The SciPy Stack

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Outline

- Numpy - Arrays, Linear Algebra, Vector Ops
- MatPlotLib - Data Plotting
- SciPy - Optimization, Scientific functions

What is Numpy?

- 3rd party module that extends the Python language
- Matrix and linear algebra operations
- General support for N-Dimensional Arrays
  - Heterogeneous elements
  - Direct mapping to C/C++/Fortran memory buffers
  - Matrix operations
  - Vectorized Algorithms
- Bindings to C and Fortran matrix math libraries
  - Requires compiled support libraries
  - Installers are platform specific

Importing Numpy

- Must install it via the SciPy stack or individually
- Most people import the numpy library “as” np
- Arrays can be created from lists or nested lists

```
>>> import numpy as np
>>> x = np.array( [1,5,10] )
>>> x
array( [1, 5, 10] )

>>> y = np.array( [ [1,2,3], [4,5,6] ]  )
>>> y
array( [ [1,2,3],
          [4,5,6] )
```

Data Types

- **Numpy stores all data in an array using a single data type**
- **Direct mapping to memory / space required**
- **The Python data types have default mappings**
- **You will most commonly use:**
  - bool - boolean, stored as a byte
  - int_ (Same as C long, either int32 or int64, architecture dependent)
  - float_ (float64)
  - complex_ (complex128)

- **Will convert python int/float/bool/complex automatically**

Data Types

- Numpy supports many different native data types
- Will convert python int/float/bool/complex automatically
- The .dtype attribute of an array tells the actual data type
- Can convert to another data type using .astype()

```
>>> x = np.array( [1,5,10] )
>>> x
array( [1, 5, 10] )
>>> x.dtype
dtype("int32")
>>> y = x.astype(np.float64)
>>> y
array( [ 1.,  5.,  10.] )
>>> y.dtype
dtype('float64')
```

Numpy Array Creation

- **Convert python "array-like" data structures**
- **Using built in array creation methods:**
  - np.zeros (shape)
  - np.ones(shape)
  - np.arange(Start, Stop, step) - Like python range
  - np.linspace(Start, Stop, number)
- **Most accept an optional dtype parameter**

```
>>> x = np.zeros( (2,2), dtype=np.int_ )
>>> x
array( [0, 0],
       [0, 0] )

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

Array = Block of Memory

- All data in the array is stored in a single block of memory
- The .shape attribute stores the size of each dimension
- You can change the shape on the fly!
  - must retain the exact number of elements
  - A 1 x 10 array and a 2 x 5 array both have 10 data items

```
>>> x = np.arange(10)
>>> x
array( [0, 1, 2, 3, 4, 5, 6, 7, 8, 9] )
>>> x.shape
(10, )
>>> x.shape = (2,5)
>>> x
array( [ 0, 1, 2, 3, 4],
         [ 5, 6, 7, 8, 9] ]  )
```

Array Indexing

- **Works like indexing in python**
  - Zero based
  - negative indexes count from the back
- **BUT, You CAN index all dimensions at once if you want!**

```
>>> x = np.arange(10)
>>> x[-1]
9
>>> x.shape = (2,5)
>>> x[1][3]
8
>>>x[1,3]
8
```

Array Slicing

- **Works like indexing in python**
  - Provide a Start:Stop:Stride
  - Can do this for multiple dimensions at once

```
>>> x = np.arange(25).reshape(5,5)
>>> x
array([[ 0,  1,  2,  3,  4],
       [ 5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14],
       [15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24] ] )

>>> x[0:5:2, 2:4]
array([[ 2,  3],
       [12, 13],
       [22, 23] ] )
```

Array Slicing - Aliasing!

- **Slices provide VIEWS**
  - Like an alias of a list
- **See array indexing if you want to copy a subset of data!**

```
>>> y = x[0:5:2, 2:4]
>>> y[0,0] = 999
>>> y
array([[999,   3],
       [ 12,  13],
       [ 22,  23]])
>>> x
array([[  0,   1, 999,   3,   4],
       [  5,   6,   7,   8,   9],
       [ 10,  11,  12,  13,  14],
       [ 15,  16,  17,  18,  19],
       [ 20,  21,  22,  23,  24]])
```

Advanced Indexing

- You can specify a set of indices with an array to select a copy of the data.

