why??

Understanding Reference Semantics II

- There is a lot going on when we type:

`x = 3`

- First, an integer **3** is created and stored in memory
- A name **x** is created
- An **reference** to the memory location storing the **3** is then assigned to the name **x**
- So: When we say that the value of **x** is **3**
- we mean that **x** now refers to the integer **3**



Understanding Reference Semantics III

- The data 3 we created is of type integer. In Python, the datatypes integer, float, and string (and tuple) are “immutable.”
- This doesn't mean we can't change the value of *x*, i.e. *change what x refers to ...*
- For example, we could increment *x*:

```
>>> x = 3
>>> x = x + 1
>>> print x
4
```

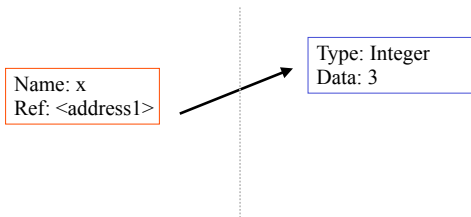
Understanding Reference Semantics IV

- If we increment `x`, then what's really happening is:

1. The reference of name `x` is looked up.

2. The value at that reference is retrieved.

```
>>> x = x + 1
```



Understanding Reference Semantics IV

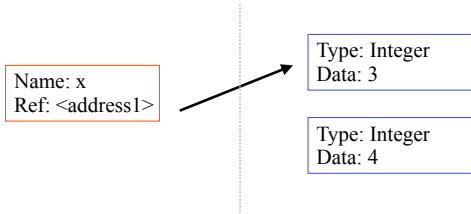
- If we increment x , then what's really happening is:

1. The reference of name x is looked up.

$\ggg \quad x = x + 1$

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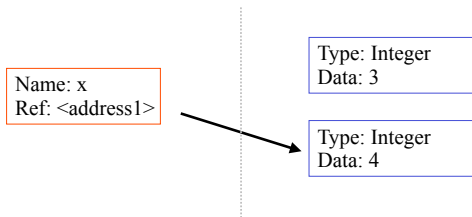
3. *The 3+1 calculation occurs, producing a new data element 4 which is assigned to a fresh memory location with a new reference.*



Understanding Reference Semantics IV

- If we increment x , then what's really happening is:

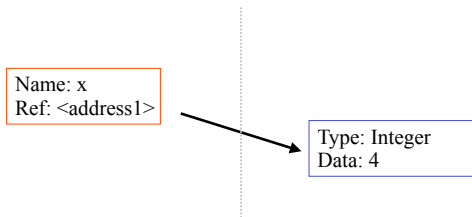
1. The reference of name x is looked up. `>>> x = x + 1`
2. The value at that reference is retrieved.
3. The $3+1$ calculation occurs, producing a new data element 4 which is assigned to a fresh memory location with a new reference.
4. *The name x is changed to point to this new reference.*



Understanding Reference Semantics IV

- If we increment **x**, then what's really happening is:

1. The reference of name **x** is looked up. >>> x = x + 1
2. The value at that reference is retrieved.
3. The 3+1 calculation occurs, producing a new data element **4** which is assigned to a fresh memory location with a new reference.
4. The name **x** is changed to point to this new reference.
5. *The old data **3** is garbage collected if no name still refers to it.*



Sequence Types

1. Tuple

- A simple *immutable* ordered sequence of items
- Items can be of mixed types, including collection types

2. Strings

- *Immutable*
- **Conceptually very much like a tuple**

3. List

- *Mutable* ordered sequence of items of mixed types

Tuples: Immutable

```
>>> t = (23, 'abc', 4.56, (2,3), 'def')
>>> t[2] = 3.14
```

```
Traceback (most recent call last):
  File "<pyshell#75>", line 1, in -toplevel-
    tu[2] = 3.14
TypeError: object doesn't support item assignment
```

You can't change a tuple.

You can make a fresh tuple and assign its reference to a previously used name.

```
>>> t = (23, 'abc', 3.14, (2,3), 'def')
```

Lists: Mutable

```
>>> li = ['abc', 23, 4.34, 23]
>>> li[1] = 45
>>> li
['abc', 45, 4.34, 23]
```

- We can change lists *in place*.
- Name *li* still points to the same memory reference when we're done.
- The mutability of lists means that they aren't as fast as tuples.

