LECTURE 6

Numerical and Scientific Packages

NUMERICAL AND SCIENTIFIC APPLICATIONS

- As you might expect, there are a number of third-party packages available for numerical and scientific computing that extend Python's basic math module.
- These include:
- NumPy/SciPy – numerical and scientific function libraries.
- Numba – Python compiler that supports JIT compilation.
- ALGLIB – numerical analysis library.
- Pandas – high-performance data structures and data analysis tools.
- PyGSL – Python interface for GNU Scientific Library.
- ScientificPython – collection of scientific computing modules.

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.

INSTALLING NUMPY AND MATPLOTLIB

- You can install NumPy and Matplotlib on our virtual machine in the following way:

```
$ sudo apt-get install python-numpy
$ sudo apt-get install python-matplotlib
```

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. ])
```

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

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

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
```

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{pmatrix}$$

- Multi-dimensional arrays support multi-dimensional indexing.

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

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 & 9 \end{pmatrix}$$

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()
0.4051793610379143
>>> 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]])
```

LINEAR ALGEBRA

```
>>> u = eye(2) # unit 2x2 matrix; "eye" represents "I"
>>> u
array([[ 1., 0.],
       [ 0., 1.]])
>>> j = array([[0.0, -1.0], [1.0, 0.0]])
>>> dot(j, j) # matrix product
array([[-1., 0.],
       [ 0., -1.]])
>>> trace(u) # trace
2.0
>>> y = array([[5.], [7.]])
>>> solve(a, y) # solve linear matrix equation
array([[-3.],
       [ 4.]])
>>> eig(j) # get eigenvalues/eigenvectors of matrix
(array([ 0.+1.j, 0.-1.j]),
 array([[ 0.70710678+0.j, 0.70710678+0.j],
        [ 0.00000000-0.70710678j, 0.00000000+0.70710678j]]))
```

MATRICES

- There is also a matrix class which inherits from the ndarray class.

  There are some slight differences but matrices are very similar to general arrays.

  In NumPy's own words, the question of whether to use arrays or matrices comes down to the short answer of "use arrays".