```
>>> x
array([ 0,  5, 10, 15, 20, 25])

>>> y = x[ np.array( [1,3,5] ) ]
>>> y
array([ 5, 15, 25])

>>> y[0] = 99
>>> y
array( [99,15,25]
>>> x
array( [ 0, 5, 10, 15, 20, 25] )
```

Advanced Indexing

- **BUT, if you assign to an array indexing operation, it modifies the original…**

```
>>> x
array([ 0,  5, 10, 15, 20, 25])

>>> y = x[ np.array( [1,3,5] ) ]
>>> y
array([ 5, 15, 25])

>>> x[ np.array( [1,3,5] ) ] += 1
>>> x
array([ 0,  6, 10, 16, 20, 26])
>>>
```

Array Broadcasting

- Element-by-element operations on two arrays typically require the arrays to have the same shape

- A scaler is treated as a 1x1 array that gets “broadcast” over all elements

```
>>> y = np.arange(1,5)
>>> y
array([1, 2, 3, 4])
>>> y * 2
array([2, 4, 6, 8], dtype=int32)
>>> y * 2.
array([ 2.,  4.,  6.,  8.])
```

Array Broadcasting

- **Arrays that are "short" in a dimension can also be broadcast!**
  - The Rule: "In order to broadcast, the size of the trailing axes for both arrays in an operation must either be the same size or one of them must be one."

```
>>> a = np.array( [ [0, 1, 2],
                    [3, 4, 5] ] )
>>> b = np.array(   [4,5,6] )
>>> c = a * b                  #Multiplication, not np.dot(a,b)
>>> c
array( [ [ 0,  5, 12],
         [12, 20, 30] ], dtype=int32)
```

Vector Algorithms:

- **Calculating y = sin(x), for 100 elements between -4 and 4**

```
>>> x = np.linspace(-4,4,100)

>>> y = np.sin(x)
```

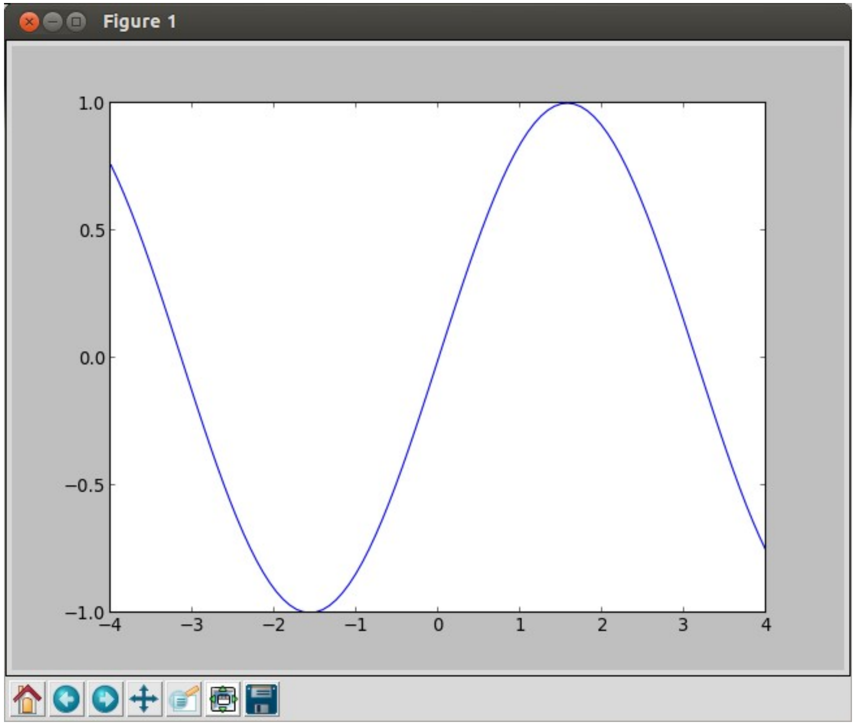
What is Matplotlib?

- **Python library that supports plotting data**
- **Many features were copied from MATLAB**
- **Easily produce Graphs/Plots of**
  - Lines
  - Histograms
  - Bargraphs
  - Scatterplots
  - 3D surfaces

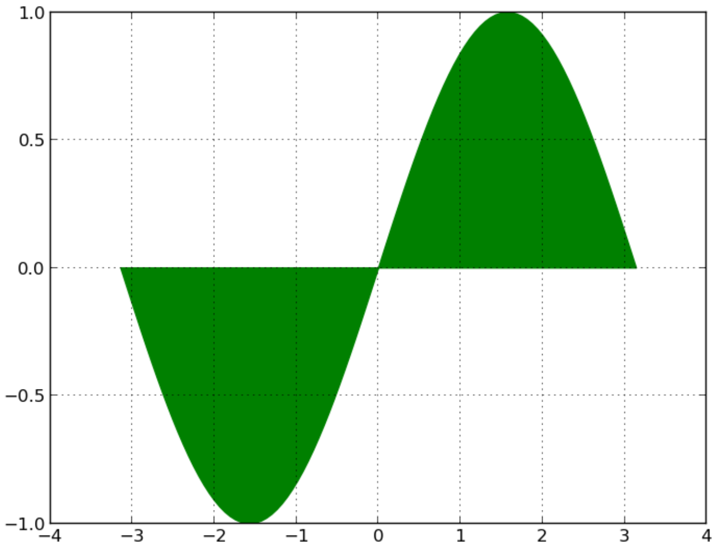
Plotting sin data

- **Plotting 2D data (x vs y) requires two lines of code**
  - Three if you count the import....

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

x = np.linspace(-4,4,100)
y = np.sin(x)

temp = plt.plot(x,y)
plt.show()
```



