Intermediate Python Programming

Feng Chen
HPC User Services
LSU HPC & LONI
sys-help@loni.org

Louisiana State University
Baton Rouge
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Outline

- **Basic Python Review**
- **Introducing Python Modules:**
  - Numpy
  - Matplotlib
  - Scipy
- **Examples**
  - Calculate derivative of a function
  - Calculate k nearest neighbor

Overview of Basic Python

- **Python is a general-purpose interpreted, interactive, object-oriented, and high-level programming language.**
- **It was created by Guido van Rossum during 1985-1990. Like Perl, Python source code is also available under the GNU General Public License (GPL).**

Advantage of using Python

- **Python is:**
  - Interpreted:
    - Python is processed at runtime by the interpreter. You do not need to compile your program before executing it. This is similar to PERL and PHP.
  - Interactive:
    - You can actually sit at a Python prompt and interact with the interpreter directly to write your programs.
  - Object-Oriented:
    - Python supports Object-Oriented style or technique of programming that encapsulates code within objects.
  - Beginner's Language:
    - Python is a great language for the beginner-level programmers and supports the development of a wide range of applications from simple text processing to browsers to games.

First “Hello World” in Python

- **Compared with other language:**
  - Fast for writing testing and developing code
  - Dynamically typed, high level, interpreted

- **First Hello World example:**

```
#!/usr/bin/env python
print "Hello World!"
```

- **Explanation of the first line shebang (also called a hashbang, hashpling, pound bang, or crunchbang) refers to the characters "`#!`":**
  - Technically, in Python, this is just a comment line, can omit if run with the python command in terminal
  - In order to run the python script, we need to tell the shell three things:
    - That the file is a script
    - Which interpreter we want to execute the script
    - The path of said interpreter

Run Hello World in Script Mode

- **On Philip (Other clusters similar):**

```
[fchen14@philip1 python]$ qsub -I -l nodes=1:ppn=1 -q single
------------------------------------------------------
Concluding PBS prologue script - 07-Oct-2016 10:09:22
------------------------------------------------------
[fchen14@philip001 ~]$ module av python
-------------/usr/local/packages/Modules/modulefiles/apps --------------
python/2.7.10-anaconda python/2.7.7/GCC-4.9.0
[fchen14@philip001 ~]$ module load python/2.7.10-anaconda
2) mpich/3.1.4/INTEL-15.0.3   4) gcc/4.9.0
[fchen14@philip001 ~]$ which python
/usr/local/packages/python/2.7.10-anaconda/bin/python
[fchen14@philip001 ~]$ cd /home/fchen14/python/
# use python to execute the script
[fchen14@philip001 python]$ python hello.py
Hello World!
# or directly run the script
[fchen14@philip001 python]$ chmod +x hello.py
[fchen14@philip001 python]$ ./hello.py
Hello World!
```

Or Run Interactively

- **On Philip (Similar on other clusters):**

```
[fchen14@philip001 python]$ python
Python 2.7.10 |Anaconda 2.3.0 (64-bit)| (default, May 28 2015, 17:02:03)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux2
...
>>> print "Hello World!"
Hello World!
```

- **Easier for todays demonstration:**

```
[fchen14@philip001 ~]$ ipython
Python 2.7.10 |Anaconda 2.3.0 (64-bit)| (default, May 28 2015, 17:02:03)
Type "copyright", "credits" or "license" for more information.
...
In [1]: %pylab
Using matplotlib backend: Qt4Agg
Populating the interactive namespace from numpy and matplotlib
In [2]:
```

Directly Run into List/Array

```
#!/usr/bin/env python
# generate array from 0-4
a = list(range(5))
print a
# len(a)=5
for idx in range(len(a)):
    a[idx] += 5
print a
```

```
[fchen14@philip001 python]$ ./loop_array.py
[0, 1, 2, 3, 4]
[5, 6, 7, 8, 9]
```

Python Tuples

- A Python tuple is a sequence of immutable Python objects. Creating a tuple is as simple as putting different comma-separated values.

```
#!/usr/bin/env python
tup1 = ('physics', 'chemistry', 1997, 2000);
tup2 = (1, 2, 3, 4, 5 );
tup3 = "a", "b", "c", "d";
# The empty tuple is written as two parentheses containing nothing
tup1 = ();
# To write a tuple containing a single value you have to include a comma,
tup1 = (50,);
# Accessing Values in Tuples
print "tup1[0]: ", tup1[0]
print "tup2[1:5]: ", tup2[1:5]
# Updating Tuples, create a new tuple as follows
tup3 = tup1 + tup2;
print tup3
# delete tuple elements
del tup3;
print "After deleting tup3 : "
print tup3
```

Practical Python Programming

Introducing Numpy

Numpy Overview

- **NumPy (Numeric Python) is the fundamental package for scientific computing in Python.**
- **It is a Python library that provides a multidimensional array object, various derived objects (such as masked arrays and matrices)**
- **An assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more.**

- **In short , NumPy package provides basic routines for manipulating large arrays and matrices of numeric data.**

Basic Array Operations

- **Simple array math using np.array**
- **Note that NumPy array starts its index from *0*, end at *N-1* (C-style)**

```
# To avoid module name collision inside package context
>>> import numpy as np
>>> a = np.array([1,2,3])
>>> b = np.array([4,5,6])
>>> a+b
array([5, 7, 9])
>>> a*b
array([ 4, 10, 18])
>>> a ** b
array([  1,  32, 729])
```

Setting Array Element Values

```
>>> a[0]
1
>>> a[0]=11
>>> a
array([11,  2,  3,  4])
>>> a.fill(0) # set all values in the array with 0
>>> a[:]=1 # why we need to use [:]?
>>> a
array([1, 1, 1, 1])
>>> a.dtype   # note that a is still int64 type !
dtype('int64')
>>> a[0]=10.6 # decimal parts are truncated, be careful!
>>> a
array([10,  1,  1,  1])
>>> a.fill(-3.7) # fill() will have the same behavior
>>> a
array([-3, -3, -3, -3])
```

Numpy Array Properties (1)

```
>>> a = np.array([0,1,2,3]) # create a from a list
# create evenly spaced values within [start, stop)
>>> a = np.arange(1,5)
>>> a
array([1, 2, 3, 4])
>>> type(a)
<type 'numpy.ndarray'>
>>> a.dtype
dtype('int64')
# Length of one array element in bytes
>>> a.itemsize
8
```

Numpy Array Properties (2)

```
# shape returns a tuple listing the length of the array
# along each dimension.
>>> a.shape # or np.shape(a)
>>> a.size  # or np.size(a), return the total number of elements
4
# return the number of bytes used by the data portion of the array
>>> a.nbytes
32
# return the number of dimensions of the array
>>> a.ndim
1
```

Numpy Array Creation Functions (1)

```
# Nearly identical to Python's
range(). Creates an array of values
in the range [start,stop) with the
specified step value. Allows non-
integer values for start, stop, and
step. Default dtype is derived from
the start, stop, and step values.
>>> np.arange(4)
array([0, 1, 2, 3])
>>> np.arange(0, 2*np.pi, np.pi/4)
array([ 0.,  0.78539816,  1.57079633,
2.35619449,  3.14159265,  3.92699082,
4.71238898,  5.49778714])
>>> np.arange(1.5,2.1,0.3)
array([ 1.5,  1.8,  2.1])
# ONES, ZEROS
# ones(shape, dtype=float64)
# zeros(shape, dtype=float64)
# shape is a number or sequence
```

```
# specifying the dimensions of the
# array. If dtype is not specified,
# it defaults to float64.
>>> a=np.ones((2,3))
>>> a
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
>>> a.dtype
dtype('float64')
>>> a=np.zeros(3)
>>> a
array([ 0.,  0.,  0.])
>>> a.dtype
dtype('float64')
```

Numpy Array Creation Functions (2)

```
# Generate an n by n identity
# array. The default dtype is
# float64.
>>> a = np.identity(4)
>>> a
array([[ 1.,  0.,  0.,  0.],
       [ 0.,  1.,  0.,  0.],
       [ 0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.]])
>>> a.dtype
dtype('float64')
>>> np.identity(4, dtype=int)
array([[1, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 1]])
# empty(shape, dtype=float64,
# order='C')
```

```
>>> a = np.empty(2)
>>> a
array([ 0.,  0.])
# fill array with 5.0
>>> a.fill(5.0)
>>> a
array([ 5.,  5.])
# alternative approach
# (slightly slower)
>>> a[:] = 4.0
>>> a
array([ 4.,  4.])
```

Numpy Array Creation Functions (3)

```
# Generate N evenly spaced elements between (and including)
# start and stop values.
>>> np.linspace(0,1,5)
array([ 0.  ,  0.25,  0.5 ,  0.75,  1.  ])
# Generate N evenly spaced elements on a log scale between
# base**start and base**stop (default base=10).
>>> np.logspace(0,1,5)
array([  1., 1.77827941, 3.16227766,   5.62341325, 10.])
```

Array from/to ASCII files

- **Useful tool for generating array from txt file**
  - `loadtxt`
  - `genfromtxt`
- **Consider the following example:**

```
#  data.txt
Index
Brain Weight
Body Weight
#here is the training set
 1     3.385    44.500 abjhk
 2     0.480    33.38  bc_00asdk
 ...
#here is the cross validation set
 6    27.660   115.000 rk
 7    14.830    98.200 fff
 ...
 9     4.190    58.000 kij
```

Using loadtxt and genfromtxt

```
>>> a= np.loadtxt('data.txt',skiprows=16,usecols={0,1,2},dtype=None,comments="#")
>>> a
array([[   1.   ,    3.385,   44.5  ],
       [   2.   ,    0.48 ,   33.38 ],
       [   3.   ,    1.35 ,    8.1  ],
       [   4.   ,  465.   ,  423.   ],
       [   5.   ,   36.33 ,  119.5  ],
       [   6.   ,   27.66 ,  115.   ],
       [   7.   ,   14.83 ,   98.2  ],
       [   8.   ,    1.04 ,    5.5  ],
       [   9.   ,    4.19 ,   58.   ]])
# np.genfromtxt can guess the actual type of your columns by using dtype=None
>>> a= np.genfromtxt('data.txt',skip_header=16,dtype=None)
>>> a
array([(1, 3.385, 44.5, 'abjhk'), (2, 0.48, 33.38, 'bc_00asdk'),
       (3, 1.35, 8.1, 'fb'), (4, 465.0, 423.0, 'cer'),
       (5, 36.33, 119.5, 'rg'), (6, 27.66, 115.0, 'rk'),
       (7, 14.83, 98.2, 'fff'), (8, 1.04, 5.5, 'zxs'),
       (9, 4.19, 58.0, 'kij')],
      dtype=[('f0', '<i8'), ('f1', '<f8'), ('f2', '<f8'), ('f3', 'S9')])
```

Reshaping arrays

```
>>> a = np.arange(6)
>>> a
array([0, 1, 2, 3, 4, 5])
>>> a.shape
(6,)
>>> a.shape = (2,3) # reshape array to 2x3
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
>>> a.reshape(3,2)  # reshape array to 3x2
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> a.reshape(2,5)  # cannot change the number of elements in the array
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: total size of new array must be unchanged
>>> a.reshape(2,-1)  # numpy determines the last dimension
```