Tuples vs. Lists

- **Lists slower but more powerful than tuples.**
 - Lists can be modified, and they have lots of handy operations we can perform on them.
 - Tuples are immutable and have fewer features.
- **To convert between tuples and lists use the `list()` and `tuple()` functions:**

```
li = list(tu)
tu = tuple(li)
```

Other containers – Python collections module

<code>namedtuple</code>	factory function for creating tuple subclasses with named fields
<code>deque</code>	list-like container with fast appends and pops on either end
<code>ChainMap</code>	dict-like class for creating a single view of multiple mappings
<code>Counter</code>	dict subclass for counting hashable objects
<code>OrderedDict</code>	dict subclass that remembers the order entries were added
<code>defaultdict</code>	dict subclass that calls a factory function to supply missing values

- book.pythontips.com/en/latest/collections.html
- docs.python.org/3.7/library/collections.html

Sources: Yasoob Khalid & Python Software Foundation (accessed on Nov 2019)

Generators, iterators and iterables

- Iterable (any object that returns an iterator or can take indices)
 - `__iter__` or `__getitem__`
- Iterator
 - `next` or `__next__`
- Generator (one time iterators where items generated on demand)
 - `yield`

```
def generator_function(n):  
  
    for i in range(n):  
        yield i  
  
    for item in generator_function():  
        print(item)
```

Source: Yasoob Khalid (accessed on Nov 2019)

Function calls with extra arguments

```
def f(a, *b, **c):  
    print(a)  
    print(b)  
    print(c)
```

> f(1, 2, c=5)

> f(a=1, b=2, c=5)

> f(1, 2, 4, 5)

> f(1, 2, 4, 5, b=3)

Function calls with extra arguments

```
def f(a, *b, **c):  
    print(a)  
    print(b)  
    print(c)
```

```
> f(1, 2, c=5)
```

```
1
```

```
(2,)
```

```
{'c': 5}
```

```
> f(a=1, b=2, c=5)
```

```
1
```

```
()
```

```
{'b': 2, 'c': 5}
```

```
> f(1, 2, 4, 5)
```

```
1
```

```
(2, 4, 5)
```

```
{}
```

```
> f(1, 2, 4, 5, b=3)
```

```
1
```

```
(2, 4, 5)
```

```
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```

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```

```
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```

```
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```
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```

```
1
```

```
()
```

```
{'b': 2, 'c': 5}
```

```
> f(1, 2, 4, 5)
```

```
1
```

```
(2, 4, 5)
```

```
{}
```

```
> f(1, 2, 4, 5, b=3)
```

```
1
```

```
(2, 4, 5)
```

```
{'b': 3}
```

```
def f(*args, **kwargs):
```

$a, *b \Rightarrow *args$

$**c \Rightarrow **kwargs$

Unpacking syntax & zip function

*: unpacks collection (to sequence of arguments)

** : unpacks dictionary (to sequence of named arguments)

zip: Makes an iterator aggregating elements from each of the input iterables

```
names = ["Joe", "James", "Zach"]
```

```
ages = [26, 39, 14]
```

```
tuples = list(zip(names, ages))
```

```
d = dict(zip(names,ages))
```

```
print(tuples) # Output: [('Joe', 26), ('James', 39), ('Zach', 14)]
```

```
print(list(zip(*tuples))) # Output: [('Joe', 'James', 'Zach'), (26, 39, 14)]
```

Unpacking syntax & zip function

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`**`: unpacks dictionary (to sequence of named arguments)

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```

```
print(list(zip(*tuples))) # Output: [('Joe', 'James', 'Zach'), (26, 39, 14)]
```

Beware of the behaviour of functions with ‘unusual inputs’

```
print(list(zip(range(5), range(3)))) # Output: [(0, 0), (1, 1), (2, 2)]
```


Functional programming & lambda function

lambda: Inline function without explicit name (anonymous)

```
add = lambda x, y: x + y
```

```
print(add(3, 5))
```

```
# Output: 8
```

```
a = [(1, 2), (4, 1), (9, 10), (13, -3)]
```

```
a.sort(key=lambda x: x[1])
```

```
print(a)
```

```
# Output: [(13, -3), (4, 1), (1, 2), (9, 10)]
```

Source: Yasoob Khalid (accessed on Nov 2019)

Functional programming & higher-order functions

Higher-order functions: Functions that accepts another function as input

- **map**

```
items = [1, 2, 3, 4, 5]
squared = list(map(lambda x: x**2, items))

print(squared) # Output: [1, 4, 9, 16, 25]
```

- **filter**

```
number_list = range(-5, 5)
less_than_zero = list(filter(lambda x: x < 0, number_list))

print(less_than_zero) # Output: [-5, -4, -3, -2, -1]
```

- **reduce**

```
from functools import reduce
product = reduce((lambda x, y: x * y), [1, 2, 3, 4])

print(product) # Output: 24
```

For with else clause

General structure:

```
for item in container:
    if search_something(item): # Found it!
        process(item)
        break
else: # Didn't find anything..
    not_found_in_container()
```

Example:

```
for n in range(2, 10):
    for x in range(2, n):
        if n % x == 0:
            print( n, 'equals', x, '*', n/x)
            break
    else:
        # loop fell through without finding a factor
        print(n, 'is a prime number')
```

Source: Yasoob Khalid (accessed on Nov 2019)

File I/O, Strings, Exceptions...

