Brief Introduction to Python

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19.10.18	Introduction	Python, Introduction
26.10.18	Learning Theory	Learning Theory
02.11.18		No Lesson
09.11.18	Machine Learning Algorithms	Machine Learning Algorithms
16.11.18	Introduction to Feed Forward Neural Networks	Introduction to Feed Forward Neural Networks
23.11.18	Introduction to Optimization	Introduction to Optimization
30.11.18	Training Neural Networks	Training Neural Networks
07.12.18	Convolutional Neural Networks	Convolutional Neural Networks
14.12.18	RNNs, LSTM, Attention Models	RNNs, LSTM, Attention Models
21.12.18		Christmas
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04.01.19	Unsupervised Learning	Unsupervised Learning
11.01.19	Reinforcement Learning	Reinforcement Learning
18.01.19	Data Analysis	Data Analysis
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19.10.18	Python, Numpy
26.10.18	Pandas, Matplotlib, Seaborn
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09.11.18	ML Algorithms
16.11.18	Feed Forward Neural Networks
23.11.18	Optimization and Hyperparameters
30.11.18	Training a NN
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Brief Introduction to Python

Python, a first Glance

Python, a first Glance

- **Open source general-purpose language.**
- **Object Oriented, Procedural, Functional**
- **Easy to prototype and interface**
- **Great interactive environment**
- **Interpreted (Bytecode to VM)**
- **Easy to learn**

- **Downloads: http://www.python.org**
- **Documentation: http://www.python.org/doc/**
- **Free book: http://www.diveintopython.org**

Python, a first Glance

- **Guido van Rossum is the author, in the late eighties and early nineties.**

- **Python is now maintained by a core development team (CWI) at the institute, although Guido van Rossum for long time still held a vital role in directing its progress (Resigned 2018).**

- **Python 1.0 was released in November 1994. In 2000, Python 2.0 was released. Python 2.7.11 is the latest edition of Python 2.**

- **Python 3.0 was released in 2008. Python 3 is not backward compatible with Python 2. Now, Python 3.7**

Python, a first Glance

- **A broad standard library**
- **Portable**
- **Extendable**
- **Databases**
- **GUI Programming**
- **Scalable**

Technical Issues

The Python Interpreter

- **Python interpreter evaluates inputs:**

```
>>> 3*(7+2)
27
```

- **Python prompts with ‘>>>’.**
- **To exit Python:**
  - CTRL-D

Running Programs on UNIX

```
% python filename.py
```

You could make the *.py file executable and add the following *#!/usr/bin/env python* **to the top to make it runnable.**

Batteries Included

- **Large collection of proven modules included in the standard distribution.**

http://docs.python.org/modindex.html

numpy

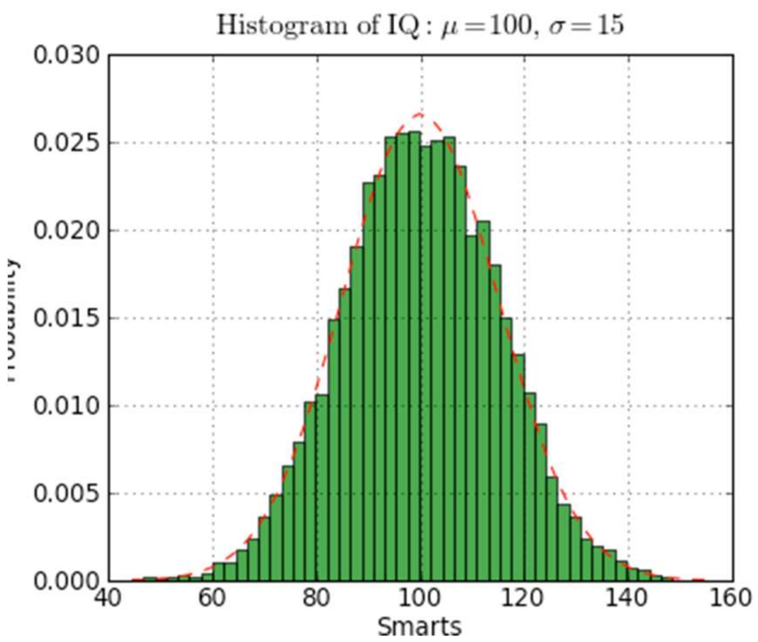
- **Offers Matlab-ish capabilities within Python**
- **Fast array operations**
- **2D arrays, multi-D arrays, linear algebra etc.**