Numpy Array Data Structure

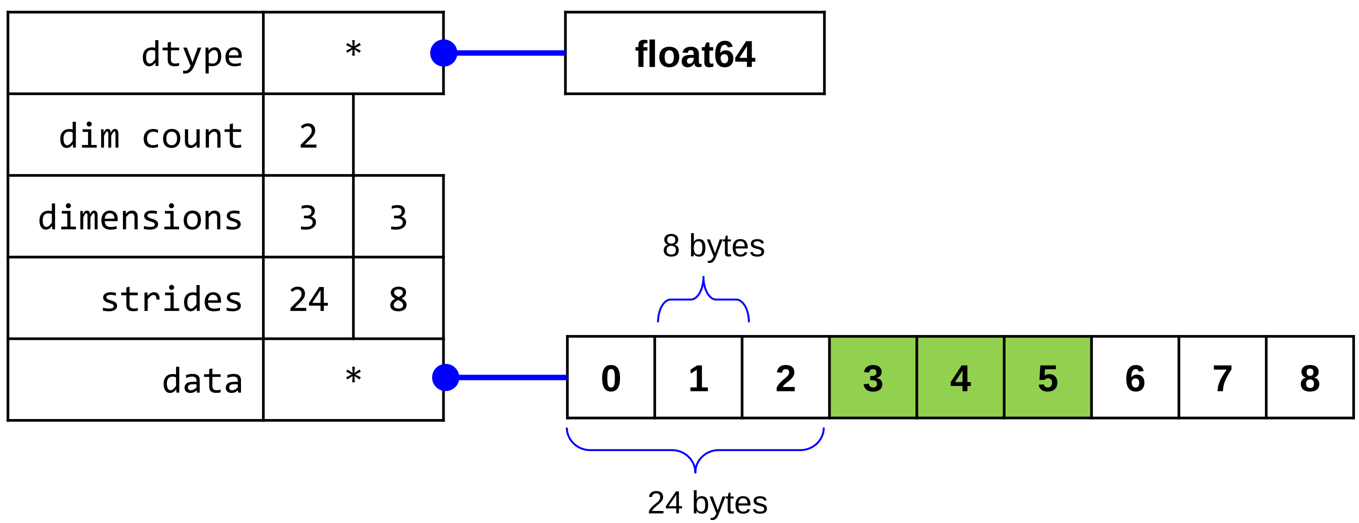
- **Numpy view of 2D array**

```
>>> a=arange(9).reshape(3,-1)
>>> a.strides
(24, 8)
>>> a.ndim
2
```

0	1	2
4	5	6
7	8	9

- **Memory block of the 2D array**

0	1	2	3	4	5	6	7	8



Flattening Multi-dimensional Arrays

```
# Note the difference between
# a.flatten() and a.flat
>>> a
array([[1, 2, 3],
       [4, 5, 6]])
# a.flatten() converts a
# multidimensional array into
# a 1-D array. The new array is a
# copy of the original data.
>>> b = a.flatten()
>>> b
array([1, 2, 3, 4, 5, 6])
>>> b[0] = 7
>>> b
array([7, 2, 3, 4, 5, 6])
>>> a
array([[1, 2, 3],
       [4, 5, 6]])
```

```
# a.flat is an attribute that
# returns an iterator object that
# accesses the data in the multi-
# dimensional array data as a 1-D
# array. It references the original
# memory.
>>> a.flat
<numpy.flatiter object at 0x1421c40>
>>> a.flat[:]
array([1, 2, 3, 4, 5, 6])
>>> b = a.flat
>>> b[0] = 7
>>> a
array([[7, 2, 3],
       [4, 5, 6]])
```

(Un)raveling Multi-dimensional Arrays

```
>>> a
array([[7, 2, 3],
       [4, 5, 6]])
# ravel() is the same as flatten
# but returns a reference of the
# array if possible
>>> b = a.ravel()
>>> b
array([7, 2, 3, 4, 5, 6])
>>> b[0] = 13
>>> b
array([13,  2,  3,  4,  5,  6])
>>> a
array([[13,  2,  3],
       [ 4,  5,  6]])
```

```
>>> at = a.transpose()
>>> at
array([[13,  4],
       [ 2,  5],
       [ 3,  6]])
>>> b = at.ravel()
>>> b
array([13,  4,  2,  5,  3,  6])
>>> b[0]=19
>>> b
array([19,  4,  2,  5,  3,  6])
>>> a
array([[13,  2,  3],
       [ 4,  5,  6]])
```

Practical Python Programming

Basic Usage of Matplotlib

Introduction

- **Matplotlib is probably the single most used Python package for 2D-graphics. (http://matplotlib.org/)**
- **It provides both a very quick way to visualize data from Python and *publication-quality* figures in many formats.**
- **Provides Matlab/Mathematica-like functionality.**

Simple plot

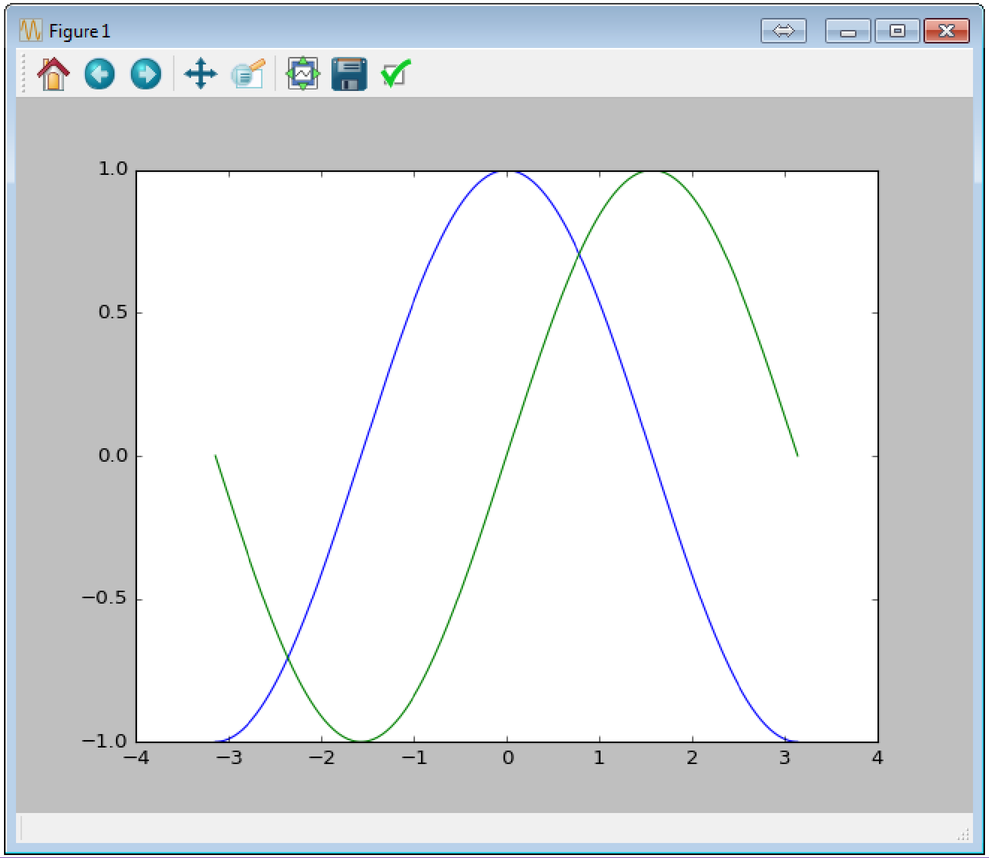
- **Draw the cosine and sine functions on the same plot.**

```
import numpy as np

# X is now a numpy array with 256 values ranging [-pi, pi]
X = np.linspace(-np.pi, np.pi, 256,endpoint=True)
# C is the cosine (256 values) and S is the sine (256 values).
C,S = np.cos(X), np.sin(X)
```

Using default settings to plot

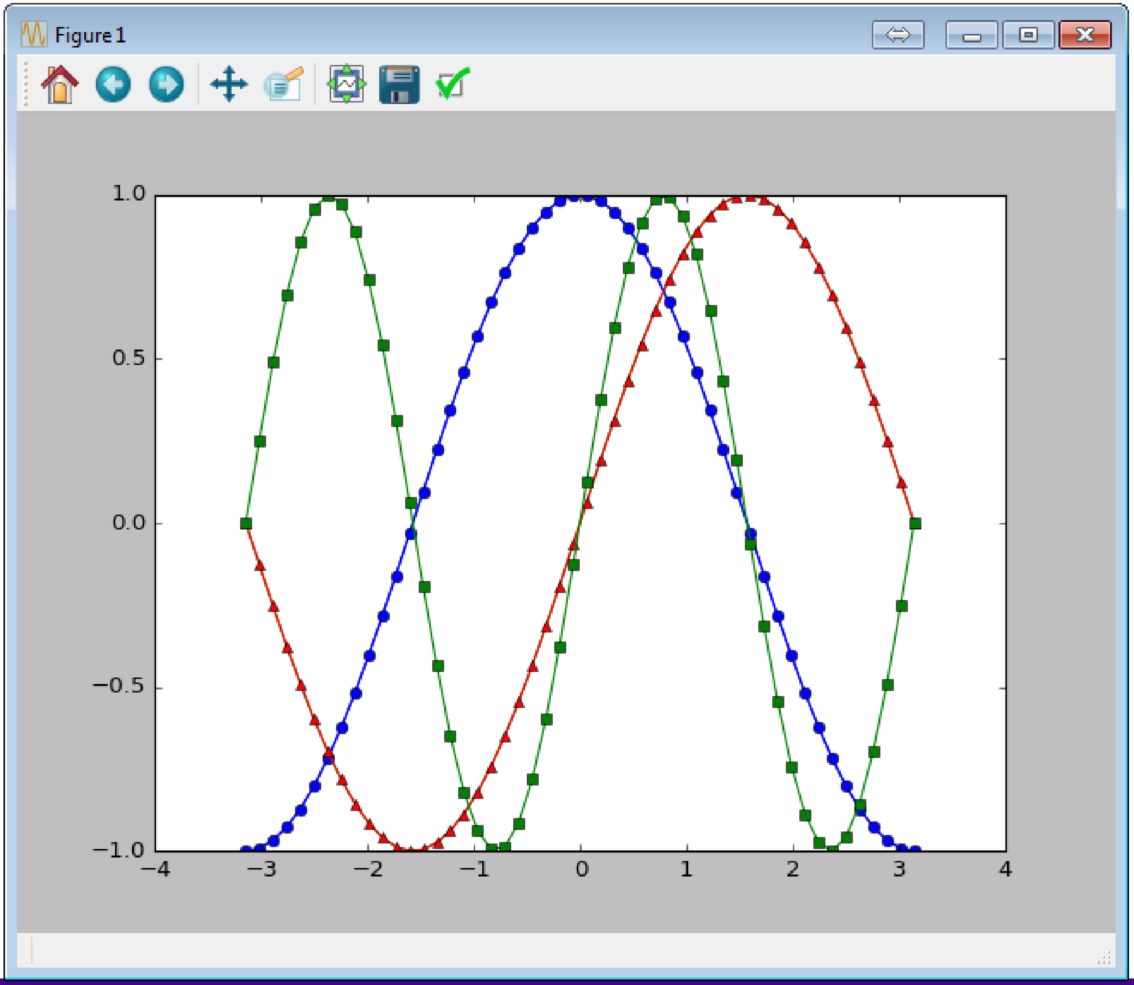
- **Plot the sine and cosine arrays using the default settings**

```
import numpy as np
import matplotlib.pyplot as plt
X = np.linspace(-np.pi, np.pi, 256,endpoint=True)
C,S = np.cos(X), np.sin(X)
# plt.plot(X,C)
# plt.plot(X,S)
plt.plot(X,C,X,S)
plt.show()
```



Line Formatting and Multiple Plot Groups

```
# plot multiple groups with different line styles
plt.plot(X,C,'b-o',X,S,'r-^',X,np.sin(2*X),'g-s')
```