```
>>> try:
...     1 / 0
... except:
...     print('That was silly!')
... finally:
...     print('This gets executed no matter what')
...
```

That was silly!

This gets executed no matter what

with open('filename') as fileptr:

```
    somestring = fileptr.read()
    for line in fileptr:
        print line
```

fileptr.closed # True

```
>>> a = 1
>>> b = 2.4          (Context management through __enter__() and __exit__() methods)
>>> c = 'Tom'
>>> '%s has %d coins worth a total of $%.02f' % (c, a, b)
'Tom has 1 coins worth a total of $2.40'
```

(OR: '%s has {} coins worth a total of \${:.02f}'.format(c, a, b))

Why Use Modules?

- **Code reuse**
 - Routines can be called multiple times within a program
 - Routines can be used from multiple programs
- **Namespace partitioning**
 - Group data together with functions used for that data
- **Implementing shared services or data**
 - Can provide global data structure that is accessed by multiple subprograms

Modules

- **Modules are functions and variables defined in separate files**
- **Items are imported using from or import**

```
from module import function  
function()
```

```
import module  
module.function()
```

- **Modules are namespaces**
 - Can be used to organize variable names, i.e.
`atom.position = atom.position - molecule.position`

What is an Object?

- **A software item that contains variables and methods**
- **Object Oriented Design focuses on**
 - Encapsulation:
 - dividing the code into a public interface, and a private implementation of that interface
 - Polymorphism:
 - the ability to overload standard operators so that they have appropriate behavior based on their context
 - Inheritance:
 - the ability to create subclasses that contain specializations of their parents

Example

```
class atom(object):
    def __init__(self,atno,x,y,z):
        self.atno = atno
        self.position = (x,y,z)
    def symbol(self):    # a class method
        return Atno_to_Symbol[atno]
    def __repr__(self): # overloads printing
        return '%d %10.4f %10.4f %10.4f' %
            (self.atno, self.position[0],
             self.position[1],self.position[2])

>>> at = atom(6,0.0,1.0,2.0)
>>> print at
6  0.0000  1.0000  2.0000
>>> at.symbol()
'C'
```


Atom Class

- **Overloaded the default constructor**
- **Defined class variables (atno,position) that are persistent and local to the atom object**
- **Good way to manage shared memory:**
 - instead of passing long lists of arguments, encapsulate some of this data into an object, and pass the object.
 - much cleaner programs result
- **Overloaded the print operator**
- **We now want to use the atom class to build molecules...**

Molecule Class

```
class molecule:
    def __init__(self,name='Generic'):
        self.name = name
        self.atomlist = []
    def addatom(self,atom):
        self.atomlist.append(atom)
    def __repr__(self):
        str = 'This is a molecule named %s\n' % self.name
        str = str+'It has %d atoms\n' % len(self.atomlist)
        for atom in self.atomlist:
            str = str + `atom` + '\n'
        return str
```

Using Molecule Class

```
>>> mol = molecule('Water')
>>> at = atom(8,0.,0.,0.)
>>> mol.addatom(at)
>>> mol.addatom(atom(1,0.,0.,1.))
>>> mol.addatom(atom(1,0.,1.,0.))
>>> print mol
This is a molecule named Water
It has 3 atoms
8  0.000 0.000 0.000
1  0.000 0.000 1.000
1  0.000 1.000 0.000
```

- **Note that the print function calls the atoms print function**
 - Code reuse: only have to type the code that prints an atom once; this means that if you change the atom specification, you only have one place to update.

Inheritance

```
class qm_molecule(molecule):  
    def addbasis(self):  
        self.basis = []  
        for atom in self.atomlist:  
            self.basis = add_bf(atom,self.basis)
```

- **`__init__`, `__repr__`, and `__addatom__` are taken from the parent class (molecule)**
- **Added a new function `addbasis()` to add a basis set**
- **Another example of code reuse**
 - Basic functions don't have to be retyped, just inherited
 - Less to rewrite when specifications change

Overloading

```
class qm_molecule(molecule):  
    def __repr__(self):  
        str = 'QM Rules!\n'  
        for atom in self.atomlist:  
            str = str + `atom` + '\n'  
        return str
```

- Now we only inherit `__init__` and `addatom` from the parent
- We define a new version of `__repr__` specially for QM

Adding to Parent Functions

- Sometimes you want to extend, rather than replace, the parent functions.

