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# Introduction to Python

**Heavily based on presentations by**  
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**...**

# Python

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- 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 ???

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- **“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**

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# **Technical Issues**

## **Installing & Running Python**

# Binaries

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- **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

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- **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

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```
% 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

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

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



# numpy

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- 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](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

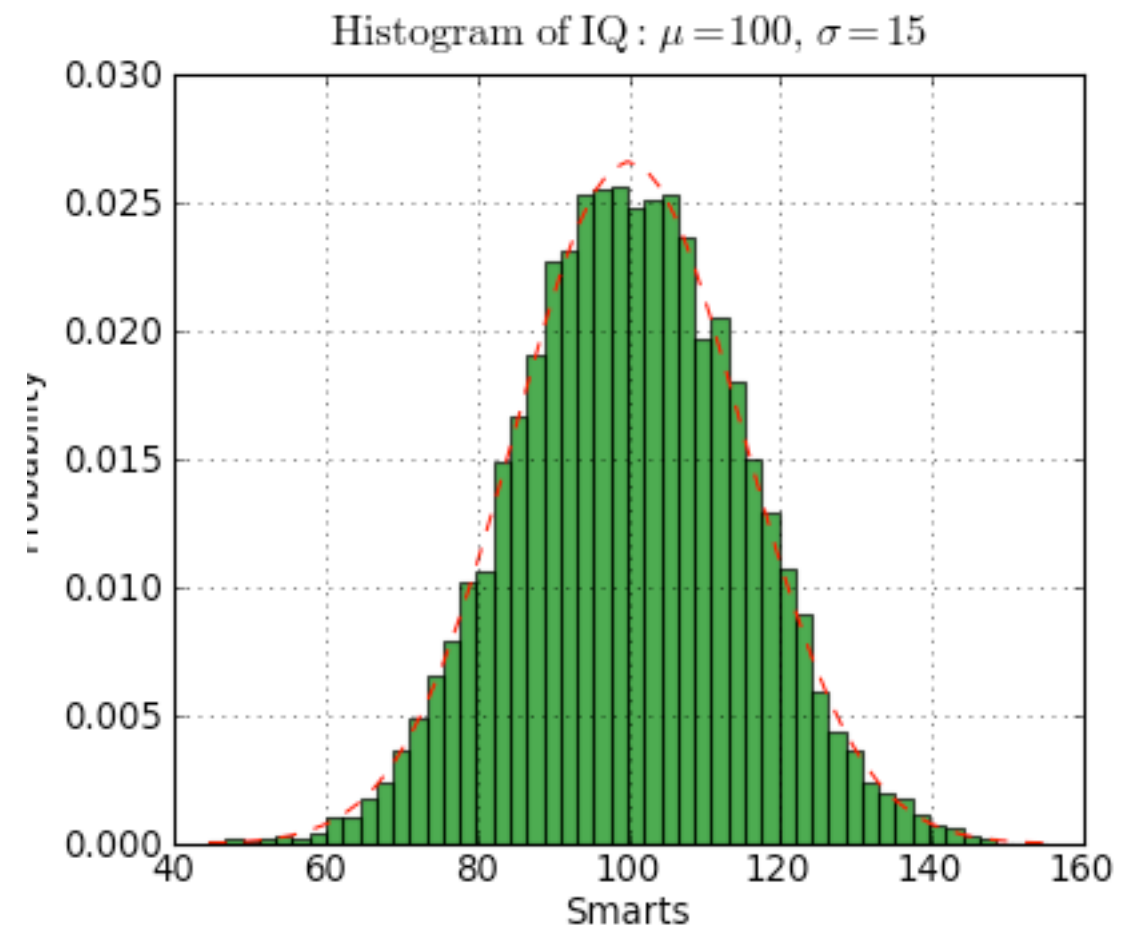
mu, sigma = 100, 15
x = mu + sigma*np.random.randn(10000)

# 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/>

# Installing Ipython

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1. IPython is a platform for Python development that contains a number of tools and environments for running Python
2. It has more features than the standard interpreter.

```
$ pip install ipython[all]
```

```
$ pip install --user ipython[all]
```

# Installing Ipython

---

1. IPython contains the powerful IPython Notebook, which allows you to write programs in a web browser.
2. It also formats your code, shows output, and allows you to annotate your scripts.

```
$ ipython3 notebook
```

# Installing scikit-learn

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1. The scikit-learn package is a machine learning library, written in Python.
2. It contains numerous algorithms, datasets, utilities, and frameworks for performing machine learning.

```
$ pip3 install -U scikit-learn
```

---

# 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

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- 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

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- **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

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- 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

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# Understanding Reference Semantics in Python



