Numerical and Scientific Packages

Scipy and friends

By far, the most commonly used packages are those in the SciPy stack. We will focus on these in this class. These packages include:

- NumPy
- SciPy
- Matplotlib – plotting library.
- IPython – interactive computing.
- Pandas – data analysis library.
- SymPy – symbolic computation library.

Numpy

Let's start with NumPy. Among other things, NumPy contains:

- A powerful N-dimensional array object.
- Sophisticated (broadcasting/universal) functions.
- Tools for integrating C/C++ and Fortran code.
- Useful linear algebra, Fourier transform, and random number capabilities.

Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data.

Numpy

The key to NumPy is the ndarray object, an *n*-dimensional array of homogeneous data types, with many operations being performed in compiled code for performance. There are several important differences between NumPy arrays and the standard Python sequences:

- NumPy arrays have a fixed size. Modifying the size means creating a new array.
- NumPy arrays must be of the same data type, but this can include Python objects.
- More efficient mathematical operations than built-in sequence types.

Numpy Datatypes

To begin, NumPy supports a wider variety of data types than are built-in to the Python language by default. They are defined by the numpy.dtype class and include:

- intc (same as a C integer) and intp (used for indexing)
- int8, int16, int32, int64
- uint8, uint16, uint32, uint64
- float16, float32, float64
- complex64, complex128
- bool_, int_, float_, complex_ are shorthand for defaults.

These can be used as functions to cast literals or sequence types, as well as arguments to numpy functions that accept the dtype keyword argument.

Numpy Datatypes

- Some examples:

```
>>> import numpy as np
>>> x = np.float32(1.0)
>>> x
1.0
>>> y = np.int_([1,2,4])
>>> y
array([1, 2, 4])
>>> z = np.arange(3,
dtype=np.uint8)
>>> z
array([0, 1, 2], dtype=uint8)
>>> z.dtype
dtype('uint8')
```

Numpy Arrays

There are a couple of mechanisms for creating arrays in NumPy:

- Conversion from other Python structures (e.g., lists, tuples).
- Built-in NumPy array creation (e.g., arange, ones, zeros, etc.).
- Reading arrays from disk, either from standard or custom formats (e.g. reading in from a CSV file).
- and others …

Numpy arrays

- In general, any numerical data that is stored in an array-like container can be converted to an ndarray through use of the array() function. The most obvious examples are sequence types like lists and tuples.

```
>>> x = np.array([2,3,1,0])
>>> x = np.array([2, 3, 1, 0])
>>> x = np.array([[1,2.0],[0,0],(1+1j,3.)])
>>> x = np.array([[ 1.+0.j, 2.+0.j], [ 0.+0.j, 0.+0.j],
[ 1.+1.j, 3.+0.j]])
```

Numpy Arrays

There are a couple of built-in NumPy functions which will create arrays from scratch.

- zeros(shape) -- creates an array filled with 0 values with the specified shape. The default dtype is float64.

```
>>> np.zeros((2, 3))
array([[ 0., 0., 0.], [ 0., 0., 0.]])
```

- ones(shape) -- creates an array filled with 1 values.
- arange() -- creates arrays with regularly incrementing values.

```
>>> np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.arange(2, 10, dtype=np.float)
array([ 2., 3., 4., 5., 6., 7., 8., 9.])
>>> np.arange(2, 3, 0.1)
array([ 2. , 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8,
2.9])
```

Numpy Arrays

- linspace() -- creates arrays with a specified number of elements, and spaced equally between the specified beginning and end values.

```
>>> np.linspace(1., 4., 6)
array([ 1. , 1.6, 2.2, 2.8, 3.4,
4. ])

>>> np.random.random((2,3))
array([[ 0.75688597, 0.41759916,
0.35007419],
       [ 0.77164187, 0.05869089,
0.98792864]])
```

- random.random(shape) – creates arrays with random floats over the interval [0,1).