```
class qm_molecule(molecule):  
    def __init__(self, name="Generic", basis="6-31G**"):  
        self.basis = basis  
        super(qm_molecule, self).__init__(name)
```

Public and Private Data

- In Python anything with two leading underscores is private

`__a, __my_variable`

- Anything with one leading underscore is semi-private, and you should feel guilty accessing this data directly.

`_b`

- Sometimes useful as an intermediate step to making data private

Public and private data – cont'd

```
class A:
    def __init__(self):
        self.__x = 1
        self._y = 2
        self.z = 3

a1 = A()
print(a1.z) # 3
print(a1._y) # 2
print(a1.__x) # AttributeError: 'A' object has no attribute '__x'
```


Instance vs class attributes & static vs class methods

- Instance attributes: attributes whose value depends on the specific instance
- Class attributes: attributes whose value is bound to the class and independent of any specific instance
- Class method can access and modify the class state (thus require a reference to the class) while static methods can not

```
class A:
    count = 0
    def __init__(self):
        self.__x = 1

    @staticmethod
    def get_count():
        return A.count

    @classmethod
    def set_count(cls):
        cls.count += 1
```

Magic methods

Internal methods, not meant to be invoked directly

- Invocation happens internally from the class on a certain action
- Syntax: `def __magicMethod__()`
- Python examples: `__init__()`, `__str__()`, `__add__()`
- For instance when you add two values using the `+` operator, internally, the `__add__()` method will be called

Source: Majeed Kassir - BGU

Garbage collection

Python objects are automatically deleted once there are no references to them

- The garbage collector removes the object instance once the reference count reaches zero

```
class Employee:
    def __init__(self):
        print("created")

    def __del__(self):
        print("destroyed")

e1 = Employee() # created
e2 = e1
print('e1 id=', id(e1)) # e1 id = 2257554491936
print('e2 id=', id(e2)) # e2 id = 2257554491936
del e1 # removes the reference e1, reducing the ref count by 1
print('e2 id=', id(e2)) # e2 id = 2257554491936
del e2 # destroyed, ref count is zero
```

Decorators

Decorators add functionality to existing functions without modifying the original code

```
def debug(func):
    def wrapper(*args, **kwargs):
        print('received arguments:', args, kwargs)
        return_values = func(*args, **kwargs)
        print('return value:', return_values)
        return return_values
    return wrapper

def add_two_elements(a, b):
    return a + b

debug_add_two_elements = debug(add_two_elements)
debug_add_two_elements(5, b=6)
# received arguments: (5,) {'b': 6}
# return value: 11
```

Functions as first class objects

- Functions can act like objects
 - referenced by another function as a variable
 - passed to another function as a variable
 - returned to another function as variable
- Functions can act as variables
 - defined inside another function
 - passed as arguments to another function
 - returned as values from another function

```
def make_divisibility_test(n):  
    def divisible_by_n(m):  
        return m % n == 0  
    return divisible_by_n  
  
is_divisible_by_five = make_divisibility_test(5)  
is_divisible_by_five(10) # True  
make_divisibility_test(7)(10) # False  
  
div_by_3 = make_divisibility_test(3)  
print(filter(div_by_3, range(10))) # 0, 3, 6, 9
```

Typing in Python

- Names for all standard built-in types are defined in *types* module
- `isinstance()` function is recommended for testing the type of an object (it takes subclasses into account)

```
type(2) # => <class 'int'>
type("Hi!") # => <class 'str'>
type(None) # => <class 'NoneType'>
type(int) # => <class 'type'>
```

```
class Plant: pass # Dummy class
class Tree(Plant): pass # Dummy class derived from Plant
tree = Tree() # A new instance of Tree class
print isinstance(tree, Tree) # True
print isinstance(tree, Plant) # True
print isinstance(tree, object) # True
print type(tree) is Tree # False
print type(tree).__name__ == "instance" # True
print tree.__class__.__name__ == "Tree" # True
```

Static vs dynamic typing

- Dynamically typed: Typing is not enforced by default in python and checked in **runtime**
- Strongly type: Once the type is detected, operations can be executed only for that detected type

```
def greeting(name: str) -> str:  
    return 'Hello ' + name
```

```
greeting(2) # Run time TypeError: must be str, not int
```

- Typing syntax could be used for annotating the code
- Type checking can be enforced with mypy package

```
$ mypy greeting.py
```

```
greeting.py:4: error: Argument 1 to "greeting" has incompatible  
type "int"; expected "str"
```

Static vs dynamic typing - cont'd

```
from typing import Dict

def get_first_name(full_name: str) -> str:
    return full_name.split(" ")[0]

fallback_name: Dict[str, str] = {
    "first_name": "UserFirstName",
    "last_name": "UserLastName"
}

raw_name: str = input("Please enter your name: ")
first_name: str = get_first_name(raw_name)

if not first_name: # If the user didn't type anything in, use the fallback name
    first_name = get_first_name(fallback_name)

print(f"Hi, first_name!")
```

```
$ mypy my_script.py
my_script.py:21: error: Argument 1 to "get_first_name" has incompatible type "Dict[str, str]"; expected "str"
```

Source: Adam Geitgey (accessed on Nov 2019)

Introspection and reflection

Ability to examine and modify an object (its attributes) at runtime

- Everything in python is an object (inherited from the built-in object class)
- Reflection-enabling functions include `type()`, `isinstance()`, `callable()`, `dir()` and `getattr()`
- *inspect* module provide more inspection functionality
- `type()`, `isinstance()`, `issubclass()` check type of an object/class