# Understanding Reference Semantics

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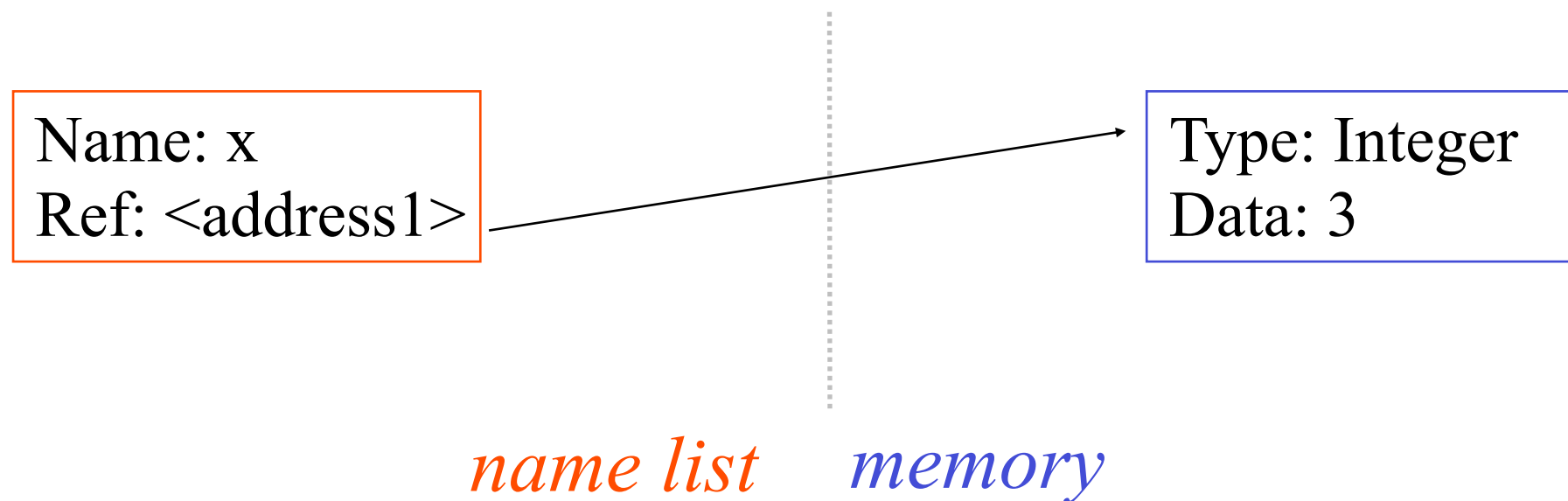
- **Assignment manipulates references**
  - $x = y$  **does not make a copy** of the object  $y$  references
  - $x = y$  makes  $x$  **reference** the object  $y$  references
- **Very useful; but beware!**
- **Example:**

```
>>> 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

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- 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
```

