Introduction to Python

Heavily based on presentations by

Matt Huenerfauth (Penn State)

Guido van Rossum (Google)

Richard P. Muller (Caltech)

...

Python

- Open source general-purpose language.
- Object Oriented, Procedural, Functional
- Easy to interface with C/ObjC/Java/Fortran
- Easy-ish to interface with C++ (via SWIG)
- Great interactive environment

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

2.5.x / 2.6.x / 3.x ???

- “Current” version is 2.6.x
- “Mainstream” version is 2.5.x
- The new kid on the block is 3.x

You probably want 2.5.x unless you are starting from scratch. Then maybe 3.x

Technical Issues

Installing & Running Python

Binaries

- Python comes pre-installed with Mac OS X and Linux.
- Windows binaries from http://python.org/

- You might not have to do anything!

The Python Interpreter

- **Interactive interface to Python**

```
% python
Python 2.5 (r25:51908, May 25 2007, 16:14:04)
[GCC 4.1.2 20061115 (prerelease) (SUSE Linux)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

- **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

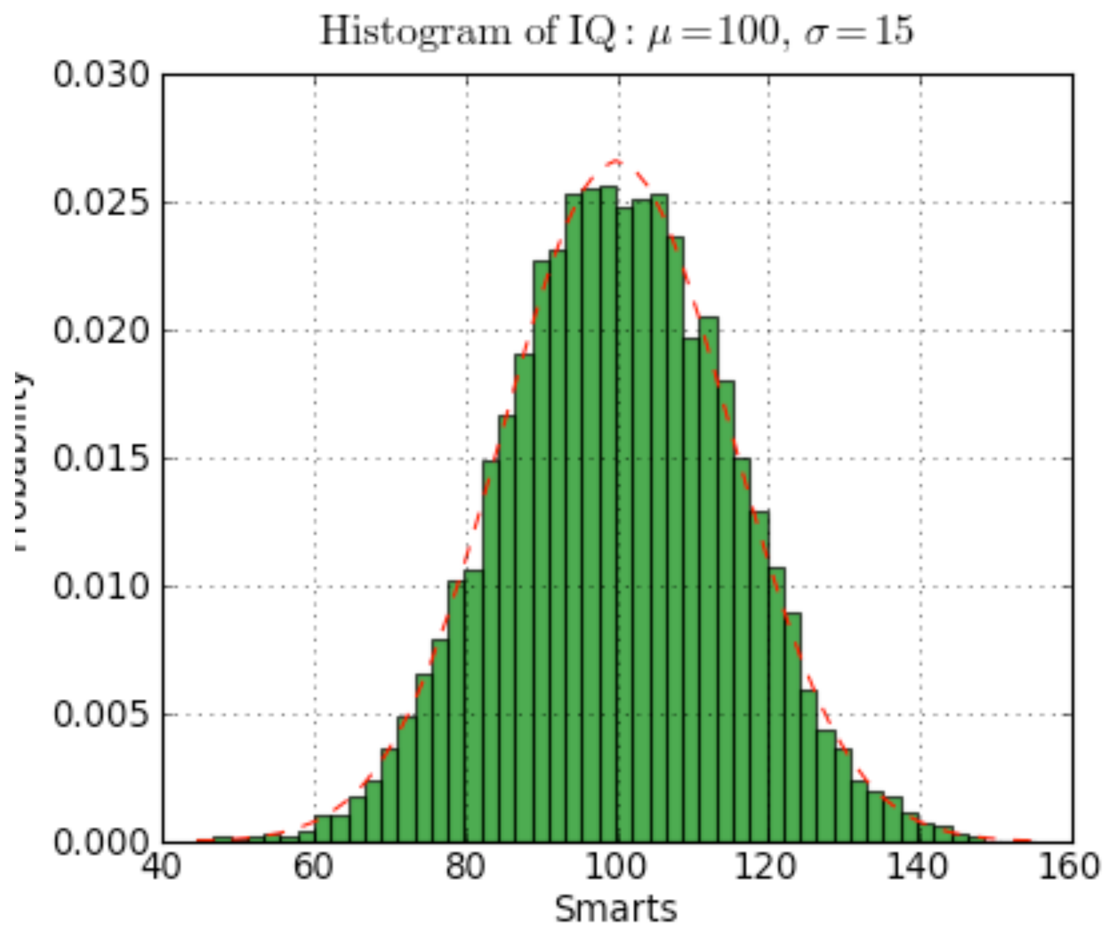
- Offers Matlab-ish capabilities within Python
- Fast array operations
- 2D arrays, multi-D arrays, linear algebra etc.

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

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/**

PyFITS

- **FITS I/O made simple:**