- **Downloads: http://numpy.scipy.org/**
- **Tutorial: http://www.scipy.org/**

matplotlib

- **High quality plotting library.**

```
#!/usr/bin/env python
import numpy as np
import matplotlib.mlab as mlab
import matplotlib.pyplot as plt

mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)

# the histogram of the data
n, bins, patches = plt.hist(x, 50, normed=1, facecolor='green',
alpha=0.75)

# add a 'best fit' line
y = mlab.normpdf( bins, mu, sigma)
l = plt.plot(bins, y, 'r--', linewidth=1)

plt.xlabel('Smarts')
plt.ylabel('Probability')
plt.title(r'$\mathrm{Histogram\ of\ IQ:}\ \mu=100,\ \sigma=15$')
plt.axis([40, 160, 0, 0.03])
plt.grid(True)

plt.show()
```



- **Downloads: http://matplotlib.sourceforge.net/**

Custom Distributions

- **Python(x,y): http://www.pythonxy.com/**
  - Python(x,y) is a free scientific and engineering development software for numerical computations, data analysis and data visualization

- **Sage: http://www.sagemath.org/**
  - Sage is a free open-source mathematics software system licensed under the GPL. It combines the power of many existing open-source packages into a common Python-based interface.

Extra Links

- iPython (better shell, distributed computing): http://ipython.scipy.org/
- SciPy (collection of science tools): http://www.scipy.org/
- Python Astronomy Modules: http://astlib.sourceforge.net/
- Python Astronomer Wiki: http://macsingularity.org/astrowiki/tiki-index.php?page=python
- AstroPy: http://www.astro.washington.edu/users/rowen/AstroPy.html
- Python for Astronomers: http://www.iac.es/sieinvens/siepedia/pmwiki.php?n=HOWTOs.EmpezandoPython

The Basics

A Code Sample

```
x = 34 - 23            # A comment.
y = "Hello"            # Another one.
z = 3.45
if z == 3.45 or y == "Hello":
    x = x + 1
    y = y + " World"   # String concat.
print x
print y
```

Enough to Understand the Code

- **Assignment uses `=` and comparison uses `==`.**
- **For numbers `+ - * / %` are as expected.**
  - Special use of `+` for string concatenation.
  - Special use of `%` for string formatting (as with printf in C)
- **Logical operators are words (`and, or, not`) *not* symbols**
- **The basic printing command is `print`.**
- **The first assignment to a variable creates it.**
  - Variable types don't need to be declared.
  - Python figures out the variable types on its own.

Basic Datatypes

- **Integers (default for numbers)**

```
z = 5 / 2    # Answer is 2, integer division.
```

- **Floats**

```
x = 3.456
```

- **Strings**
  - Can use “” or ‘’ to specify.
    `“abc”  ‘abc’` (Same thing.)
  - Unmatched can occur within the string.
    `“matt’s”`
  - Use triple double-quotes for multi-line strings or strings than contain both ‘ and “ inside of them:
    `“““a‘b“c”””`

Whitespace

Whitespace is meaningful in Python: especially indentation and placement of newlines.

- **Use a newline to end a line of code.**
  - Use `\` when must go to next line prematurely.
- **No braces `{ }` to mark blocks of code in Python… Use *consistent* indentation instead.**
  - The first line with *less* indentation is outside of the block.
  - The first line with *more* indentation starts a nested block
- **Often a colon appears at the start of a new block. (E.g. for function and class definitions.)**

Comments

- Start comments with # – the rest of line is ignored.
- Can include a “documentation string” as the first line of any new function or class that you define.
- The development environment, debugger, and other tools use it: it’s good style to include one.

```
def my_function(x, y):
  """This is the docstring. This
  function does blah blah blah."""
  # The code would go here...
```

Assignment

- ***Binding a variable*** **in Python means setting a** ***name*** **to hold a** ***reference*** **to some** ***object*****.**
  - *Assignment creates references, not copies*
- **Names in Python do not have an intrinsic type. Objects have types.**
  - Python determines the type of the reference automatically based on the data object assigned to it.
- **You create a name the first time it appears on the left side of an assignment expression:**

```
x = 3
```

- **A reference is deleted via garbage collection after any names bound to it have passed out of scope.**

Accessing Non-Existent Names

- **If you try to access a name before it's been properly created (by placing it on the left side of an assignment), you'll get an error.**

```
>>> y

Traceback (most recent call last):
  File "<pyshell#16>", line 1, in -toplevel-
    y
NameError: name ‘y' is not defined
>>> y = 3
>>> y
3
```

Multiple Assignment

- **You can also assign to multiple names at the same time.**

```
>>> x, y = 2, 3
>>> x
2
>>> y
3
```