```
>>> A = matrix('1.0 2.0; 3.0 4.0')
>>> A
[[ 1.  2.]
 [ 3.  4.]]
>>> type(A)
<class 'numpy.matrixlib.defmatrix.matrix'>
>>> A.T # transpose
[[ 1.  3.]
 [ 2.  4.]]
>>> X = matrix('5.0 7.0')
>>> Y = X.T
>>> print (A*Y)   # matrix multiplication
[[19.]
 [43.]]
>>> print (A.I) # inverse
[[-2.  1. ]
 [ 1.5 -0.5]]
>>> solve(A, Y) # solving linear equation
matrix([[-3.], [ 4.]])
```

NUMPY DOCS

- There is a very nice table of NumPy equivalent operations for MATLAB users. However, even if you do not know MATLAB, this is a pretty handy overview of NumPy functionality.

  There is also a pretty comprehensive list of example usage of all the NumPy functions here.

SCIPY

- Now we move on to SciPy. In it's own words:

> SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension of Python. It adds significant power to the interactive Python session by providing the user with high-level commands and classes for manipulating and visualizing data. With SciPy an interactive Python session becomes a data-processing and system-prototyping environment rivaling sytems such as MATLAB, IDL, Octave, R-Lab, and SciLab.

- Basically, SciPy contains various tools and functions for solving common problems in scientific computing.

SCIPY

SciPy's functionality is implemented in a number of specific sub-modules. These include:

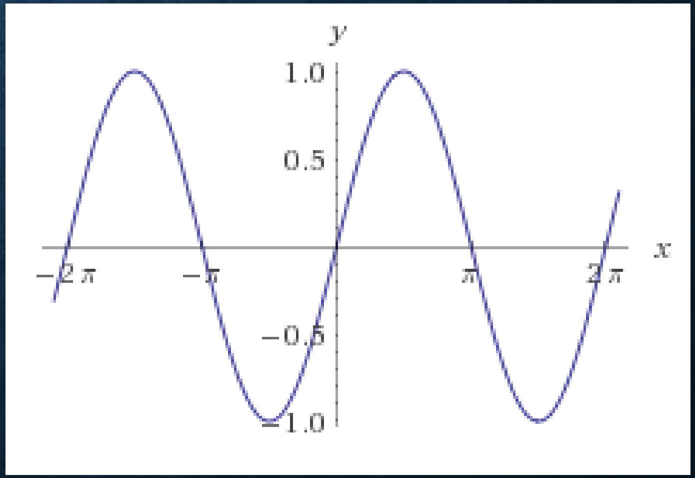
Special mathematical functions (scipy.special) -- airy, elliptic, bessel, etc.
Integration (scipy.integrate)
Optimization (scipy.optimize)
Interpolation (scipy.interpolate)
Fourier Transforms (scipy.fftpack)
Signal Processing (scipy.signal)
Linear Algebra (scipy.linalg)
Compressed Sparse Graph Routines (scipy.sparse.csgraph)
Spatial data structures and algorithms (scipy.spatial)
Statistics (scipy.stats)
Multidimensional image processing (scipy.ndimage)
Data IO (scipy.io)
Weave (scipy.weave)
and more!

SCIPY

- We can't possibly tour all of the SciPy library and, even if we did, it might be a little boring. So let's just look at some example modules with SciPy to see how it can be used in a Python program.

  Let's start with a simple little integration example.
  Say we wanted to compute the following:

$$\int_a^b \sin x \, dx$$



- Obviously, the first place we should look is scipy.integrate!

SCIPY.INTEGRATE

- Methods for Integrating Functions given a function object:
- `quad` -- General purpose integration.
  `dblquad` -- General purpose double integration.
  `tplquad` -- General purpose triple integration.
  `fixed_quad` -- Integrate func(x) using Gaussian quadrature of order n.
  `quadrature` -- Integrate with given tolerance using Gaussian quadrature.
  `romberg` -- Integrate func using Romberg integration.
- Methods for Integrating Functions given a fixed set of samples:
- `trapz` -- Use trapezoidal rule to compute integral from samples.
  `simps` -- Use Simpson's rule to compute integral from samples.
  `romb` -- Use Romberg Integration to compute integral from (2**k + 1) evenly-spaced samples.

SCIPY.INTEGRATE

We have a function object – np.sin defines the sin function for us. We can compute the definite integral from $x = 0$ to $x = \pi$ using the quad function.

- ```
  >>> result = scipy.integrate.quad(np.sin, 0, np.pi)
  >>> print (result)
  (2.0, 2.220446049250313e-14) # 2 with a very small error margin!
  >>> result = scipy.integrate.quad(np.sin, -np.inf, +np.inf)
  >>> print (result)
  (0.0, 0.0) # Integral does not converge
  ```
  ```

SCIPY.INTEGRATE

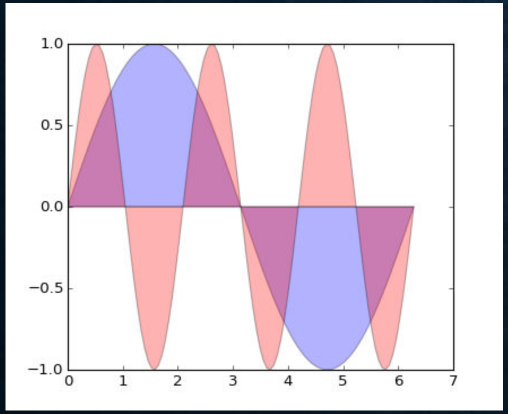
Let's say that we don't have a function object, we only have some (x,y) samples that "define" our function. We can estimate the integral using the trapezoidal rule.