```
>>> import pyfits
>>> hdulist = pyfits.open('input.fits')
>>> hdulist.info()
Filename: test1.fits
No. Name Type Cards Dimensions Format
0 PRIMARY PrimaryHDU 220 () Int16
1 SCI ImageHDU 61 (800, 800) Float32
2 SCI ImageHDU 61 (800, 800) Float32
3 SCI ImageHDU 61 (800, 800) Float32
4 SCI ImageHDU 61 (800, 800) Float32
>>> hdulist[0].header['targname']
'NGC121'
>>> scidata = hdulist[1].data
>>> scidata.shape
(800, 800)
>>> scidata.dtype.name 'float32'
>>> scidata[30:40,10:20] = scidata[1,4] = 999
```

- **Downloads: http://www.stsci.edu/resources/software_hardware/pyfits**

pyds9 / python-sao

- Interaction with DS9
- Display Python 1-D and 2-D arrays in DS9
- Display FITS files in DS9

- Downloads: Ask Eric Mandel :-)
- Downloads: http://code.google.com/p/python-sao/

Wrappers for Astronomical Packages

- CasaPy (Casa)
- PYGILDAS (GILDAS)
- ParselTongue (AIPS)
- PyRAF (IRAF)
- PyMIDAS (MIDAS)
- PyIMSL (IMSL)

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 Astronomy 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

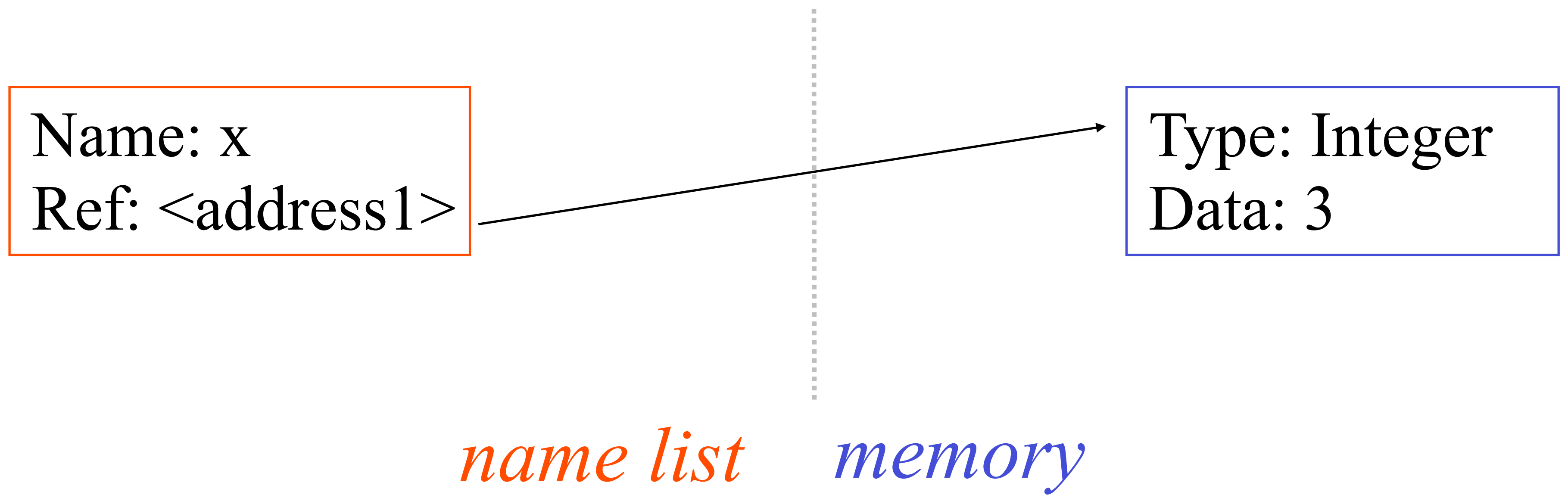
- **Assignment manipulates references**
  - x = y **does not make a copy** of the object y references
  - x = y makes x **reference** the object y references
- **Very useful; but beware!**
- **Example:**