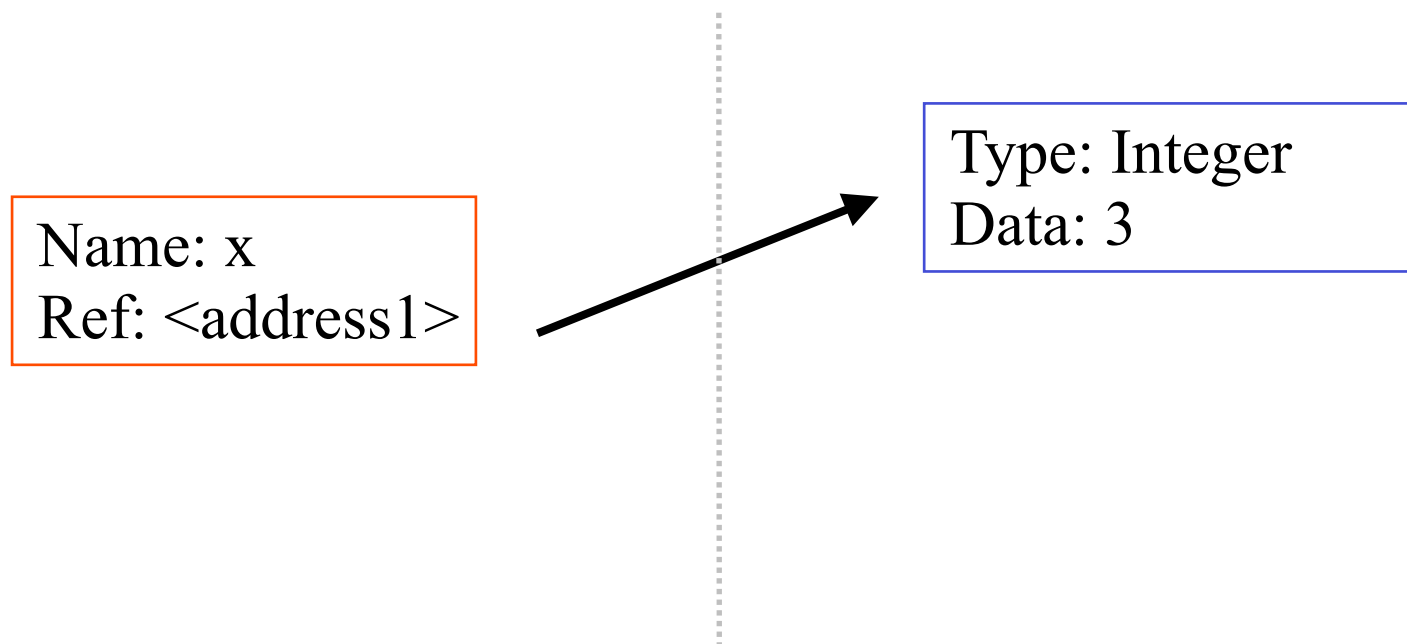
# Understanding Reference Semantics IV

---

- 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

---

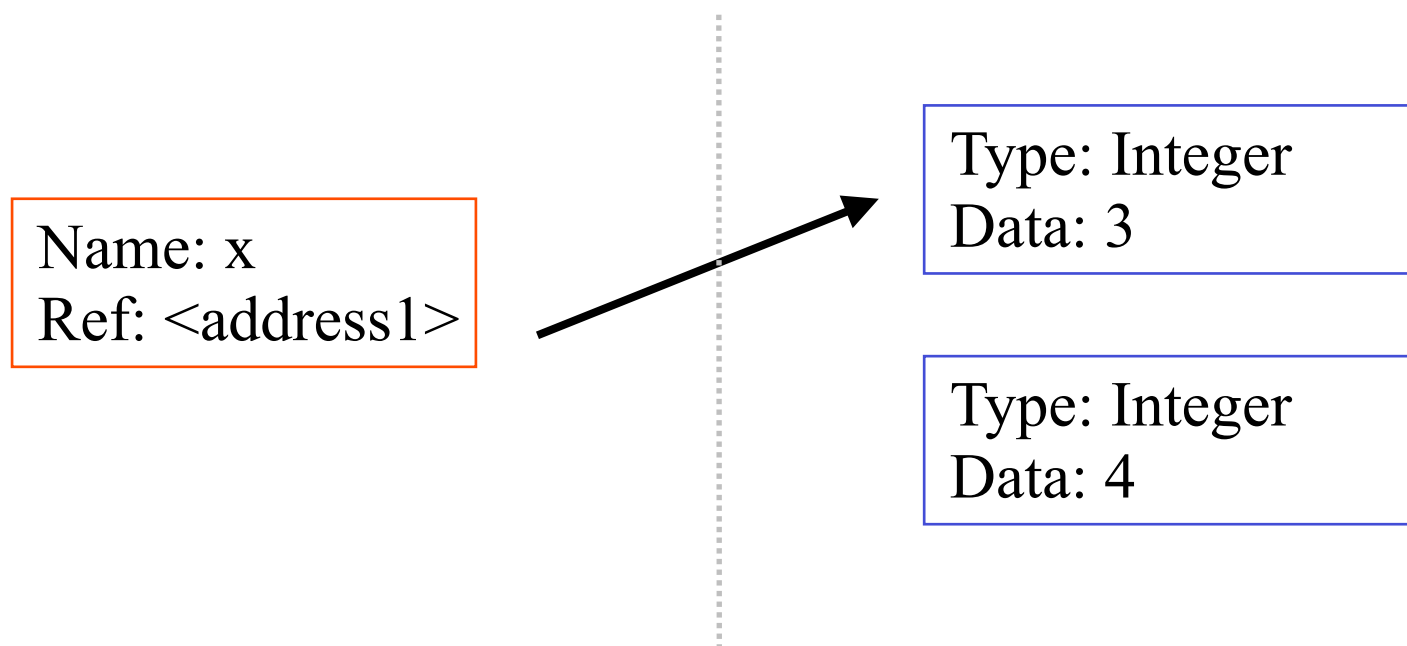
- If we increment  $x$ , then what's really happening is:

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.*

$\ggg x = x + 1$

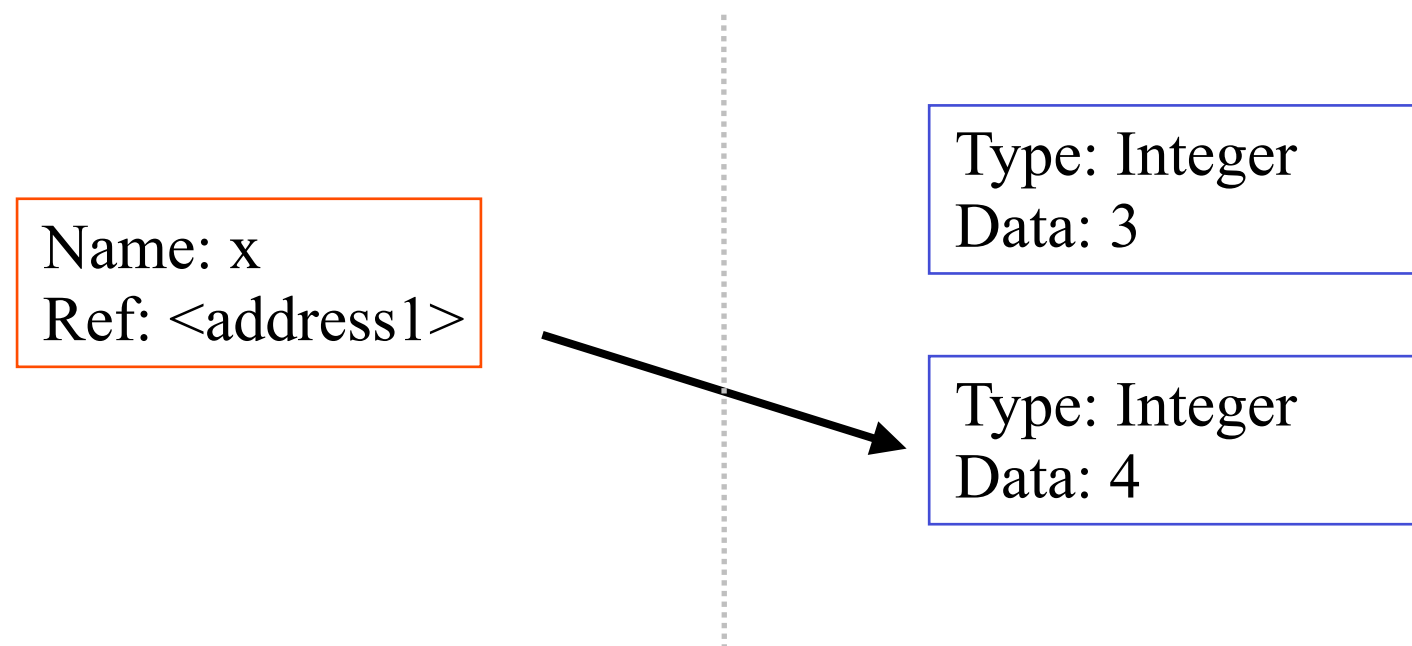


# Understanding Reference Semantics IV

- 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.*

$\ggg x = x + 1$



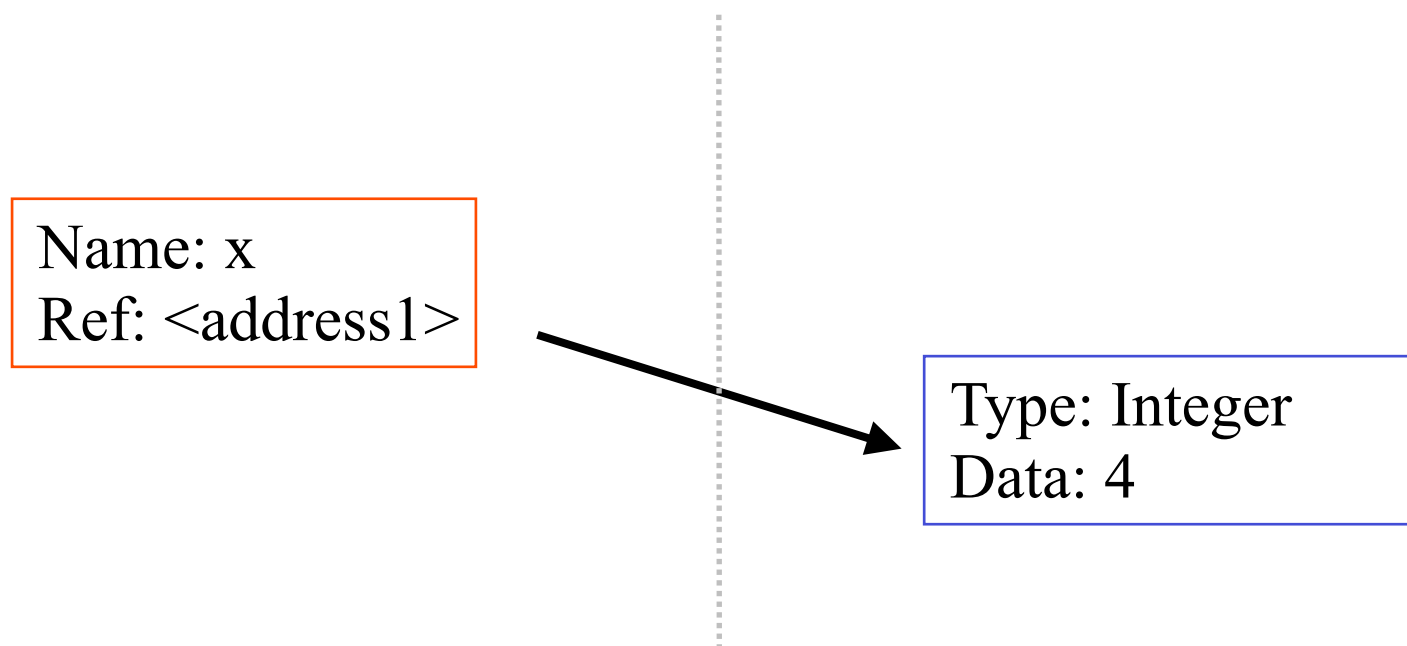
# Understanding Reference Semantics IV

---

- 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.
