LECTURE 19

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, 0.9879286 4]])
```

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]]]
```

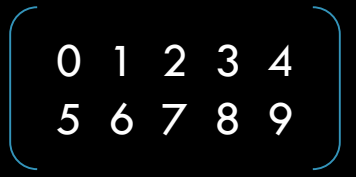
INDEXING

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]])
```

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!

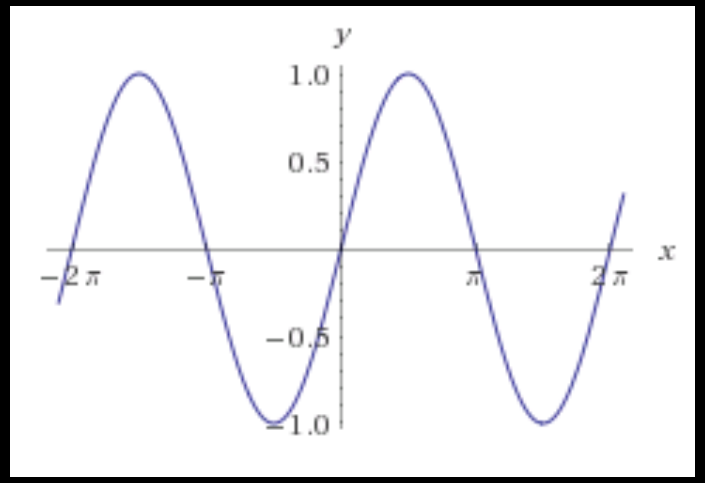
SCIPY

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
```

PLOTTING

Before we can look at some more sophisticated examples, we need to get some plotting under our belt.

We'll start the next lecture by introducing the matplotlib plotting package and see how we can build more complex scientific applications.