```
>>> 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

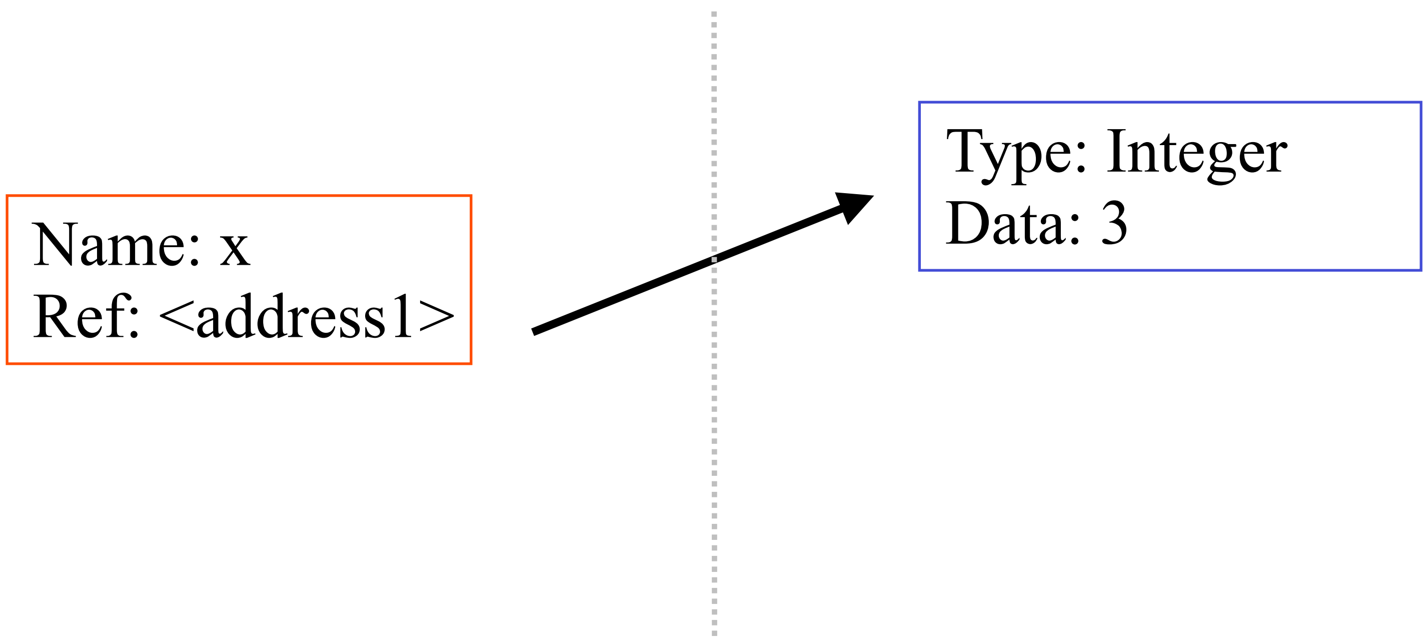
- The data 3 we created is of type integer. In Python, the datatypes integer, float, and string (and tuple) are "immutable."
- This doesn't mean we can't change the value of x, i.e. *change what x refers to* …
- For example, we could increment x:

```
>>> 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.*