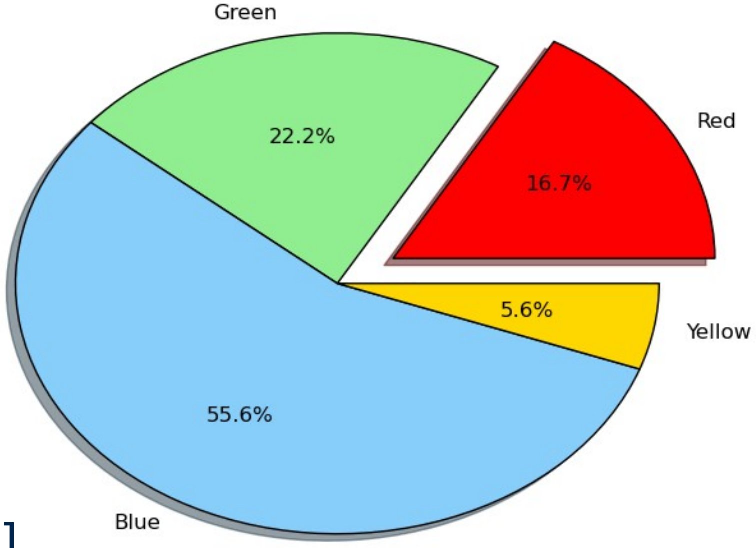
Filled Plot




```
import numpy as np
import matplotlib.pyplot as plt
x = np.linspace(-np.pi, np.pi,100)
y = np.sin(x)

temp = plt.fill(x,y, color="green")
plt.grid(True)
plt.show()
```

Other plots

- **Pie charts**




```
import matplotlib.pyplot as plt

labels = [ 'Red', 'Green', 'Blue', 'Yellow' ]
colors = [ 'red', 'lightgreen', 'lightskyblue', 'gold']
values = [3,4,10,1]
explode = (0.2, 0, 0, 0)

plt.pie(values, explode=explode, colors=colors,
        labels=labels, shadow=True, autopct='%1.1f%%')

plt.show()
```

