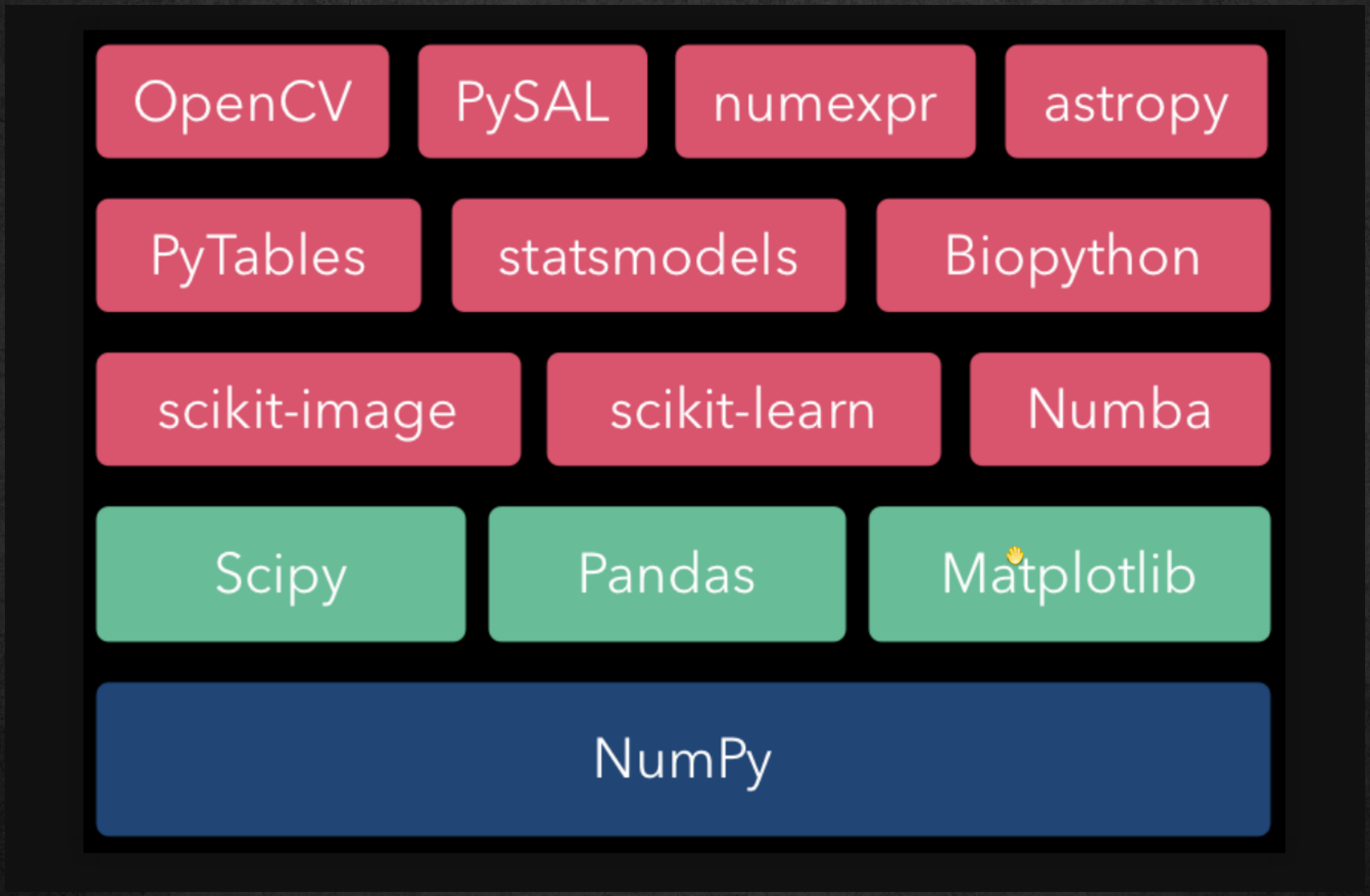
Unit 1:
Python for Data Mining

Numpy ecosystem



Python packages

- Numpy and Scipy: Fundamental scientific computing
- Pandas: Data manipulation and analysis
- Matplotlib: Plotting and visualization
  - Seaborn: Higher level library
- Scikit-learn: Machine learning and data mining
- StatsModels: Statistical modeling, testing and analysing

Section 1: Numpy

What is NumPy?

- Python is a fabulous language
  - Easy to extend
  - Great syntax which encourages easy to write and maintain code
  - Incredibly large standard-library and third-party tools
- No built-in multi-dimensional array (but it supports the needed syntax for extracting elements from one)
- NumPy provides a fast built-in object (ndarray) which is a multi-dimensional array of a homogeneous data-type.

NumPy

- Website -- http://numpy.scipy.org/
- Offers Matlab-ish capabilities within Python
- NumPy replaces Numeric and Numarray
- Initially developed by Travis Oliphant (building on the work of dozens of others)
- Over 30 svn "committers" to the project
- NumPy 1.0 released October, 2006
- ~20K downloads/month from Sourceforge.
  - This does not count:
    - Linux distributions that include NumPy
    - Enthought distributions that include NumPy
    - Mac OS X distributions that include NumPy
    - Sage distributes that include NumPy

Overview of NumPy

N-D ARRAY (NDARRAY)

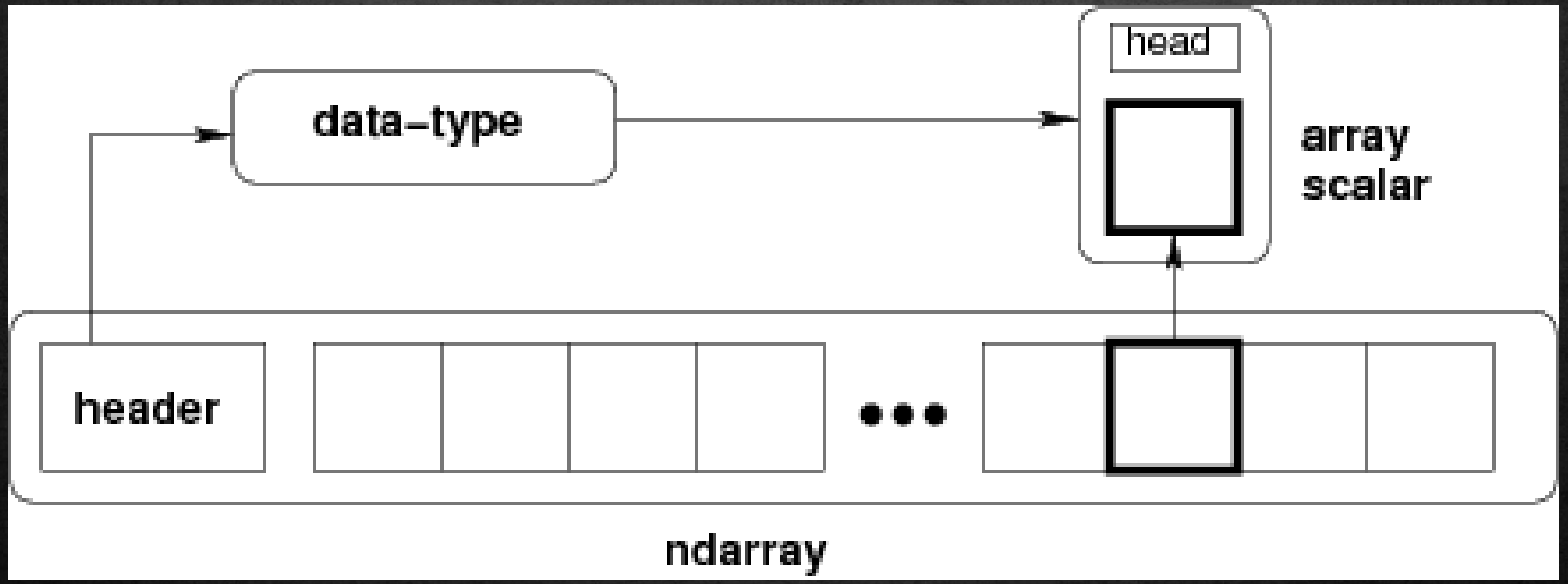
- N-dimensional array of rectangular data
- Element of the array can be C-structure or simple data-type.
- Fast algorithms on machine data-types (int, float, etc.)

UNIVERSAL FUNCTIONS (UFUNC)

- functions that operate element-by-element and return result
- fast-loops registered for each fundamental data-type
- sin(x) = [sin(xi) i=0..N]
- x+y = [xi + yi i=0..N]

NumPy Array

- A NumPy array is an N-dimensional homogeneous collection of "items" of the same "kind". The kind can be any arbitrary structure and is specified using the data-type.



NumPy Array

A NumPy array is a homogeneous collection of "items" of the same "data-type" (dtype)

```
>>> import numpy as N
>>> a = N.array([[1,2,3],[4,5,6]],float)
>>> print a
[[1. 2. 3.]
 [4. 5. 6.]]
>>> print a.shape, "\n", a.itemsize
(2, 3)
8
>>> print a.dtype, a.dtype.type
'<f8' <type 'float64scalar'>
>>> type(a[0,0])
<type 'float64scalar'>
>>> type(a[0,0]) is type(a[1,2])
True
```

Introducing NumPy Arrays

SIMPLE ARRAY CREATION

```
>>> a = array([0,1,2,3])
>>> a
array([0, 1, 2, 3])
```

CHECKING THE TYPE

```
>>> type(a)
<type 'array'>
```

NUMERIC 'TYPE' OF ELEMENTS

```
>>> a.dtype
dtype('int32')
```

BYTES PER ELEMENT

```
>>> a.itemsize # per element
4
```

ARRAY SHAPE

```
# shape returns a tuple
# listing the length of the
# array along each dimension.
>>> a.shape
(4,)
>>> shape(a)
(4,)
```

ARRAY SIZE

```
# size reports the entire
# number of elements in an
# array.
>>> a.size
4
>>> size(a)
4
```

Introducing NumPy Arrays

BYTES OF MEMORY USED

```
# returns the number of bytes
# used by the data portion of
# the array.
 >>> a.nbytes
12
```

NUMBER OF DIMENSIONS

```
>>> a.ndim
1
```

ARRAY COPY

```
# create a copy of the array
>>> b = a.copy()
>>> b
array([0, 1, 2, 3])
```

CONVERSION TO LIST

```
# convert a numpy array to a
# python list.
>>> a.tolist()
[0, 1, 2, 3]

# For 1D arrays, list also
# works equivalently, but
# is slower.
>>> list(a)
[0, 1, 2, 3]
```

Setting Array Elements

ARRAY INDEXING

```
>>> a[0]
0
>>> a[0] = 10
>>> a
[10, 1, 2, 3]
```

FILL

```
# set all values in an array.
>>> a.fill(0)
>>> a
[0, 0, 0, 0]

# This also works, but may
# be slower.
>>> a[:] = 1
>>> a
[1, 1, 1, 1]
```

BEWARE OF TYPE COERSION

```
>>> a.dtype
dtype('int32')

# assigning a float to an int32 array
will
# truncate decimal part.
>>> a[0] = 10.6
>>> a
[10, 1, 2, 3]

# fill has the same behavior
>>> a.fill(-4.8)
>>> a
[-4, -4, -4, -4]
```

Multi-Dimensional Arrays

MULTI-DIMENSIONAL ARRAYS

```
>>> a = array([[ 0, 1, 2, 3],
               [10,11,12,13]])
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,13]])
```

(ROWS,COLUMNS)

```
>>> a.shape
(2, 4)
>>> shape(a)
(2, 4)
```

ELEMENT COUNT

```
>>> a.size
8
>>> size(a)
8
```

NUMBER OF DIMENSIONS

```
>>> a.ndims
2
```

GET/SET ELEMENTS

```
>>> a[1,3]
13
```

```
>>> a[1,3] = -1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```

ADDRESS FIRST ROW USING SINGLE INDEX

```
>>> a[1]
array([10, 11, 12, -1])
```

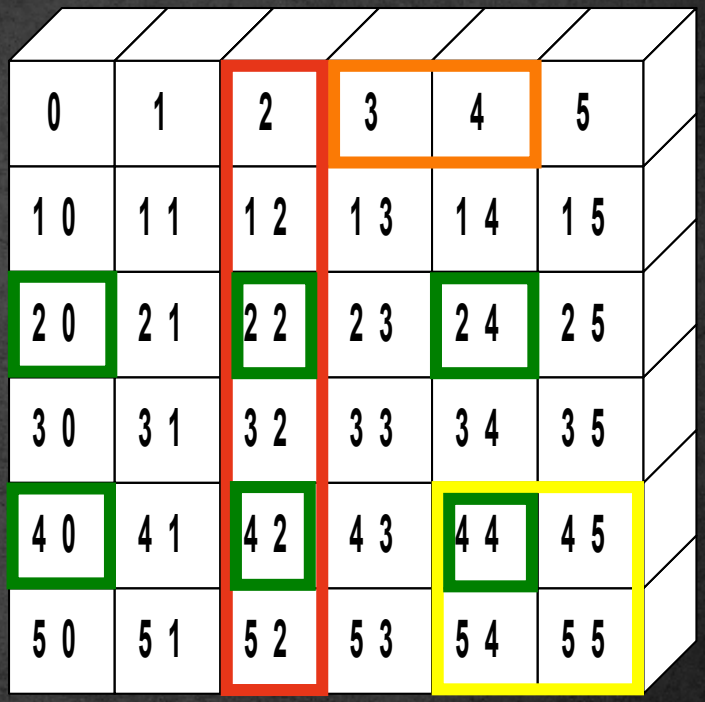
Array Slicing

SLICING WORKS MUCH LIKE STANDARD PYTHON SLICING

```
>>> a[0,3:5]
array([3, 4])

>>> a[4:,4:]
array([[44, 45],
       [54, 55]])

>>> a[:,2]
array([2,12,22,32,42,52])
```

STRIDES ARE ALSO POSSIBLE

```
>>> a[2::2,::2]
array([[20, 22, 24],
       [40, 42, 44]])
```



Memory Model

```
>>> print a.strides
(24, 8)
>>> print a.flags.fortran, a.flags.contiguous
False True
>>> print a.T.strides
(8, 24)
>>> print a.T.flags.fortran, a.T.flags.contiguous
True False
```

- Every dimension of an ndarray is accessed by stepping (striding) a fixed number of bytes through memory.
- If memory is contiguous, then the strides are "pre-computed" indexing-formulas for either Fortran-order (first-dimension varies the fastest), or C-order (last-dimension varies the fastest) arrays.

Array slicing (views)

- Memory model allows "simple indexing" (integers and slices) into the array to be a **view** of the same data.