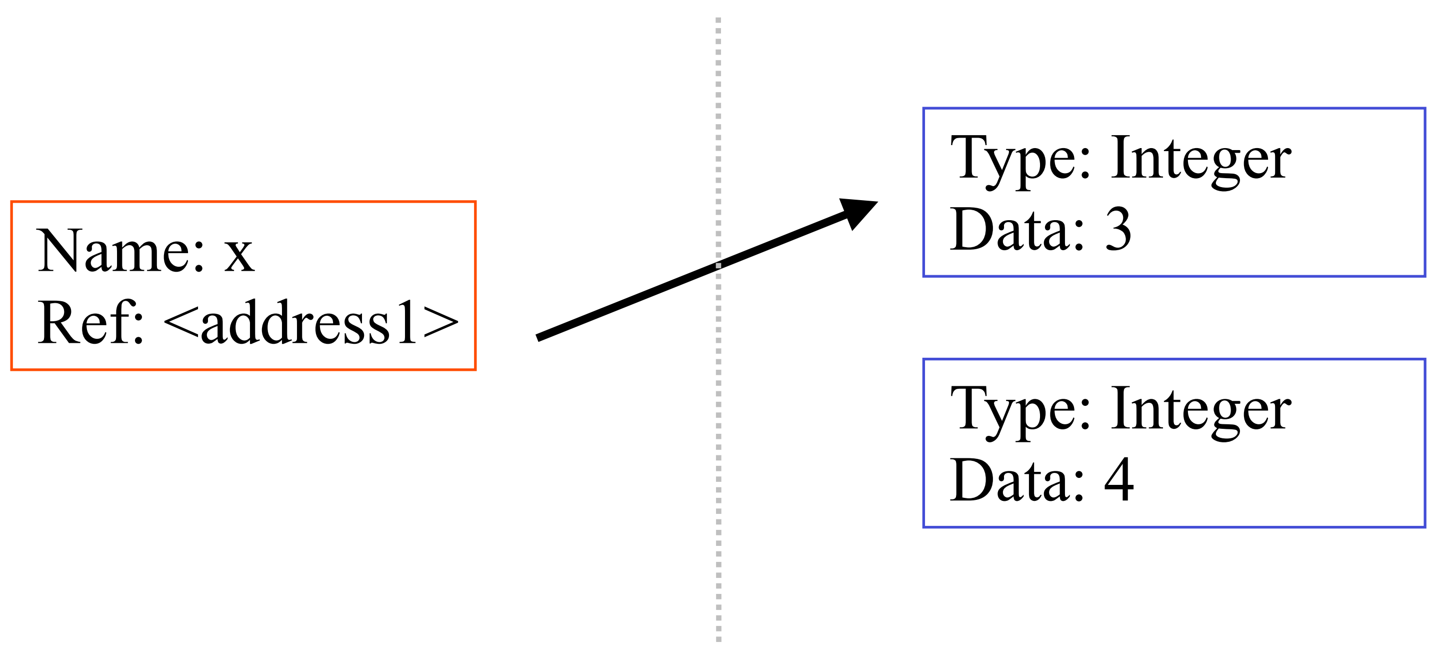
```
>>> x = x + 1
```



Understanding Reference Semantics IV

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

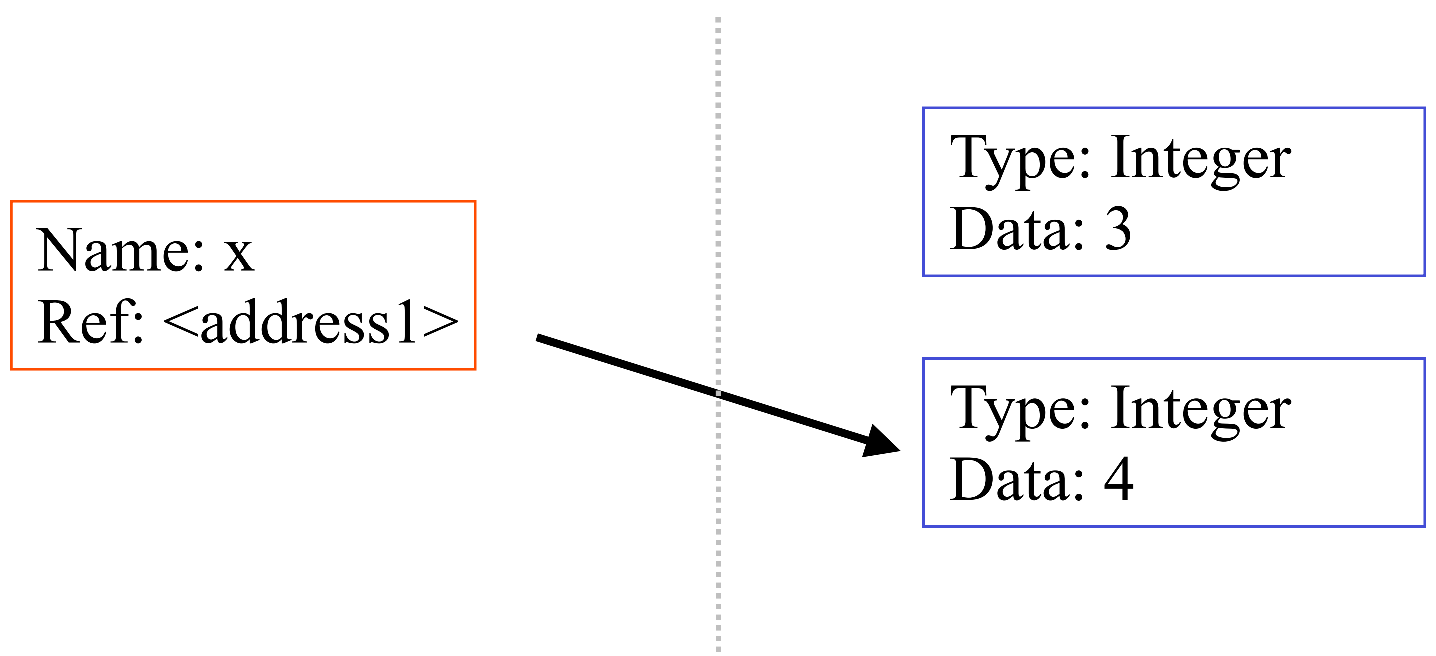
```
>>> x = x + 1
```



Understanding Reference Semantics IV

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

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

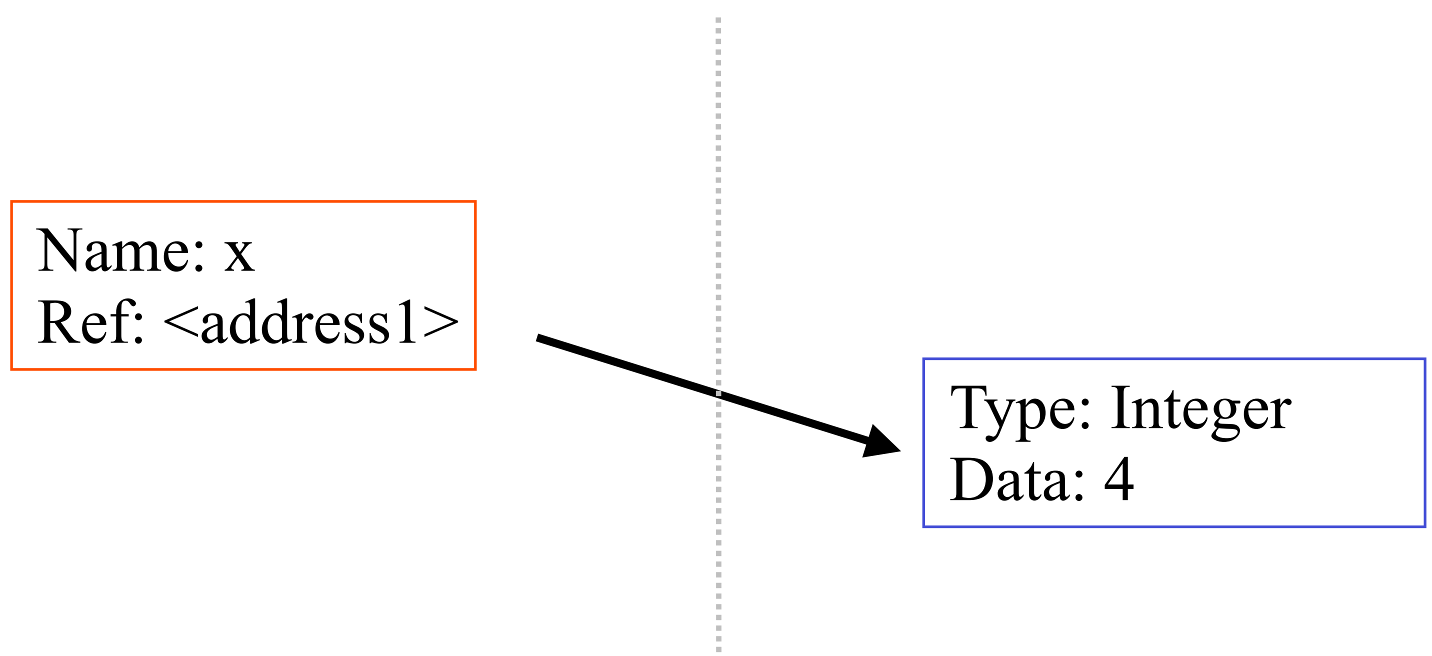