Numpy Arrays

- Printing an array can be done with the print statement.

```
>>> import numpy as np
>>> a = np.arange(3)
>>> print a
[0 1 2]
>>> a
array([0, 1, 2])
>>> b =
np.arange(9).reshape(3,3)
>>> print b
[[0 1 2]
 [3 4 5]
 [6 7 8]]
>>> c =
np.arange(8).reshape(2,2,2)
>>> print c
[[[0 1]
  [2 3]]

 [[4 5]
  [6 7]]]
```

Indexing

- Single-dimension indexing is accomplished as usual.

```
>>> x = np.arange(10)
>>> x[2]
2
>>> x[-2]
8
```

- Multi-dimensional arrays support multi-dimensional indexing.

```
>>> x.shape = (2,5) # now x is 2-dimensional
>>> x[1,3]
8
>>> x[1,-1]
9
```

Indexing

- Using fewer dimensions to index will result in a subarray.

```
>>> x[0]
array([0, 1, 2, 3, 4])
```

- This means that `x[i, j] == x[i][j]` but the second method is less efficient.

Indexing

- Slicing is possible just as it is for typical Python sequences.

```
>>> x = np.arange(10)
>>> x[2:5]
array([2, 3, 4])
>>> x[:-7]
array([0, 1, 2])
>>> x[1:7:2]
array([1, 3, 5])
>>> y = np.arange(35).reshape(5,7)
>>> y[1:5:2,::3]
array([[ 7, 10, 13], [21, 24, 27]])
```

Array operations

```
>>> a = np.arange(5)
>>> b = np.arange(5)
>>> a+b
array([0, 2, 4, 6, 8])
>>> a-b
array([0, 0, 0, 0, 0])
>>> a**2
array([ 0,  1,  4,  9, 16])
>>> a>3
array([False, False, False,
False,  True], dtype=bool)
>>> 10*np.sin(a)
array([ 0.,
8.41470985, 9.09297427, 1.41120008, -
7.56802495])
>>> a*b
array([ 0,  1,  4,  9, 16])
```

- Basic operations apply element-wise. The result is a new array with the resultant elements.

Operations like *= and += will modify the existing array.

Array operations

- Since multiplication is done element-wise, you need to specifically perform a dot product to perform matrix multiplication.

```
>>> a = np.zeros(4).reshape(2,2)
>>> a
array([[ 0.,  0.],
       [ 0.,  0.]])
>>> a[0,0] = 1
>>> a[1,1] = 1
>>> b = np.arange(4).reshape(2,2)
>>> b
array([[0, 1],
       [2, 3]])
>>> a*b
array([[ 0.,  0.],
       [ 0.,  3.]])
>>> np.dot(a,b)
array([[ 0.,  1.],
       [ 2.,  3.]])
```

Array operations

- There are also some built-in methods of ndarray objects.

  Universal functions which may also be applied include exp, sqrt, add, sin, cos, etc…

```
>>> a = np.random.random((2,3))
>>> a
array([[ 0.68166391, 0.98943098,
0.69361582],
       [ 0.78888081, 0.62197125,
0.40517936]])
>>> a.sum()
4.1807421388722164
>>> a.min()
0.405179361037914 3
>>> a.max(axis=0)
array([ 0.78888081, 0.98943098,
0.69361582])
>>> a.min(axis=1)
array([ 0.68166391, 0.40517936])
```

Array operations

- An array shape can be manipulated by a number of methods.

  resize(size) will modify an array in place.

  reshape(size) will return a copy of the array with a new shape.

```
>>> a =
np.floor(10*np.random.random((3,4)))
>>> print a
[[ 9. 8. 7. 9.]
 [ 7. 5. 9. 7.]
 [ 8. 2. 7. 5.]]
>>> a.shape
(3, 4)
>>> a.ravel()
array([ 9., 8., 7., 9., 7., 5., 9., 7., 8.,
2., 7., 5.]) >>> a.shape = (6,2)
>>> print a
[[ 9. 8.]
 [ 7. 9.]
 [ 7. 5.]
 [ 9. 7.]
 [ 8. 2.]
 [ 7. 5.]]
>>> a.transpose()
array([[ 9., 7., 7., 9., 8., 7.],
       [ 8., 9., 5., 7., 2., 5.]])
```