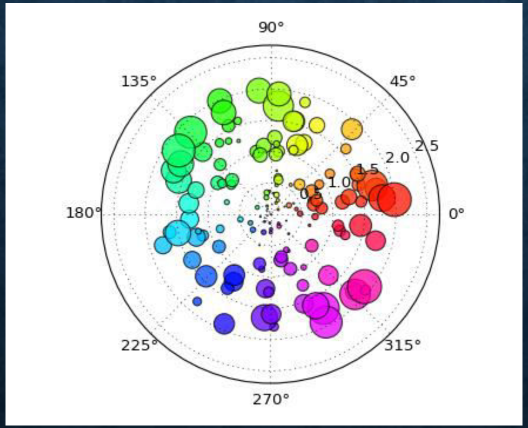
```
>>> sample_x = np.linspace(0, np.pi, 1000)
>>> sample_y = np.sin(sample_x) # Creating 1,000 samples
>>> result = scipy.integrate.trapz(sample_y, sample_x)
>>> print (result)
1.99999835177
>>> sample_x = np.linspace(0, np.pi, 1000000)
>>> sample_y = np.sin(sample_x) # Creating 1,000,000 samples
>>> result = scipy.integrate.trapz(sample_y, sample_x)
>>> print (result)
2.0
```

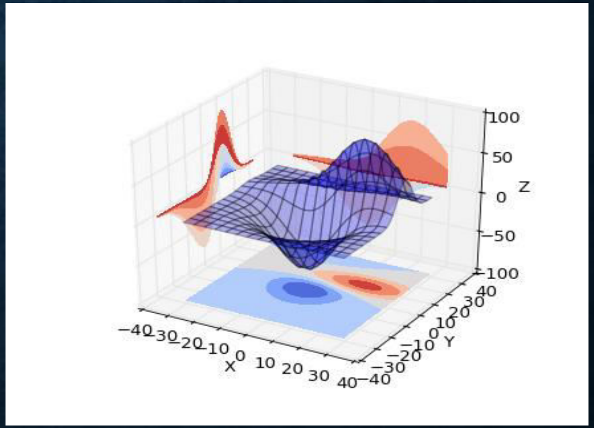
MATPLOTLIB

- We're going to continue our discussion of scientific computing with matplotlib.

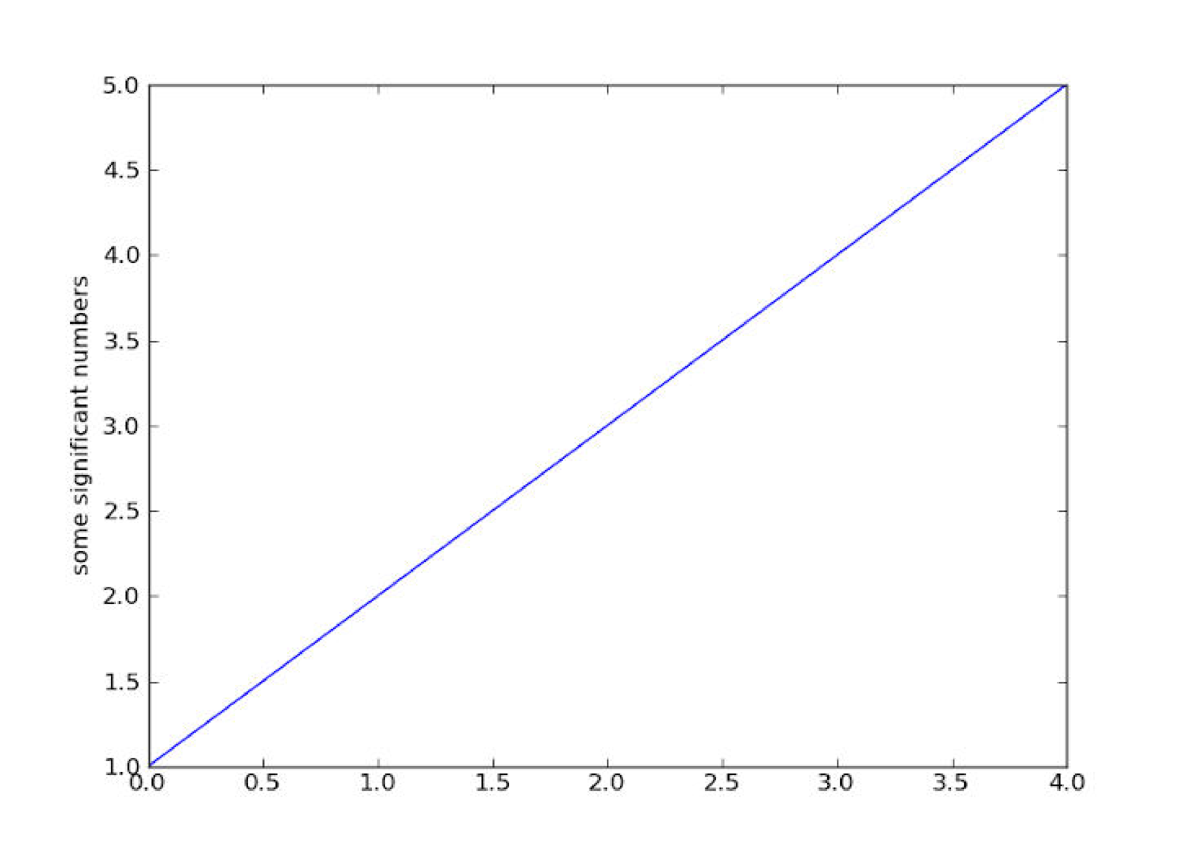
  Matplotlib is an incredibly powerful (and beautiful!) 2-D plotting library. It's easy to use and provides a huge number of examples for tackling unique problems.