Understanding Reference Semantics IV

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

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

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.
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

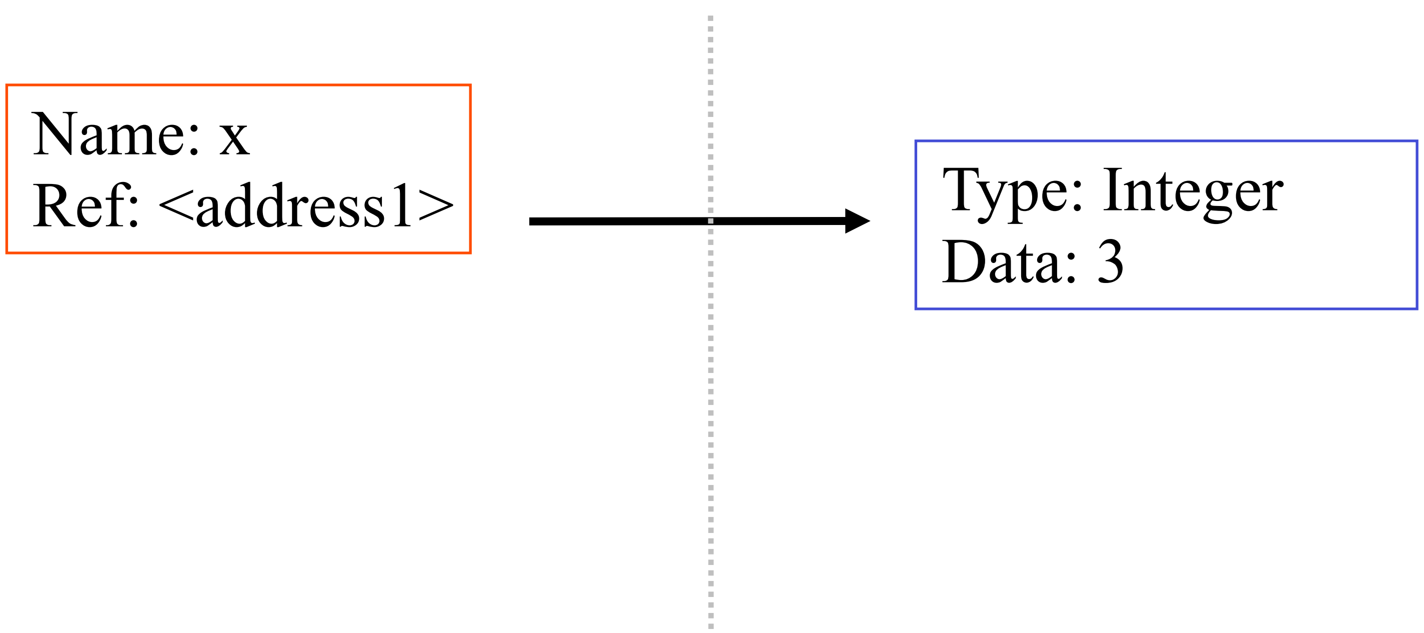
- **So, for simple built-in datatypes (integers, floats, strings), assignment behaves as you would expect:**