```
# Check the type/class of an object
```

```
type(my_object)
```

```
my_object.__class__
```

```
# check is the object is a specific type or class
```

```
isinstance(my_str, str)
```

```
# check if an object's class is a subclass of a parent class
```

```
issubclass(my_object.__class__, ParentClass)
```

Source: *Bonne Nuit Metrics Blog* (accessed on Nov 2019)

Introspection and reflection – cont'd

- `dir()` returns the list of names of attributes of an object, including its methods

```
class A:
    def __init__(self):
        self.__x = 1

a1 = A()
print(dir(a1))
# ['__class__', '__delattr__', '__dict__', '__dir__', '__doc__',
'__eq__', '__format__', '__ge__', '__getattribute__', '__gt__',
'__hash__', '__init__', '__init_subclass__', '__le__', '__lt__',
'__module__', '__ne__', '__new__', '__reduce__', '__reduce_ex__',
'__repr__', '__setattr__', '__sizeof__', '__str__', '__subclasshook__',
'__weakref__', '_A__x']

print(a1._A__x) # 1
```

Source: Bonne Nuit Metrics Blog (accessed on Nov 2019)

Introspection and reflection – cont'd

- `callable()` determines whether the object can be called

```
callable([1,2].pop) # True
```

- a class can be made callable by providing a `__call__()` method

```
class Sq:  
    def __call__(self, x):  
        return x**2
```

```
f = Sq()  
f(2) # 4
```

- `getattr()` returns the value of an attribute of an object using the attribute name passed as a string

```
getattr(3, "__add__")(2) # 5
```

Source:

Introspection and reflection – cont'd

```
class MyClass:
    def __getattr__(self, attr):
        greeting = " ".join(attr.split('_')[1:])
        return greeting.capitalize()

m = MyClass()
m.say_hello() # TypeError: 'str' object is not callable
m.say_hello # 'Hello'
```

```
class MyClass:
    def __getattr__(self, attr):
        def _call():
            greeting = " ".join(attr.split('_')[1:])
            return greeting.capitalize()
        return _call

m = MyClass()
m.say_hello() # 'Hello'
m.say_bye_bye() # 'Bye bye'
```

Introspection and reflection – cont'd

```
class MyClass:
```

```
    def __init__(self):  
        self.say_hello = 0
```

```
    def __getattr__(self, attr):  
        def _call():  
            greeting = " ".join(attr.split('_')[1:])  
            return greeting.capitalize()  
        return _call
```

```
    def say_hello(self):  
        return 'Hi'
```

```
m = MyClass()
```

```
m.say_hello # 0
```

```
m.say_hello() # TypeError: 'int' object is not callable
```

```
m.say_bye_bye() # 'Bye bye'
```

Instance attribute (self.say_hello) takes precedence over class attribute (say_hello(self))

Introspection and reflection – cont'd

Instance attributes 'usually' take precedence over class attributes

(See this Stackoverflow post)

```
class Foo(object):

    def __init__(self, lst):
        self.lst = lst

    def sum(self):
        self.sum = sum(self.lst)
        return self.sum

f = Foo([1,2,3])
print(f.sum()) # None ⇒ self.sum = 6
print(f.sum()) # TypeError: 'int' object is not callable ⇒ print(6())
```

Source: Stackoverflow Blckknight (accessed on Nov 2019)

Introspection and reflection – cont'd

```
def capit(func):  
    def wrapper(*args, **kwargs):  
        return func(*args, **kwargs).capitalize()  
    return wrapper
```

```
class MyClass:
```

```
    def __getattr__(self, attr):  
        @capit # decorator  
        def _call():  
            greeting = " ".join(attr.split('_')[1:])  
            return greeting  
        return _call
```

```
m = MyClass()  
m.say_hello() # 'Hello'  
m.say_bye_bye() # 'Bye bye'
```

Introspection and reflection – cont'd

```
class GreetMe:
    def __init__(self, name):
        self.name = name

    def __getattr__(self, attr):
        allowed = ['hello', 'bye', 'nice_to_meet_you', 'good_bye', 'goodnight']

        def call_(name=None):
            if attr in allowed:
                greeting = attr.replace('_', ' ')
                target = name if name else self.name
                return f"{target, greeting.capitalize()}"
            else:
                raise ValueError(f"Invalid name or greeting: name, attr")
        return call_

greet = GreetMe('Luna')
greet.hello() # Outputs: 'Luna, Hello'
greet.bye(name='John') # Outputs: 'John, Bye'
greet.nice_to_meet_you(name='Jane') # Outputs: 'Jane, Nice to meet you'
```


Unit testing

Defining tests using unittest module

```
import unittest
class TestStatisticalFunctions(unittest.TestCase):
    def test_average(self):
        self.assertEqual(average([20, 30, 70]), 40.0)
        self.assertEqual(round(average([1, 5, 7]), 1), 4.3)
        with self.assertRaises(ZeroDivisionError):
            average([])
        with self.assertRaises(TypeError):
            average(20, 30, 70)

unittest.main() # Calling from the command line invokes all tests
```

Source: Paul Fodor - SBU (accessed on Nov 2019)

Debugging & profiling

Debugging using pdb package