PYPLOT



- At the center of most matplotlib scripts is pyplot. The pyplot module is stateful and tracks changes to a *figure*. All pyplot functions revolve around creating or manipulating the state of a figure.

```
import matplotlib.pyplot as plt
plt.plot([1,2,3,4,5])
plt.ylabel('some significant numbers')
plt.show()
```

When a single sequence object is passed to the plot function, it will generate the x-values for you starting with 0.

PYPLOT

- The plot function can actually take any number of arguments. Common usage of plot:

```
plt.plot(x_values, y_values, format_string [, x, y, format, ])
```

- The format string argument associated with a pair of sequence objects indicates the color and line type of the plot (e.g. 'bs' indicates blue squares and 'ro' indicates red circles).

  Generally speaking, the `x_values` and `y_values` will be numpy arrays and if not, they will be converted to numpy arrays internally.

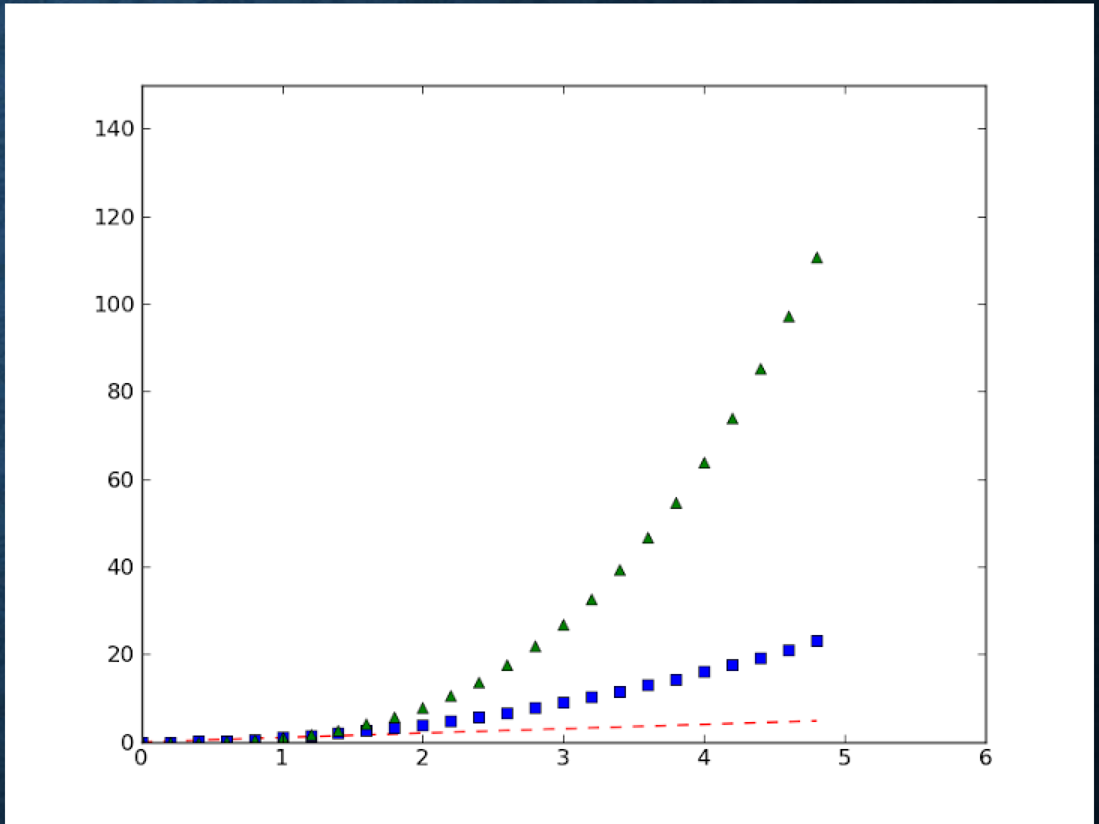
  Line properties can be set via keyword arguments to the plot function. Examples include `label`, `linewidth`, `animated`, `color`, etc…