Linear algebra

- One of the most common reasons for using the NumPy package is its linear algebra module.

```
>>> from numpy import *
>>> from numpy.linalg import *
>>> a = array([[1.0, 2.0], [3.0,
4.0]])
>>> print a
[[ 1. 2.]
 [ 3. 4.]]
>>> a.transpose()
array([[ 1., 3.],
       [ 2., 4.]])
>>> inv(a) # inverse
array([[-2. , 1. ],
       [ 1.5, -0.5]])
```

What is pandas ?

- ***Pandas*** is Python package for **data analysis**.
- It Provides built-in data structures which simplify the manipulation and analysis of data sets.
- Pandas is easy to use and powerful, but “with great power comes great responsibility”
- We cannot teach you all things Pandas, we must focus on how it works, so you can figure out the rest on your own.
- http://pandas.pydata.org/pandas-docs/stable/

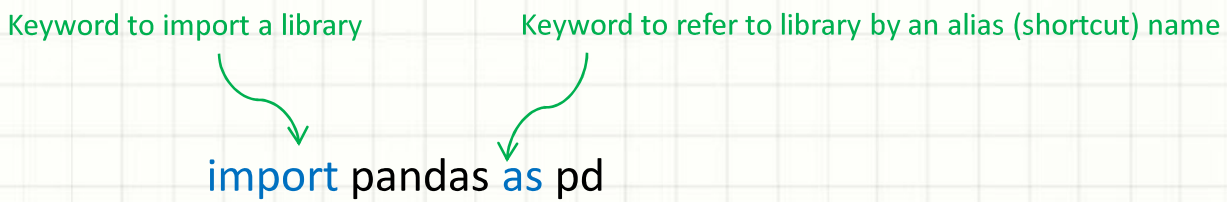
Watch Me Code 1

Pandas Basics

- Series
- DataFrame
- Creating a DataFrame from a dict
- Select columns, Select rows with Boolean indexing

Libraries - Pandas

- **A popular library for importing and managing datasets in Python for Machine Learning is 'pandas'.**