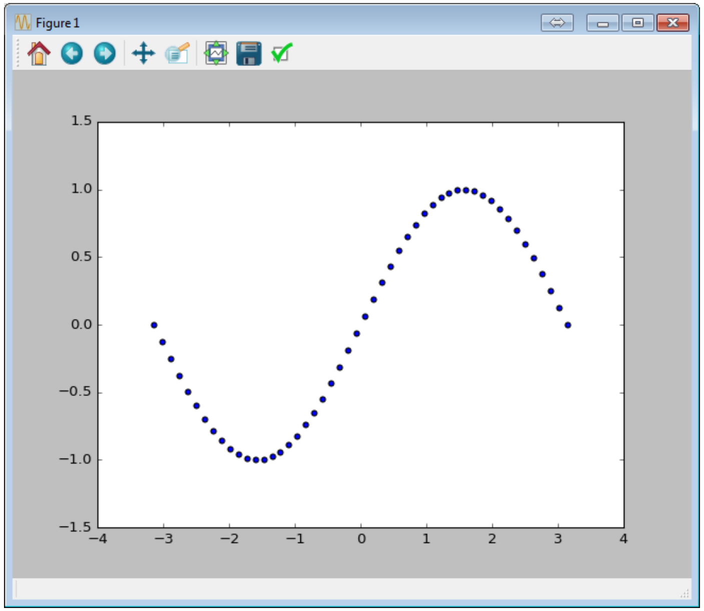
Scatter Plots

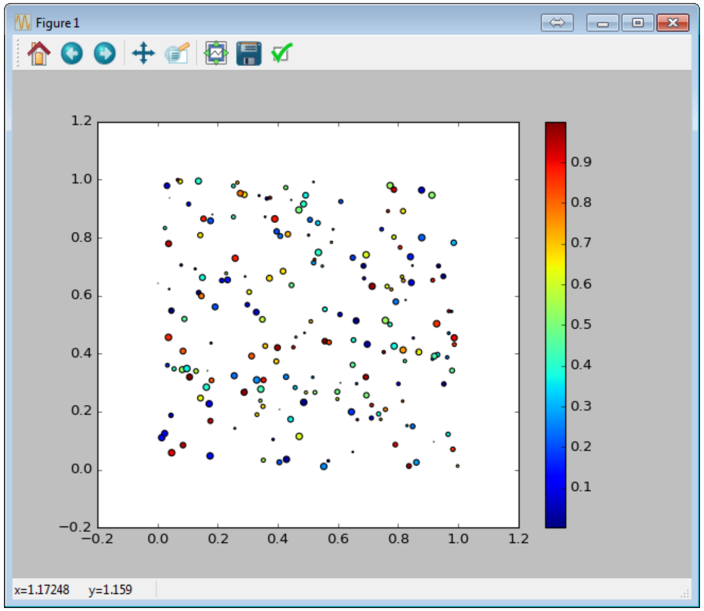
- **Simple Scatter Plot**

```
plt.scatter(X,S)
plt.show()
```

- **Scatter Plot with Colormap**

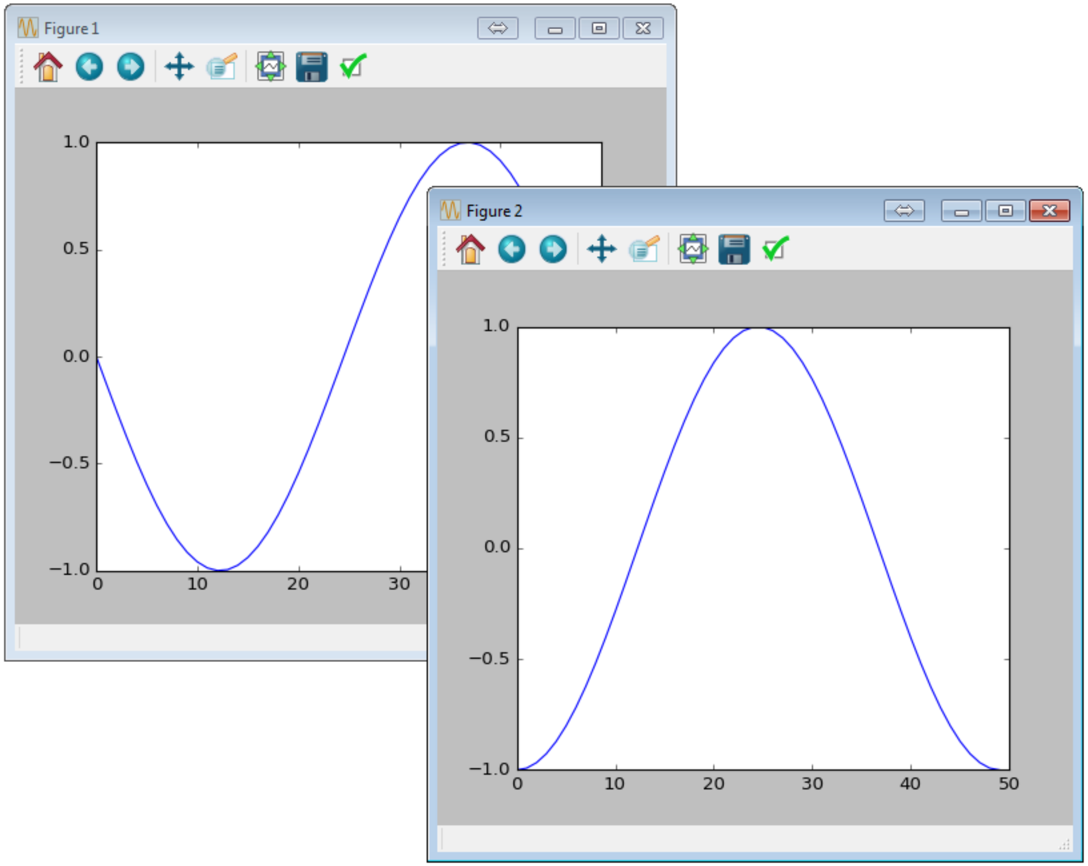
```
x = np.random.rand(200)
y = np.random.rand(200)
size = np.random.rand(200)*30
color = np.random.rand(200)
plt.scatter(x, y, size, color)
plt.colorbar()
```





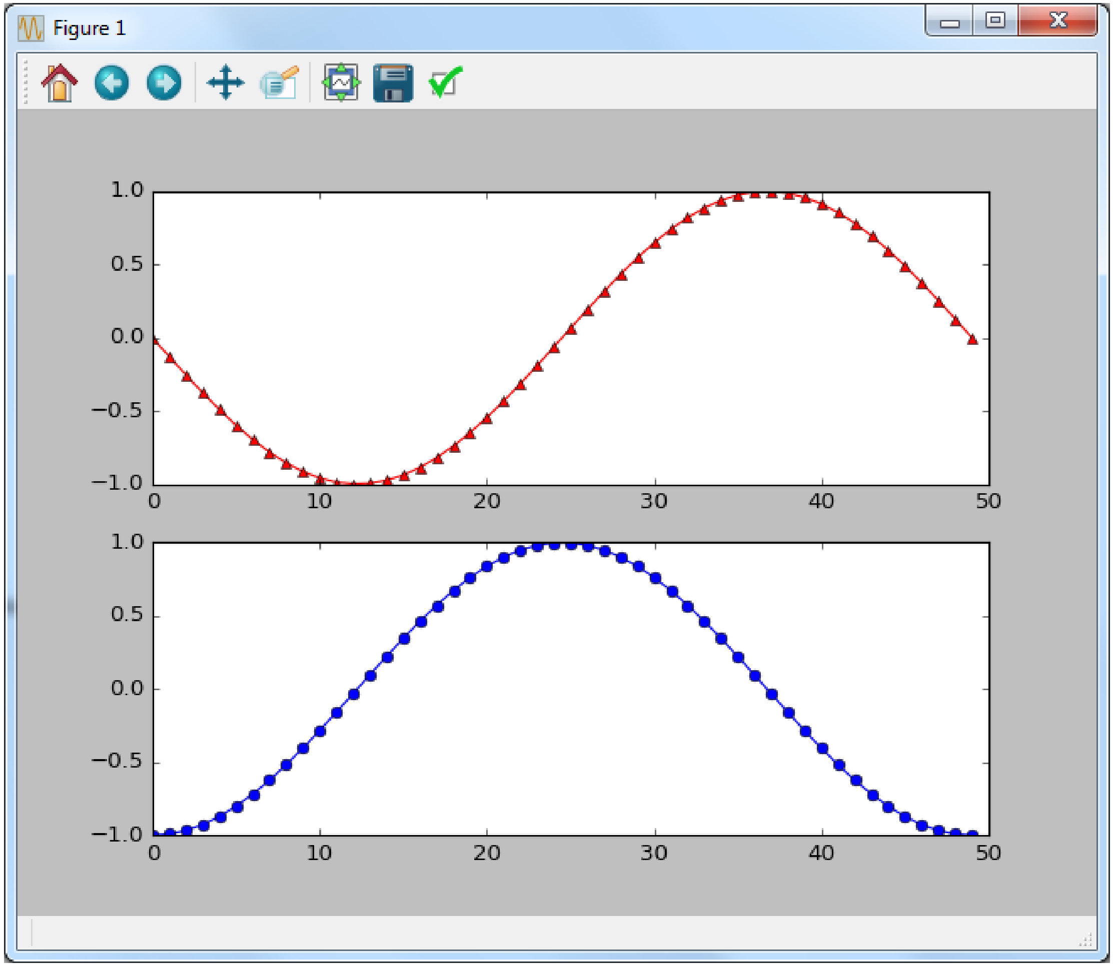
Multiple Figures

```
X = np.linspace(-np.pi, np.pi, 50,endpoint=True)
C,S = np.cos(X), np.sin(X)
# create a figure
plt.figure()
plt.plot(S)
# create a new figure
plt.figure()
plt.plot(C)
plt.show()
```



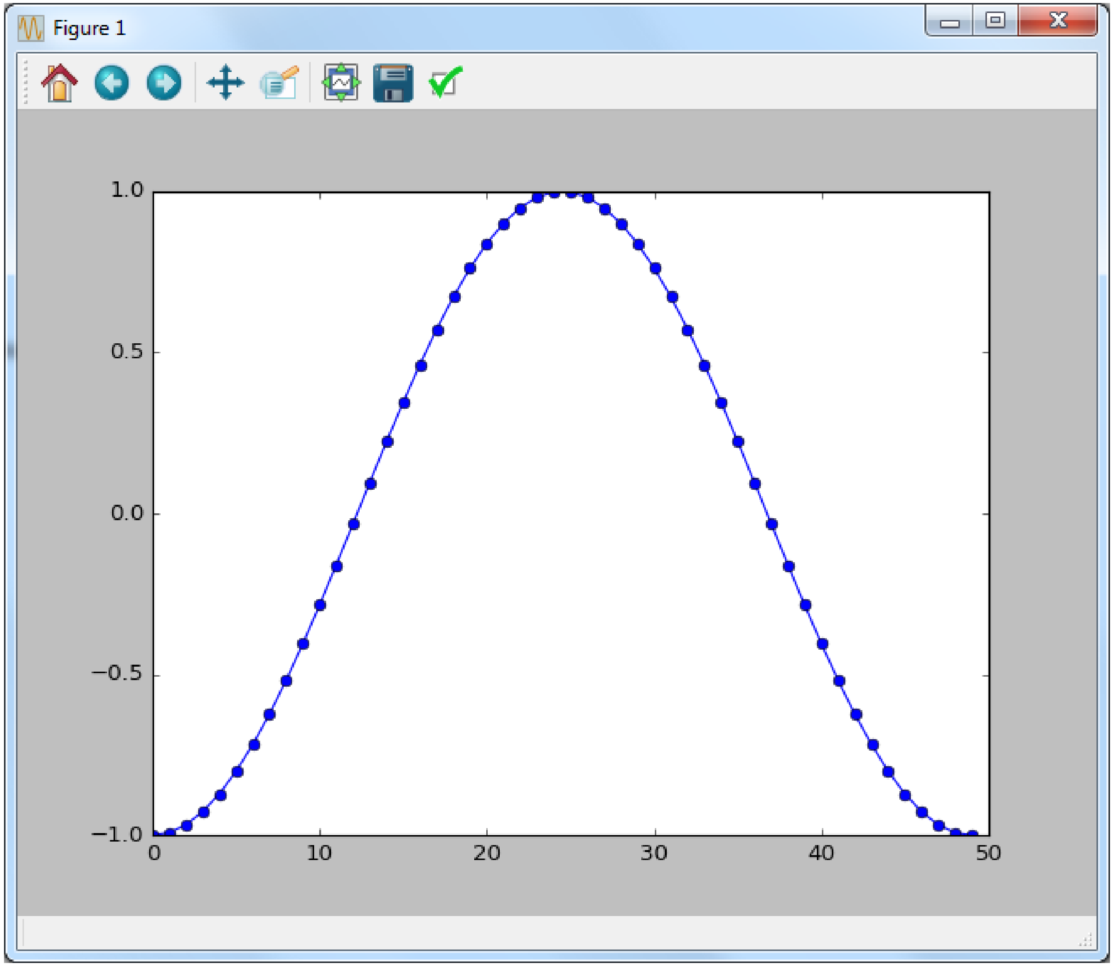
Multiple Plots Using subplot

```
# divide the plotting area in 2 rows and 1 column(s)
# subplot(rows, columns, active_plot)
plt.subplot(2, 1, 1)
plt.plot(S, 'r-^')
# create a new figure
plt.subplot(2, 1, 2)
plt.plot(C, 'b-o')
plt.show()
```