Naming Rules

- **Names are case sensitive and cannot start with a number. They can contain letters, numbers, and underscores.**

```
bob   Bob   _bob   _2_bob_   bob_2   BoB
```

- **There are some reserved words:**

```
and, assert, break, class, continue, def, del, elif,
else, except, exec, finally, for, from, global, if,
import, in, is, lambda, not, or, pass, print, raise,
return, try, while
```

Understanding Reference Semantics in Python

Understanding Reference Semantics

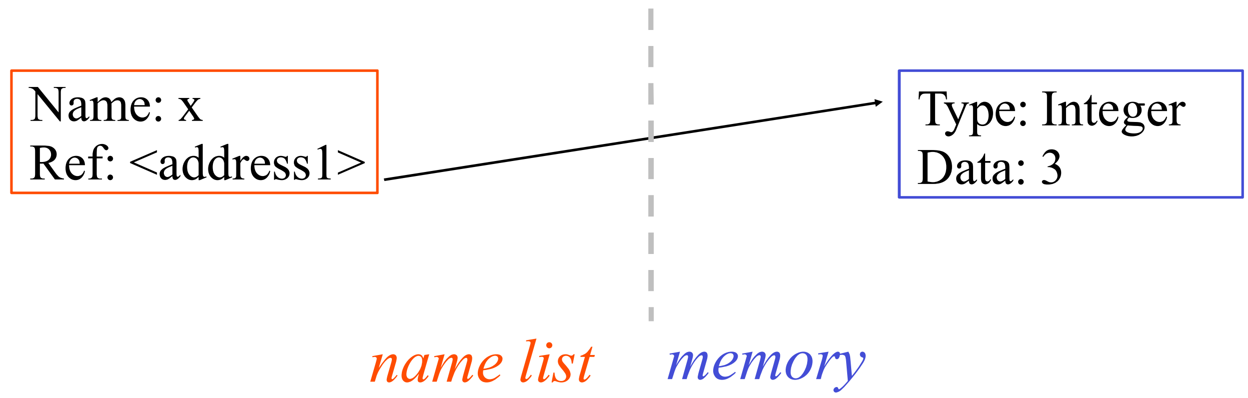
- **Assignment manipulates references**
  - x = y **does not make a copy** of the object y references
  - x = y makes x **reference** the object y references
- **Very useful; but beware!**
- **Example:**

```
>>> 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

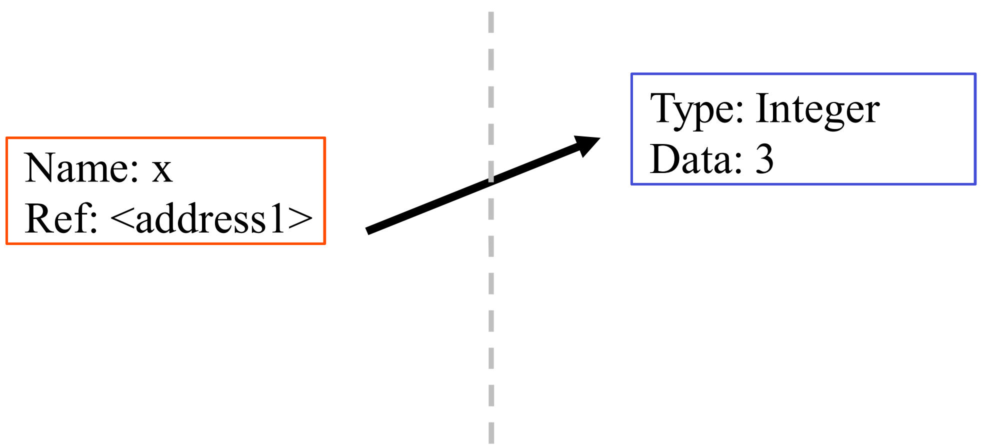
- **The data 3 we created is of type integer. In Python, the datatypes integer, float, and string (and tuple) are “immutable.”**
- **This doesn’t mean we can’t change the value of x, i.e. *change what x refers to* …**
- **For example, we could increment x:**

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

Understanding Reference Semantics IV

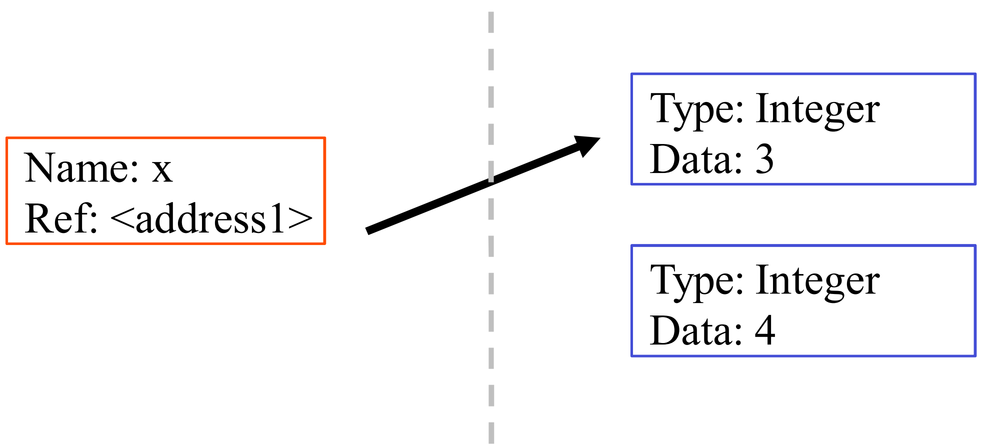
- **If we increment x, then what's really happening is:**
  1. *The reference of name* ***x*** *is looked up.*
  2. *The value at that reference is retrieved.*

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



Understanding Reference Semantics IV

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



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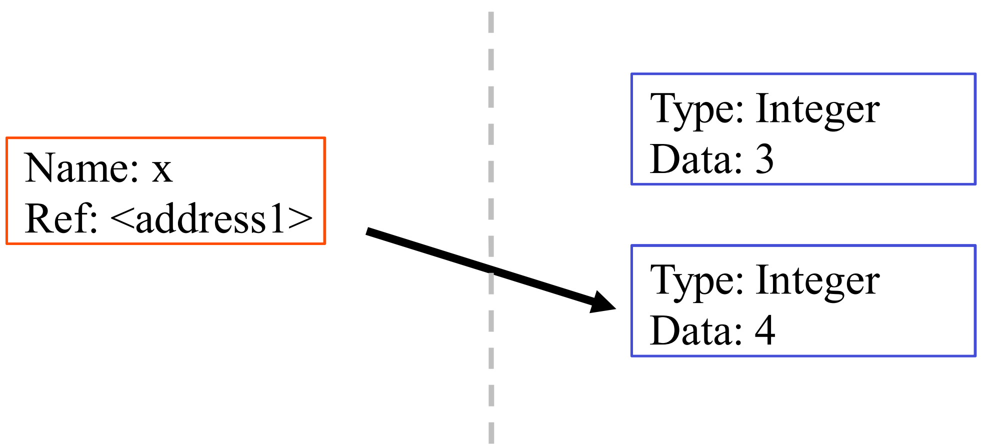

Understanding Reference Semantics IV

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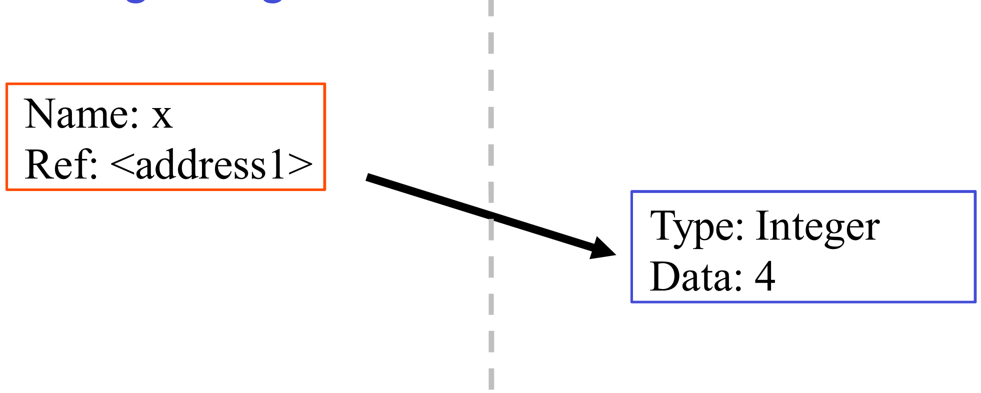
4. *The name **x** is changed to point to this new reference.*
5. *The old data 3 is garbage collected if no name still refers to it.*



Assignment 1

- **So, for simple built-in datatypes (integers, floats, strings), assignment behaves as you would expect:**