PYPLOT

```
import numpy as np
import matplotlib.pyplot as plt

# evenly sampled time at .2 intervals
t = np.arange(0., 5., 0.2)

# red dashes, blue squares and green triangles
plt.plot(t, t, 'r--', t, t**2, 'bs', t, t**3, 'g^')
plt.axis([0, 6, 0, 150]) # x and y range of axis
plt.show()
```



BEHIND THE SCENES

- It's important to note that a figure is a separate idea from how it is rendered. Pyplot convenience methods are used for creating figures and immediately displaying them in a pop up window. An alternative way to create this figure is shown below.

```
import numpy as np
import matplotlib.figure as figure

t = np.arange(0, 5, .2)

f = figure.Figure()
axes = f.add_subplot(111)
axes.plot(t, t, 'r--', t, t**2, 'bs', t, t**3, 'g^')
axes.axis([0, 6, 0, 150])
```

PYPLOT

A script can generate multiple figures, but
typically you'll only have one.

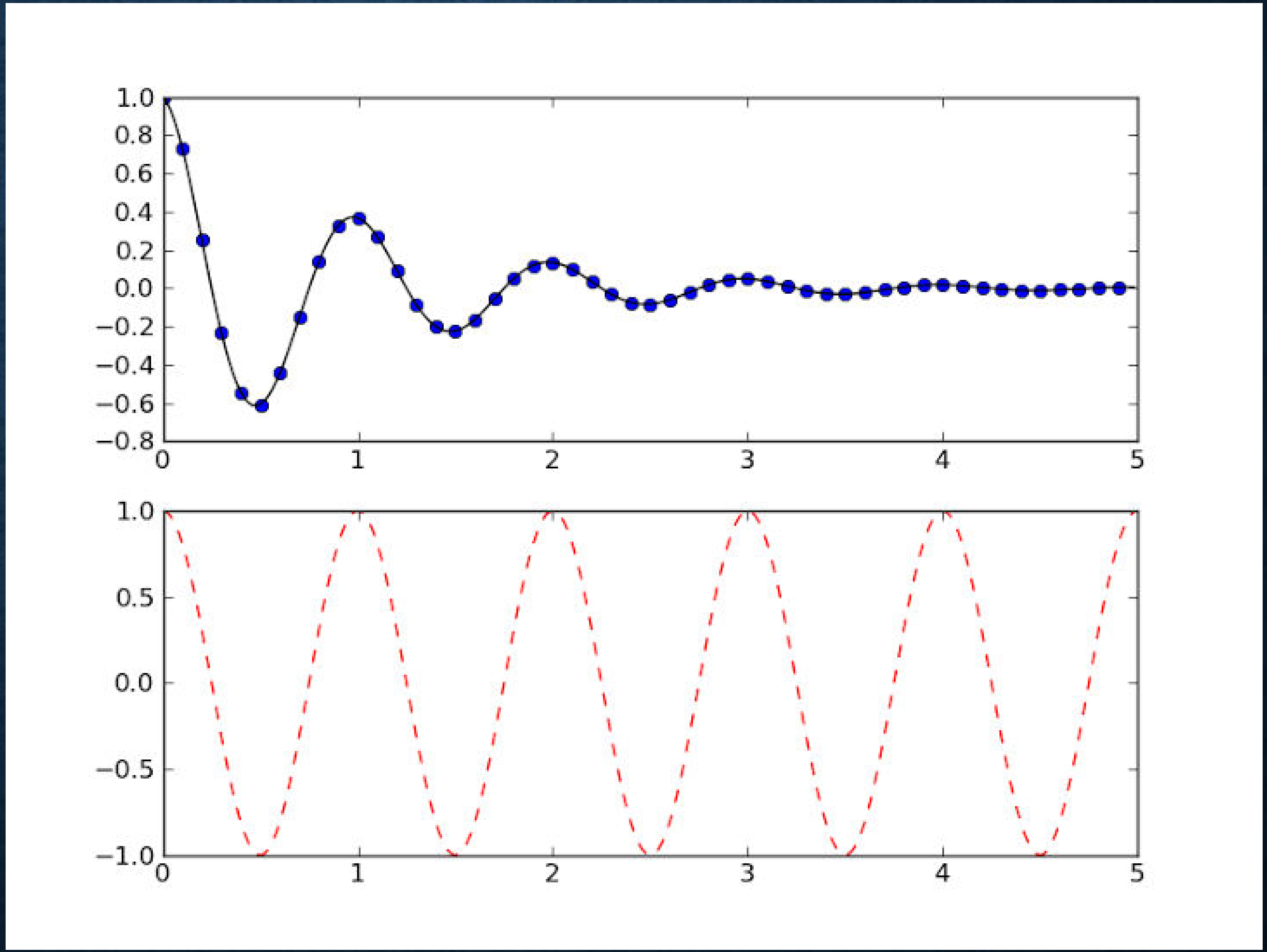
To create multiple plots within a figure, either use the `subplot()` function which manages the layout of the figure or use `add_axes()`.

```
import numpy as np
import matplotlib.pyplot as plt

def f(t):
    return np.exp(-t) * np.cos(2*np.pi*t)

t1 = np.arange(0.0, 5.0, 0.1)
t2 = np.arange(0.0, 5.0, 0.02)
plt.figure(1) # Called implicitly but can use
              # for multiple figures
plt.subplot(211) # 2 rows, 1 column, 1st plot
plt.plot(t1, f(t1), 'bo', t2, f(t2), 'k')

plt.subplot(212) # 2 rows, 1 column, 2nd plot
plt.plot(t2, np.cos(2*np.pi*t2), 'r--')
plt.show()
```


1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
0
1
2
3
4
5
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5

PYPLOT

- The `text()` command can be used to add text in an arbitrary location
- `xlabel()` adds text to x-axis.
- `ylabel()` adds text to y-axis.
- `title()` adds title to plot.
- `clear()` removes all plots from the axes.

All methods are available on pyplot and on the axes instance generally.