Erase the Previous Curves

```
plt.plot(S, 'r-^')
# whether to keep the old plot use hold(True/False)
plt.hold(False)
plt.plot(C, 'b-o')
plt.show()
```



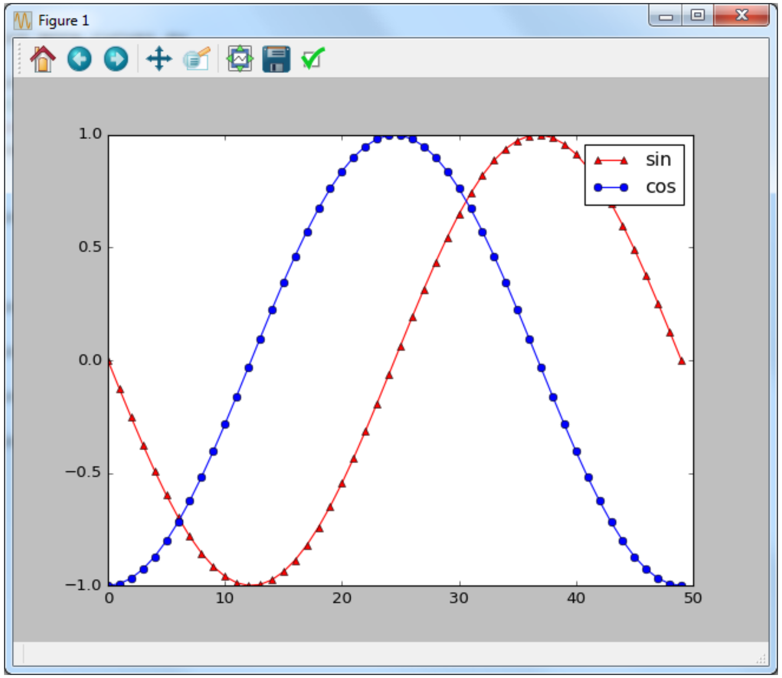
Adding Legend to Plot

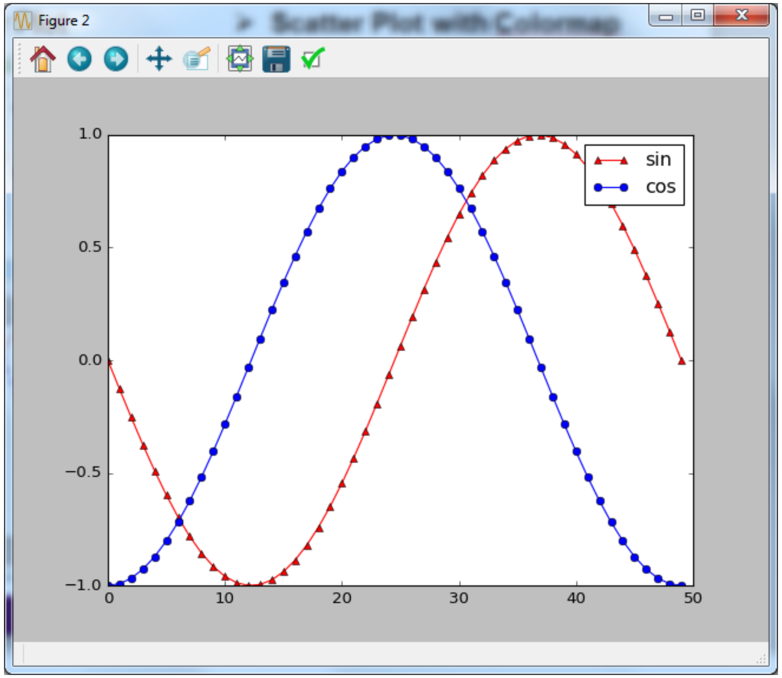
- **Legend labels with plot**

```
# Add labels in plot command
plt.plot(S, 'r-^', label='sin')
plt.plot(C, 'b-o', label='cos')
plt.legend()
```

- **Label with** `plt.legend`

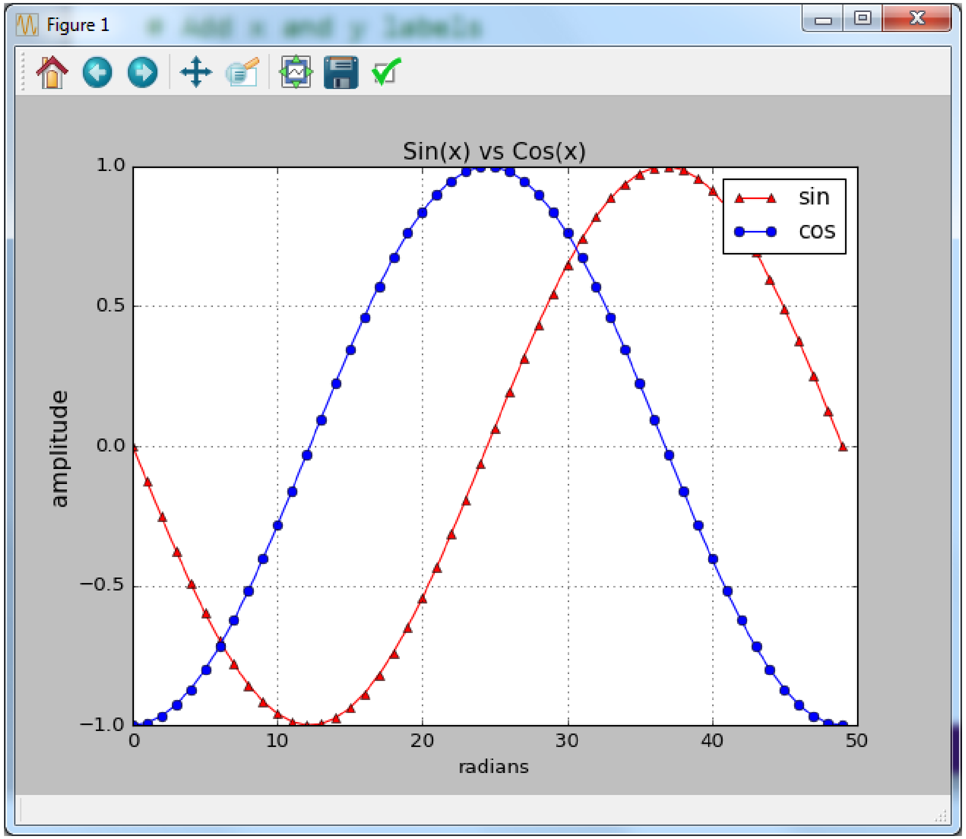
```
# Add labels via list in legend.
plt.plot(S, 'r-^', C, 'b-o')
plt.legend(['sin','cos'])
```





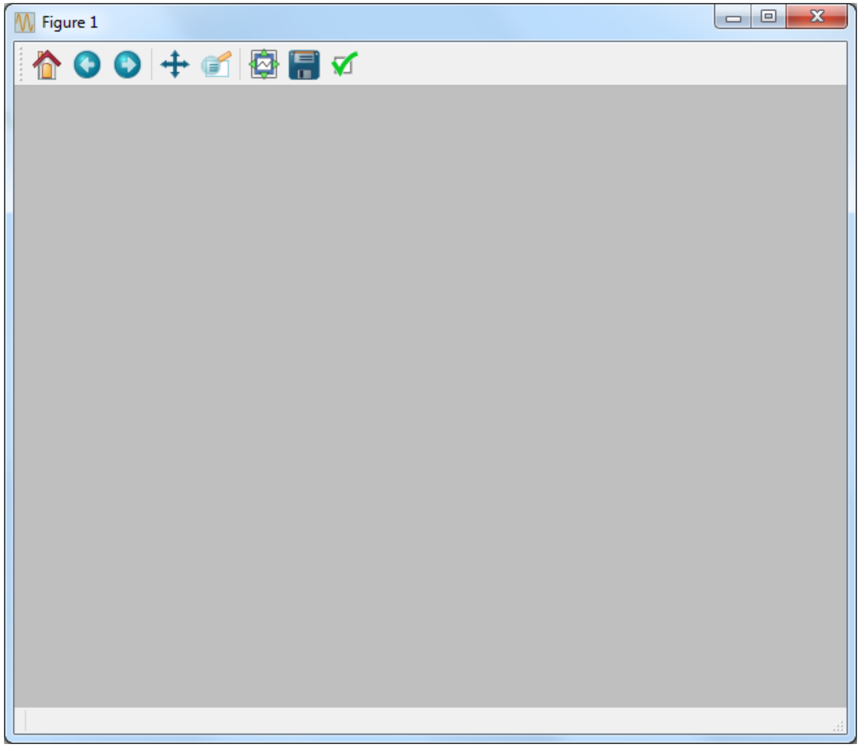
Adding Titles and Grid

```
# Add x and y labels
plt.xlabel('radians')
# Keywords set text properties.
plt.ylabel('amplitude', fontsize='large')
# Add title and show grid
plt.title('Sin(x) vs Cos(x)')
plt.grid()
plt.show()
```

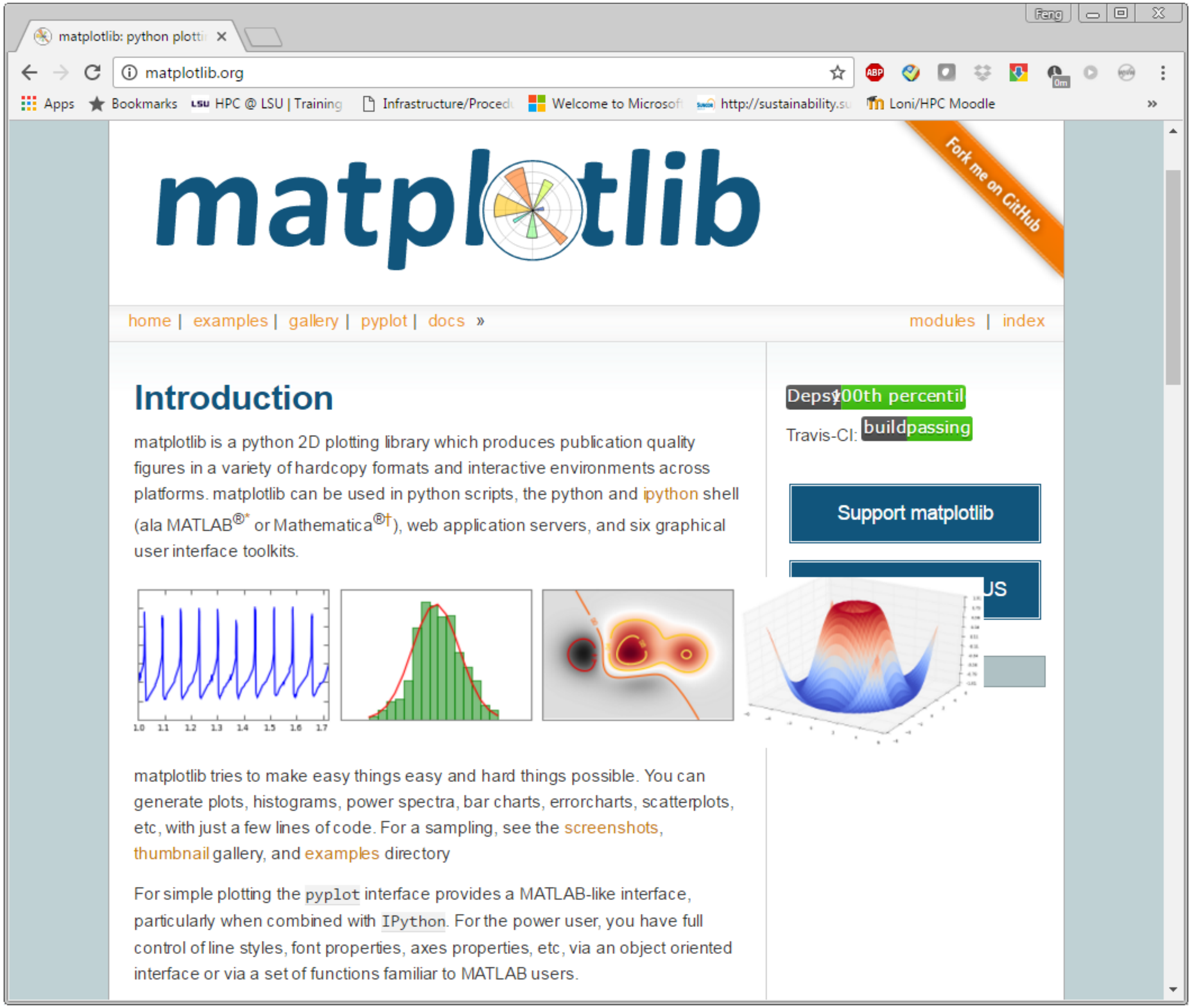


Clearing and Closing Plots

```
# Plot some curves command
plt.plot(S, 'r-^', label='sin')
plt.plot(C, 'b-o', label='cos')
# clf will clear the current plot (figure).
plt.clf()
plt.show()
# close() will close the currently
# active plot window.
plt.close()
# close('all') closes all the plot
# windows.
plt.close('all')
```