```
>>> x = 3          # Creates 3, name x refers to 3
>>> y = x          # Creates name y, refers to 3.
>>> y = 4          # Creates ref for 4. Changes y.
>>> print x        # No effect on x, still ref 3.
3
```

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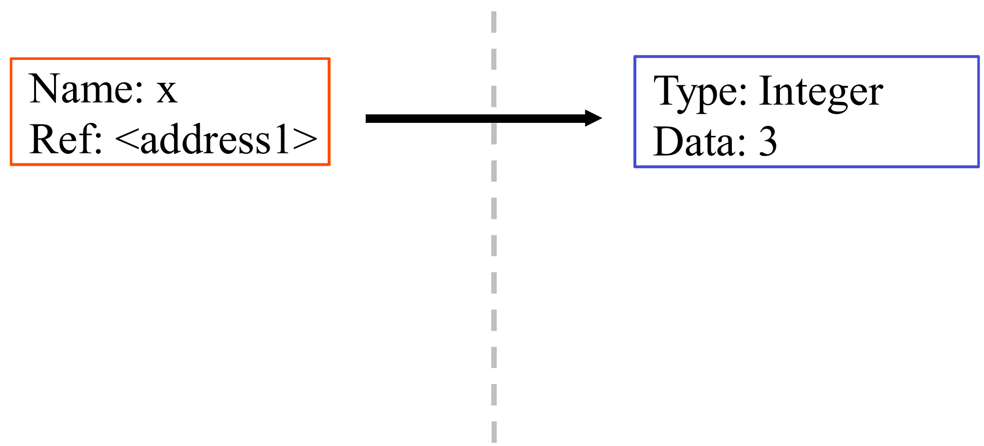

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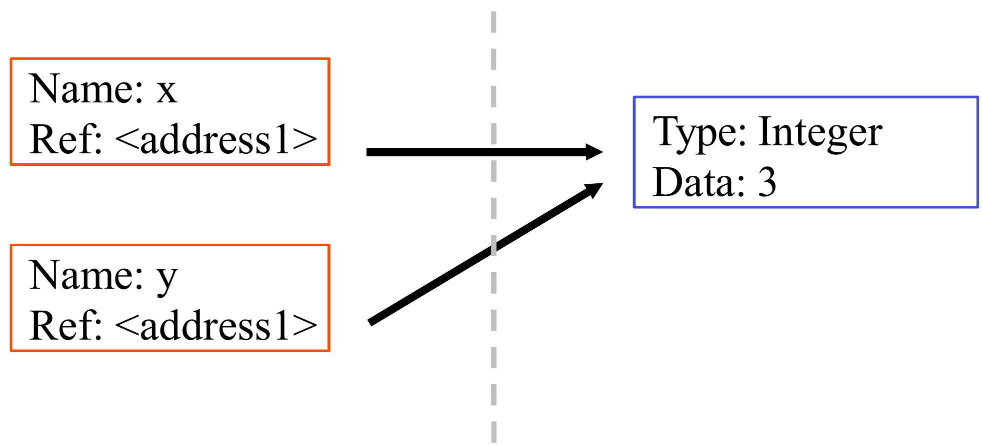

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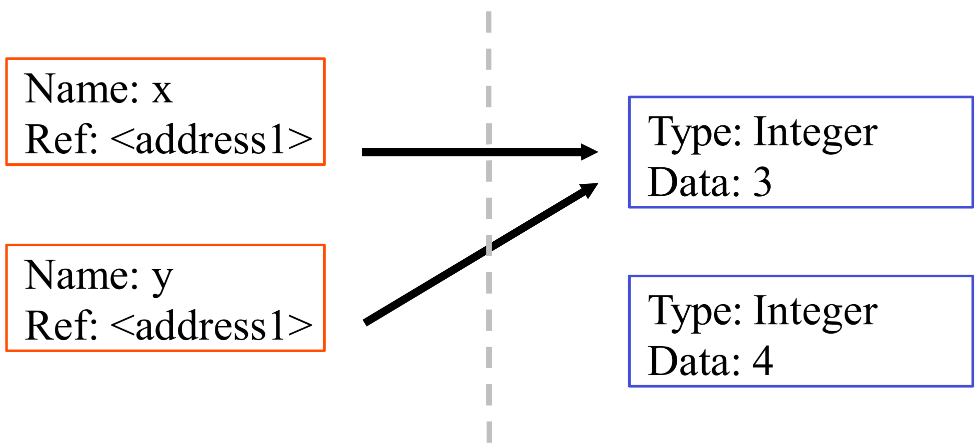
3
```