```
>>> b = a[:,::2]
>>> b[0,1] = 100
>>> print a
[[   1.    2.  100.]]
 [   4.    5.    6.]]
>>> c =
a[:,::2].copy()
>>> c[1,0] = 500
>>> print a
[[   1.    2.  100.]]
 [   4.    5.    6.]]
```

Other uses of view

```
>>> b = a.view('i8')
>>> [hex(val.item()) for
val in b.flat]
['0x3FF0000000000000L',
 '0x4000000000000000L',
 '0x4059000000000000L',
 '0x4010000000000000L',
 '0x4014000000000000L',
 '0x4018000000000000L']
```

Slices Are References

Slices are references to memory in original array. Changing values in a slice also changes the original array.

```
>>> a = array((0,1,2,3,4))

# create a slice containing only the
# last element of a
>>> b = a[2:4]
>>> b[0] = 10

# changing b changed a!
>>> a
array([ 1,  2, 10,  3,  4])
```

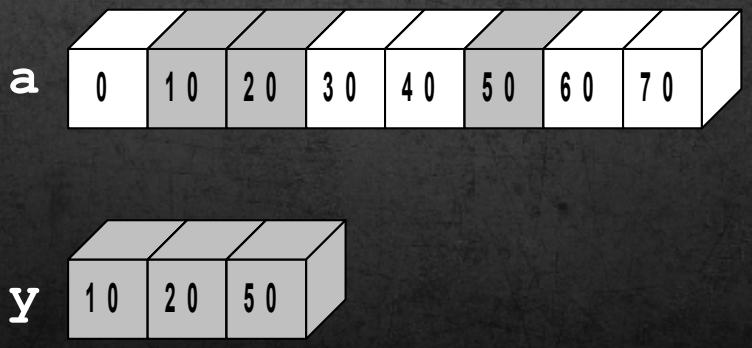
Fancy Indexing

INDEXING BY POSITION

```
>>> a = arange(0,80,10)


# fancy indexing
>>> y = a[[1, 2, -3]]
>>> print y
[10 20 50]

# using take
>>> y = take(a,[1,2,-3])
>>> print y
[10 20 50]
```

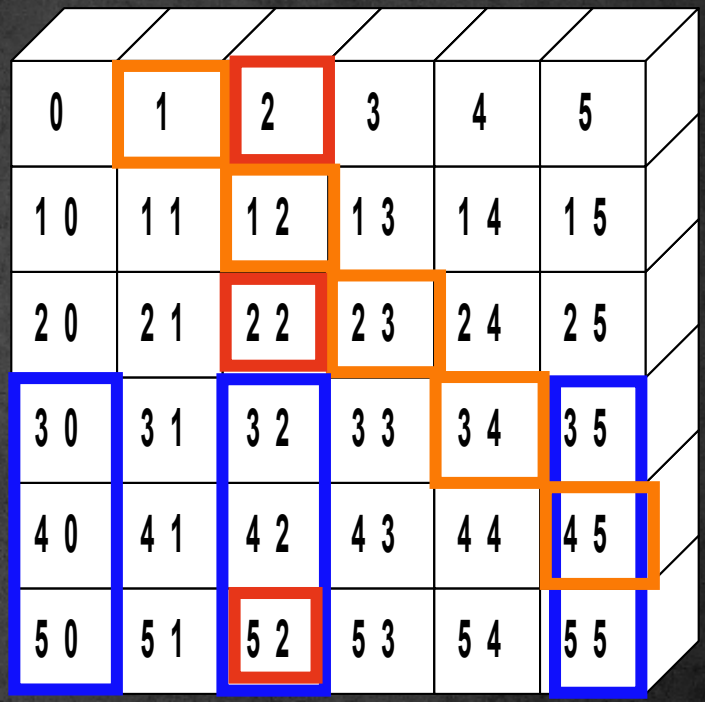
INDEXING WITH BOOLEANS

```
>>> mask = array([0,1,1,0,0,1,0,0],
...              dtype=bool)

# fancy indexing
>>> y = a[mask]
>>> print y
[10,20,50]

# using compress
>>> y = compress(mask, a)
>>> print y
[10,20,50]
```



Fancy Indexing in 2D

```
>>> a[(0,1,2,3,4),(1,2,3,4,5)]
array([ 1, 12, 23, 34, 45])

>>> a[3:,[0, 2, 5]]
array([[30, 32, 35],
       [40, 42, 45]])
       [50, 52, 55]])

>>> mask = array([1,0,1,0,0,1],
                 dtype=bool)
>>> a[mask,2]
array([2,22,52])
```



Unlike slicing, fancy indexing creates copies instead of views into original arrays.

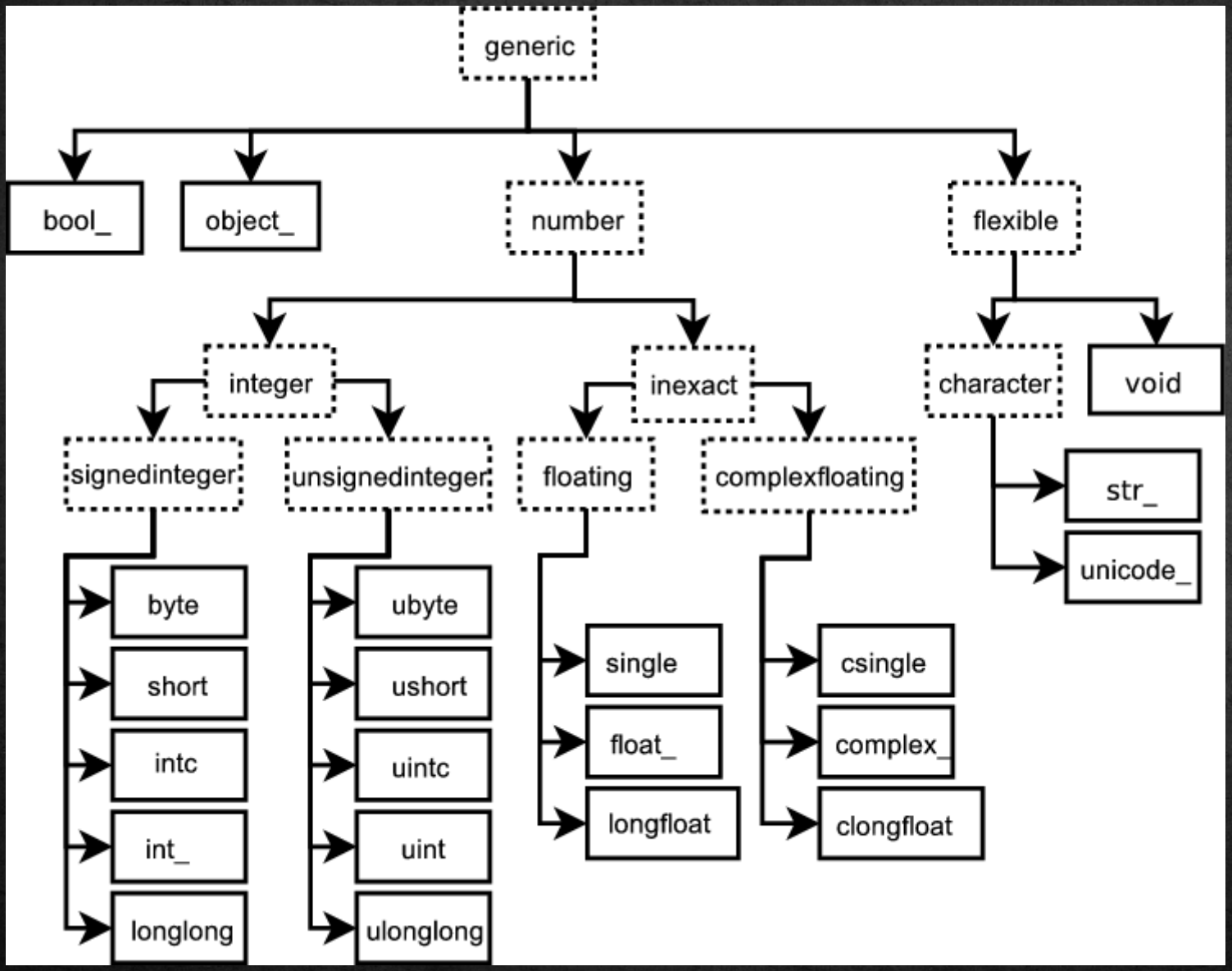
Data-types

- There are two related concepts of “type”
  - The data-type object (dtype)
  - The Python “type” of the object created from a single array item (hierarchy of scalar types)
- The dtype object provides the details of how to interpret the memory for an item. It's an instance of a single dtype class.
- The “type” of the extracted elements are true Python classes that exist in a hierarchy of Python classes
- Every dtype object has a type attribute which provides the Python object returned when an element is selected from the array

NumPy dtypes

Basic Type	Available NumPy types	Comments
Boolean	bool	Elements are 1 byte in size
Integer	int8, int16, int32, int64, int128, int	int defaults to the size of int in C for the platform
Unsigned Integer	uint8, uint16, uint32, uint64, uint128, uint	uint defaults to the size of unsigned int in C for the platform
Float	float32, float64, float, longfloat,	Float is always a double precision floating point value (64 bits). longfloat represents large precision floats. Its size is platform dependent.
Complex	complex64, complex128, complex	The real and complex elements of a complex64 are each represented by a single precision (32 bit) value for a total size of 64 bits.
Strings	str, unicode	Unicode is always UTF32 (UCS4)
Object	object	Represent items in array as Python objects.
Records	void	Used for arbitrary data structures in record arrays.

Built-in "scalar" types



Data-type object (dtype)

- There are 21 "built-in" (static) data-type objects
- New (dynamic) data-type objects are created to handle
  - Alteration of the byteorder
  - Change in the element size (for string, unicode, and void built-ins)
  - Addition of fields
  - Change of the type object (C-structure arrays)
- Creation of data-types is quite flexible.
- New user-defined "built-in" data-types can also be added (but must be done in C and involves filling a function-pointer table)

Data-type fields

- An item can include fields of different data-types.
- A field is described by a data-type object and a byte offset --- this definition allows nested records.
- The array construction command interprets tuple elements as field entries.

```
>>> dt = N.dtype("i4,f8,a5")
>>> print dt.fields
{'f1': (dtype('<i4'), 0), 'f2': (dtype('<f8'), 4),
'f3': (dtype('|S5'), 12)}
>>> a = N.array([(1,2.0,"Hello"), (2,3.0,"World")],
dtype=dt)
>>> print a['f3']
[Hello World]
```

Array Calculation Methods

SUM FUNCTION

```
>>> a = array([[1,2,3],
               [4,5,6]], float)

# Sum defaults to summing all
# *all* array values.
>>> sum(a)
21.

# supply the keyword axis to
# sum along the 0th axis.
>>> sum(a, axis=0)
array([5., 7., 9.])

# supply the keyword axis to
# sum along the last axis.
>>> sum(a, axis=-1)
array([6., 15.])
```

SUM ARRAY METHOD

```
# The a.sum() defaults to
# summing *all* array values
>>> a.sum()
21.