Visit Matplotlib Website for More



Four Tools in Numpy

- **Removing loops using NumPy**
  1) Ufunc (Universal Function)
  2) Aggregation
  3) Broadcasting
  4) Slicing, masking and fancy indexing

Numpy's Universal Functions

- **Numpy's universal function (or ufunc for short) is a function that operates on ndarrays in an element-by-element fashion**
- **Ufunc is a "vectorized" wrapper for a function that takes a fixed number of scalar inputs and produces a fixed number of scalar outputs.**
  - Vectorization (simplified): is the process of rewriting a loop so that instead of processing a single element of an array N times, it processes (say) 4 elements of the array simultaneously N/4 times.
- **Many of the built-in functions are implemented in compiled C code.**
  - They can be much faster than the code on the Python level

Ufunc: Math Functions on Numpy Arrays

```
>>> x = np.arange(5.)
>>> x
array([ 0.,  1.,  2.,  3.,  4.])
>>> c = np.pi
>>> x *= c
array([  0.        ,   3.14159265,   6.28318531,   9.42477796,
12.56637061])
>>> y = np.sin(x)
>>> y
array([  0.00000000e+00,   1.22464680e-16,  -2.44929360e-16,
         3.67394040e-16,  -4.89858720e-16])
>>> import math
>>> y = math.sin(x) # must use np.sin to perform array math
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: only length-1 arrays can be converted to Python scalars
```

Ufunc: Many ufuncs available

- **Arithmetic Operators:** `+ - * / // % **`
- **Bitwise Operators:** `& | ~ ^ >> <<`
- **Comparison Oper's:** `< > <= >= == !=`
- **Trig Family:** `np.sin, np.cos, np.tan ...`
- **Exponential Family:** `np.exp, np.log, np.log10 ...`
- **Special Functions:** `scipy.special.*`
- **. . . and many, many more.**

Aggregation Functions

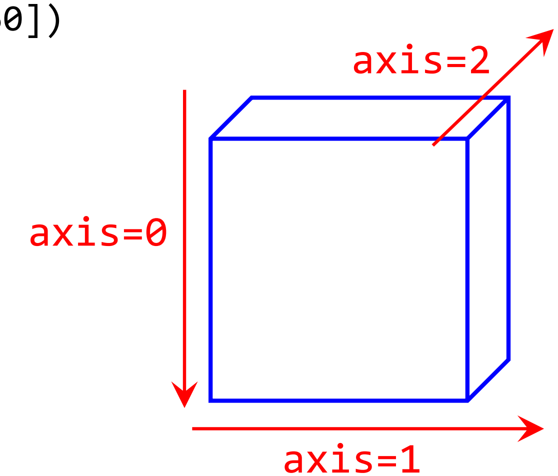
- **Aggregations are functions which summarize the values in an array (e.g. min, max, sum, mean, etc.)**
- **Numpy aggregations are much faster than Python built-in functions**

Numpy Aggregation - Array Calculation

```
>>> a=np.arange(6).reshape(2,-1)
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
# by default a.sum() adds up all values
>>> a.sum()
15
# same result, functional form
>>> np.sum(a)
15
# note this is not numpy’s sum!
>>> sum(a)
array([3, 5, 7])
# not numpy’s sum either!
>>> sum(a,axis=0)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: sum() takes no keyword
arguments
```

```
# sum along different axis
>>> np.sum(a,axis=0)
array([3, 5, 7])
>>> np.sum(a,axis=1)
array([ 3, 12])
>>> np.sum(a,axis=-1)
array([ 3, 12])
# product along different axis
>>> np.prod(a,axis=0)
array([ 0,  4, 10])
>>> a.prod(axis=1)
array([ 0, 60])
```

The **axes** of an array describe the order of indexing into the array, e.g., axis=0 refers to the first index coordinate, axis=1 the second, etc.



Numpy Aggregation – Statistical Methods

```
>>> np.set_printoptions(precision=4)
# generate 2x3 random float array
>>> a=np.random.random(6).reshape(2,3)
>>> a
array([[ 0.7639,  0.6408,  0.9969],
       [ 0.5546,  0.5764,  0.1712]])
>>> a.mean(axis=0)
array([ 0.6592,  0.6086,  0.5841])
>>> a.mean()
0.6173086542501534‍7
>>> np.mean(a)
0.61730865425015347
# average can use weights
>>> np.average(a,weights=[1,2,3],axis=1)
array([ 0.8394,  0.3702])
# standard deviation
>>> a.std(axis=0)
array([ 0.1046,  0.0322,  0.4129])
```

```
# variance
>>> np.var(a, axis=1)
array([ 0.0218,  0.0346])
>>> a.min()
0.17118969968007625
>>> np.max(a)
0.99691892655137737
# find index of the minimum
>>> a.argmin(axis=0)
array([1, 1, 1])
>>> np.argmax(a,axis=1)
array([2, 1])
# this will return flattened index
>>> np.argmin(a)
5
>>> a.argmax()
2
```

Numpy's Aggregation - Summary

- **All have the same call style.**
  - `np.min() np.max() np.sum() np.prod()`
  - `np.argsort()`
  - `np.mean() np.std() np.var() np.any()`
  - `np.all() np.median() np.percentile()`
  - `np.argmin() np.argmax() . . .`
  - `np.nanmin() np.nanmax() np.nansum(). . .`

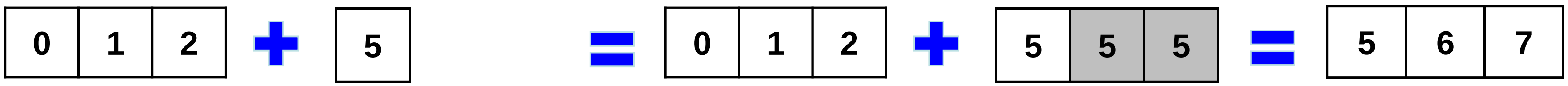
Array Broadcasting

- **Broadcasting is a set of rules by which ufuncs operate on arrays of different sizes and/or dimensions.**
- **Broadcasting allows NumPy arrays of different dimensionality to be combined in the same expression.**
- **Arrays with smaller dimension are broadcasted to match the larger arrays, without copying data.**

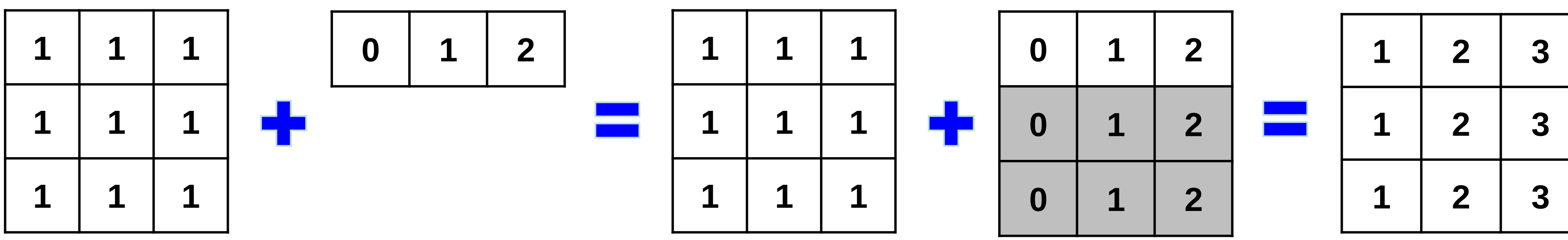
Broadcasting Rules

1. If array shapes differ, left-pad the smaller shape with 1s
2. If any dimension does not match, broadcast the dimension with size=1
3. If neither non-matching dimension is 1, raise an error.

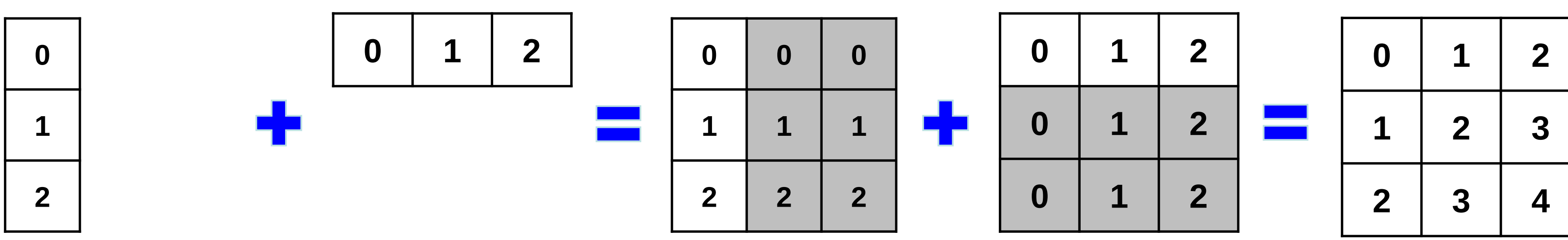
```
np.arange(3) + 5
```




```
np.ones((3,3)) + np.arange(3)
```




```
np.arange(3).reshape(3,1) + np.arange(3)
```



Broadcasting Rules – 1D array

```
np.arange(3) + 5
```

0	1	2	+	5

1. **If array shapes differ, left-pad the smaller shape with 1s**

```
1) shape=(3,)      shape=()
2) shape=(3,)      shape=(1,)
3) shape=(3,)      shape=(3,)
4) final shape=(3,)
```

2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**

0	1	2	+	5	5	5	=	5	6	7

Broadcasting Rules – 2D array (1)

```
np.ones((3,3)) + np.arange(3)
```

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 2 \\ 0 & 1 & 2 \\ 0 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix}$$

```
1) shape=(3,3)     shape=(3,)
2) shape=(3,3)     shape=(1,3)
3) shape=(3,3)     shape=(3,3)
final shape=(3,3)
```

1. **If array shapes differ, left-pad the smaller shape with 1s**
2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**

Broadcasting Rules – 2D array (2)

```
np.arrange(3).reshape(3,1) + np.arange(3)
```

0	0	0
1	1	1
2	2	2

+

0	1	2
0	1	2
0	1	2

=

0	1	2
1	2	3
2	3	4

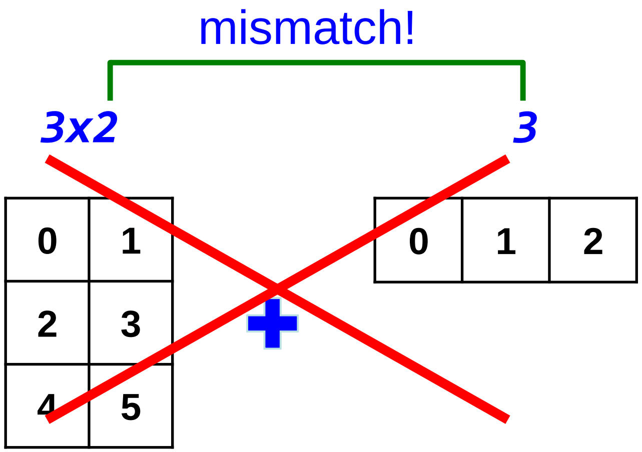
```
1) shape=(3,1)     shape=(3)
2) shape=(3,1)     shape=(1,3)
3) shape=(3,3)     shape=(3,3)
final shape=(3,3)
```