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>>> y = 4        # Creates ref for 4. Changes y.
>>> print x      # No effect on x, still ref 3.
3
```
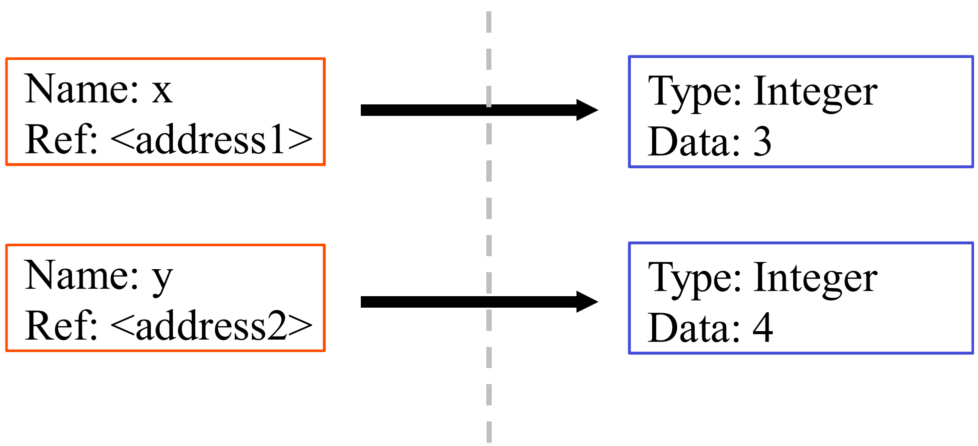



Assignment 2

- **For other data types (lists, dictionaries, user-defined types), assignment works differently.**
  - These datatypes are **"mutable."**
  - When we change these data, we do it *in place.*
  - We don't copy them into a new memory address each time.
  - If we type y=x and then modify y, both x and y are changed.

immutable

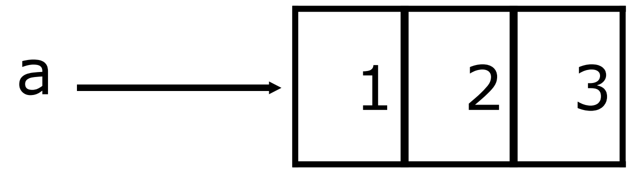
```
>>> x = 3