5. *The old data  $3$  is garbage collected if no name still refers to it.*

$\ggg x = x + 1$



# 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
```



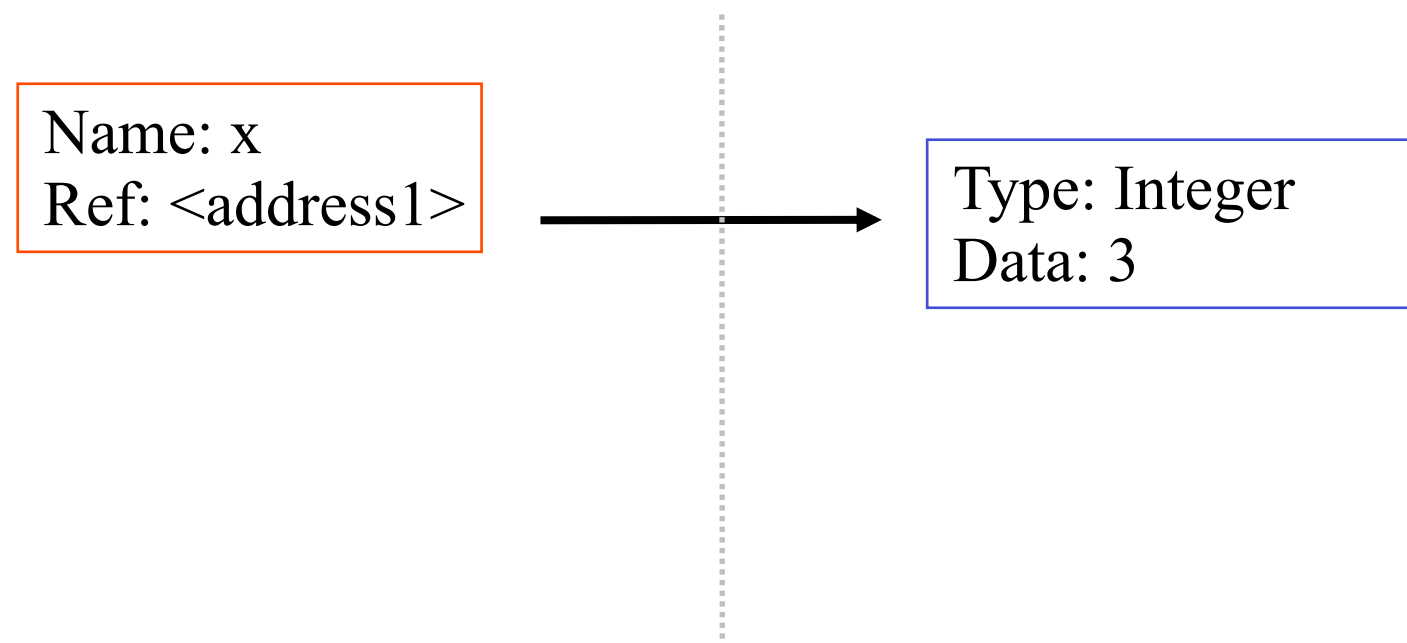
# Assignment 1

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→ 

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



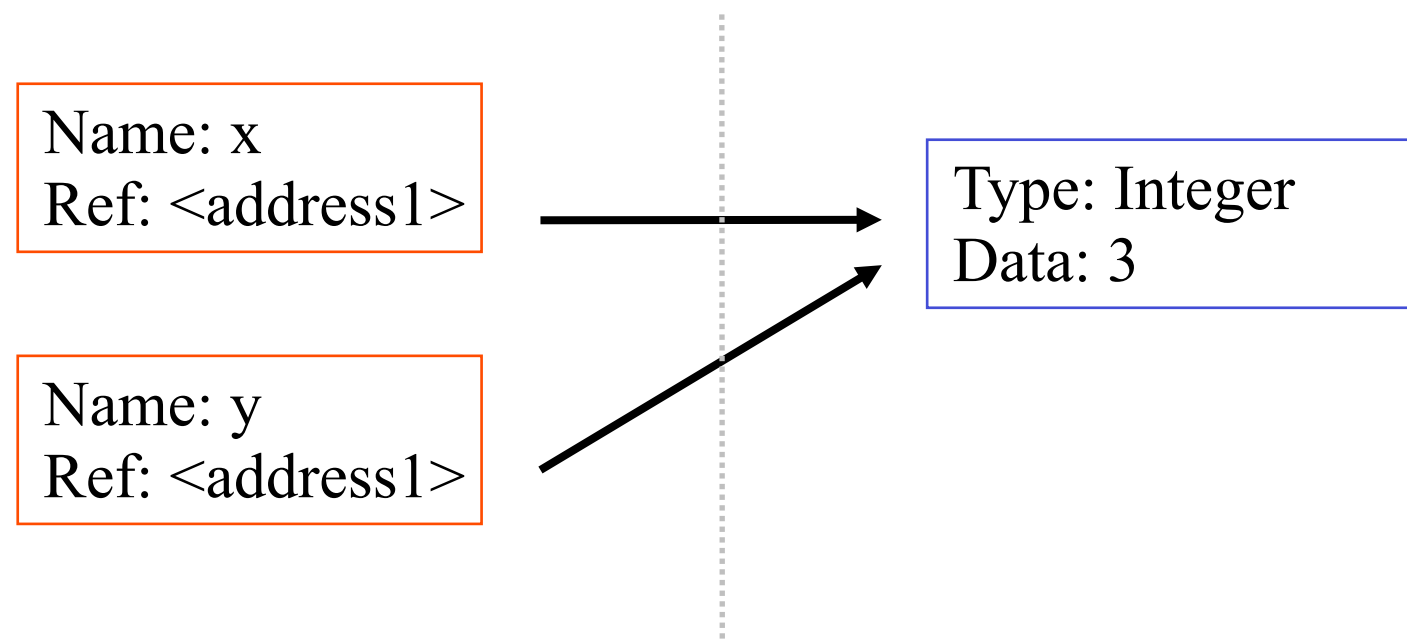
# Assignment 1

---

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→ 