1. **If array shapes differ, left-pad the smaller shape with 1s**
2. **If any dimension does not match, broadcast the dimension with size=1**
3. **If neither non-matching dimension is 1, raise an error.**

Broadcasting Rules – Error

- **The trailing axes of either arrays must be 1 or both must have the same size for broadcasting to occur. Otherwise, a "ValueError: operands could not be broadcast together with shapes" exception is thrown.**

```
>>> a=np.arange(6).reshape(3,2)
>>> a
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> b=np.arange(3)
>>> b
array([0, 1, 2])
>>> a+b
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: operands could not be broadcast together with shapes (3,2) (3,)
```



Slicing, Masking and Fancy Indexing

- **See next few slides...**

Array Slicing (1)

- `arr[lower:upper:step]`
- **Extracts a portion of a sequence by specifying a lower and upper bound. The lower-bound element is included, but the upper-bound element is not included. Mathematically: `[lower, upper)`. The step value specifies the stride between elements.**

```
# indices:          0  1  2  3  4
# negative indices:-5 -4 -3 -2 -1
>>> a =  np.array([10,11,12,13,14])
# The following slicing results are the same
>>> a[1:3]
array([11, 12])
>>> a[1:-2]
array([11, 12])
>>> a[-4:3]
array([11, 12])
```

Array Slicing (2)

- **Omitting Indices: omitted boundaries are assumed to be the beginning or end of the list, compare the following results**

```
>>> a[:3] # first 3 elements
array([10, 11, 12])
>>> a[-2:] # last 2 elements
array([13, 14])
>>> a[1:]  # from 1st element to the last
array([11, 12, 13, 14])
>>> a[:-1] # from 1st to the second to last
array([10, 11, 12, 13])
>>> a[:]   # entire array
array([10, 11, 12, 13, 14])
>>> a[::2] # from 1st, every other element (even indices)
array([10, 12, 14])
>>> a[1::2] # from 2nd, every other element (odd indices)
array([11, 13])
```

Multidimensional Arrays

- **A few 2D operations similar to the 1D operations shown above**

```
>>> a = np.array([[ 0, 1, 2, 3],[10,11,12,13]], float)
>>> a
array([[  0.,   1.,   2.,   3.],
       [ 10.,  11.,  12.,  13.]])
>>> a.shape # shape = (rows, columns)
(2, 4)
>>> a.size  # total elements in the array
8
>>> a.ndim  # number of dimensions
2
>>> a[1,3]  # reference a 2D array element
13
>>> a[1,3] = -1 # set value of an array element
>>> a[1]    # address second row using a single index
array([10., 11., 12., -1.])
```

2D Array Slicing

```
>>> a = np.arange(1,26)
>>> a = a.reshape(5,5) # generate the 2D array
>>> a[0,3:5]
array([4, 5])
>>> a[0,3:4]
array([4])
>>> a[4:,4:]
array([[25]])
>>> a[3:,3:]
array([[19, 20],
       [24, 25]])
>>> a[:,2]
array([ 3,  8, 13, 18, 23])
>>> a[2::2,::2]
array([[11, 13, 15],
       [21, 23, 25]])
```

1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

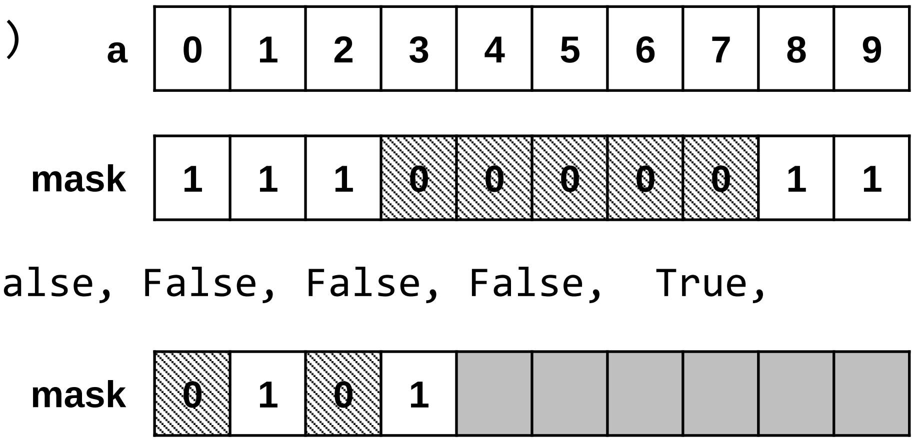
Slices Are References

- **Slices are references to memory in the original array**
- **Changing values in a slice also changes the original array !**

```
>>> a = np.arange(5)
>>> a
array([0, 1, 2, 3, 4])
>>> b = a[2:4]
>>> b
array([2, 3])
>>> b[0]=7
>>> a
array([0, 1, 7, 3, 4])
```

Masking

```
>>> a=np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
# creation of mask using ufunc
>>> mask=np.abs(a-5)>2
>>> mask
array([ True,  True,  True, False, False, False, False, False,  True,
True], dtype=bool)
>>> a[mask]
array([0, 1, 2, 8, 9])
>>> mask=np.array([0,1,0,1],dtype=bool)
# manual creation of mask
>>> mask
array([False,  True, False,  True], dtype=bool)
>>> a[mask]
array([1, 3])
```

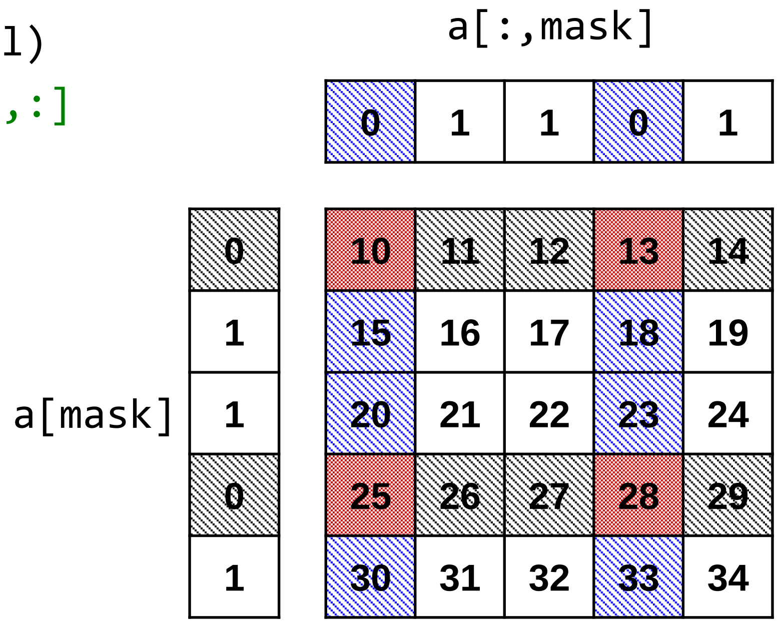


Masking and where

```
>>> a=np.arange(8)**2
>>> a
array([ 0,  1,  4,  9, 16, 25, 36, 49])
>>> mask=np.abs(a-9)>5
>>> mask
array([ True,  True, False, False,  True,  True,  True,  True], 
dtype=bool)
# find the locations in array where expression is true
>>> np.where(mask)
(array([0, 1, 4, 5, 6, 7]),)
>>> loc=np.where(mask)
>>> a[loc]
array([ 0,  1, 16, 25, 36, 49])
```

Masking in 2D

```
>>> a=np.arange(25).reshape(5,5)+10
>>> a
array([[10, 11, 12, 13, 14],
       [15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24],
       [25, 26, 27, 28, 29],
       [30, 31, 32, 33, 34]])
>>> mask=np.array([0,1,1,0,1],dtype=bool)
>>> a[mask]   # on rows, same as a[mask,:]
array([[15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24],
       [30, 31, 32, 33, 34]])
>>> a[:,mask] # on columns
array([[11, 12, 14],
       [16, 17, 19],
       [21, 22, 24],
       [26, 27, 29],
       [31, 32, 34]])
```



Fancy Indexing - 1D

- NumPy offers more indexing facilities than regular Python sequences.
- In addition to indexing by integers and slices, arrays can be indexed by arrays of integers and arrays of Booleans (as seen before).

```
>>> a=np.arange(8)**2
>>> a
array([ 0,  1,  4,  9, 16, 25, 36, 49])
# indexing by position
>>> i=np.array([1,3,5,1])
>>> a[i]
array([ 1,  9, 25,  1])
>>> b=(np.arange(6)**2).reshape(2,-1)
>>> b
array([[ 0,  1,  4],
       [ 9, 16, 25]])
>>> i=[0,1,0]
>>> j=[0,2,1]
>>> b[i,j] # indexing 2D array by position
array([ 0, 25,  1])
```

Fancy Indexing - 2D

```
>>> b=(np.arange(12)**2).reshape(3,-1)
>>> b
array([[  0,   1,   4,   9],
       [ 16,  25,  36,  49],
       [ 64,  81, 100, 121]])
>>> i=[0,2,1]
>>> j=[0,2,3]
# indexing 2D array
>>> b[i,j]
array([  0, 100,  49])
# note the shape of the resulting array
>>> i=[[0,2],[2,1]]
>>> j=[[0,3],[3,1]]
# When an array of indices is used,
# the result has the same shape as the indices;
>>> b[i,j]
array([[  0, 121],
       [121,  25]])
```

idx	0	1	2	3
0	0	1	4	9
1	16	25	36	49
2	64	81	100	121

Change RGB Image to Grayscale

Using Numpy to Process Image

- **RGB to Grayscale Conversion:**
  - Using simple average

$$V_{Gray} = \left(V_{Red} + V_{Green} + V_{Blue}\right)/3$$

  - Using weighted average (https://en.wikipedia.org/wiki/Grayscale)

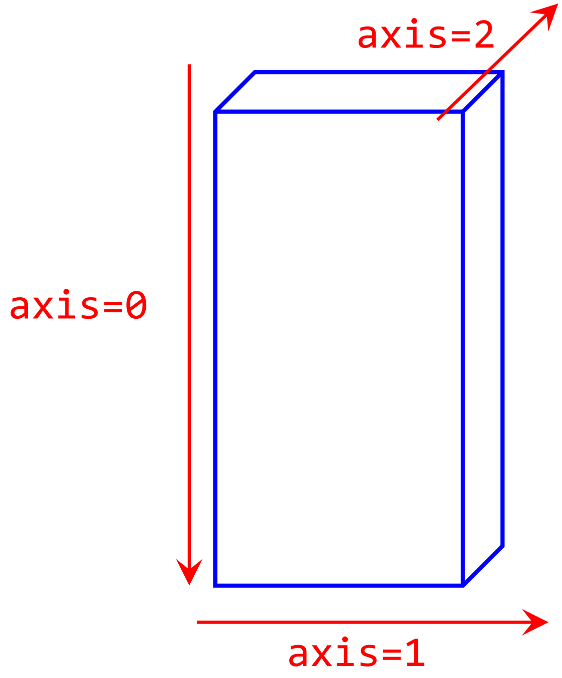
$$V_{Gray} = \left(0.299V_{Red} + 0.587V_{Green} + 0.114V_{Blue}\right)/3$$