```
$ python -m pdb my_script.py
```

```
import pdb

def make_bread():
    pdb.set_trace()
    return "I don't have time"

print(make_bread())
```

- c: continue execution
- w: shows the context of the current line it is executing
- a: prints the argument list of the current function
- s: executes the current line and stop at the first possible occasion
- n: continue execution until the next line in the current function is reached or it returns

Profiling using cProfile package

```
$ python -m cProfile my_script.py
```

Memoization: Caching Technique

- A technique to **speed** up Python programs using **caching**.
 - A cache **stores** the results of an operation for **later** use.
- It caches a function output based on the given input parameters.
 - It will compute the output **once** for each input set of parameters.
 - Every **consequent** call after the first will be quickly retrieved from a cache!
- When to use?
 - Only in cases where the code is expensive to run.
 - Expensive code in terms of storage space and execution time.

Memoization: Implementation

- Implementing Memoization:
 - Set up a cache data structure for function results
 - Every time the function is called, do one of the following:
 - Return the cached result, if any; or
 - Call the function to compute the missing result, and then update the cache before returning the result to the caller
 - Given enough cache storage this virtually guarantees that function results for a specific set of function arguments will only be computed once.
- As soon as we have a cached result we won't have to re-run the memoized function for the same set of inputs.
 - Instead, we can just fetch the cached result and return it right away!

Python Decorators: Memoization Decorator

```
1 # Memoization Decorator
2 def memoize(func):
3     cache = dict()
4     def memoized_func(*args):
5         if args in cache:
6             return cache[args]
7         result = func(*args)
8         cache[args] = result
9         return result
10    return memoized_func
```

```
1 def fibonacci(n):
2     if n == 0:
3         return 0
4     elif n == 1:
5         return 1
6     return fibonacci(n - 1) + fibonacci(n - 2)
7
8 import timeit
9
10 # Normal Fibonacci
11 print('normal run')
12 print(timeit.timeit('fibonacci(35)', globals=globals(),
13 number=1))
14 print(timeit.timeit('fibonacci(35)', globals=globals(),
15 number=1))
16
17 # Memoized Fibonacci
18 print('memoized run')
19 m_fibonacci = memoize(fibonacci)
20 print(timeit.timeit('m_fibonacci(35)', globals=globals(),
21 number=1))
22 print(timeit.timeit('m_fibonacci(35)', globals=globals(),
23 number=1))
```

lru_cache (Python 3.2+)

```
from functools import lru_cache

@lru_cache(maxsize=32)
def fib(n):
    if n < 2:
        return n
    return fib(n-1) + fib(n-2)

>>> print([fib(n) for n in range(10)])
# Output: [0, 1, 1, 2, 3, 5, 8, 13, 21, 34]
```

Memoization Caveats

- Memoize **deterministic** functions only!
 - Caching non-deterministic functions will return incorrect or unexpected results.
- Ensure **caching space** complexity is much smaller than function execution complexity!
 - It is best to have a **bounded** (max size) caching storage.
- Bounded caches require a **smart purge** once it is full:
 - By gathering usage statistics
 - Discarding older entries
 - Discarding least frequently unused entries, etc

Using `__slot__` for reducing memory usage

- Python uses a dict to store an object's instance attributes
- Creating a lot of objects ($>> 100,000$) uses large memory due to the storage of (default) attributes
- `__slot__` can be used to tell Python not to use a dict and only allocate space for a fixed set of attributes
- Could give upto 50% reduction in memory usage (see PyPy which does this kind of optimizations by default)

```
class MyClass(object):  
  
    __slots__ = ['name', 'identifier']  
  
    def __init__(self, name, identifier):  
        self.name = name  
        self.identifier = identifier  
        self.set_up()  
  
# ...
```


Python General Good Programming Practices

- We will follow PEP8 coding conventions for good programming practices
 - Complete guidelines: <https://www.python.org/dev/peps/pep-0008/>
- Spacing:
 - 4 spaces to indent. No tabs.
 - Use blank lines to separate functions and logical sections inside functions.
 - Use spaces around operators and after commas, but not directly inside delimiters
- Commenting:
 - Comment all nontrivial functions.
 - Add header comments at the top of files before any imports.
 - If possible, put comments on a line of their own.

Python General Good Programming Practices

- Naming:
 - snake_case for variables/functions
 - CamelCase for classes
 - CAPS_CASE for constants
- Decomposition and Logic:
 - Simple is better than complex.
 - Seek abstractions and clean design.
- Automated Code Style Checking: (PEP8)
 - PyLintOnline: Captures mechanical violations (naming, spacing); advanced suggestions.
 - pycodestyle: install using `pip install pycodestyle`

Python Good Programming Practices

- Swapping two variables:

```
1 # Bad  
2 temp = a  
3 a = b  
4 b = temp
```

```
1 # Good  
2 a, b = b, a
```

Python Good Programming Practices

- Loop unpacking:

```
1 # Bad
2 for bundle in zip([1,2,3], 'abc'):
3     num, let = bundle
4     print(let * num)
5 # Bad
6 for key in d:
7     val = d[key]
8     print('{}: {}'.format(key, val))
```

```
1 # Good
2 for num, let in zip([1,2,3], 'abc'):
3     print(let * num)
4
5 # Good
6 for key, val in d.items():
7     print('{}->{}'.format(key, val))
```

Python Good Programming Practices

- Enumerate Iterables:

```
1 # Bad
2 for index in range(len(arr)):
3     elem = arr[index]
4     print(elem)
5 # Bad
6 for index in range(len(arr)):
7     elem = array[index]
8     print(index, elem)
```

```
1 # Good
2 for elem in arr:
3     print(elem)
4
5 # Good
6 for index, elem in
7     enumerate(arr):
8         print(index, elem)
```

Python Good Programming Practices

- Joining Strings:

```
1 # Bad
2 s = ''
3 for color in colors:
4     s += color
5
6 # Bad
7 s = ''
8 for color in colors:
9     s += color + ', '
10 s = s[:-2]
```

```
1 # Good
2 s = ''.join(colors)
3
4 # Good
5 s = ', '.join(colors)
```

Python Good Programming Practices

- Reduce In-Memory Buffering:

```
1 # Bad
2 ', '.join([color.upper() for color in colors])
3 # Bad
4 map(lambda x: int(x) ** 2, [line.strip() for line in
5 file])
6 # Bad
7 sum([n ** 2 for n in range(1000)])
```

```
1 # Good
2 ', '.join((color.upper() for color in colors))
3 # Good
4 map(lambda x: int(x) ** 2, (line.strip() for line in
5 file))
6 # Good
7 sum(n ** 2 for n in range(1000))
```

Python Good Programming Practices

- Chained Comparison Tests:

```
1 # Bad
2     return 0 < x and x < 10
3 # Bad
4 if a < x and x < b:
5     return x
```

```
1 # Good
2     return 0 < x < 10
3 # Good
4 if a < x < b:
5     return x
```


Python Good Programming Practices

- Using in:

```
1 # Bad
2 if d.has_key(key):
3     print("Here!")
4 # Bad
5 if x == 1 or x == 2 or x == 3:
6     return True
7 # Bad
8 if 'hello'.find('lo') != -1:
9     print("Found")
```

```
1 # Good
2 if key in d:
3     print("Here!")
4 # Good
5 if x in [1, 2, 3]:
6     return True
7 # Good
8 if 'lo' in 'hello':
9     print("Found")
```

Python Good Programming Practices

- Boolean Tests:

```
1 # Bad
2 if x == True:
3     print("Yes")
4 # Bad
5 if len(items) > 0:
6     print("Nonempty")
7 # Bad
8 if items != []:
9     print("Nonempty")
10 # Bad
11 if x != None:
12     print("Something")
```

```
1 # Good
2 if x:
3     print("Yes")
4 # Good
5 if items:
6     print("Nonempty")
7 # Good
8 if items:
9     print("Nonempty")
10 # Good
11 if x is not None:
12     print("Something")
```

Python Good Programming Practices

- Ignore values using underscore:

```
1 # Bad
2 for i in range(10):
3     x = input("> ")
4     print(x[::-1])
```

```
1 # Good
2 for _ in range(10):
3     x = input("> ")
4     print(x[::-1])
```

Python Good Programming Practices

- Looping Correctly:

```
1 # Bad
2 for i in range(len(colors)):
3     color = colors[i]
4     name = names[i]
5     print(color, name)
6 # Bad
7 for ind in range(len(elems) - 1, -1, -1):
8     print(elems[ind])
```

```
1 # Good
2 for color, name in zip(colors, names):
3     print(color, name)
4
5 # Good
6 for elem in reversed(elems):
7     print(elem)
```

Python Good Programming Practices

- Initializing Lists:

```
1 # Bad
2 nones = [None, None, None, None]
3 # Bad
4 two_dim = [[None] * 4] * 5
5
6 # Good
7 nones = [None] * 4
8 # Good
9 two_dim = [[None] * 4 for _ in range(5)]
```

Python Good Programming Practices

- **Avoid** mutable default parameters:

```
1 # Bad
2 def init_list(x, li=[]):
3     li.append(x)
4     print(li)
5
6
7 init_list(1, [4]) # =>
8 [4, 1]
9 init_list(3) # => [3]
10 init_list(3) # => [3, 3]
11 init_list(3) # => [3, 3,
12 3]
```