# Supply an axis argument to
# sum along a specific axis.
>>> a.sum(axis=0)
array([5., 7., 9.])
```

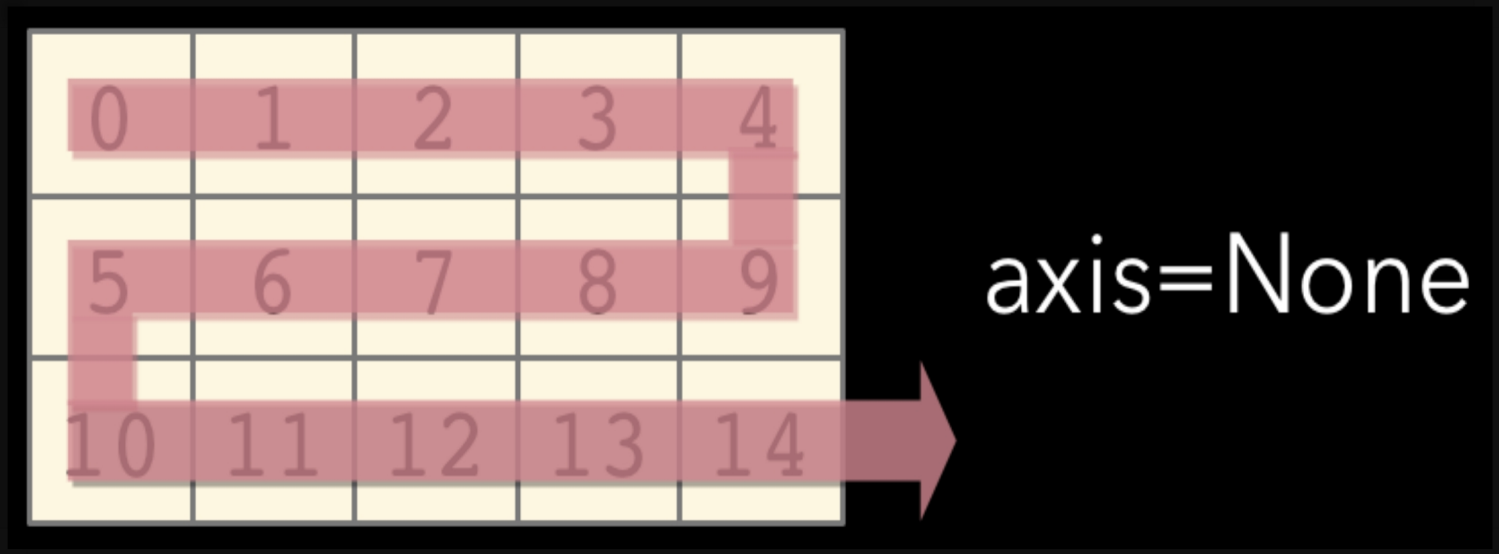
PRODUCT

```
# product along columns.
>>> a.prod(axis=0)
array([ 4., 10., 18.])

# functional form.
>>> prod(a, axis=0)
array([ 4., 10., 18.])
```

Axis

- Array method reductions take an optional axis parameter that specifies over which axes to reduce
- axis=None reduces into a single scalar

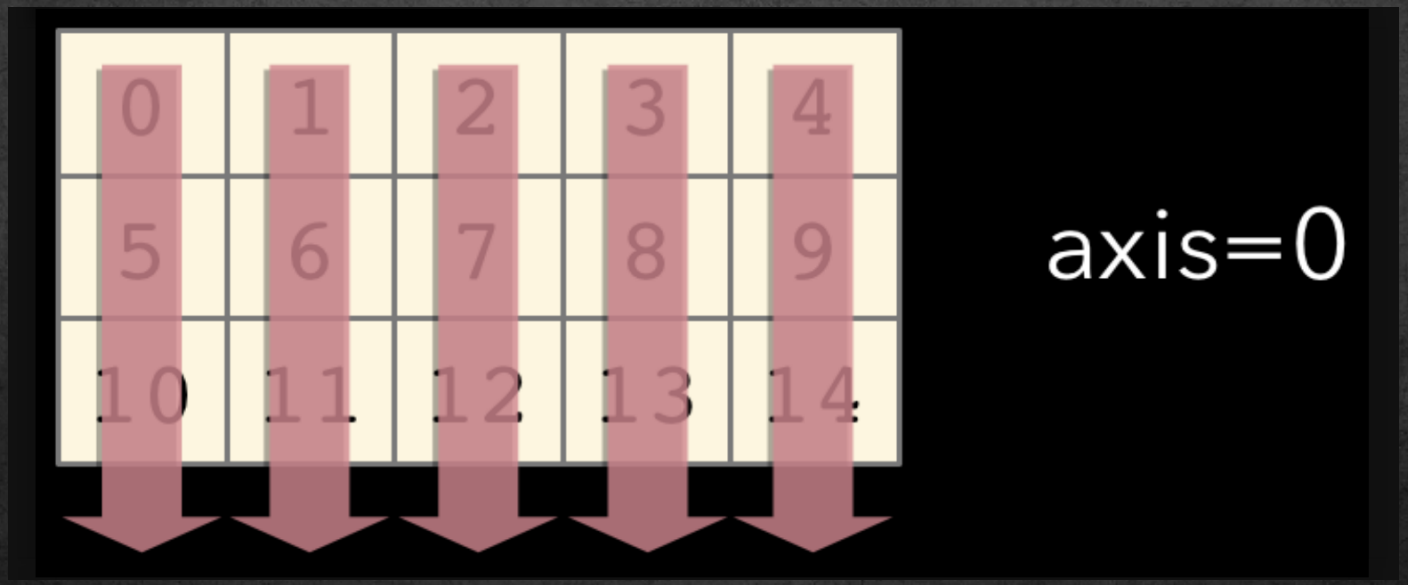
```
In [7]: a.sum
()
Out[7]: 105
```



Axis = 0

- axis=0 reduces into the zeroth dimension

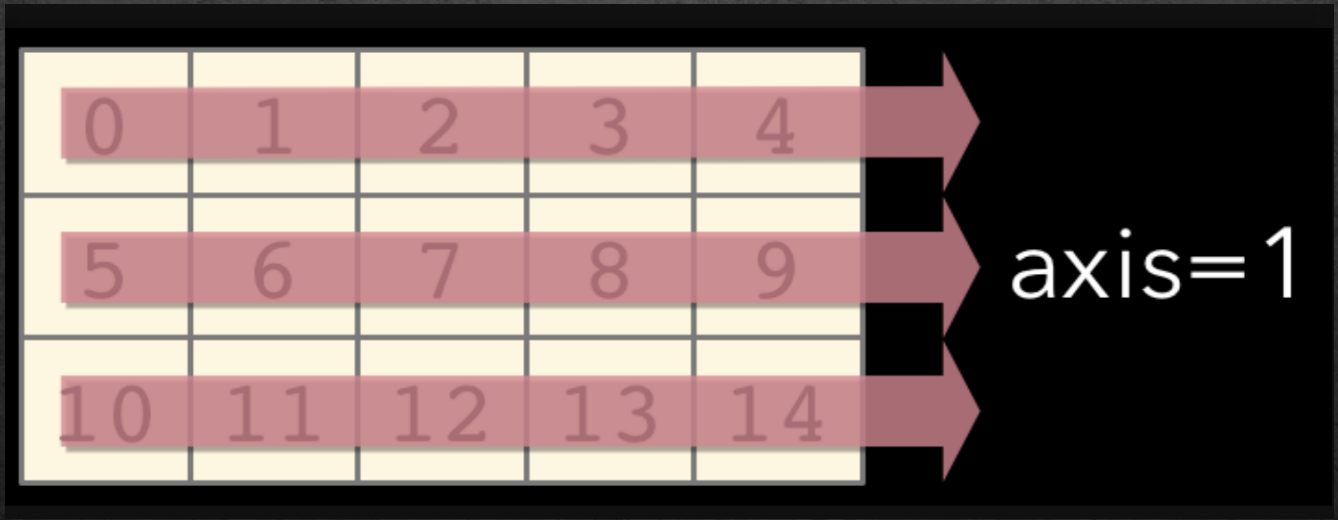
```
In [8]: a.sum(axis=0)
Out[8]: array([15, 18, 21, 24,
27])
```



Axis = 1

- axis=1 reduces into the first dimension

```
In [9]: a.sum(axis=1)
Out[9]: array([10, 35, 60])
```



Min/Max

MIN

```
>>> a = array([2.,3.,0.,1.]) >>>
a.min(axis=0)
0.
# use Numpy's amin() instead
# of Python's builtin min()
# for speed operations on
# multi-dimensional arrays.
>>> amin(a, axis=0)
0.
```

ARGMIN

```
# Find index of minimum value.
>>> a.argmin(axis=0)
2
# functional form
>>> argmin(a, axis=0)
2
```

MAX

```
>>> a = array([2.,1.,0.,3.]) >>>
a.max(axis=0)
3.

# functional form
>>> amax(a, axis=0)
3.
```

ARGMAX

```
# Find index of maximum value.
>>> a.argmax(axis=0)
1
# functional form
>>> argmax(a, axis=0)
1
```

Statistics Array Methods

MEAN

```
>>> a = array([[1,2,3],
              [4,5,6]], float)

# mean value of each column
>>> a.mean(axis=0)
array([ 2.5,  3.5,  4.5])
>>> mean(a, axis=0)
array([ 2.5,  3.5,  4.5])
>>> average(a, axis=0)
array([ 2.5,  3.5,  4.5])

# average can also calculate
# a weighted average
>>> average(a, weights=[1,2],
...         axis=0)
array([ 3.,  4.,  5.])
```

STANDARD DEV./VARIANCE

```
# Standard Deviation
>>> a.std(axis=0)
array([ 1.5,  1.5,  1.5])

# Variance
>>> a.var(axis=0)
array([2.25, 2.25, 2.25])
>>> var(a, axis=0)
array([2.25, 2.25, 2.25])
```

Other Array Methods

CLIP

```
# Limit values to a range

>>> a = array([[1,2,3],
               [4,5,6]], float)

# Set values < 3 equal to 3.
# Set values > 5 equal to 5.
>>> a.clip(3,5)
>>> a
array([[ 3.,  3.,  3.],
       [ 4.,  5.,  5.]])
```

ROUND

```
# Round values in an array.
# Numpy rounds to even, so
# 1.5 and 2.5 both round to 2.
>>> a = array([1.35, 2.5, 1.5])
>>> a.round()
array([ 1.,  2.,  2.])

# Round to first decimal place.
>>> a.round(decimals=1)
array([ 1.4,  2.5,  1.5])
```

POINT TO POINT

```
# Calculate max - min for
# array along columns
>>> a.ptp(axis=0)
array([ 3.0,  3.0,  3.0])
# max - min for entire array.
>>> a.ptp(axis=None)
5.0
```

Summary of (most) array attributes/methods

BASIC ATTRIBUTES

a.dtype - Numerical type of array elements. float32, uint8, etc.
a.shape - Shape of the array. (m,n,o,...)
a.size - Number of elements in entire array.
a.itemsize - Number of bytes used by a single element in the array.
a.nbytes - Number of bytes used by entire array (data only).
a.ndim - Number of dimensions in the array.

SHAPE OPERATIONS

a.flat - An iterator to step through array as if it is 1D.
a.flatten() - Returns a 1D copy of a multi-dimensional array.
a.ravel() - Same as flatten(), but returns a 'view' if possible.
a.resize(new_size) - Change the size/shape of an array in-place.
a.swapaxes(axis1, axis2) - Swap the order of two axes in an array. a.transpose(*axes) - Swap the order of any number of array axes. a.T - Shorthand for a.transpose()
a.squeeze() - Remove any length=1 dimensions from an array.

Summary of (most) array attributes/methods

FILL AND COPY

a.copy() - Return a copy of the array.
a.fill(value) - Fill array with a scalar value.

CONVERSION / COERSION

a.tolist() - Convert array into nested lists of values.
a.tostring() - raw copy of array memory into a python string.
a.astype(dtype) - Return array coerced to given dtype.
a.byteswap(False) - Convert byte order (big <-> little endian).

COMPLEX NUMBERS

a.real - Return the real part of the array.
a.imag - Return the imaginary part of the array.
a.conjugate() - Return the complex conjugate of the array.
a.conj()- Return the complex conjugate of an array.(same as conjugate)

Summary of (most) array attributes/methods

SAVING

a.dump(file) - Store a binary array data out to the given file.
a.dumps() - returns the binary pickle of the array as a string.
a.tofile(fid, sep="", format="%s") Formatted ascii output to file.

SEARCH / SORT

a.nonzero() - Return indices for all non-zero elements in a.
a.sort(axis=-1) - Inplace sort of array elements along axis.
a.argsort(axis=-1) - Return indices for element sort order along axis. a.searchsorted(b) - Return index where elements from b would go in a.

ELEMENT MATH OPERATIONS

a.clip(low, high) - Limit values in array to the specified range.
a.round(decimals=0) - Round to the specified number of digits.
a.cumsum(axis=None) - Cumulative sum of elements along axis.
a.cumprod(axis=None) - Cumulative product of elements along axis.

Summary of (most) array attributes/methods

REDUCTION METHODS

All the following methods "reduce" the size of the array by 1 dimension by carrying out an operation along the specified axis. If axis is None, the operation is carried out across the entire array.

a.sum(axis=None) - Sum up values along axis.
a.prod(axis=None) - Find the product of all values along axis.
a.min(axis=None)- Find the minimum value along axis.
a.max(axis=None) - Find the maximum value along axis.
a.argmin(axis=None) - Find the index of the minimum value along axis.
a.argmax(axis=None) - Find the index of the maximum value along axis.
a.ptp(axis=None) - Calculate a.max(axis) - a.min(axis)
a.mean(axis=None) - Find the mean (average) value along axis.
a.std(axis=None) - Find the standard deviation along axis.
a.var(axis=None) - Find the variance along axis.

a.any(axis=None) - True if any value along axis is non-zero. (or)
a.all(axis=None) - True if all values along axis are non-zero. (and)

Array Operations

SIMPLE ARRAY MATH

```
>>> a = array([1,2,3,4])
>>> b = array([2,3,4,5])
>>> a + b
array([3, 5, 7, 9])
```

Numpy defines the following constants:

pi = 3.14159265359

e = 2.71828182846

MATH FUNCTIONS

```
# Create array from 0 to 10
>>> x = arange(11.)