>>> y = x
>>> y = 4
>>> print x
3
```

mutable

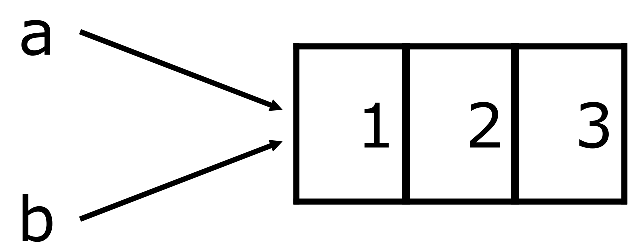
```
x = some mutable object
y  =  x
Make a  change to  y
look at x
x will be changed as well
```

Why? Changing a Shared List

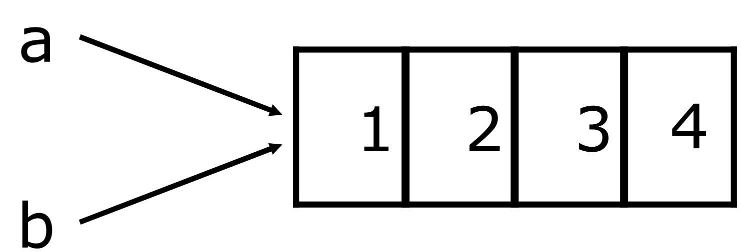
```
a = [1, 2, 3]
```




```
b = a
```




```
a.append(4)
```



Our surprising example surprising no more...

- **So now, here's our code:**

```
>>> 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…
```

Sequence Types:
Tuples, Lists, and Strings

Sequence Types

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

2. Strings
   - ***Immutable***

3. List
   - ***Mutable*** ordered sequence of items of mixed types

Similar Syntax

- **All three sequence types (tuples, strings, and lists) share much of the same syntax and functionality.**

- Key difference:
  - **Tuples and strings are *immutable***
  - **Lists are *mutable***
- The operations shown in this section can be applied to *all* sequence types
  - **most examples will just show the operation performed on one**

Sequence Types 1

- **Tuples are defined using parentheses (and commas).**

```
>>> tu = (23, 'abc', 4.56, (2,3), 'def')
```

- **Lists are defined using square brackets (and commas).**

```
>>> li = ["abc", 34, 4.34, 23]
```

- **Strings are defined using quotes (", ', or """).**

```
>>> st = "Hello World"
>>> st = 'Hello World'
>>> st = """This is a multi-line
string that uses triple quotes."""
```

Sequence Types 2

- **We can access individual members of a tuple, list, or string using square bracket “array” notation.**
- ***Note that all are 0 based…***

```
>>> tu = (23, ‘abc’, 4.56, (2,3), ‘def’)
>>> tu[1]      # Second item in the tuple.
 ‘abc’

>>>  li =  [“abc”,  34, 4.34, 23]
>>>  li[1]        #  Second item in
                     the list
 34

>>>  st = “Hello World”
>>>  st[1]     # Second character in  string.
‘e’
```

Positive and negative indices

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

Positive index: count from the left, starting with 0.