```
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>>> 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
```



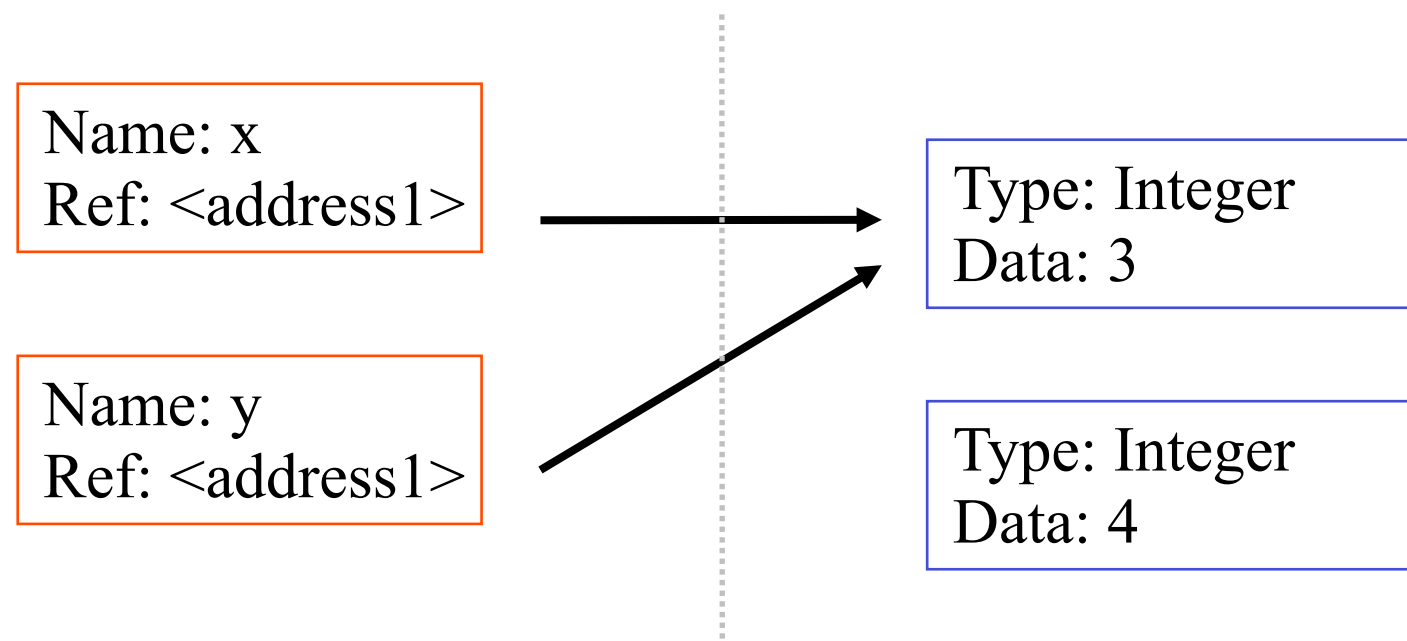
# Assignment 1

---

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→ 

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>>> 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
```