# multiply entire array by
# scalar value
>>> a = (2*pi)/10.
>>> a
0.628318530717958 62
>>> a*x
array([ 0.,0.628,...,6.283])

# inplace operations
>>> x *= a
>>> x
array([ 0.,0.628,...,6.283])

# apply functions to array.
>>> y = sin(x)
```

Universal Functions

- ufuncs are objects that rapidly evaluate a function element-by-element over an array.
- Core piece is a 1-d loop written in C that performs the operation over the largest dimension of the array
- For 1-d arrays it is equivalent to but much faster than list comprehension

```
>>> type(N.exp)
<type 'numpy.ufunc'>
>>> x = array([1,2,3,4,5])
>>> print N.exp(x)
[   2.71828183    7.3890561    20.08553692
54.59815003  148.4131591 ]
>>> print [math.exp(val) for val in x]
[2.718281828459045,
7.3890560989306504,20.085536923187668,
 54.598150033144236,148.4131591025766]
```

Mathematic Binary Operators

```
a + b  ☾  add(a,b)
a - b  ☾  subtract(a,b)
a % b  ☾  remainder(a,b)
```

```
a * b  ☾  multiply(a,b)
a / b  ☾  divide(a,b)
a ** b ☾  power(a,b)
```

MULTIPLY BY A SCALAR

```
>>> a = array((1,2))
>>> a*3.
array([3., 6.])
```

ELEMENT BY ELEMENT ADDITION

```
>>> a = array([1,2])
>>> b = array([3,4])
>>> a + b
array([4, 6])
```

ADDITION USING AN OPERATOR FUNCTION

```
>>> add(a,b)
array([4, 6])
```

IN PLACE OPERATION

```
# Overwrite contents of a.
# Saves array creation
# overhead
>>> add(a,b,a) # a += b
array([4, 6])
>>> a
array([4, 6])
```

Comparison and Logical Operators

equal	(==)	not_equal	(!=)	greater	(>)
greater_equal	(>=)	less	(<)	less_equal	(<=)
logical_and		logical_or		logical_xor	
logical_not					

2D EXAMPLE

```
>>> a = array(((1,2,3,4),(2,3,4,5)))
>>> b = array(((1,2,5,4),(1,3,4,5)))
>>> a == b
array([[True, True, False, True],
       [False, True, True, True]])
# functional equivalent
>>> equal(a,b)
array([[True, True, False, True],
       [False, True, True, True]])
```

Bitwise Operators

bitwise_and	(&)	invert	(~)	right_shift(a,shifts)	
bitwise_or	(|)	bitwise_xor		left_shift (a,shifts)	

BITWISE EXAMPLES

```
>>> a = array((1,2,4,8))
>>> b = array((16,32,64,128))
>>> bitwise_or(a,b)
array([ 17,  34,  68, 136])

# bit inversion
>>> a = array((1,2,3,4), uint8)
>>> invert(a)
array([254, 253, 252, 251], dtype=uint8)

# left shift operation
>>> left_shift(a,3)
array([ 8, 16, 24, 32], dtype=uint8)
```

Trig and Other Functions

TRIGONOMETRIC

sin(x)	sinh(x)
cos(x)	cosh(x)
arccos(x)	arccosh(x)
arctan(x)	arctanh(x)
arcsin(x)	arcsinh(x)
arctan2(x,y)	

OTHERS

exp(x)	log(x)
log10(x)	sqrt(x)
absolute(x)	conjugate(x)
negative(x)	ceil(x)
floor(x)	fabs(x) hypot(x,y)
	fmod(x,y)
maximum(x,y)	minimum(x,y)

`hypot(x,y)`

Element by element distance calculation using $\sqrt{x^2 + y^2}$

Broadcasting

- When there are multiple inputs, then they all must be "broadcastable" to the same shape.
  - All arrays are promoted to the same number of dimensions (by pre-prending 1's to the shape)
  - All dimensions of length 1 are expanded as determined by other inputs with non-unit lengths in that dimension.

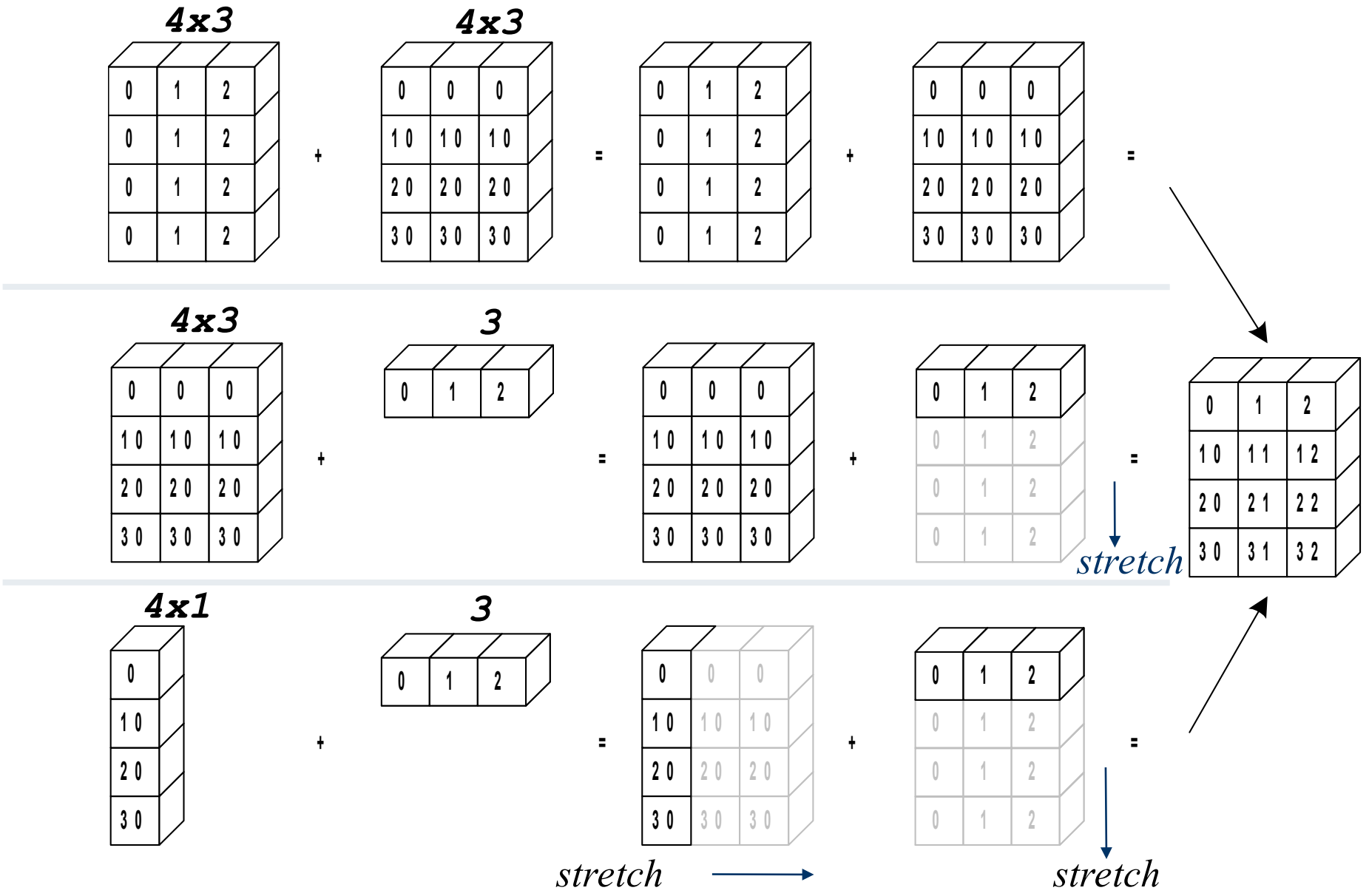
```
>>> x = [1,2,3,4];
>>> y = [[10],[20],
[30]]
>>> print N.add(x,y)
[[11 12 13 14]
 [21 22 23 24]
 [31 32 33 34]]
>>> x = array(x)
>>> y = array(y)
>>> print x+y
[[11 12 13 14]
 [21 22 23 24]
 [31 32 33 34]]
```

X HAS SHAPE (4,) THE UFUNC SEES IT AS HAVING SHAPE (1,4)

Y HAS SHAPE (3,1)

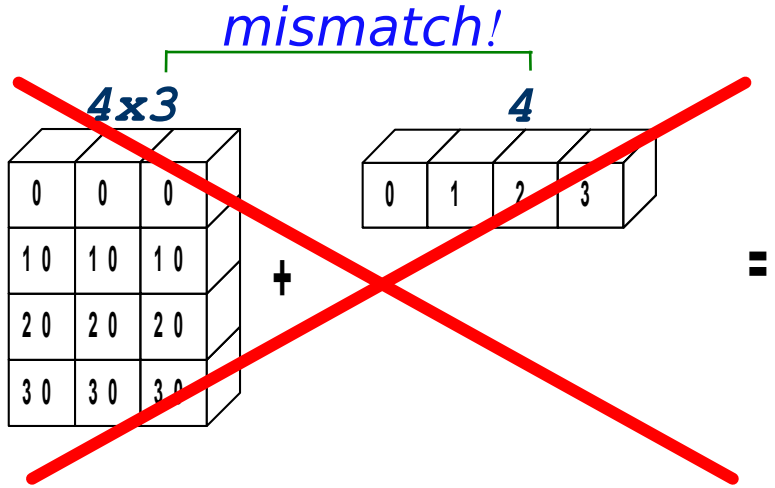
THE UFUNC RESULT HAS SHAPE (3,4)

Array Broadcasting



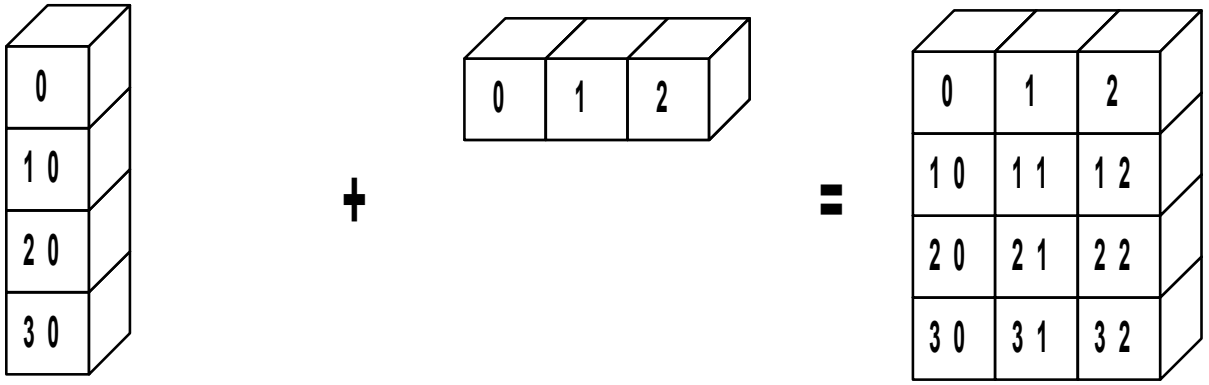
Broadcasting Rules

✗The trailing axes of both arrays must either be 1 or have the same size for broadcasting to occur. Otherwise, a "ValueError: frames are not aligned" exception is thrown.



Broadcasting in Action

```
>>> a = array((0,10,20,30))
>>> b = array((0,1,2))
>>> y = a[:, None] + b
```



Universal Function Methods

- The mathematic, comparative, logical, and bitwise operators that
- take two arguments (binary operators) have special methods that operate on arrays:

```
op.reduce(a,axis=0)
op.accumulate(a,axis=0)
op.outer(a,b)
op.reduceat(a,indices)
```

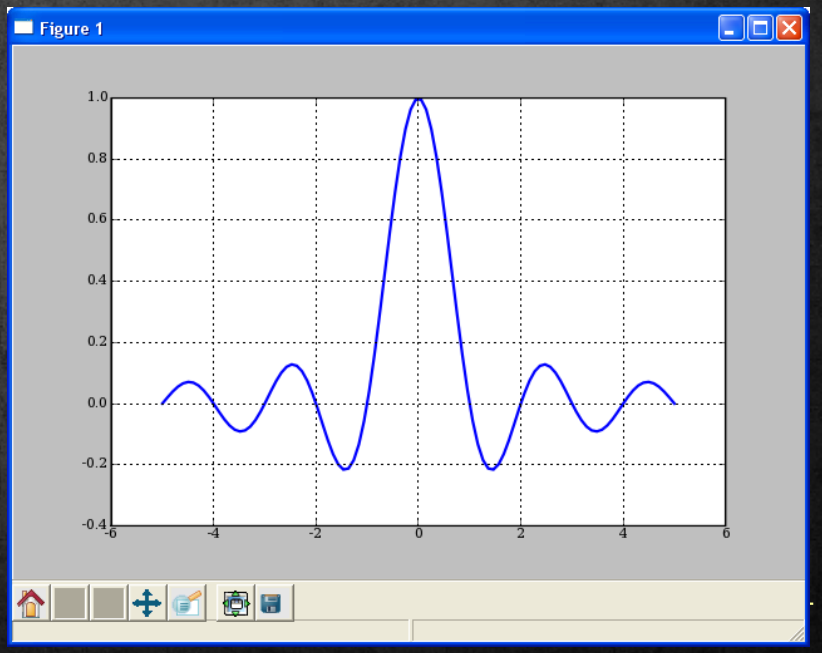
Vectorizing Functions

VECTORIZING FUNCTIONS

Example

