



CS135

Introduction to Machine Learning

Lecture 1: Python Programming for ML

Overview:

- ☐ Python Installation
- ☐ Python Basics
- ☐ Advanced Data Type
- ☐ Functions
- ☐ Control Flow
- ☐ Modules
- ☐ Classes and Objects (Supplemental)

Python

- ❑ Open source **general-purpose** language.
 - ❑ Object Oriented, Procedural, Functional
 - ❑ Powerful library of Modules
 - ❑ Great interactive environment
-
- ❑ Downloads: <https://www.anaconda.com/download/#macos>
 - ❑ Documentation: <https://docs.python.org/3/>
 - ❑ Pep8 Style Guidelines: <https://www.python.org/dev/peps/pep-0008/>
 - ❑ Hitchhiker's Guide: <http://docs.python-guide.org/en/latest/writing/style/>
 - ❑ The Hitchhiker's Guide to Python: <http://docs.python-guide.org/en/latest/>

Batteries Included

- ❑ Advanced data structures (lists, dictionaries) part of language
- ❑ Numerical, math, statistics
 - ❑ numpy, scipy: matlab-like functionality
 - ❑ pandas: R-like data frames
 - ❑ matplotlib: beautiful plots
- ❑ File and directory access
- ❑ Data compression and archiving
- ❑ Cryptography
- ❑ Multithreading, OS
- ❑ Networking/Internet/WWW protocols
- ❑ Multimedia
- ❑ Optimization
- ❑ ...

Python Installation

❑ Anaconda Installation

<https://docs.anaconda.com/anaconda/install/>

Silent mode install

You can use [silent mode](#) to automatically accept default settings and have no screen prompts appear during installation.

Installing Anaconda on a non-networked machine

1. Obtain a local copy of the appropriate Anaconda installer for the non-networked machine. You can copy the Anaconda installer to the target machine using many different methods including, but not limited to, a portable hard drive, USB drive or CD.
2. After copying the installer to the non-networked machine, follow the installation instructions for your operating system.

Detailed installation information

For installation instructions, see the following:

- [Installing on Windows](#)
- [Installing on macOS](#)
- [Installing on Linux](#)
- [Installing on Linux POWER8](#)
- [Verifying your installation](#)
- [Anaconda installer file hashes](#)
- [Updating from older versions](#)
- [Uninstalling Anaconda](#)

Python IDE

 PyCharm



SingaporeScript - [C:\Users\Ernst.Haagsman\PycharmProjects\SingaporeScript] - analyze.py - PyCharm 2017.1 EAP

File Edit View Navigate Code Refactor Run Tools VCS Window Help

SingaporeScript analyze.py

```
1 import pandas as pd
2 from pylab import show
3
4 aircraft_arrivals = pd.read_csv('aircraft-arrivals-departures.csv')
5 exports = pd.read_csv('domestic-exports-by-area-annual.csv')
6
7 # Set aircraft_arrival's index to a DateTimeIndex
8 aircraft_arrivals = aircraft_arrivals\
9     .set_index(pd.DatetimeIndex(aircraft_arrivals['month']))
10
11 # Set exports' index to DateTimeIndex, and ensure numeric values are numeric
12 exports = exports.set_index(
13     pd.DatetimeIndex(exports['year']).apply(
14         lambda x: pd.to_datetime(x, format='%Y'))))
15
16 exports['domestic_exports'] = exports['domestic_exports']\
17     .apply(lambda x: pd.to_numeric(x, errors='coerce'))
18
19 # Add an 'aircraft_movements' column to aircraft_arrivals
20 aircraft_arrivals = aircraft_arrivals\
21     .assign(aircraft_movements=
22         lambda x: x['aircraft_arrivals'] + x['aircraft_departures'])
23
24 annual_movements = aircraft_arrivals.resample('A').sum()
25
26 del annual_movements['aircraft_departures']
27 del annual_movements['aircraft_arrivals']
28
29 annual_exports = exports.resample('A').sum()
30
31 del annual_exports['year']
32
33 singapore_data = pd.merge(annual_movements, annual_exports,
34                             left_index=True, right_index=True)
35
36 singapore_data.plot()
37 show()
```