- **Loading and Displaying Images**

Load Image

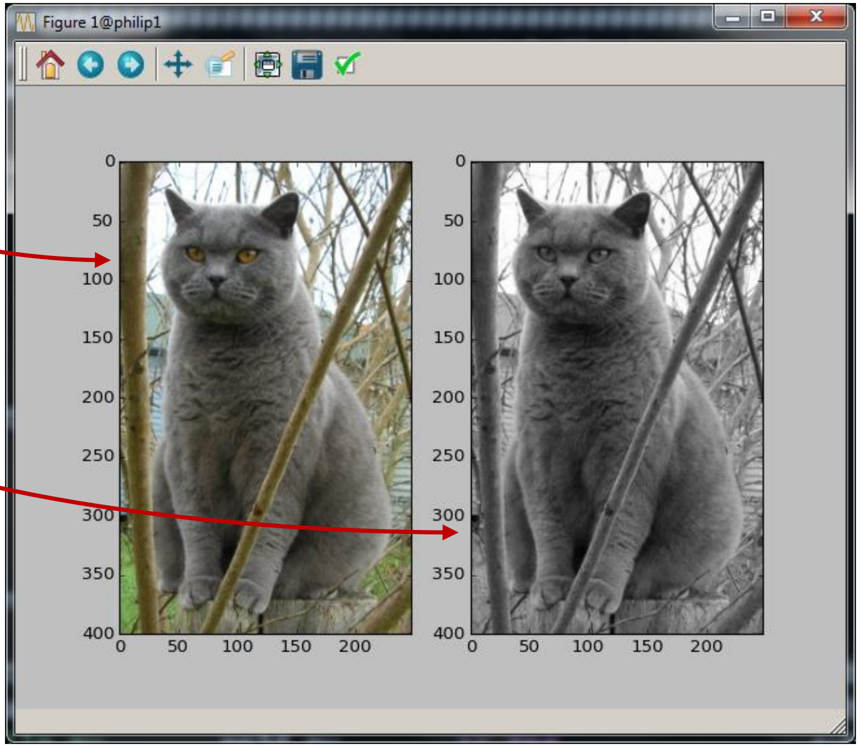
```
# import necessary images
import numpy as np
from scipy.misc import imread, imresize
import matplotlib.pyplot as plt
# To load an image, we use imread method from scipy's misc modules:
img = imread('cat.jpg')
print img.shape
```

```
Shape of the loaded image in ipython:
In [2]: imread('cat.jpg')
Out[2]:
array([[[132, 128, 117],
        [155, 151, 139],
        [181, 175, 161],
        ...,
        [ 91,  76,  57],
        [ 89,  74,  55],
        [ 86,  71,  50]]], dtype=uint8)
```



Averaging The RGB Channel Values

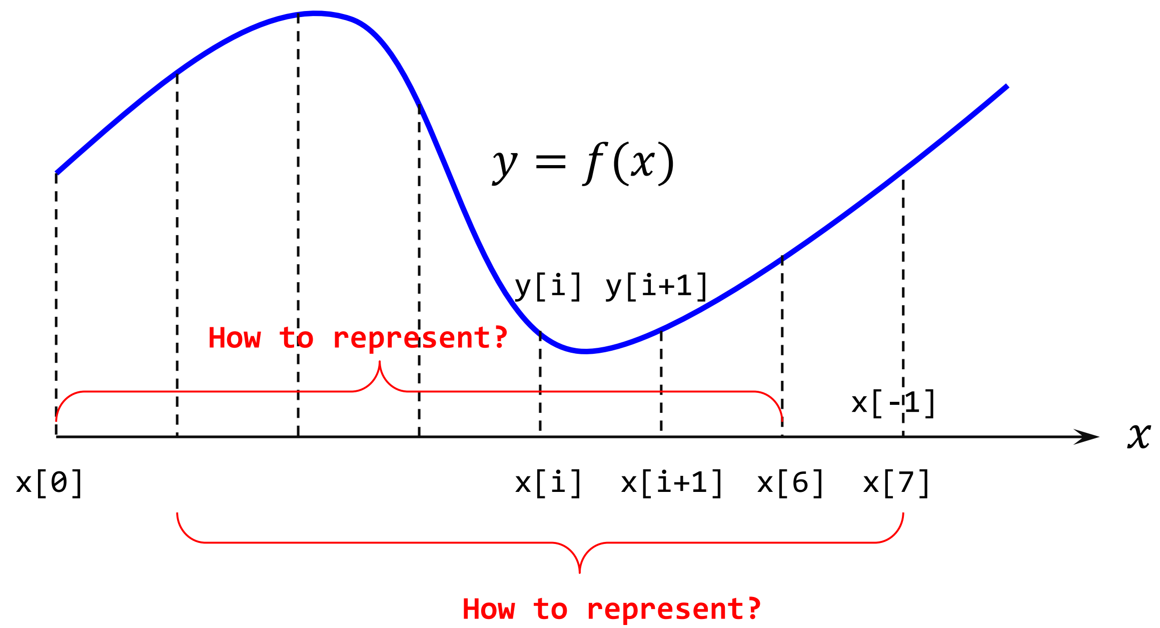
```
# This is simple average along axis=2
# img_tinted = np.average(img,axis=2)
# This is weighted average along axis=2
img_tinted = np.average(img,weights=[0.299,0.587,0.114],axis=2)
print img_tinted.shape
print img.shape
# plot the original image on the left
plt.subplot(1, 2, 1)
plt.imshow(img)
# plot the grayscale image on the left
plt.subplot(1, 2, 2)
plt.imshow(np.uint8(img_tinted),
    cmap='gray')
plt.show()
```



Practical Python Programming

Calculate Derivative/Integration

Problem Description



- **Numerical Derivative and Integration:**

$$y' = \frac{dy}{dx} \approx \frac{\Delta y}{\Delta x} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

$$\int_a^b f(x)dx = \sum_{i=1}^{N} \frac{1}{2}\left(y_i + y_{i+1}\right) \cdot \Delta x$$

- **How to get a vector of Δy and Δx ?**

Calculate Derivative - Solution

- **Using Numpy slicing:**

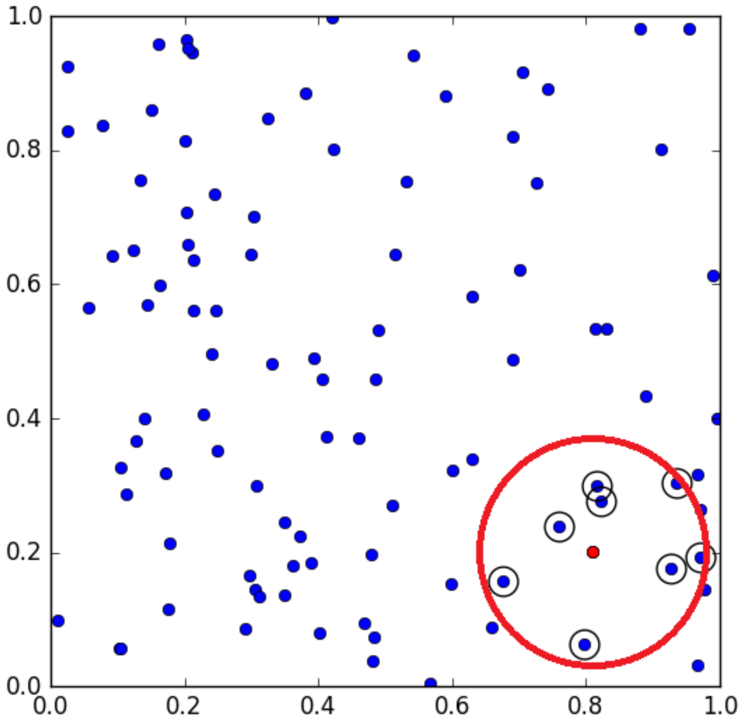
```
import numpy as np
import matplotlib.pyplot as plt

# calculate the sin() function on evenly spaced data.
x = np.linspace(0,2*np.pi,101)
y = np.sin(x)

# use slicing to get dy and dx
dy=y[1:]-y[:-1]
dx=x[1:]-x[:-1]

dy_dx = dy/dx
```

Calculate Integration - Solution

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

# calculate the sin() function on evenly spaced data.
x = np.linspace(0,2*np.pi,101)
y = np.sin(x)

# use slicing to get dy and dx
cx = 0.5*(x[1:]+x[:-1])
dy_by_2=0.5*(y[1:]+y[:-1])

# note the trapezoid rule with cumsum
area = np.cumsum(dx*dy_by_2)
analytical = -np.cos(x) + np.cos(0)
```

Example using Numpy: Nearest Neighbors

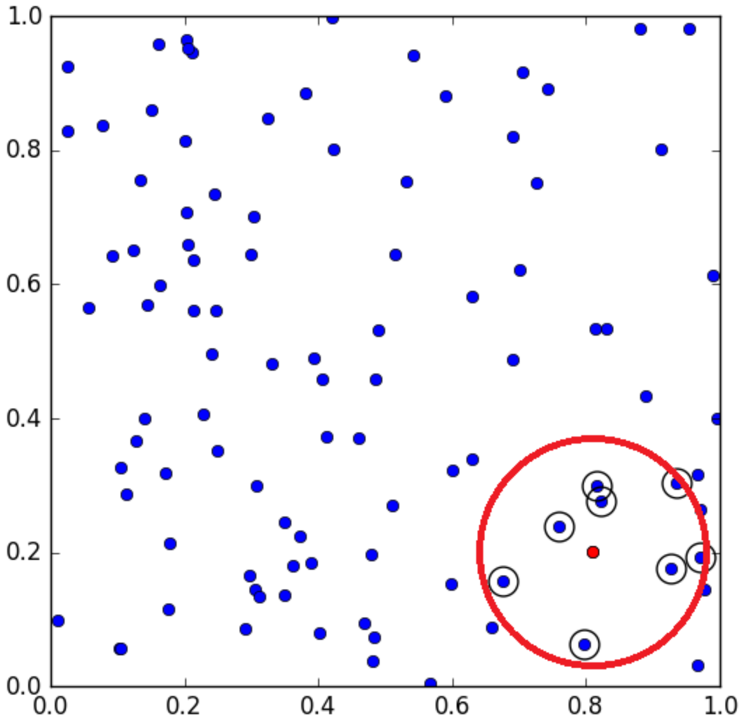
- **A k-nearest neighbor search identifies the top k nearest neighbors to a query.**
- **The problem is: given a dataset D of vectors in a d-dimensional space and a query point x in the same space, find the closest point in D to x.**
  - Molecular Dynamics
  - K-means clustering



Nearest Neighbors - Naive Implementation

- **Using for loops…?**

$$d_{i,j}^2 = \left(x_i - x_j\right)^2 + \left(y_i - y_j\right)^2$$



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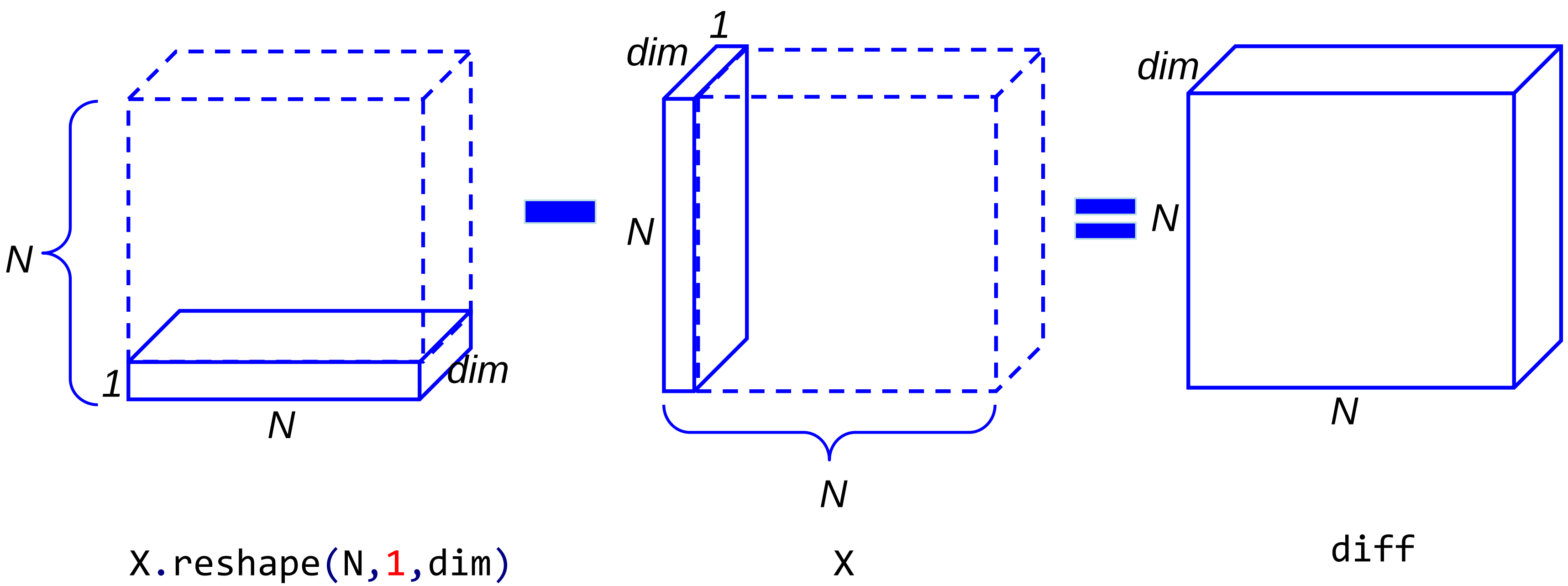
Nearest Neighbors - Better Implementation