```
>>> t[1]
'abc'
```

Negative lookup: count from right, starting with –1.

```
>>> t[-3]
4.56
```

Slicing: Return Copy of a Subset 1

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

Return a copy of the container with a subset of the original members. Start copying at the first index, and stop copying *before* the second index.

```
>>> t[1:4]
('abc', 4.56, (2,3))
```

You can also use negative indices when slicing.

```
>>> t[1:-1]
('abc', 4.56, (2,3))
```

Slicing: Return Copy of a Subset 2

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

Omit the first index to make a copy starting from the beginning of the container.

```
>>> t[:2]
(23, 'abc')
```

Omit the second index to make a copy starting at the first index and going to the end of the container.

```
>>> t[2:]
(4.56, (2,3), 'def')
```

Copying the Whole Sequence

To make a *copy* of an entire sequence, you can use `[:]`.

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

Note the difference between these two lines for mutable sequences:

```
>>> list2 = list1     # 2 names refer to 1 ref
                      # Changing one affects both

>>> list2 = list1[:] # Two independent copies, two refs
```

The 'in' Operator

- **Boolean test whether a value is inside a container:**

```
>>> t = [1, 2, 4, 5]
>>> 3 in t
False
>>> 4 in t
True
>>> 4 not in t
False
```

- **For strings, tests for substrings**

```
>>> a = 'abcde'
>>> 'c' in a
True
>>> 'cd' in a
True
>>> 'ac' in a
False
```

- **Be careful: the *in* keyword is also used in the syntax of *for loops* and *list comprehensions*.**

The +Operator

- **The + operator produces a *new* tuple, list, or string whose value is the concatenation of its arguments.**

```
>>>  (1, 2, 3) +  (4, 5, 6)
 (1, 2, 3, 4, 5, 6)

>>>  [1, 2, 3] + [4, 5, 6]

 [1, 2, 3, 4, 5, 6]

>>> "Hello" + " " + "World"
 'Hello World'
```

The *Operator

- **The * operator produces a *new* tuple, list, or string that “repeats” the original content.**

```
>>> (1, 2, 3) * 3
(1, 2, 3, 1, 2, 3, 1, 2, 3)

>>> [1, 2, 3] * 3
[1, 2, 3, 1, 2, 3, 1, 2, 3]

>>> “Hello” * 3
‘HelloHelloHello’
```

Mutability: Tuples vs. Lists

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.**

Operations on Lists Only 1

```
>>> li = [1, 11, 3, 4, 5]

>>> li.append(‘a’)     # Our first exposure to method syntax
>>> li
[1, 11, 3, 4, 5, ‘a’]

>>> li.insert(2, ‘i’)

>>>li

[1, 11, ‘i’, 3, 4, 5, ‘a’]
```

The *extend* method vs the + operator.

- **+ creates a fresh list (with a new memory reference)**
- ***extend* operates on list `li` in place.**

```
>>> li.extend([9, 8, 7])
>>>li
[1, 2, 'i', 3, 4, 5, 'a', 9, 8, 7]
```

***Confusing*:**

- **Extend takes a list as an argument.**
- **Append takes a singleton as an argument.**

```
>>> li.append([10,  11, 12])
>>> li

[1, 2, 'i', 3, 4, 5, 'a', 9, 8, 7, [10, 11, 12]]
```

Operations on Lists Only 3

```
>>> li = ['a', 'b', 'c', 'b']

>>> li.index('b')      # index of first occurrence
1

>>> li.count('b')      # number of occurrences
2

>>> li.remove('b')     # remove first Occurrence

>>> li
['a', 'c', 'b']
```

Operations on Lists Only 4

```
>>> li = [5, 2, 6, 8]

>>> li.reverse()     # reverse the list *in place*
>>> li
  [8, 6, 2, 5]

>>> li.sort()        # sort the list *in place*
>>> li
  [2, 5, 6, 8]

>>> li.sort(some_function)
    # sort in place using user-defined comparison
```

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)
```

Dictionaries

Dictionaries: A Mapping type

- **Dictionaries store a mapping between a set of keys and a set of values.**
  - Keys can be any immutable type.
  - Values can be any type
  - A single dictionary can store values of different types

- **You can define, modify, view, lookup, and delete the key-value pairs in the dictionary.**