Data View

aircraft_movements	domestic_exports
75971	25806.00000
71365	29452.00000
68159	29158.00000
67594	29207.00000
70674	33052.00000
73223	32576.00000
73022	32063.00000
76276	39070.00000
82930	49556.00000
87421	55253.00000
97675	62754.00000
108728	66031.00000
125526	66336.80000
136762	75394.00000
145334	88533.20000
156334	98472.70000
166749	103588.80000
172672	107535.20000
165242	105917.60000
165961	138614.80000
173956	157806.70000
179360	137677.60000
174820	137354.40000
154346	174149.70000
184933	209473.50000
204138	238991.20000
214224	260301.30000
220746	268136.70000
231926	279331.40000
240360	224844.00000
263593	281122.10000
301711	315389.40000

singapore_data Format: %

Debugger Console

Frames

- MainThread
- <module>, analyze.py:28
- execfile_pydev_execfile.py:18
- run_pydev.py:1001
- <module>, pydevd.py:1624

Variables

Special Variables

- aircraft_arrivals = (DataFrame)
- annual_exports = (DataFrame)
- annual_movements = (DataFrame)
- exports = (DataFrame)
- singapore_data = (DataFrame)

2:74 CRLF UTF-8

Running Python: The Python Interpreter

```
$python
Python 2.7.10 (default, Jul 14 2015, 19:46:27)
[GCC 4.2.1 Compatible Apple LLVM 6.0 (clang-600.0.39)] on darwin
Type "help", "copyright", "credits" or "license" for more
information.
>>> 3*(7+2)
27
>>> CTRL-D           # to exit
>>> CTRL-Z           # to exit (Windows)
```

Executing Python programs

- ❑ Write a program in pycharm
 - ❑ Save it with a .py file extension

- ❑ To execute:
 - ❑ From the command line type
python <filename>.py
 - ❑ Press 'Run' in PyCharm
 - ❑ Press 'Debug' in PyCharm (debug mode)

A Simple Example

```
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)
```

Output:

```
12  
Hello World
```

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 **do not** 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 if statements, 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 like `help()` 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 Statements

```
>>> a = 1
>>> b = 1.5
>>> c = 'banana'
>>> d = "apple"
>>> print(a,b,c,d)
1 1.5 banana apple
>>> e = (a >= b)
>>> print(e)
False
```

#int

#float

#str

#"..." same as '...'

#Boolean expression

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
```

```
NameError: name 'y' is not defined
```

```
>>> y = 3
```

```
>>> y
```

```
3
```

Multiple Simultaneous Assignments

```
>>> 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

- ❑ 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

Basic Operators

❑ Binary ops on numbers

```
>>> a = 1
>>> b = 1.5
>>> print(a+b, a-b, a/b, a*b, 2**b)
2.5 -0.5 0.666666666666667 1.5 2.8284271247461903
>>> print(5/2, 1.*5/2, 5%2, 5.1//2)
2 2.5 1 2.0
```

❑ Some overloaded to work on strings

```
>>> 'banana'+'_'+ 'apple'      #concatenation
'banana_apple'
>>> 4*('appricot'+ ' ')        #replication
'appricot appricot appricot appricot '
```

Casting

```
>>> a = '1.5'
>>> b = float(a)+2                                #cast as number
>>> print('Bank Balance: $' + str(b))            #cast as str
Bank Balance: $3.5

>>> print(eval('1+2*(1/3.0)'))
                                #evaluate string as python expression
1.666666666667
```

Print to console

```
>>> b = 3
```

```
>>> print(f'Bank Balance: ${b}')           #f str
```

```
Bank Balance: $3
```

```
>>> print('Bank Balance: {}'.format(b))    #format str
```

```
Bank Balance: $3
```

```
>>> print('Bank Balance: $' + b)          #concat str
```

```
Bank Balance: $3
```

Overview

- ☐ Python Basics
- ☒ **Advanced Data Types**
- ☐ Functions
- ☐ Control Flow
- ☐ Modules
- ☐ Classes and Objects (Supplemental)

Sequence Types (a.k.a. Collections, Containers)

1. Tuple

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

2. String

- *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*
- ❑ Most operations shown in this section can be applied to all sequence types

Definitions

❑ **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."""
```


Accessing Elements

- ❑ 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 first element, starting with 0.

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

Negative lookup: count from last element, starting with -1.

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

Slicing: Return a Copy of a Subset

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

Get subsequence.

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

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

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

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')
```

Copy the Entire Sequence

To make a copy of the entire sequence, use [:].