```
# A better implementation
N=100
dim=2
# generate N random points in 2D
X = np.random.random((N,dim))
```

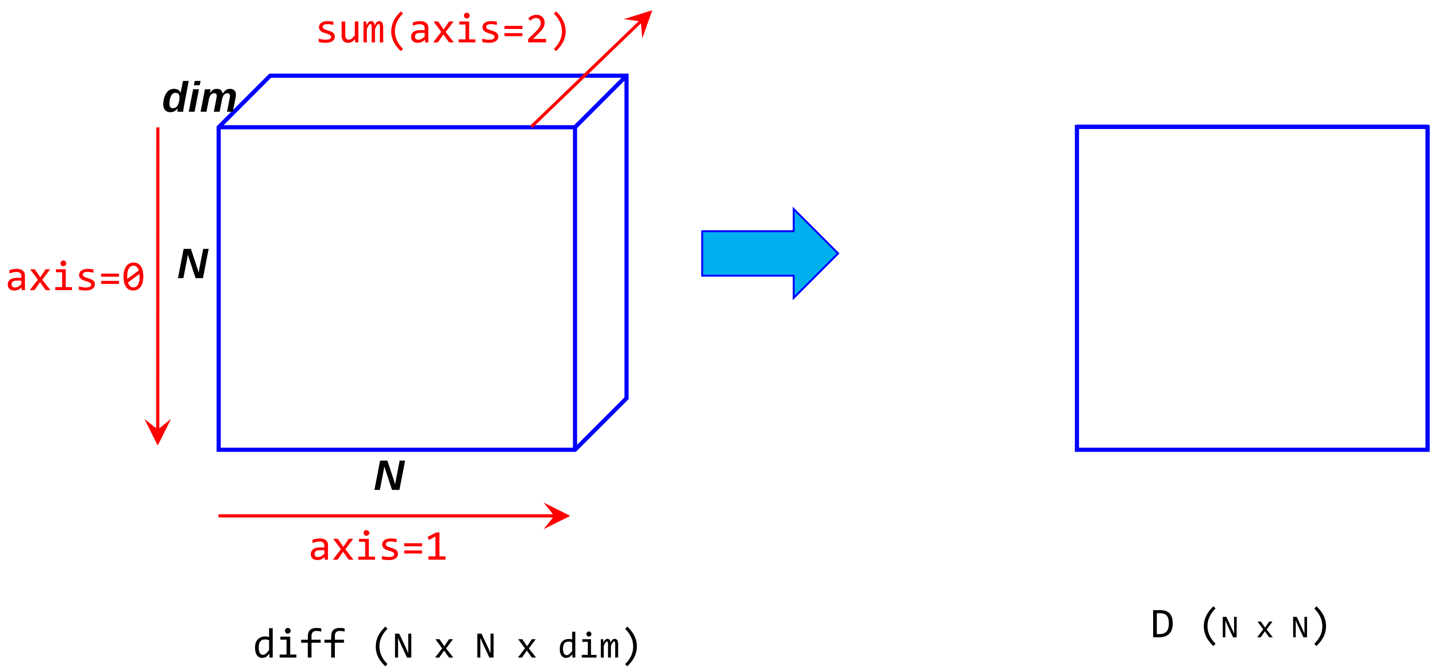
Nearest Neighbors - Pairwise differences

```
# find pairwise difference using broadcasting
diff = X.reshape(N,1,dim)-X
                (N,1,dim)      (N,dim)
                (N,1,dim)    (1,N,dim)
                (N,N,dim)    (N,N,dim)
```



Nearest Neighbors - argsum

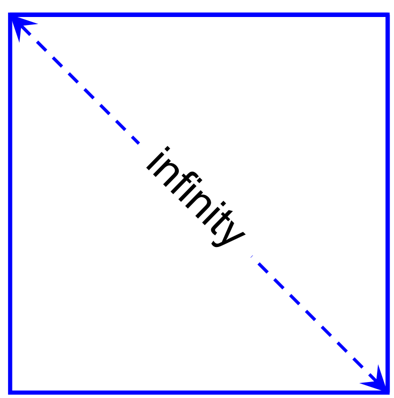
```
# Calculate the sum of diff using the aggregate function
D = (diff**2).sum(axis=2)
```



Nearest Neighbors - Diagonal Values

- **In order to avoid the self-self neighbors, set the diagonal values to infinity using numpy's pre-defined values**

```
# set diagonal to infinity to skip self-neighbors
i = np.arange(N)
# using advanced (integer) indexing
D[i,i]=np.inf
```



D(N x N)

Nearest Neighbors - Obtain the Indices

- An example of the D matrix (N=5)

```
Index:        0           1           2           3           4
[[         inf  0.06963122  0.44504047  0.04605534  0.36092231]
 [ 0.06963122          inf  0.23486059  0.06682903  0.31504998]
 [ 0.44504047  0.23486059         inf  0.23614707  0.12082747]
 [ 0.04605534  0.06682903  0.23614707         inf  0.14981131]
 [ 0.36092231  0.31504998  0.12082747  0.14981131         inf]]
```

- For p=1, the nearest neighbor is 3

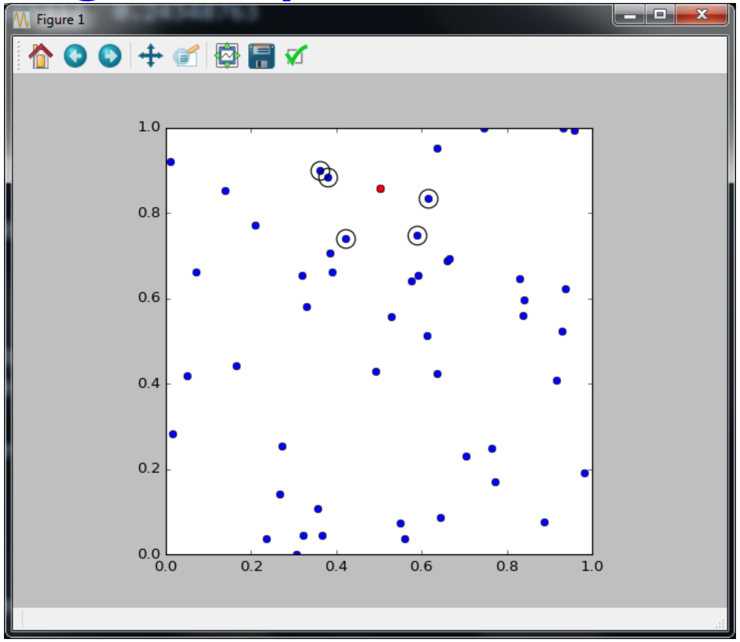
Nearest Neighbors – k nearest neighbor

- **How to get the k nearest neighbors?**

```
# this will return all the nearest neighbors matrix (nnm)
nnm = D.argsort(axis=1)
```

Verify Results using Matplotlib

```
# plot all the random points
plt.plot(X[:,0],X[:,1],'ob')
# plot pth point in red
p = N/2
plt.plot(X[p,0],X[p,1],'or')
```




```
k = 5
# plot k neighbors in circles
plt.plot(X[nnm[p,:k],0],X[nnm[p,:k],1],'o',markerfacecolor='None',markersize=15,markeredgewidth=1)
# equalize the x and y scale
plt.gca().set_aspect('equal', adjustable='box')
plt.show()
```

Practical Python Programming

Introducing Scipy

Numerical Methods with Scipy

- **Scipy package (SCIentific PYthon) provides a multitude of numerical algorithms built on Numpy data structures**
- **Organized into subpackages covering different scientific computing areas**
- **A data-processing and prototyping environment almost rivaling MATLAB**

Major modules from scipy

- **Available sub-packages include:**
  - constants: physical constants and conversion factors
  - cluster: hierarchical clustering, vector quantization, K-means
  - integrate: numerical integration routines
  - interpolate: interpolation tools
  - io: data input and output
  - linalg: linear algebra routines
  - ndimage: various functions for multi-dimensional image processing
  - optimize: optimization algorithms including linear programming
  - signal: signal processing tools
  - sparse: sparse matrix and related algorithms
  - spatial: KD-trees, nearest neighbors, distance functions
  - special: special functions
  - stats: statistical functions
  - weave: tool for writing C/C++ code as Python multiline strings

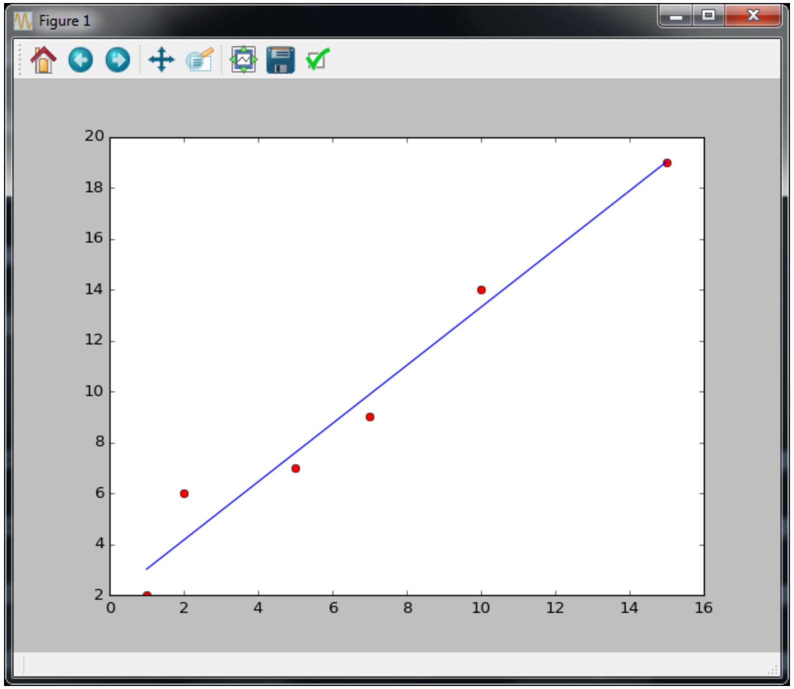
Scipy Example: Integration

$$\int_1^3 x^2 dx = \frac{1}{3} x^3 \Big|_1^3$$

```
#!/usr/bin/env python
import scipy.integrate as integrate
import scipy.special as special
result_integ, err = integrate.quad(lambda x: x**2, 1, 3)
result_real = 1./3.*(3.**3-1**3)

print "result_real=", result_real
print "result_integ=", result_integ
```

Scipy Example: Regression




```
#!/usr/bin/env python

from scipy import stats
import numpy as np
import matplotlib.pyplot as plt

x = np.array([1, 2, 5, 7, 10, 15])
y = np.array([2, 6, 7, 9, 14, 19])
slope, intercept, r_value, p_value, std_err = stats.linregress(x,y)

plt.plot(x,y,'or')
yh = x*slope + intercept
plt.plot(x, yh, '-b')
plt.show()
```

Future Trainings

- **Next week training: Machine Learning in HPC Environments**
  - Wednesday April 5, 2017, Frey Computing Service Center 307
- **Programming/Parallel Programming workshops in Summer**
- **Keep an eye on our webpage: www.hpc.lsu.edu**