```
1 # Good
2 def init_list(x, li=None):
3     if li is None:
4         li = []
5     li.append(x)
6     print(li)
7
8 init_list(1, [4]) # => [4, 1]
9 init_list(3) # => [3]
10 init_list(3) # => [3]
11 init_list(3) # => [3]
```

Python Good Programming Practices

- Use Comprehensions:

```
1 # Bad
2 out = []
3 for word in lex:
4     if word.endswith('py'):
5         out.append(word[:-2])
6 # Bad
7 lengths = set()
8 for word in lex:
9     lengths.add(len(word))
```

```
1 # Good
2 out = [word[:-2] for word in lex if
3 word.endswith('py')]
4
5 # Good
6 lengths = {len(word) for word in lex}
```

Python Good Programming Practices

- Use Context Managers:

```
1 # Bad
2 f = open('path/to/file')
3 try:
4     raw = f.read()
5
6 except IOError as e:
7     print('IOError:', e)
8 finally:
9     f.close()
```

```
1 # Good
2 with open('path/to/file') as f:
3     raw = f.read()
```


Python Good Programming Practices

- In python, EAFP > LBYL:
 - EAFP: It's easier to ask for forgiveness than permission.
 - LBYL: Look before you leap

```
1 # LBYL
2 def safe_div(m, n):
3     if n == 0:
4         print("Can't divide by 0")
5         return None
6     return m / n
7
8 # EAFP
9 def safe_div(m, n):
10    try:
11        return m / n
12    except ZeroDivisionError:
13        print("Can't divide by 0")
14    return None
```

Python Good Programming Practices

- **Avoid** using Catch-Alls:

```
1 # Bad
2 try:
3     n = int(input("> "))
4 except:
5     print("Invalid input.")
6 else:
7     return n ** 2
8
9 # Good
10 try:
11     n = int(input("> "))
12 except ValueError:
13     print("Invalid input.")
14 else:
15     return n ** 2
```

Python Good Programming Practices

- Use Custom Made Exceptions:

```
1 # Bad
2 if not self.available_cheeses:
3     raise ValueError("No cheese!")
4
5 # Good
6 class NoCheeseError(ValueError):
7     pass
8 if not self.available_cheeses:
9     raise NoCheeseError("I'm afraid we're right out, sir.")
```

Python Good Programming Practices

- Always implement Magic Methods for the defined Class:

```
1 class Vector():
2     def __init__(self, elems):
3         self.elems = elems
4     def size(self):
5         return len(self.elems)
6
7 v = Vector([1,2])
8 len(v) # => fails!
```

```
1 class Vector():
2     def __init__(self, elems):
3         self.elems = elems
4     def __len__(self):
5         return len(self.elems)
6
7 v = Vector([1,2])
8 len(v) # => succeeds!
```

Serialization using Pickle

```
# Importing pickle
try:
    import cPickle as pickle # Python 2
except ImportError:
    import pickle # Python 3

# Creating Pythonic object:
class Family(object):
    def __init__(self, names):
        self.sons = names
    def __str__(self):
        return ' '.join(self.sons)

my_family = Family(['John', 'David'])

# Dumping to string
pickle_data = pickle.dumps(my_family, pickle.HIGHEST_PROTOCOL)
```

Source: Python notes for professionals (accessed on Nov 2019)

Serialization using JSON

```
import json

families = ([ 'John'], [ 'Mark', 'David', 'name': 'Avraham'])

# Dumping it into string
json_families = json.dumps(families)
# [{"John"}, ["Mark", "David", "name": "Avraham"]]
# Pretty printing
print(json.dumps(json_families, indent = 4, sort_keys=True))

# Dumping it to file
with open('families.json', 'w') as json_file:
    json.dump(families, json_file)

# Loading it from string
json_families = json.loads(json_families)

# Loading it from file
with open('families.json', 'r') as json_file:
    json_families = json.load(json_file)
```

XML parsing

- xml.etree.ElementTree

```
import xml.etree.ElementTree as ET
tree = ET.parse('country_data.xml')
root = tree.getroot()

for child in root:
    print(child.tag, child.attrib)

for neighbor in root.iter('neighbor'):
    print(neighbor.attrib)

for country in root.findall('country'):
    rank = country.find('rank').text
    name = country.get('name')
    print(name, rank)
```

Sources: Python documentation (accessed on Nov 2019)

XML parsing – 3rd party

- **untangle**

```
import untangle

obj = untangle.parse('path/to/file.xml')
obj.root.child['my_attr']
```

- **xmltodict**

```
import xmltodict

with open('path/to/file.xml') as fd:
    doc = xmltodict.parse(fd.read())

doc['my_tag']['my_attr']
```

Source: THGtP (accessed on Nov 2019)

- Native C calls in Python (extending Python with C)
 - <https://docs.python.org/3.7/extending/extending.html>
 - <https://www.csestack.org/calling-c-functions-from-python/>
- Multiprocessing
<https://docs.python.org/3.7/library/multiprocessing.html>
- Logging
<https://docs.python.org/3.7/howto/logging-cookbook.html>