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

Note the difference between these two assignments

```
>>> list2 = list1      # 2 names refer to same list  
                        # Changing one affects both
```

```
>>> list2 = list1[:] # Creates new independent copy
```

Membership test

Boolean test whether a value is inside a container:

```
>>> t = [1,2,3,4,5]
>>> 3 in t
True
>>> 6 in t
False
>>> 6 not in t
True
```

For strings, also tests for substrings

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

Note: `in` also used in syntax of `for` loops and *list comprehensions*

Concatenation

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"
```

Replication

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 are Immutable

```
>>> t = (23, 'abc', 4.56, (2,3), 'def')
>>> t[2] = 3.14
Traceback (most recent call last):
  File "", 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 variable name.

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


Mutability: Lists are Mutable

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

- ❑ You can change a list *in place*. (i.e., no additional memory used)
- ❑ Variable `li` still points to the same memory location after assignment
- ❑ No free lunch: supporting mutability makes lists *slower* than tuples.

Operations Only on Lists

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

```
>>> li.append('a')           # Our first exposure to an object method
```

```
>>> li
[1, 11, 3, 4, 5, 'a']
```

```
>>> li.insert(2, 'i')
```

```
>>> li
[1, 11, 'i', 3, 4, 5, 'a']
```

```
>>> li.sort()
[1, 3, 4, 5, 11, 'a', 'i']
```

```
>>> help(li)                 # see all methods that can be applied to a list
```

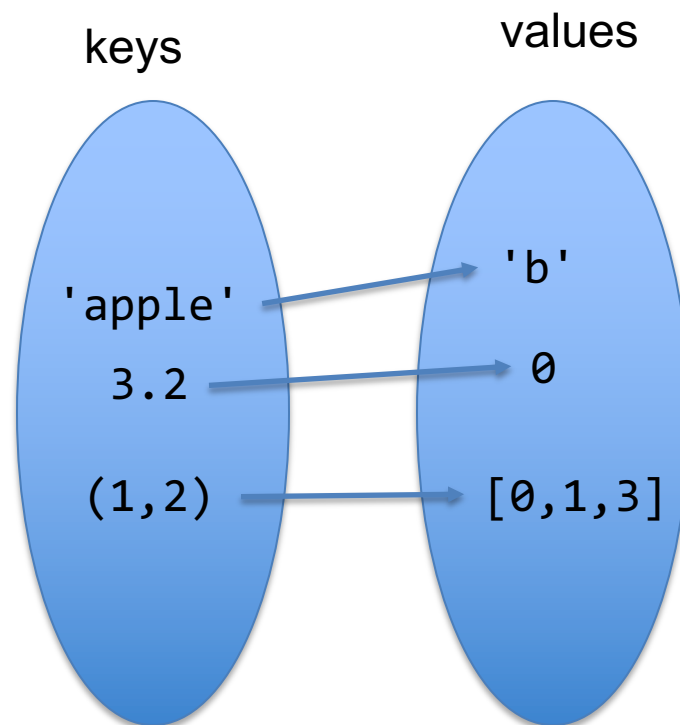
Tuples vs. Lists

- ❑ **Lists are slower but more powerful than tuples**
- ❑ **Is your data going to be *accessed* but *not changed*?**
 - **Use tuple**
- ❑ **Do you need to support modifications?**
 - **Use list**
- ❑ **Convert between tuples and lists through casting:**

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

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



Dictionary Examples

```
>>> d = {'user':'bozo', 'pswd':1234}
>>> d['user']
'bozo'
>>> d['pswd']
1234
>>> d['banana']
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
KeyError: 'banana'
```

```
# Change value for existing key
>>> d = {'user':'bozo', 'pswd':1234}
>>> d['user'] = 'clown'
>>> d
{'pswd': 1234, 'user': 'clown'}
```

```
# Add new key-value pair
>>> d['id'] = 25
>>> d
{'id': 25, 'pswd': 1234, 'user': 'clown'}
```

```
# remove key-value map
>>> d = {'user':'bozo', 'p':1234, 'i':34}
>>> del d['user']
>>> d
{'i': 34, 'p': 1234}
>>> d.clear()
>>> d
{}
```

```
#change value for existing key
>>> d = {'user':'bozo', 'p':1234, 'i':34}
>>> d.keys()           # List of keys
['i', 'p', 'user']
>>> d.values()         # List of values
[34, 1234, 'bozo']
>>> d.items()          # List of pairs as tuples.
[('i', 34), ('p', 1234), ('user', 'bozo')]
```