3D Plots require 3D data

- **Numpy meshgrid function allows you to create arrays with all possible X or Y coordinates**

```
>>> x = np.arange(0,5,1)
>>> y = np.arange(0,4,1)
>>> x
array([0, 1, 2, 3, 4])
>>> y
array([0, 1, 2, 3])
>>> NX,NY = np.meshgrid(x,y)
>>> NX
array([[0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4]])
>>> NY
array([[0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [2, 2, 2, 2, 2],
       [3, 3, 3, 3, 3]])
```

3D Plots require 3D data

- **These arrays can be used to calculate a 3rd (Z) axis based upon a formula, such as euclidean distance from origin.**
  - Note the distance at point (4,3) is 5 (3x4x5 triangle)

```
>>> D = np.sqrt( NX**2 + NY**2 )
>>> D
array([[ 0.      ,  1.      ,  2.      ,  3.      ,  4.      ],
       [ 1.      ,  1.4142,  2.2360,  3.1622,  4.1231],
       [ 2.      ,  2.2360,  2.8284,  3.6055,  4.4721],
       [ 3.      ,  3.1622,  3.6055,  4.2426,  5.      ]])
>>>
```

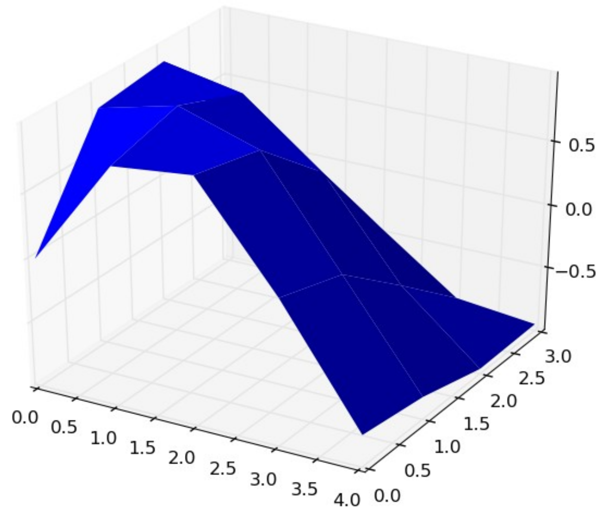
3D Plots require 3D data

- **And you could calculate the sin of the distance…**

```
>>> Z = np.sin(D)
>>> Z
array([[ 0.       ,  0.84147,  0.90929,  0.14112, -0.7568   ],
       [ 0.84147,  0.98776,  0.78674, -0.02068, -0.83133 ],
       [ 0.90929,  0.78674,  0.30807, -0.44749, -0.97127 ],
       [ 0.14112, -0.02068, -0.44749, -0.89168, -0.95892 ]])
```

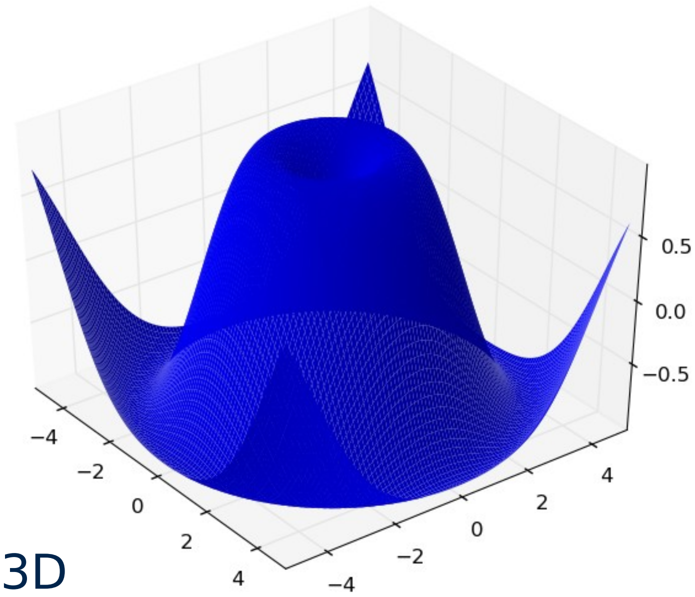
3D surface Plot

```
>>> import matplotlib.pyplot as plt
>>> from mpl_toolkits.mplot3d import Axes3D
>>> fig = plt.figure()
>>> ax = fig.gca(projection='3d')  #Requires Axes3D import!
>>> surf = ax.plot_surface(NX,NY, Z, rstride=1,  cstride=1,
linewidth=0 )
>>> plt.show()
```