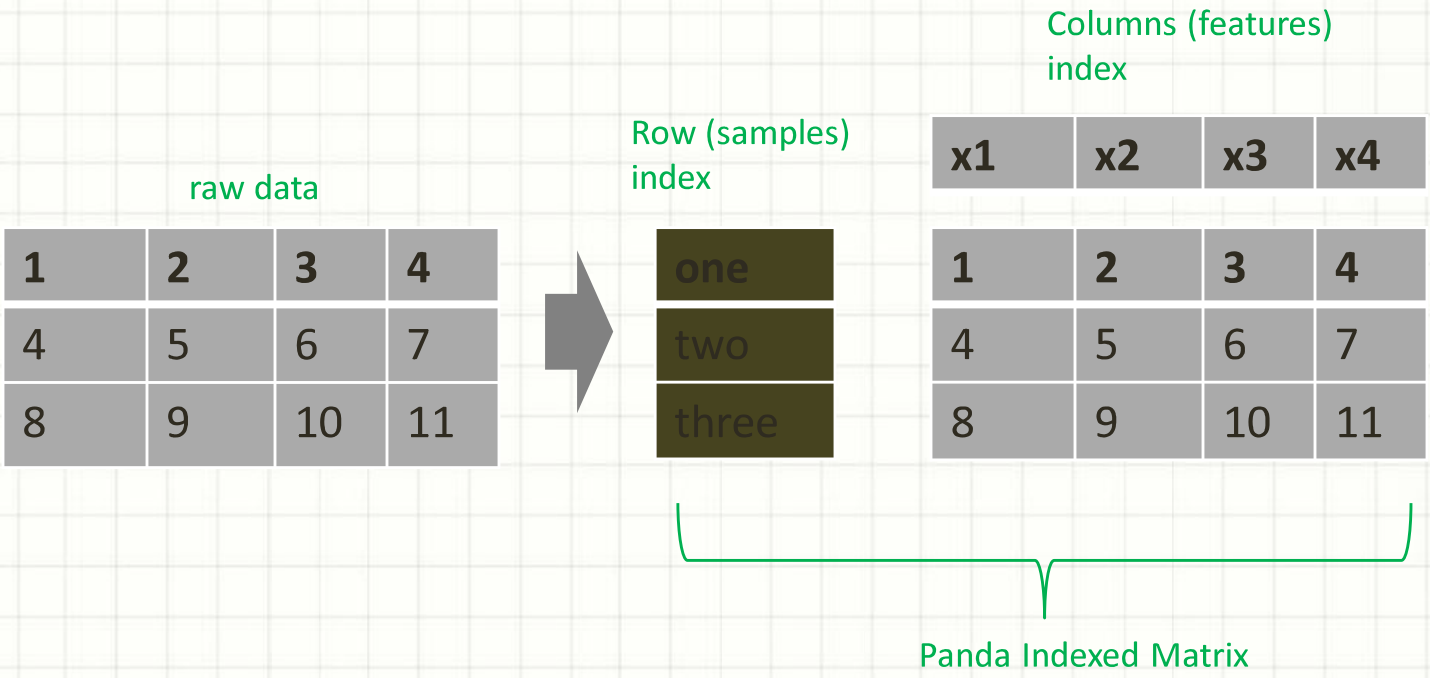
Used for:

- **Data Analysis**
- **Data Manipulation**
- **Data Visualization**

PyData.org : high-performance, easy-to-use data structures and data analysis tools for the Python programming language.

Pandas – Indexed Arrays

- **Pandas are used to build indexed arrays (1D) and matrices (2D), where columns and rows are labeled (named) and can be accessed via the labels (names).**

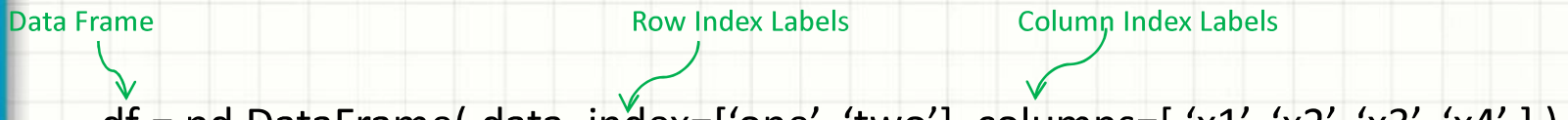


Pandas – Series and Data Frames

- **Pandas Indexed Arrays are referred to as Series (1D) and Data Frames (2D).**

- **Series is a 1D labeled (indexed) array and can hold any data type, and mix of data types.**

- **Data Frame is a 2D labeled (indexed) matrix and can hold any data type, and mix of data types.**



Pandas: Essential Concepts

- A **Series** is a named Python list (dict with list as value).

```
{ ‘grades’ : [50,90,100,45] }
```

- A **DataFrame** is a dictionary of Series (dict of series):

```
{  { ‘names’ :
[‘bob’,’ken’,’art’,’joe’]}
   { ‘grades’ : [50,90,100,45] }
 }
```

Check Yourself: Series or DataFrame?