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if statement

```
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'."
```

#indentation defines blocks!

while statement

Fibonacci Series:

```
>>> a, b = 0, 1
>>> while a < 10:
    print(a)
    a, b = b, a+b
```

#multiple var assignment

#indentation defines block!

```
0
1
1
2
3
5
8
```


for loop

Primality Test:

```
for n in range(2, 10):
    for x in range(2, n):
        if n % x == 0:
            print(n, 'equals', x, '*', n//x)
            break
        else:
            # executed only if loop does not break early
            print(n, 'is a prime number')
```

```
2 is a prime number
3 is a prime number
4 equals 2 * 2
5 is a prime number
6 equals 2 * 3
7 is a prime number
8 equals 2 * 4
9 equals 3 * 3
```

Lists made out of other lists: List Comprehension

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

```
squares = [x**2 for x in li]
print squares
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

```
even_squares = [x for x in squares if x%2==0]
[0, 4, 16, 36, 64]
```

```
[(x,1) for x in even_squares]
[(0, 1), (4, 1), (16, 1), (36, 1), (64, 1)]
```

```
[range(x) for x in range(4)]
[[], [0], [0, 1], [0, 1, 2]]
```

```
[y for x in range(4) for y in range(x)]           # "nested" for loop
[0, 0, 1, 0, 1, 2]
```

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Function Definitions

- ❑ **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
```

Optional Arguments

- ❑ Can define default values 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 return a value:

- ❑ If no return statement, function returns None

❑ Functions can be used like *any other data type*! They can be

- ❑ Arguments to other functions
- ❑ Return values of other functions
- ❑ Assigned to variables
- ❑ Parts of tuples, lists, etc.

```
def square(x):  
    return x * x
```

```
>>> z = square
```

```
>>> z(2)
```

```
4
```

```
>>> map(square, [1,2,3,4])  
[1, 4, 9, 16]
```

```
# map's 1st input is a function!
```

Anonymous Functions: the `lambda` operator

```
def square(x):  
    return x * x
```

```
>>> map(square, [1,2,3,4])  
[1, 4, 9, 16]
```

```
>>> map(lambda x: x*x , [1,2,3,4])  
[1, 4, 9, 16]
```

```
def power_generator(n):  
    return lambda x : x ** n      #power_generator returns a function!
```

```
>>> square = power_generator(2)  
>>> cube = power_generator(3)
```

```
>>> map(square, [1,2,3,4])  
[1, 4, 9, 16]  
>>> map(cube, [1,2,3,4])  
[1, 8, 27, 64]
```

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Python Modules

- ❑ Modules comprise functions and variables defined in separate files
- ❑ Functions or variables from a module are imported using from or import

```
from numpy import sqrt          #imports only sqrt
sqrt(2343523)
```

```
import numpy                    #imports entire module
numpy.sqrt(2343523)
```

```
import numpy as np             #imports entire module as "np"
np.sqrt(2343523)
```

```
from numpy import *            #imports everything in module
sqrt(1243)
exp(-1.23)
```

- ❑ Type `help(module)` to see module functionality

numpy

- ❑ Functions galore:

`exp, log, log10, sin, cos, tan, sqrt, ...`

- ❑ Numerical Arrays and Matrices!

```
import numpy as np
```

```
a = np.array([1.0, 2.0, 2.1])
```

```
b = np.array([2.0, 1.0, -3.1])
```

```
print a + b
```

```
[ 3.  3. -1.]
```

`#vector addition`

```
print np.dot(a,b)
```

```
-2.51
```

`#vector dot product`

```
print np.outer(a,b)
```

```
[[ 2.   1.  -3.1 ]
```

```
 [ 4.   2.  -6.2 ]
```

```
 [ 4.2  2.1 -6.51]]
```

`#vector outer product`

numpy.linalg

`help(numpy.linalg)`

NAME

`numpy.linalg`

FILE

`/Library/Python/2.7/site-packages/numpy-1.11.0-py2.7-macosx-10.10-intel.egg/numpy/linalg/__init__.py`

DESCRIPTION

Core Linear Algebra Tools

Linear algebra basics:

- `norm` Vector or matrix norm
- `inv` Inverse of a square matrix
- `solve` Solve a linear system of equations
- `det` Determinant of a square matrix
- `lstsq` Solve linear least-squares problem
- `pinv` Pseudo-inverse (Moore-Penrose) calculated using a singular value decomposition
- `matrix_power` Integer power of a square matrix

Eigenvalues and decompositions:

- `eig` Eigenvalues and vectors of a square matrix
- `eigh` Eigenvalues and eigenvectors of a Hermitian matrix
- `eigvals` Eigenvalues of a square matrix
- `eigvalsh` Eigenvalues of a Hermitian matrix
- `qr` QR decomposition of a matrix
- `svd` Singular value decomposition of a matrix
- `cholesky` Cholesky decomposition of a matrix

Tensor operations:

- `tensorsolve` Solve a linear tensor equation
- `tensorinv` Calculate an inverse of a tensor

A few useful modules

❑ See documentation for following modules:

<code>scipy</code>	<code># Numerical integration, linear algebra, # signal processing, Fourier transforms</code>
<code>numpy.random</code>	<code># Sample random numbers</code>
<code>argparse</code>	<code># parse command line arguments</code>
<code>sklearn</code>	<code># Machine learning algorithms</code>
<code>sklearn.linear_model</code>	<code># Linear & logistic regression</code>
<code>sys</code>	<code># I/O</code>
<code>time</code>	<code># time utilities</code>
<code>matplotlib.pyplot</code>	<code># plotting tools</code>

Use Docstrings!

```
class atom(object):  
    """This will be shown whenever someone calls help(atom), along  
    with list of public methods """  
  
    def symbol(self):  
        """This will be shown whenever someone  
        calls help(atom.symbol) or help(x.symbol)  
        where x is an atom object"""  
        return Atno_to_Symbol[atno]
```

Overview

- ☐ Python Basics
- ☐ Advanced Data Types
- ☐ Control Flow
- ☐ Functions
- ☐ Modules
- ☒ Classes & Objects (Supplemental)

What is an Object?

- ❑ A data structure that contains *variables* and *methods*
- ❑ Object Oriented Design abides by the principles of:
 - **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 __str__(self): # overloads str() function
        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`) and a class method (`symbol`)
 - accessed as `self.atno` within the class definition
 - accessed as `at.atno` outside class for atom `at`
- ❑ 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, easier to interpret programs result
- ❑ **Overloaded** the `str()` operator
- ❑ We now want to use the atom class to build molecules...

Molecules

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

Using the Molecule Class

```
>>> mol = molecule('Water')
>>> 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      0.0000      0.0000      0.0000
1      0.0000      0.0000      1.0000
1      0.0000      1.0000      0.0000
```

- ❑ Note that the str function calls the atoms str 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 dna_molecule(molecule):  
    def clone(self):  
        new_molecule = dna_molecule(molecule.name)  
        for at in self.atomlist:  
            new_molecule.addatom(atom(at.atno,  
                                       at.position[0],  
                                       at.position[1],  
                                       at.position[2]))  
  
        return new_molecule
```

- ❑ `__init__`, `__str__`, and `addatom` are *inherited* from the parent class (`molecule`)!
- ❑ `dna_molecule` is augmented with an additional method (`clone`)
- ❑ Another example of code reuse

Overriding Parent Methods

```
class dna_molecule(molecule):
    def __init__(self, name='DNA molecule', isOrganic=True):
        self.isOrganic=isOrganic
        super(dna_molecule, self).__init__(name)
    def clone(self):
        new_molecule = dna_molecule(molecule.name)
        for at in self.atomlist:
            new_molecule.addatom(atom(at.atno,
                                         at.position[0],
                                         at.position[1],
                                         at.position[2]))
        return new_molecule
```

- ❑ A parent method (`__init__`) gets a new definition, using also the parent definition

Private and public variables and methods

- ❑ In Python anything with two leading underscores is private

`__a`, `__my_variable`

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

`_b`

- ❑ Sometimes useful as an intermediate step to making variable private

Overloading Operators

__contains__(...)

$x._\text{contains}__(y) \iff y \text{ in } x$

__eq__(...)

$x._\text{eq}__(y) \iff x==y$

__ge__(...)

$x._\text{ge}__(y) \iff x \geq y$

__add__(...)

$x._\text{add}__(y) \iff x+y$

__lt__(...)

$x._\text{lt}__(y) \iff x < y$

__mul__(...)

$x._\text{mul}__(n) \iff x*n$