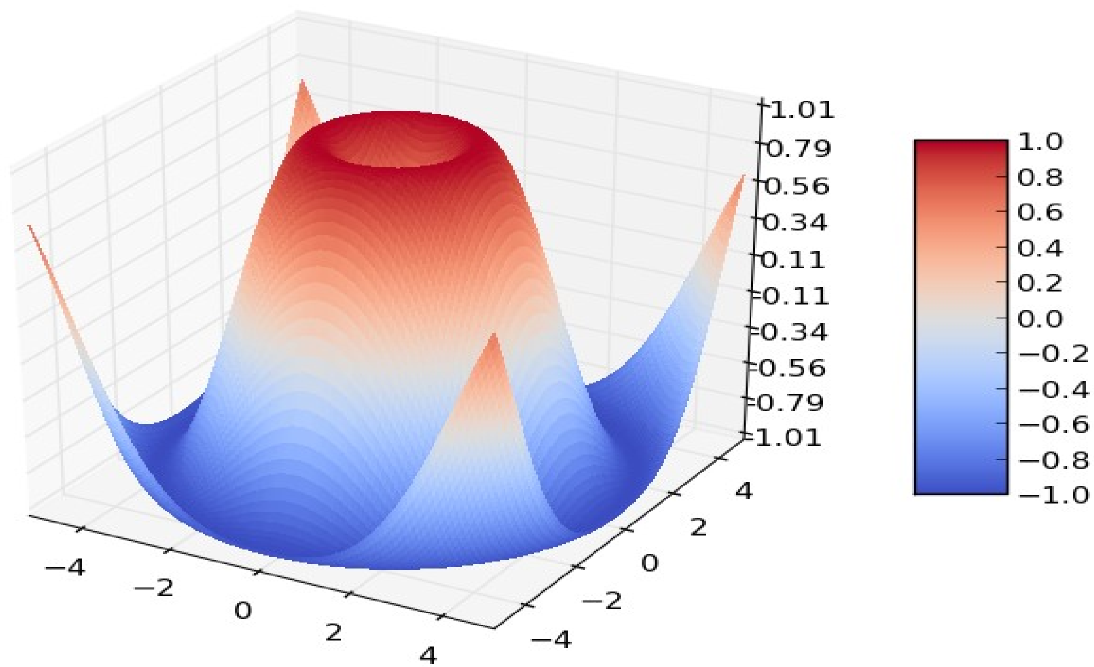
Surface Plot - more points

```
import numpy as np

X = np.arange(-5, 5, 0.1)
Y = np.arange(-5, 5, 0.1)
NX,NY = np.meshgrid(X, Y)
D = np.sqrt(NX**2 + NY**2)
Z = np.sin(D)


import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
fig = plt.figure()
ax = fig.gca(projection='3d')

surf = ax.plot_surface(NX,NY, Z, rstride=1,  cstride=1,
linewidth=0 )
plt.show()
```



Adding more bling…

- Add a colormap and colorbar (key)
- Customizing the Z axis



Colormap & Z-axis scale

```
from matplotlib.ticker import LinearLocator, FormatStrFormatter
from matplotlib import cm

...
ax = fig.gca(projection='3d')

surf = ax.plot_surface(NX,NY, Z, rstride=1,  cstride=1,
linewidth=0, cmap=cm.coolwarm  )

#Colorbar requires the surface to have a colormap.
fig.colorbar(surf, shrink=0.5, aspect=5)

#Customize Z-axis
ax.set_zlim(-1.01, 1.01)
ax.zaxis.set_major_locator(LinearLocator(10))
ax.zaxis.set_major_formatter(FormatStrFormatter('%.02f'))
```