```
# special.sinc already available
# This is just for show.
def sinc(x):
    if x == 0.0:
        return 1.0
    else:
        w = pi*x
        return sin(w) / w
```

```
# attempt
>>> sinc([1.3,1.5])
TypeError: can't multiply sequence to non-int
>>> x = r_[-5:5:100j]
>>> y = vsinc(x)
>>> plot(x, y)
```



SOLUTION

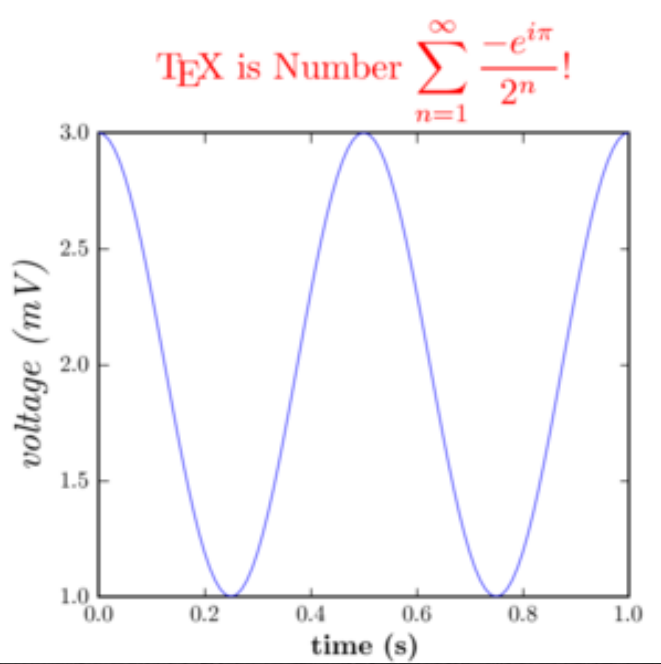
```
>>> from numpy import vectorize
>>> vsinc = vectorize(sinc)
>>> vsinc([1.3,1.5])
array([-0.1981, -0.2122])
```

Interface with C/C++/Fortan

- Python excels at interfacing with other languages
  - weave (C/C++)
  - f2py (Fortran)
  - pyrex
  - ctypes (C)
  - SWIG (C/C++)
  - Boost.Python (C++)
  - RPy / RSPython (R)

Matplotlib

- Requires NumPy extension. Provides powerful plotting commands.
- http://matplotlib.sourceforge.net



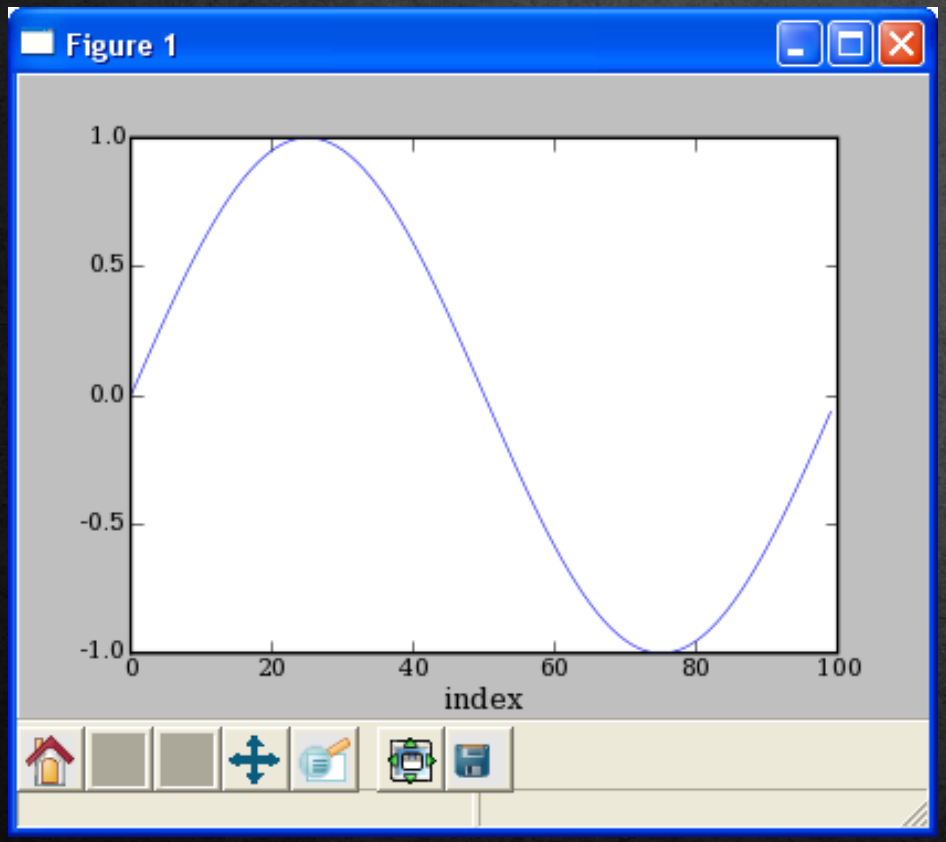
Recommendations

- Matplotlib for day-to-day data exploration.
  - Matplotlib has a large community, tons of plot types, and is well integrated into ipython. It is the de-facto standard for 'command line' plotting from ipython.
- Chaco for building interactive plotting applications
  - Chaco is architected for building highly interactive and configurable plots in python. It is more useful as plotting toolkit than for making one-off plots.

Line Plots

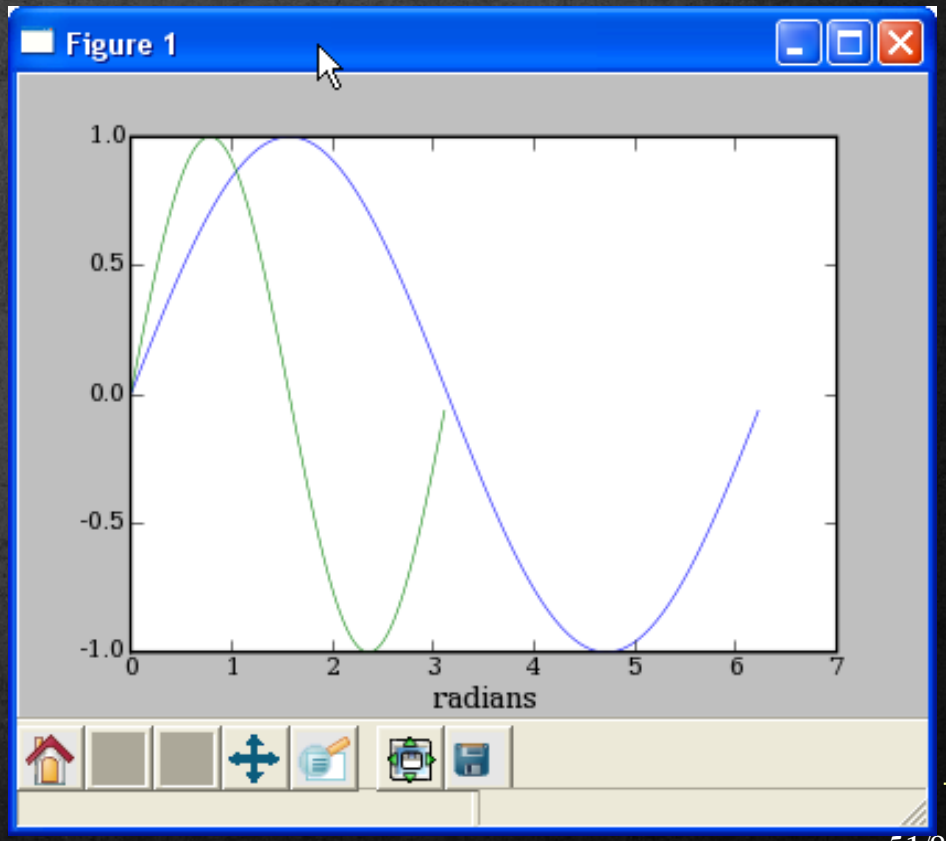
PLOT AGAINST INDICES

```
>>> x = arange(50)*2*pi/50.
>>> y = sin(x)
>>> plot(y)
>>> xlabel('index')
```



MULTIPLE DATA SETS

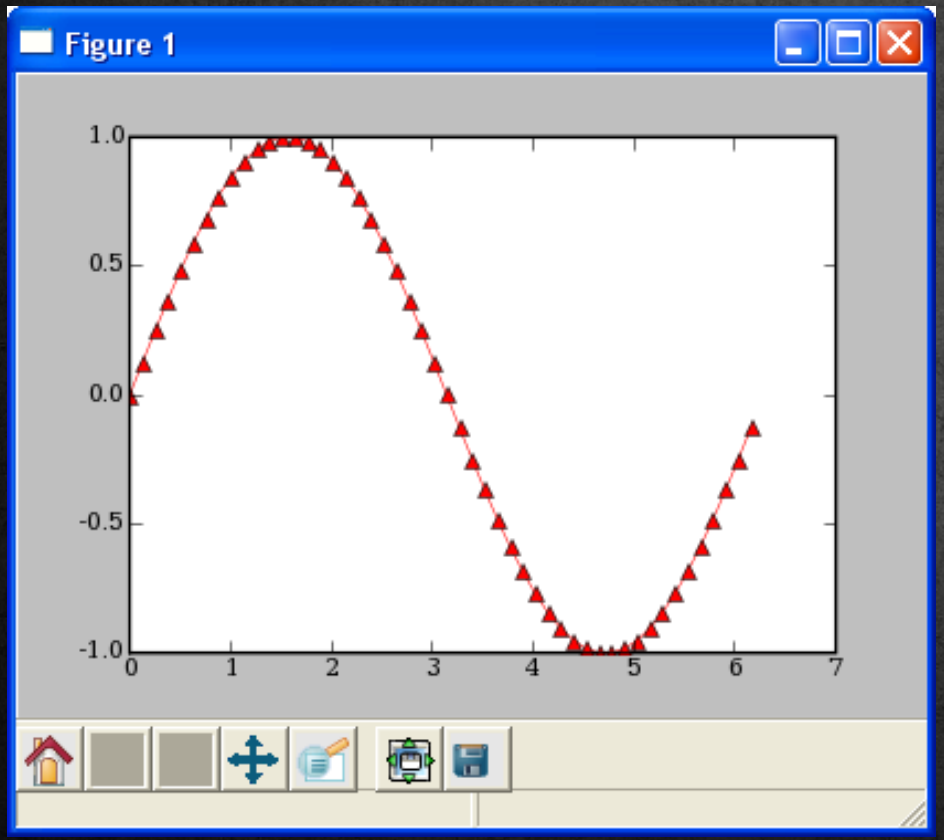
```
>>> plot(x,y,x2,y2)
>>> xlabel('radians')
```



Line Plots

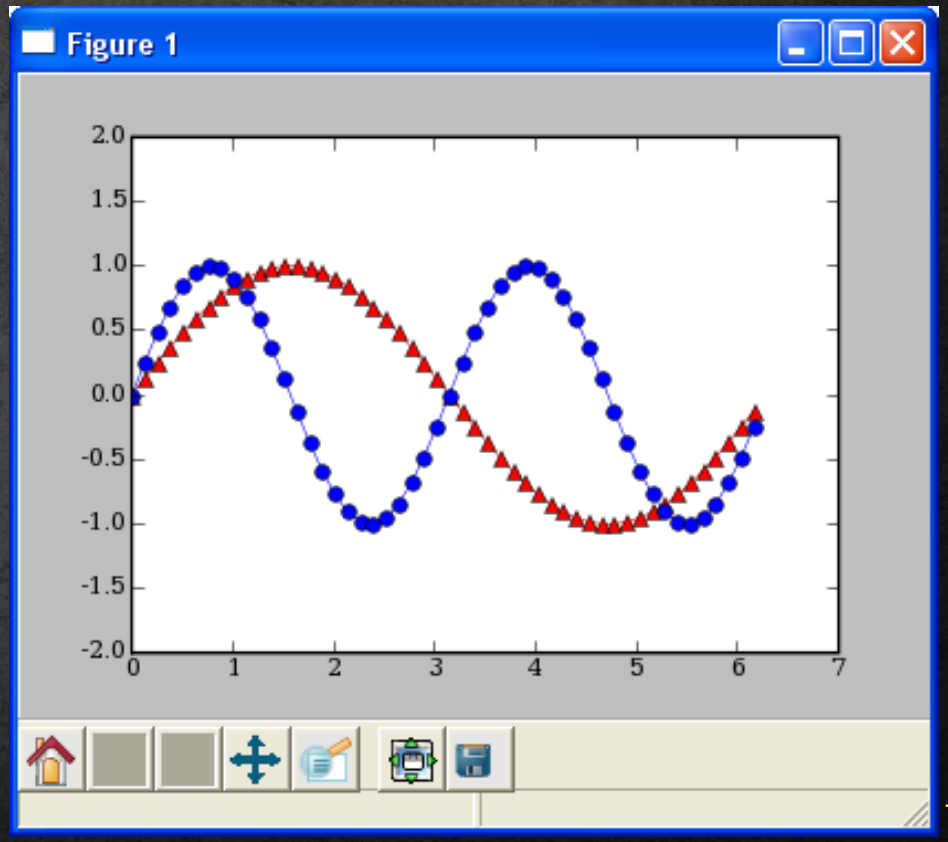
LINE FORMATTING