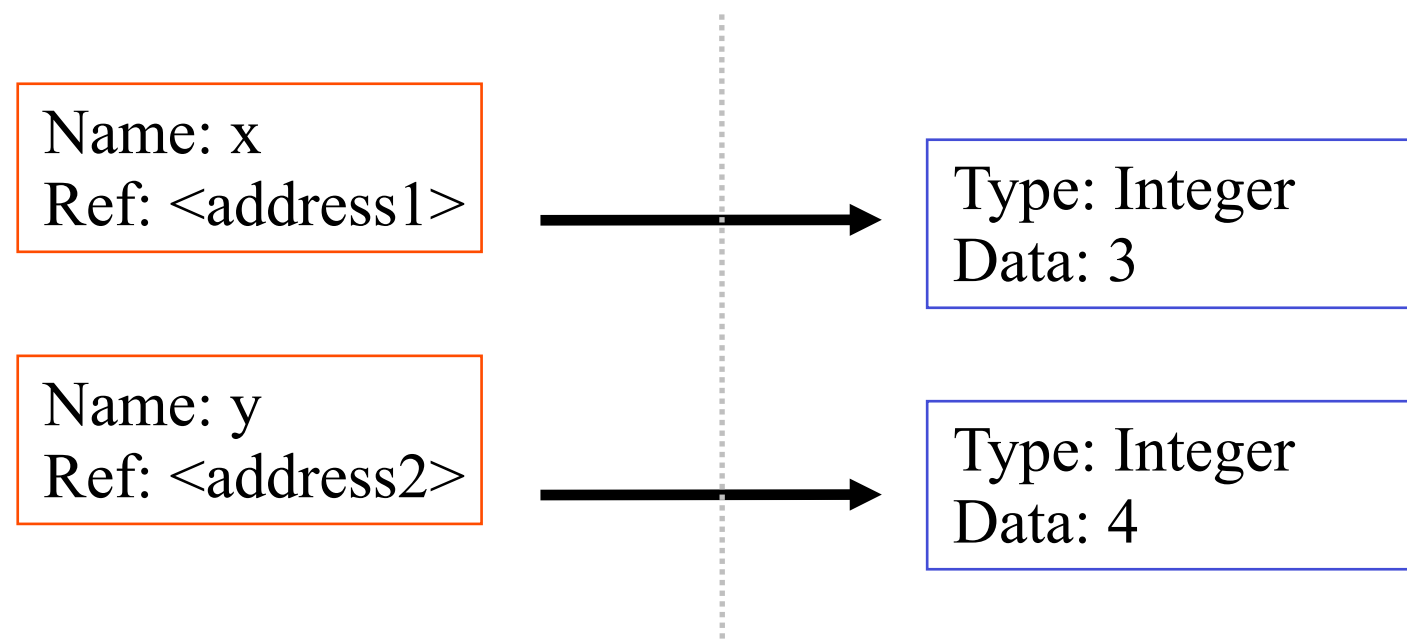


# Assignment 1

---

- 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
```

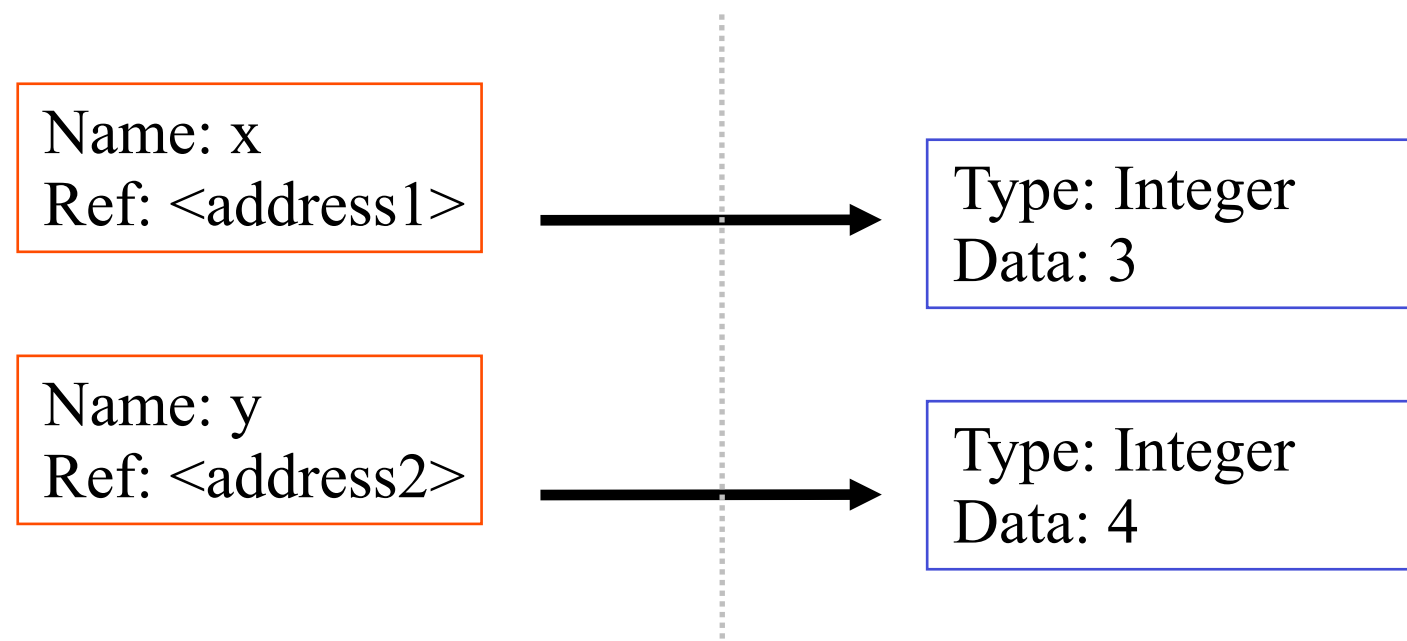


# Assignment 1

---

- 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
```

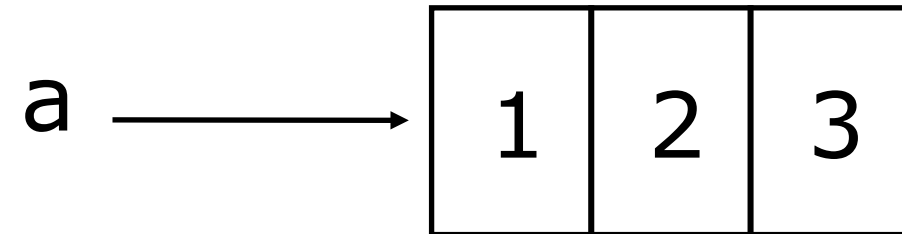