```
>>> 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
```

Assignment 1

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

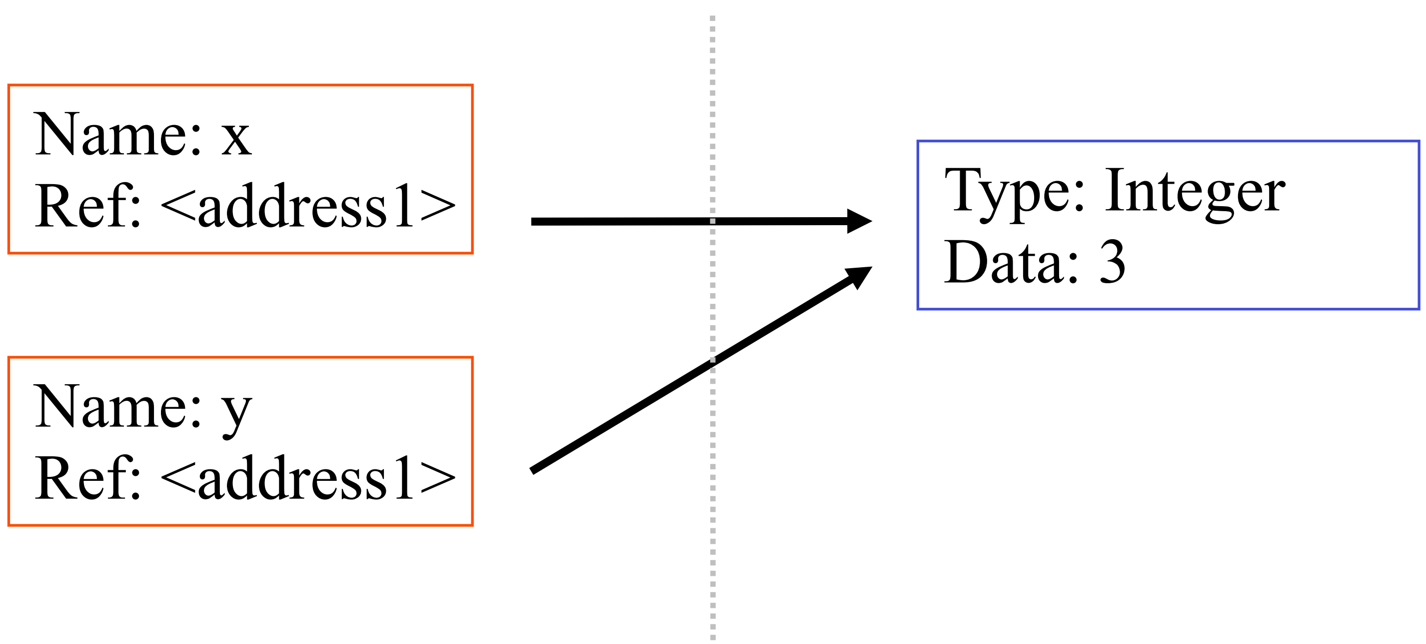
```
>>> x = 3         # Creates 3, name x refers to 3
>>> y = x         # Creates name y, refers to 3.
>>> y = 4         # Creates ref for 4. Changes y.
>>> print x       # No effect on x, still ref 3.
3
```



Assignment 1

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

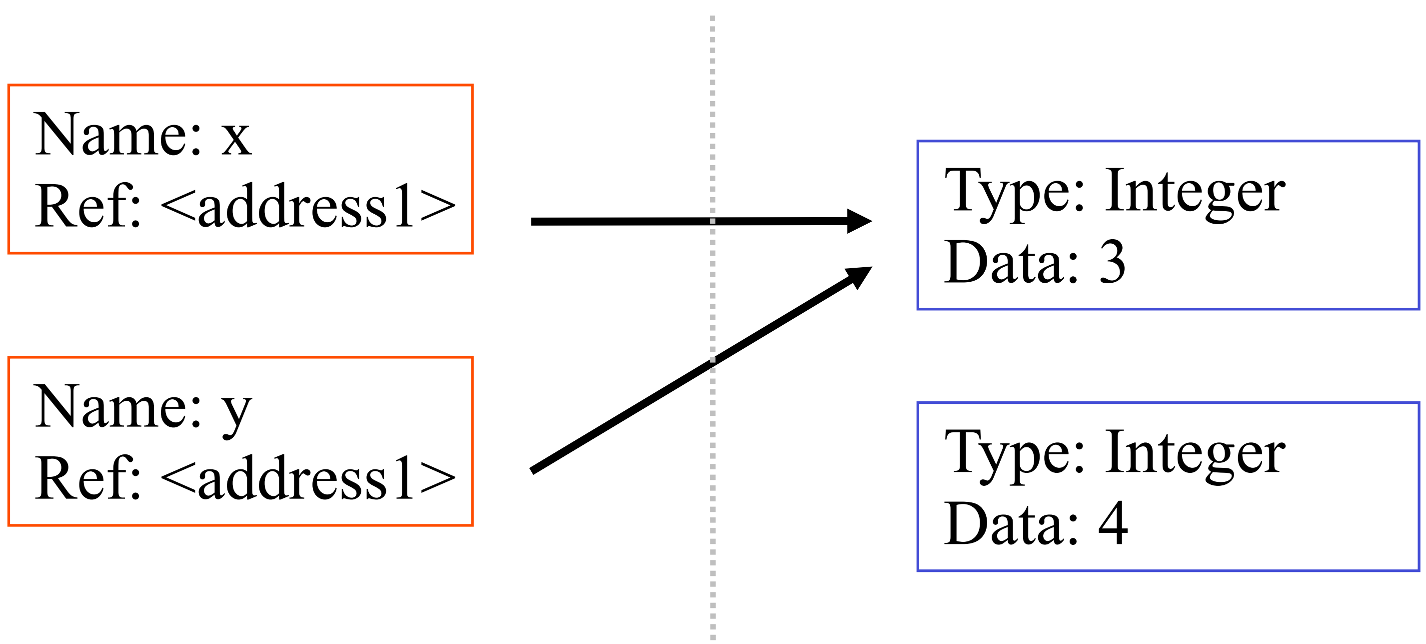
```
>>> x = 3          # Creates 3, name x refers to 3
>>> y = x          # Creates name y, refers to 3.
>>> y = 4          # Creates ref for 4. Changes y.
>>> print x        # No effect on x, still ref 3.
3
```