```
# red, dot-dash, triangles
>>> plot(x,sin(x),'r-^')
```



MULTIPLE PLOT GROUPS

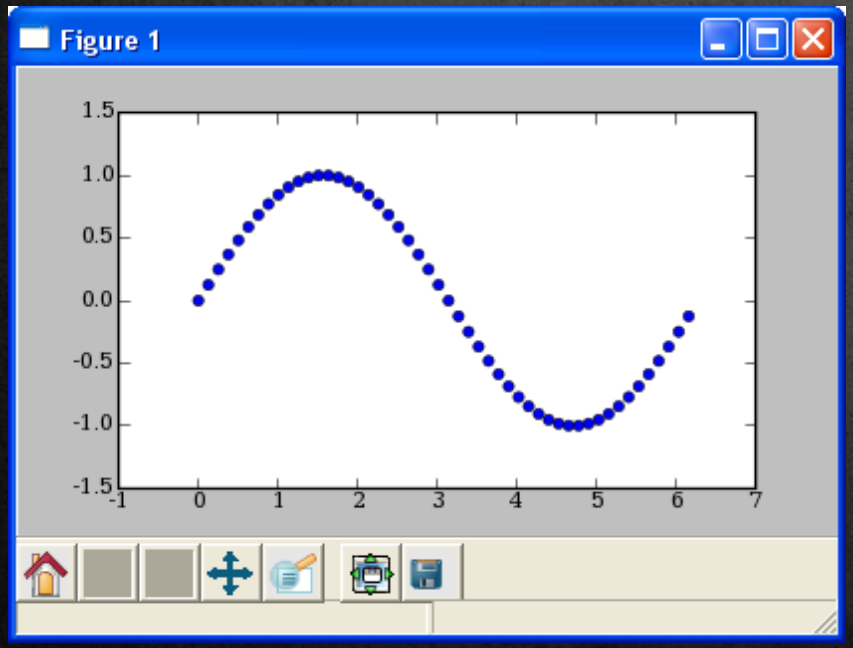
```
>>> plot(x,y1,'b-o', x,y2), r-^')
>>> axis([0,7,-2,2])
```



Scatter Plots

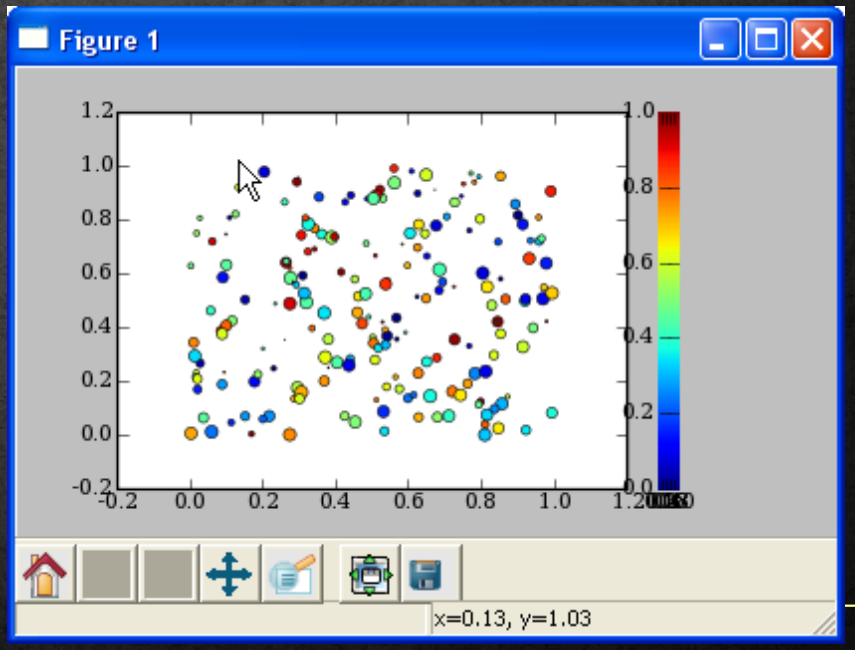
SIMPLE SCATTER PLOT

```
>>> x = arange(50)*2*pi/50.
>>> y = sin(x)
>>> scatter(x,y)
```



COLORMAPPED SCATTER

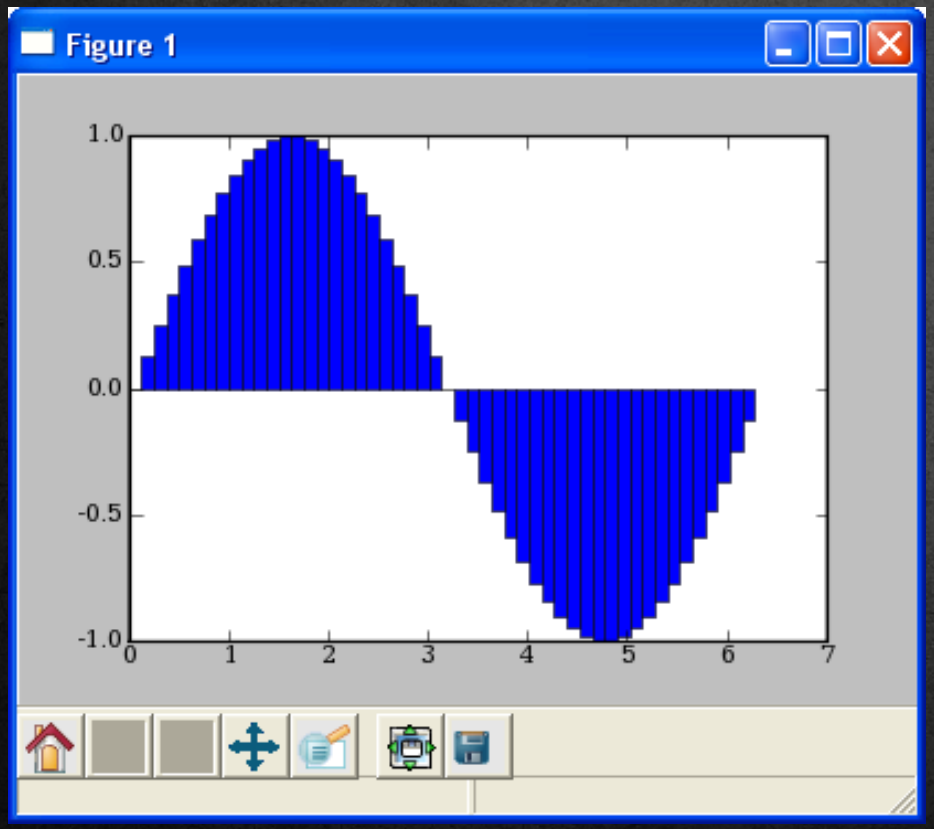
```
# marker size/color set with data
>>> x = rand(200)
>>> y = rand(200)
>>> size = rand(200)*30
>>> color = rand(200)
>>> scatter(x, y, size, color)
>>> colorbar()
```



Bar Plots

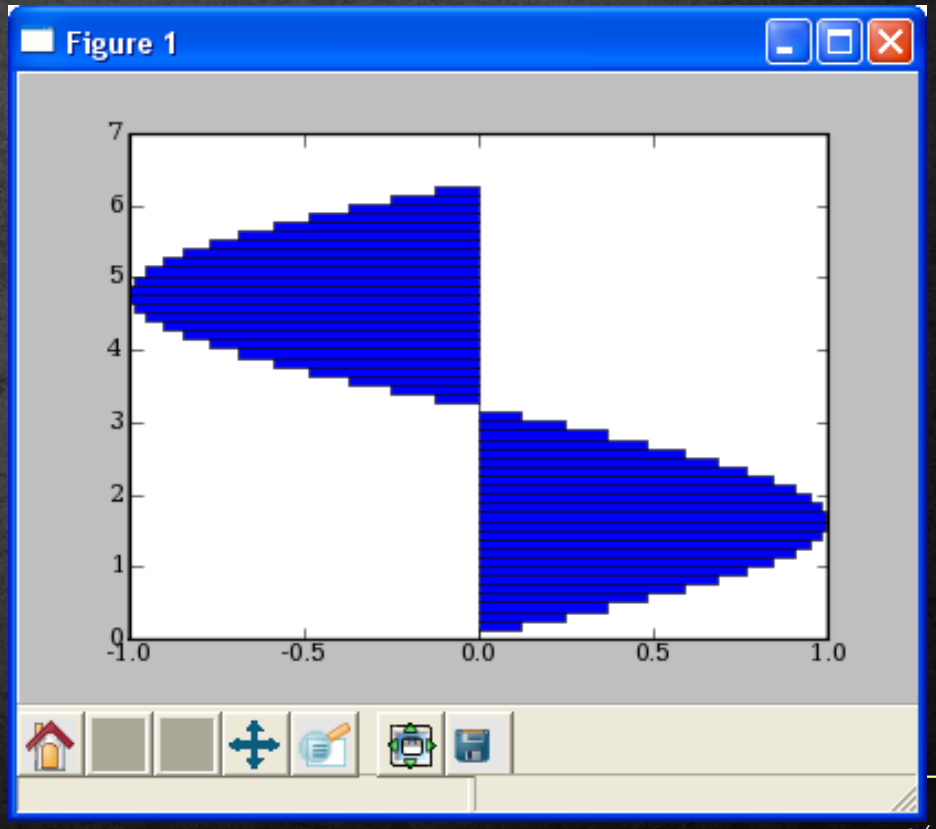
BAR PLOT

```
>>> bar(x,sin(x),
...      width=x[1]-x[0])
```



HORIZONTAL BAR PLOT

```
>>> hbar(x,sin(x),
...      height=x[1]-x[0],
...     orientation='horizontal')
```



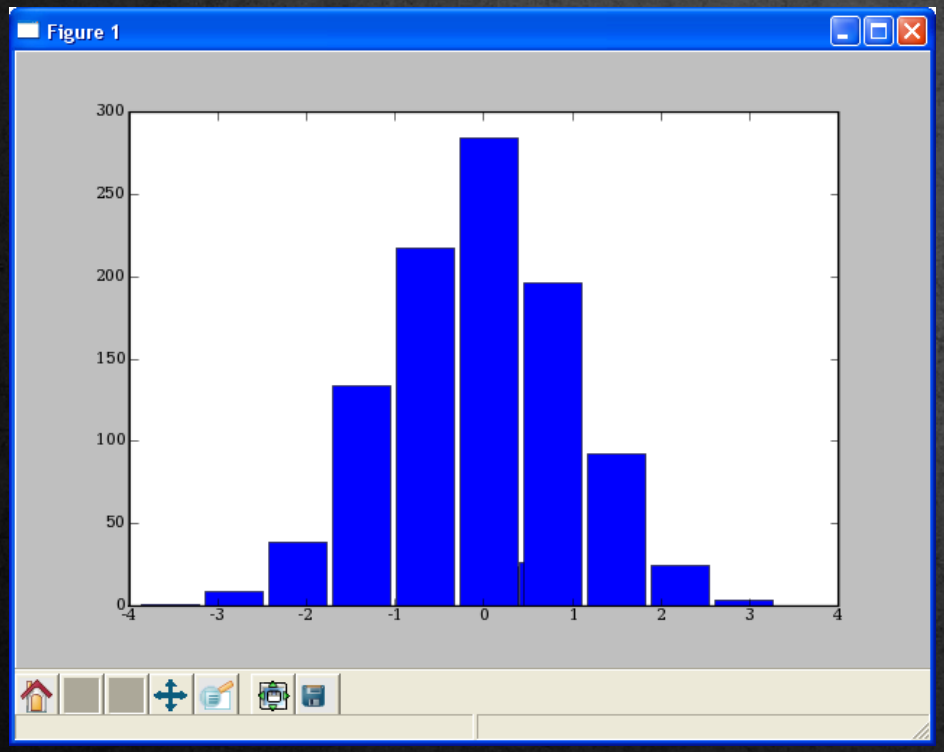
Bar Plots

DEMO/MATPLOTLIB_PLOTTING/BARCHART_DEMO.PY

HISTOGRAMS

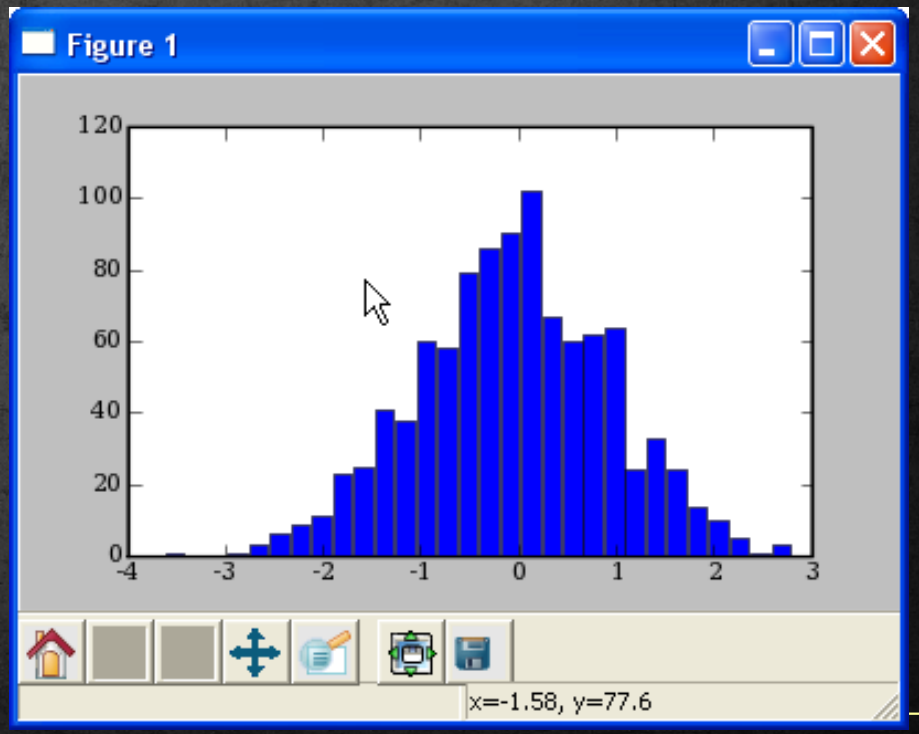
HISTOGRAM