*mutable*

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

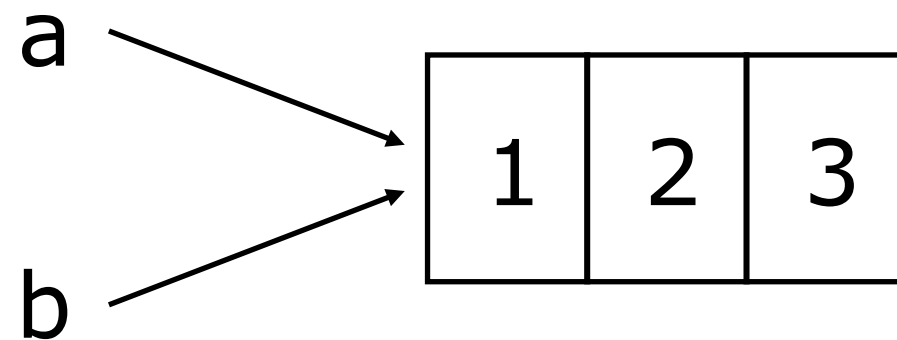
# Why? Changing a Shared List

---

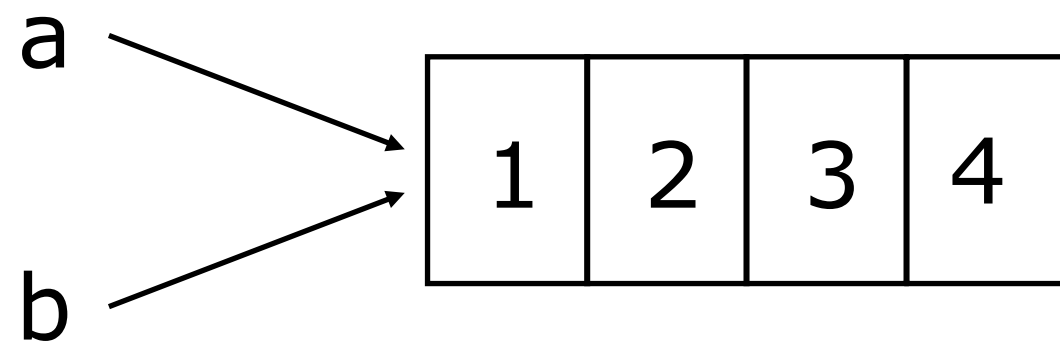
`a = [1, 2, 3]`



`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'
```