Assignment 1

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

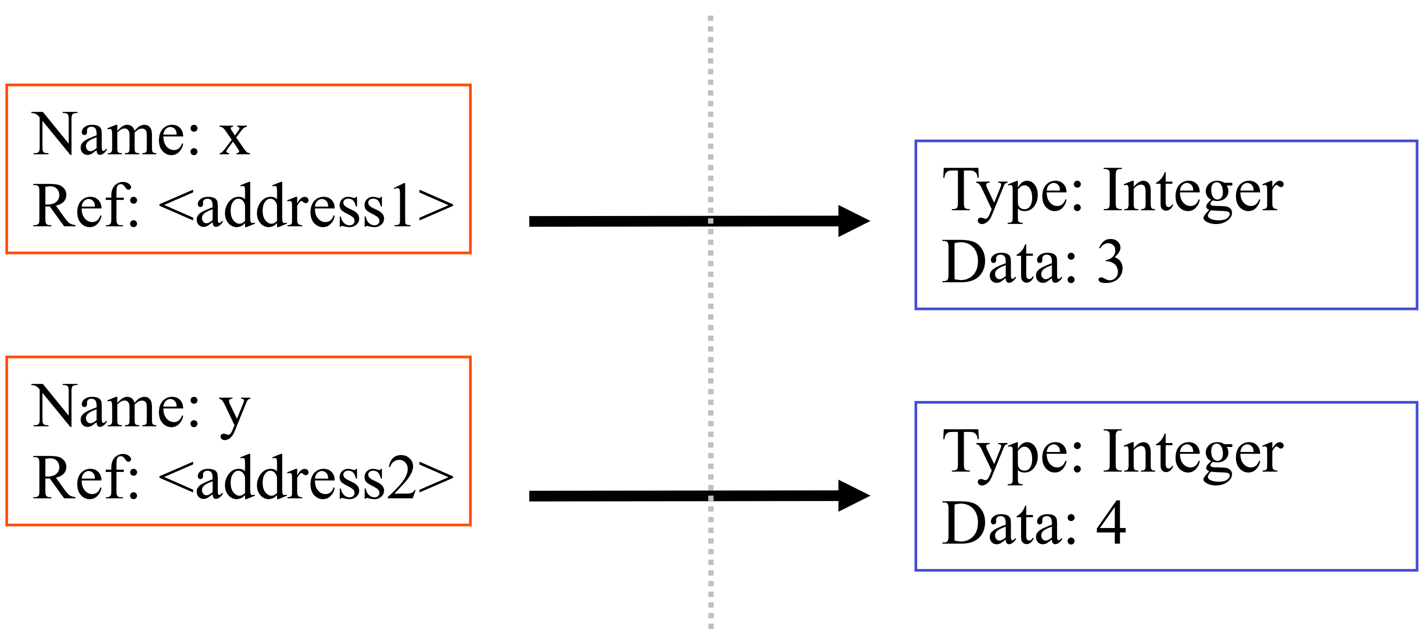
```
>>> x = 3          # Creates 3, name x refers to 3
>>> y = x          # Creates name y, refers to 3.
>>> y = 4          # Creates ref for 4. Changes y.
>>> print x        # No effect on x, still ref 3.
3
```



Assignment 1

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

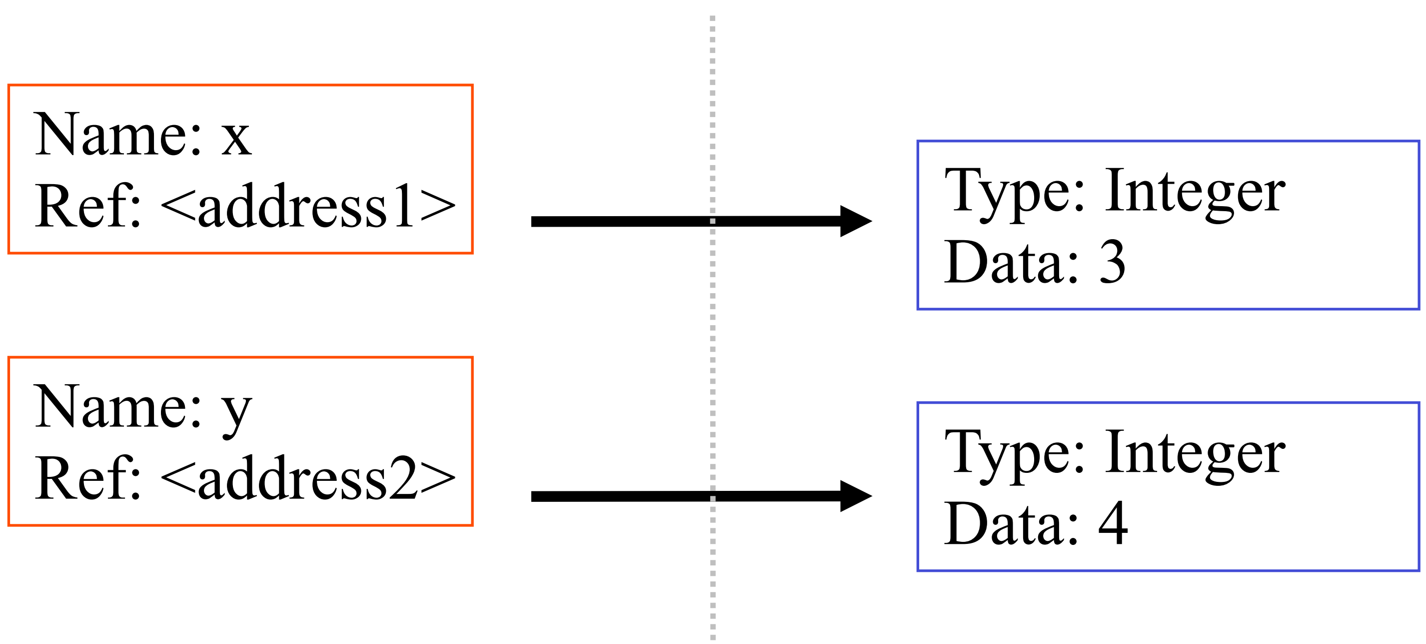
```
>>> x = 3          # Creates 3, name x refers to 3
>>> y = x          # Creates name y, refers to 3.
>>> y = 4          # Creates ref for 4. Changes y.
>>> print x        # No effect on x, still ref 3.
3
```



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
```