```
# plot histogram
# default to 10 bins
>>> hist(randn(1000))
```



HISTOGRAM 2

```
# change the number of bins
>>> hist(randn(1000), 30)
```



Multiple Plots using Subplot

DEMO/MATPLOTLIB_PLOTTING/EXAMPLES/SUBPLOT_DEMO.PY

```
def f(t):
    s1 = cos(2*pi*t)
    e1 = exp(-t)
    return multiply(s1,e1)

t1 = arange(0.0, 5.0, 0.1)
t2 = arange(0.0, 5.0, 0.02)
t3 = arange(0.0, 2.0, 0.01)

subplot(211)
l = plot(t1, f(t1), 'bo', t2, f(t2),
        'k--')
setp(l, 'markerfacecolor', 'g')
grid(True)
title('A tale of 2 subplots')
ylabel('Damped oscillation')

subplot(212)
plot(t3, cos(2*pi*t3), 'r.')
grid(True)
xlabel('time (s)')
ylabel('Undamped')
show()
```

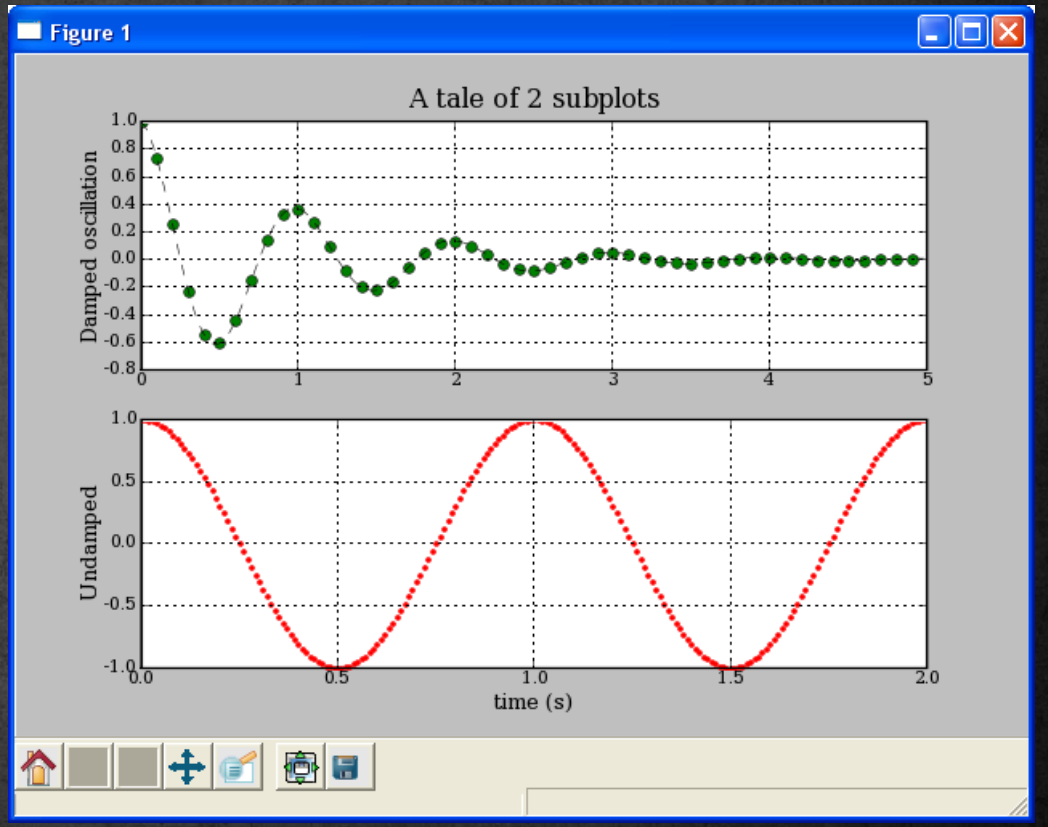
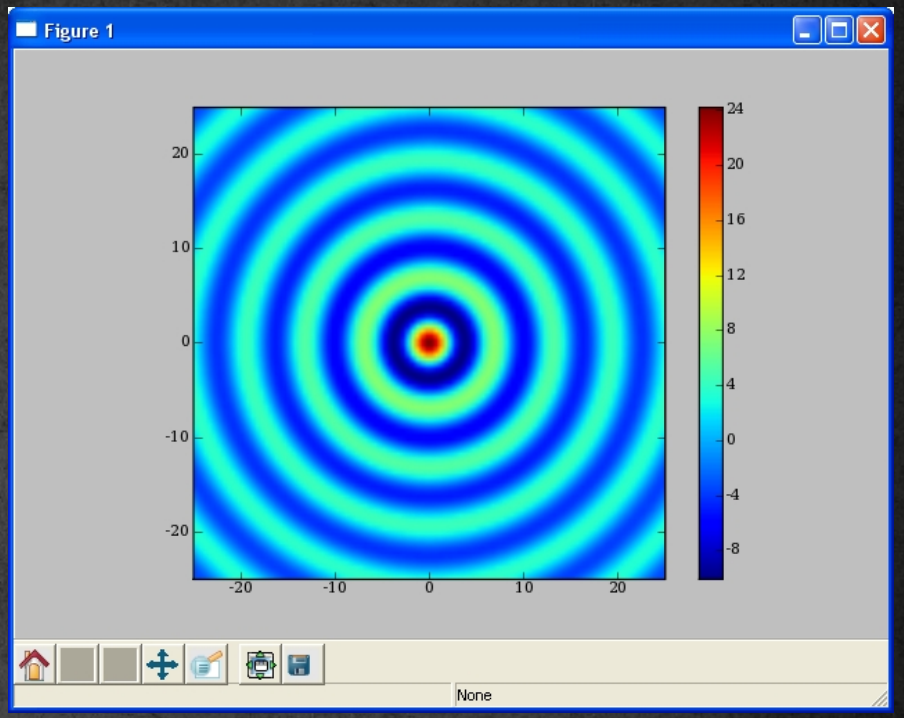


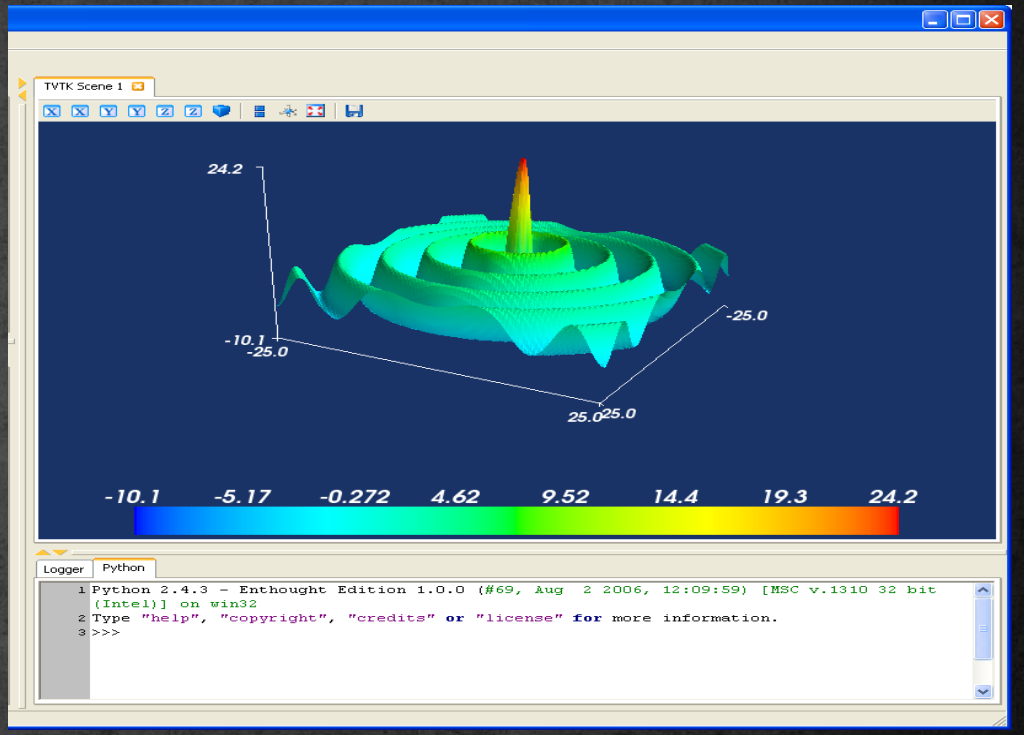
Image Display

```
# Create 2d array where values
# are radial distance from
# the center of array.
>>> from numpy import mgrid
>>> from scipy import special
>>> x,y = mgrid[-25:25:100j,
...             -25:25:100j]
>>> r = sqrt(x**2+y**2)
# Calculate bessel function of
# each point in array and scale
>>> s = special.j0(r)*25

# Display surface plot.
>>> imshow(s, extent=[-25,25,-25,25])
>>> colorbar()
```



Surface plots with mlab

```
# Create 2d array where values
# are radial distance from
# the center of array.
>>> from numpy import mgrid
>>> from scipy import special
>>> x,y = mgrid[-25:25:100j,
...             -25:25:100j]
>>> r = sqrt(x**2+y**2)
# Calculate bessel function of
# each point in array and scale
>>> s = special.j0(r)*25