Using dictionaries

```
>>> d = {'user':'bozo', 'pswd':1234}
>>> d['user']
'bozo'
>>> d['pswd']
1234
>>> d['bozo']

Traceback (innermost last):
  File '<interactive input>' line 1, in ?
KeyError: bozo
```

```
>>> d = {'user':'bozo', 'pswd':1234}
>>> d['user'] = 'clown'
>>> d
{'user':'clown', 'pswd':1234}
```

```
>>> d['id'] = 45
>>> d
{'user':'clown', 'id':45, 'pswd':1234}
```

```
>>> d = {'user':'bozo', 'p':1234, 'i':34}
>>> del d['user']             # Remove one.
>>> d
{'p':1234, 'i':34}
>>> d.clear()                 # Remove all.
>>> d
{}
```

```
>>> d = {'user':'bozo', 'p':1234, 'i':34}
>>> d.keys()              # List of keys.
['user', 'p', 'i']
>>> d.values()            # List of values.
['bozo', 1234, 34]
>>> d.items()        # List of item tuples.
[('user','bozo'), ('p',1234), ('i',34)]
```

Functions

Functions

- ***def* creates a function and assigns it a name**
- **return sends a result back to the caller**
- **Arguments are passed by assignment**
- **Arguments and return types are not declared**

```
def <name>(arg1, arg2, ..., argN):
  <statements>
  return <value>

def times(x,y):
  return x*y
```

Passing Arguments to Functions

- ***Arguments are passed by assignment***
- ***Passed arguments are assigned to local names***
- ***Assignment to argument names doesn't affect the caller***
- ***Changing a mutable argument may affect the caller***

```
def changer (x,y):
  x = 2                   # changes local value of x only
  y[0] = 'hi'             # changes shared object
```

Optional Arguments

- **Can define defaults for arguments that need not be passed**

```
def func(a, b, c=10, d=100):  print a, b, c, d

>>> func(1,2)  1 2 10 100

>>> func(1,2,3,4)  1,2,3,4
```

Gotchas

- **All functions in Python have a return value**
  - even if no return line inside the code.
- **Functions without a return, return the special value *None*.**
- **There is no function overloading in Python.**
  - Two different functions can't have the same name, even if they have different arguments.
- **Functions can be used as any other data type. They can be:**
  - Arguments to function
  - Return values of functions
  - Assigned to variables
  - Parts of tuples, lists, etc

Control of Flow

Examples

```
if x == 3:
    print "X equals 3."
elif x == 2:
    print "X equals 2."
else:
    print "X equals something else."
print "This is outside the 'if'."
```

```
assert(number_of_players < 5)
```

```
x = 3
while x < 10:
   if x > 7:
       x += 2
       continue
   x = x + 1
   print "Still in the loop."
   if x == 8:
       break
print "Outside of the loop."
```

```
for x in range(10):
   if x > 7:
       x += 2
       continue
   x = x + 1
   print "Still in the loop."
   if x == 8:
       break
print "Outside of the loop."
```

Modules

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
```

Classes and Objects

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

The Extra Stuff...

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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
```

```
fileptr = open('filename')
somestring = fileptr.read()
for line in fileptr:
   print line
fileptr.close()
```

```
>>> a = 1
>>> b = 2.4
>>> c = 'Tom
>>> '%s has %d coins worth a total of $%.02f' % (c, a, b)
'Tom has 1 coins worth a total of $2.40'
```

Sources

Sources

https://www.tutorialspoint.com/python3/python_files_io.htm

http://tdc-www.harvard.edu/Python.pdf

https://www.youtube.com/watch?v=IROo4norCG0

Termin	Teil 1: 13:15-14.00	Teil 2: 14:15-15:00	Übung 15:15-17:30
19.10.18	Introduction	Python, Introduction	Python, Numpy
26.10.18	Learning Theory	Learning Theory	Pandas, Matplotlib, Seaborn
02.11.18		No Lesson	
09.11.18	Machine Learning Algorithms	Machine Learning Algorithms	ML Algorithms
16.11.18	Introduction to Feed Forward Neural Networks	Introduction to Feed Forward Neural Networks	Feed Forward Neural Networks
23.11.18	Introduction to Optimization	Introduction to Optimization	Optimization and Hyperparameters
30.11.18	Training Neural Networks	Training Neural Networks	Training a NN
07.12.18	Convolutional Neural Networks	Convolutional Neural Networks	CNN
14.12.18	RNNs, LSTM, Attention Models	RNNs, LSTM, Attention Models	RNNs, LSTM
21.12.18		Christmas	
28.12.18			
04.01.19	Unsupervised Learning	Unsupervised Learning	GANs
11.01.19	Reinforcement Learning	Reinforcement Learning	Reinforcement Learning
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