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

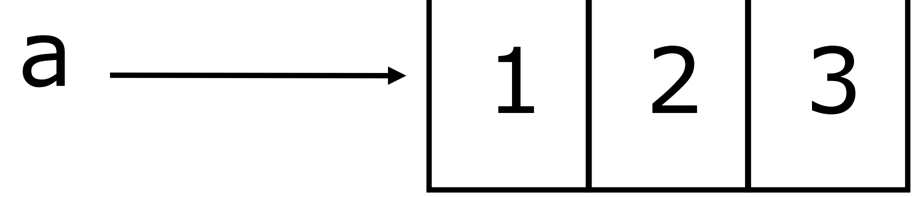
```
>>> x = 3
>>> y = x
>>> y = 4
>>> print x
3
```

mutable

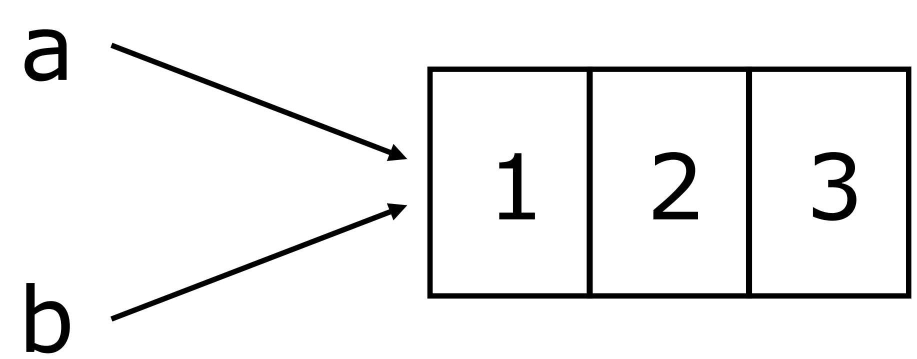
```
x = some mutable object
y = x
make a change to y
look at x
x will be changed as well
```

Why? Changing a Shared List

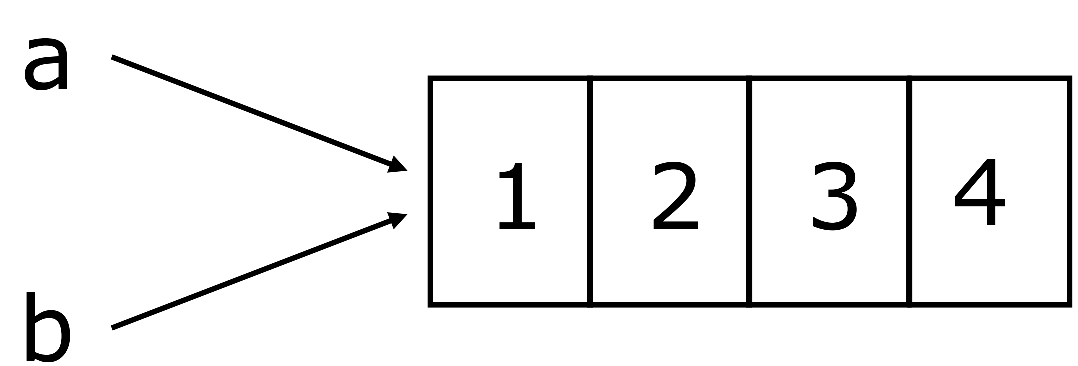
a = [1, 2, 3]



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

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 don'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...

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'
```