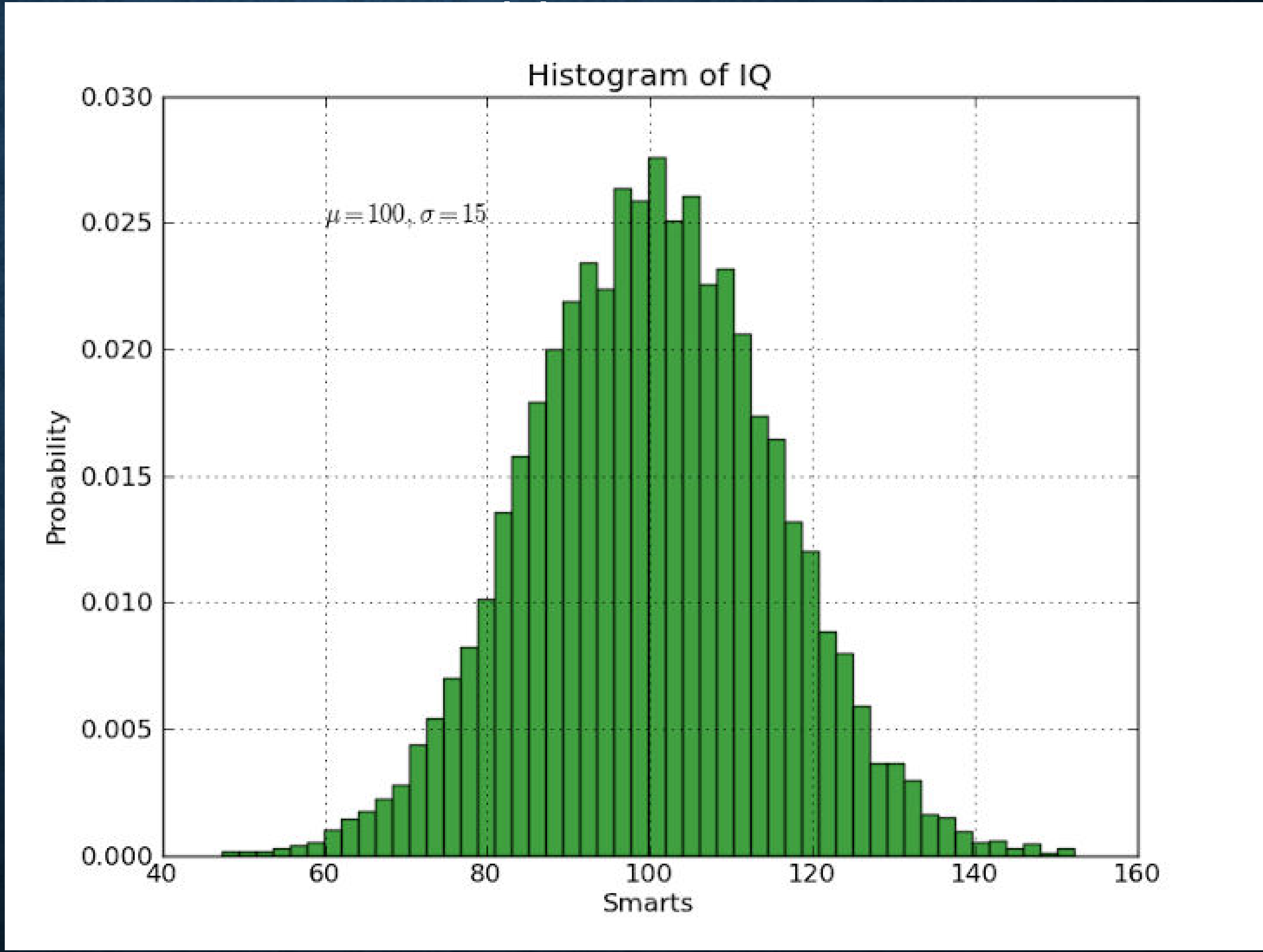
PYPLOT

```
import numpy as np
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='g', alpha=0.75)

plt.xlabel('Smarts')
plt.ylabel('Probability')
plt.title('Histogram of IQ')
plt.text(60, .025, r'$\mu=100,\ \sigma=15$') #TeX equations
plt.axis([40, 160, 0, 0.03])
plt.grid(True)
plt.show()
```


Histogram of IQ
$\mu=100,\ \sigma=15$
Probability
Smarts
0.030
0.025
0.020
0.015
0.010
0.005
0.000
40
60
80
100
120
140
160

PYPLOT

- There are tons of specialized functions – check out the API here. Also check out the examples list to get a feel for what matploblib is capable of (it's a lot!).

  You can also embed plots into GUI applications.

  For PyQt4, use `matplotlib.backends.backend_qt4agg`.
- Let's do a little demonstration.

PLOT GUI

- The two most important classes from matplotlib.backends.backend_qt4agg:
- `FigureCanvasQTAgg(`*`fig`*`)`: returns the canvas the figure *fig* renders into.
- `NavigationToolbar2QT(`*`canvas, prnt`*`)`: creates a navigation toolbar for *canvas* which has the parent *prnt*.

Furthermore, a canvas object has the following method defined:

- `canvas.draw()`: redraws the updated figure on the canvas.