Match the code to the result. One result is a Series, the other a DataFrame

```
1.df['Quarter']
2.df[
   ['Quarter'] ]
```

	Quarter	Sold
0	Q1	100
1	Q2	120
2	Q3	90
3	Q4	150

Check Yourself: Boolean Index

Which rows are included in this Boolean index?

```
df[ df['Sold']
< 110 ]
```

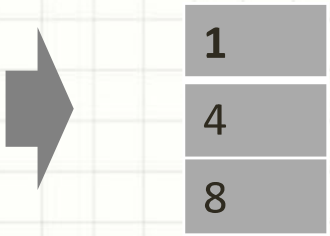
	Quarter	Sold
0	Q1	100
1	Q2	120
2	Q3	90
3	Q4	150

Pandas – Selecting

- **Selecting One Column**

Selects column labeled x1 for all rows

```
x1 = df[ 'x1' ]
```



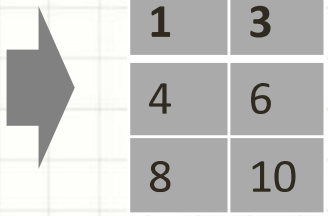
1
4
8

- **Selecting Multiple Columns**

Note: df['x1':'x3'] this python syntax does not work!

Selects columns labeled x1 and x3 for all rows

```
x1 = df[ [ 'x1', 'x3' ] ]
```

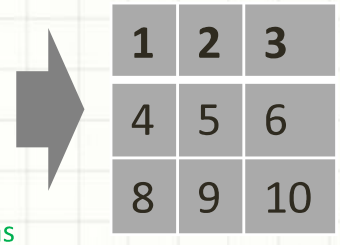


1	3
4	6
8	10

Selects columns labeled x1 through x3 for all rows

```
x1 = df.ix[ :, 'x1':'x3' ]
```

Slicing function — rows (all) — columns

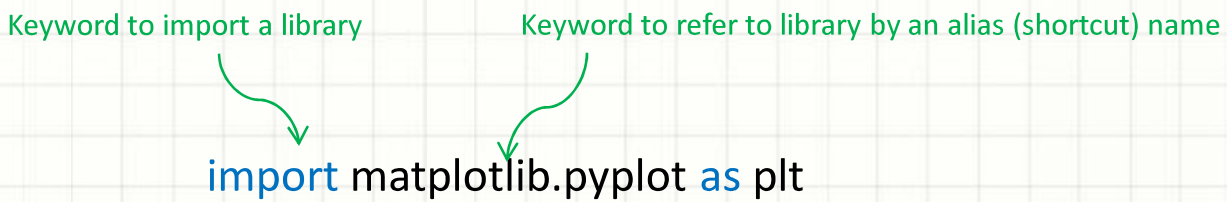


1	2	3
4	5	6
8	9	10

And many more functions: merge, concat, stack, …

Libraries - Matplotlib

- **A popular library for plotting and visualizing data in Python**



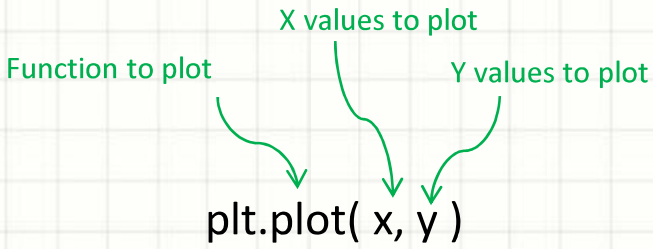
Used for:

- **Plots**
- **Histograms**
- **Bar Charts**
- **Scatter Plots**
- **etc**

matplotlib.org: Matplotlib is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms.