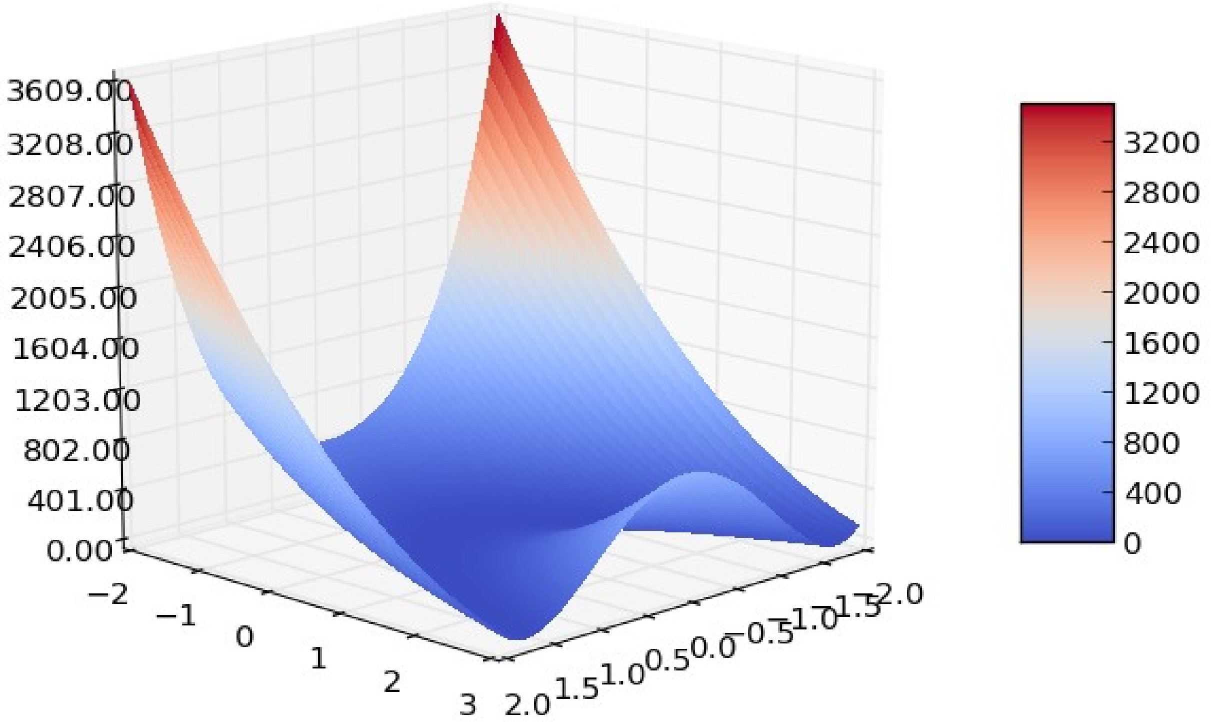
What is SciPy?

- **Python library that builds upon Numpy arrays**
- **Provides higher level math support for**
  - Optimization
  - Linear Algebra
  - Interpolation
  - FFT
  - Ordinary Differential Equation Solvers

SciPy

$$f(x, y) = (1 - x)^2 + 100(y - x^2)^2.$$

- **Function minimization**
- **Classic example function: Rosenbrock**



Source code in handout: rosenbrock_demo.py

Function Minimization

- **Define the function to accept a sequence (of parameters)**

```
def rosenbrock(parms):
   x,y = parms
   return (1-x)**2 + 100 * (y-x**2)**2
```

Source code in handout: rosenbrock_minimum.py

Function Minimization

- Import and call fmin from scipy.optimize
- Provide a starting point, and GO!

```
import numpy as np
from scipy.optimize import fmin

x0 = np.array( [4,-3]) #Try starting at (4,-3)
res = fmin( rosenbrock, x0, xtol=1e-8)

print res
```

Source code in handout: rosenbrock_minimum.py

Function Minimization

Optimization terminated successfully.
Current function value: 0.000000
Iterations: 90
Function evaluations: 174

[1. 1.]

Source code in handout: rosenbrock_minimum.py

Fin

Questions?