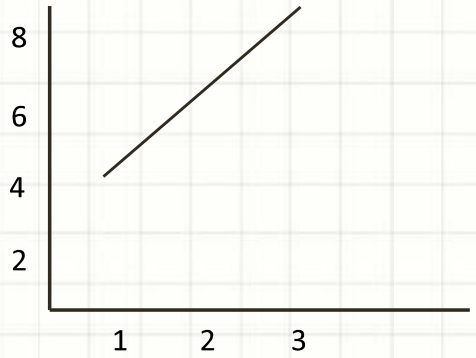
Matplotlib - Plot

- **The function plot plots a 2D graph.**



- **Example:**

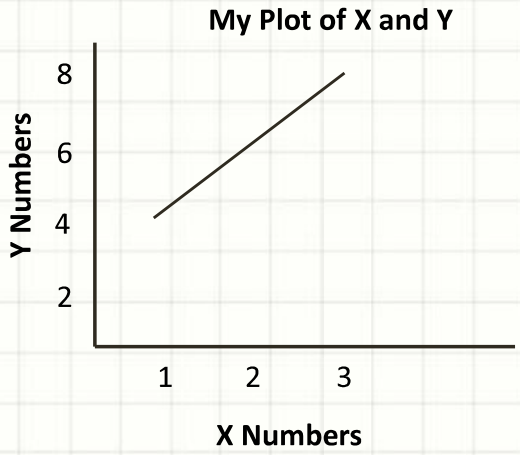
```
plt.plot( [ 1, 2, 3 ], [ 4, 6, 8 ] )  # Draws plot in the background
plt.show()                             # Displays the plot
```



Matplotlib – Plot Labels

- **Add Labels for X and Y Axis and Plot Title (caption)**

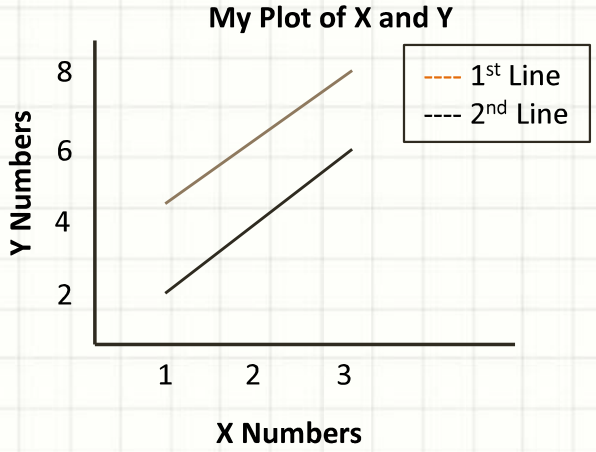
```
plt.plot( [ 1, 2, 3 ], [ 4, 6, 8 ] )
plt.xlabel( “X Numbers” )          # Label on the X-axis
plt.ylabel( “Y Numbers” )          # Label on the Y-axis
plt.title( “My Plot of X and Y”)   # Title for the Plot
plt.show()
```



Matplotlib – Multiple Plots and Legend

- **You can add multiple plots in a Graph**

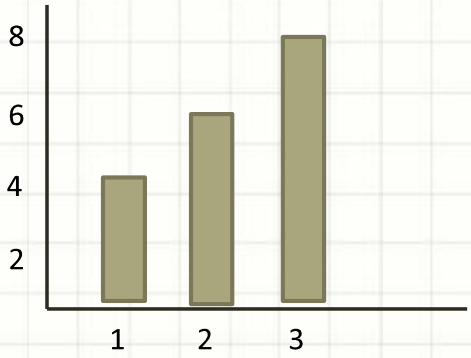
```
plt.plot( [ 1, 2, 3 ], [ 4, 6, 8 ], label=‘ 1st Line’ )     # Plot for 1st Line
plt.plot( [ 1, 2, 3 ], [ 2, 4, 6 ], label=‘2nd Line’ )     # Plot for 2nd Line
plt.xlabel( “X Numbers” )
plt.ylabel( “Y Numbers” )
plt.title( “My Plot of X and Y”)
plt.legend()                                               # Show Legend for the plots
plt.show()
```



Matplotlib – Bar Chart

- **The function bar plots a bar graph.**

```
plt.plot( [ 1, 2, 3 ], [ 4, 6, 8 ] ) # Plot for 1st Line
plt.bar()                             # Draw a bar chart
plt.show()
```



And many more functions: hist, scatter, …