# Display surface plot.
>>> from enthought.mayavi \
      import mlab
>>> mlab.surf(x,y,s)
>>> mlab.scalarbar()
>>> mlab.axes()
```



SciPy Overview

- Available at www.scipy.org
- Open Source BSD Style License
- Over 30 svn "committers" to the project

CURRENT PACKAGES

- Special Functions (scipy.special)
- Signal Processing (scipy.signal)
- Image Processing (scipy.ndimage)
- Fourier Transforms (scipy.fftpack)
- Optimization (scipy.optimize)
- Numerical Integration (scipy.integrate)
- Linear Algebra (scipy.linalg)

Input/Output (scipy.io)

Statistics (scipy.stats)

Fast Execution (scipy.weave)

Clustering Algorithms (scipy.cluster)

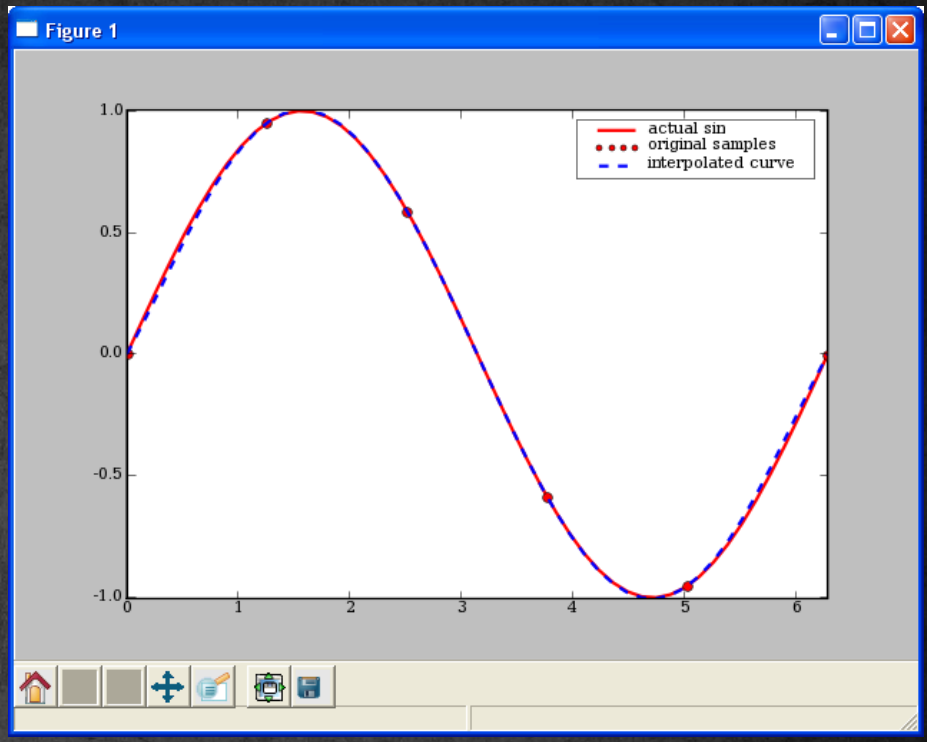
Sparse Matrices (scipy.sparse)

Interpolation (scipy.interpolate)

More (e.g. scipy.odr, scipy.maxentropy)

1D Spline Interpolation

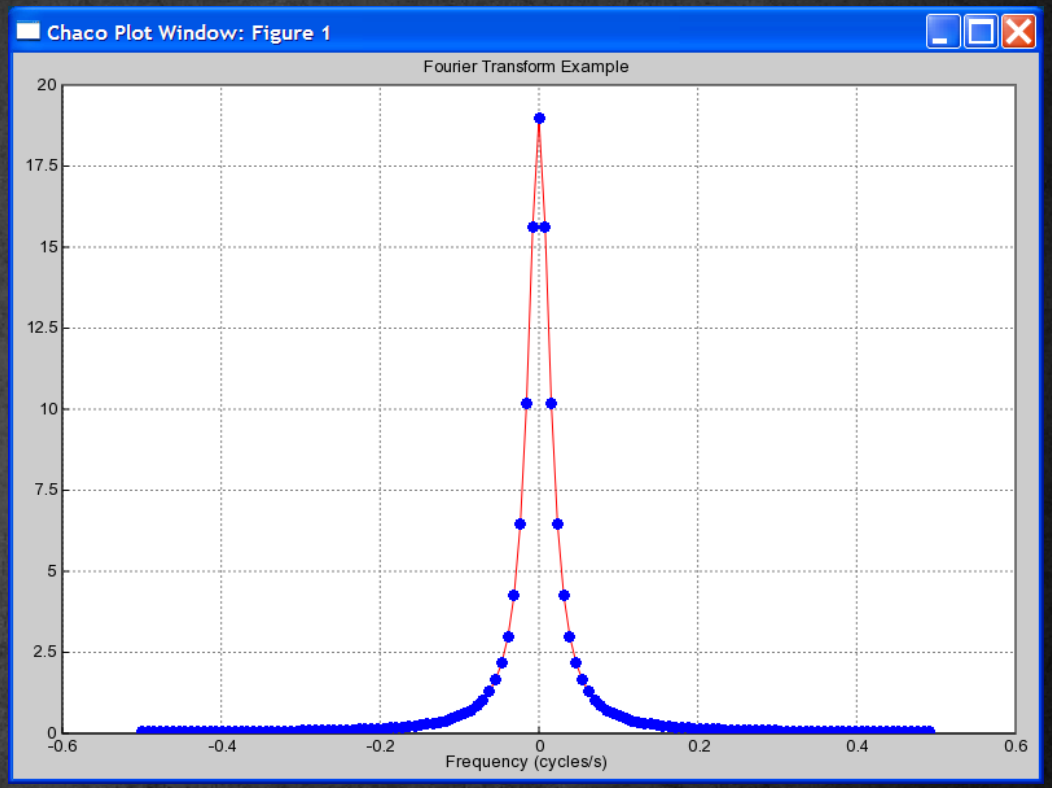
```
# demo/interpolate/spline.py
from scipy.interpolate import interpld
from pylab import plot, axis, legend
from numpy import linspace

# sample values
x = linspace(0,2*pi,6)
y = sin(x)

# Create a spline class for interpolation.
# kind=5 sets to 5th degree spline.
# kind=0 -> zeroth order hold.
# kind=1 or 'linear' -> linear interpolation.
# kind=2 or
spline_fit = interpld(x,y,kind=5)
xx = linspace(0,2*pi, 50)
yy = spline_fit(xx)

# display the results.
plot(xx, sin(xx), 'r-', x,y,'ro',xx,yy, 'b--',linewidth=2)
axis('tight')
legend(['actual sin', 'original samples', 'interpolated curve'])
```



FFT

scipy.fft --- FFT and related functions

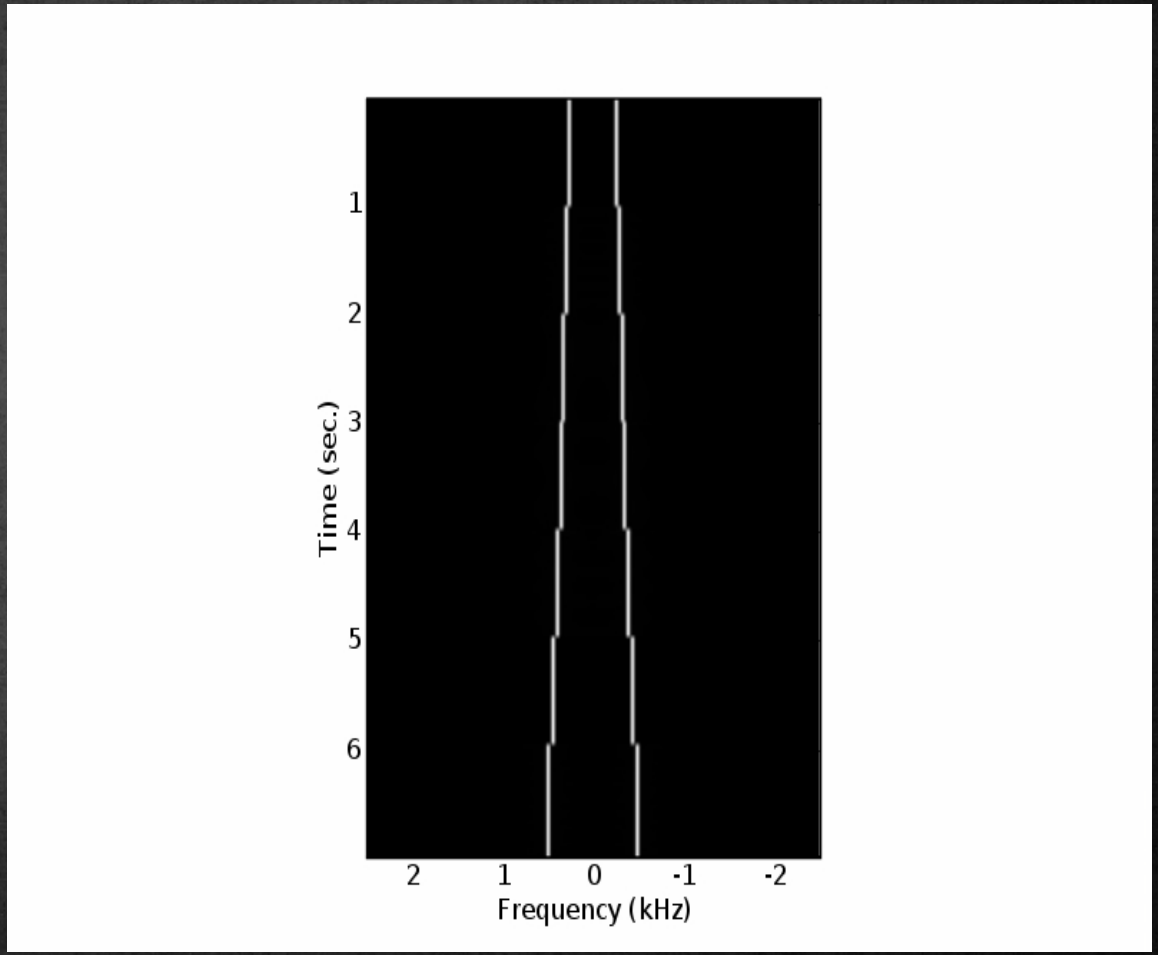
```
>>> n = fftfreq(128)*128
>>> f = fftfreq(128)
>>> ome = 2*pi*f
>>> x = (0.9)**abs(n)
>>> X = fft(x)
>>> z = exp(1j*ome)
>>> Xexact = (0.9**2 - 1)/0.9*z /   \
...          (z-0.9) / (z-1/0.9)
>>> f = fftshift(f)
>>> plot(f, fftshift(X.real),'r-',
...      f, fftshift(Xexact.real),'bo')
>>> title('Fourier Transform Example')
>>> xlabel('Frequency (cycles/s)')
>>> axis(-0.6,0.6, 0, 20)
```



FFT

EXAMPLE --- Short-Time Windowed Fourier Transform

```
rate, data = read('scale.wav')
dT, T_window = 1.0/rate, 50e-3
N_window = int(T_window * rate)
N_data = len(data)
window = get_window('hamming', N_window)
result, start = [], 0
# compute short-time FFT for each block
while (start < N_data - N_window):
        end = start + N_window
    val = fftshift(fft(window*data[start:end]))
    result.append(val)
    start = end
lastval = fft(window*data[-N_window:])
result.append(fftshift(lastval))
result = array(result,result[0].dtype)
```



Signal Processing

scipy.signal --- Signal and Image Processing

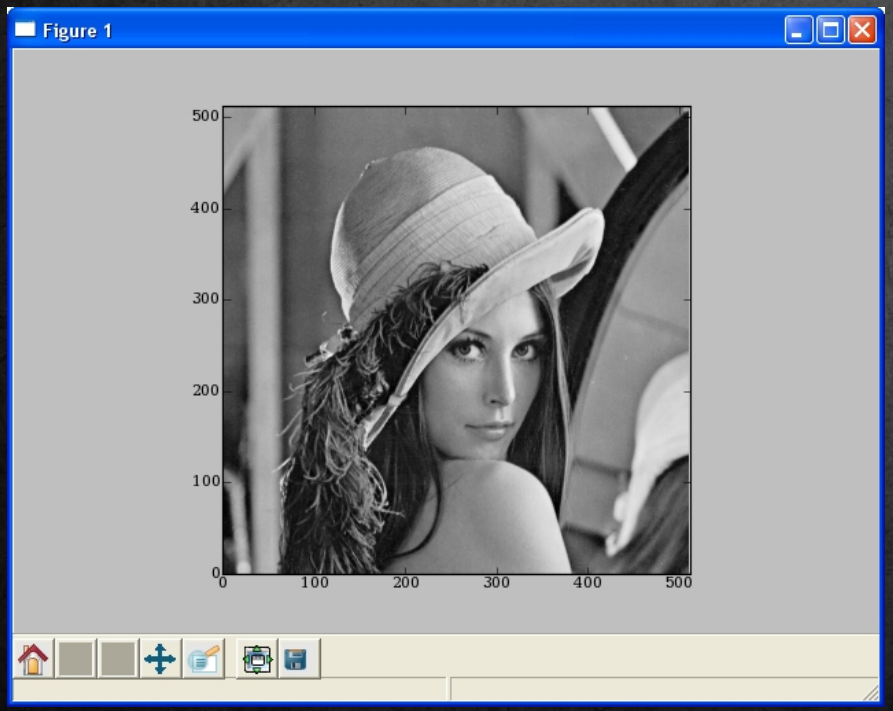
What's Available?

- Filtering
- General 2-D Convolution (more boundary conditions)
- N-D convolution
- B-spline filtering
- N-D Order filter, N-D median filter, faster 2d version,
- IIR and FIR filtering and filter design
- LTI systems
- System simulation
- Impulse and step responses
- Partial fraction expansion

Image Processing

```
# The famous lena image is packaged with scipy
>>> from scipy import lena, signal
>>> lena = lena().astype(float32)
>>> imshow(lena, cmap=cm.gray)
# Blurring using a median filter
>>> fl = signal.medfilt2d(lena, [15,15])
>>> imshow(fl, cmap=cm.gray)
```

LENA IMAGE



MEDIAN FILTERED IMAGE

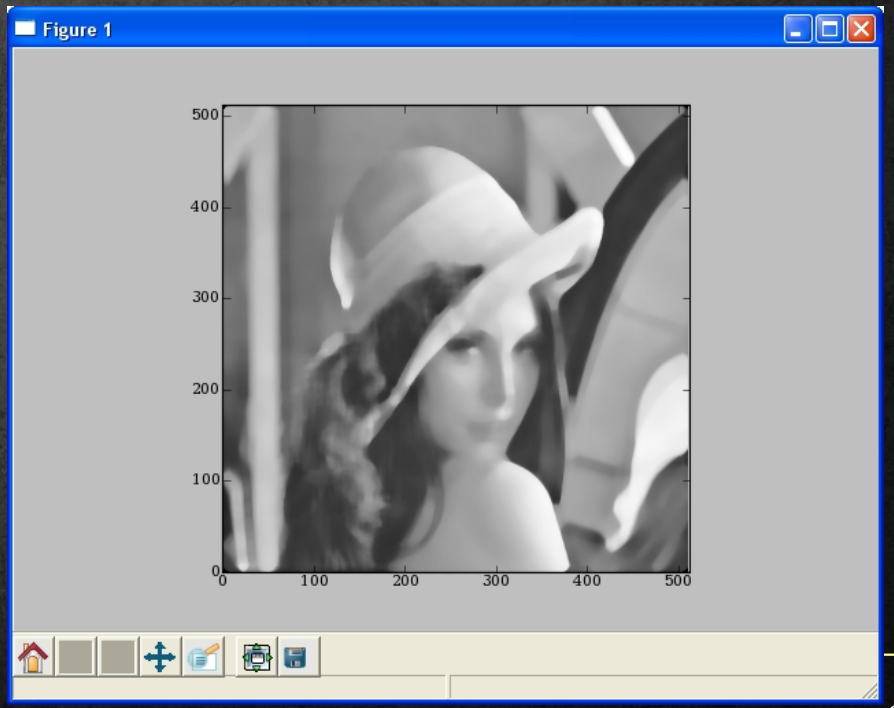
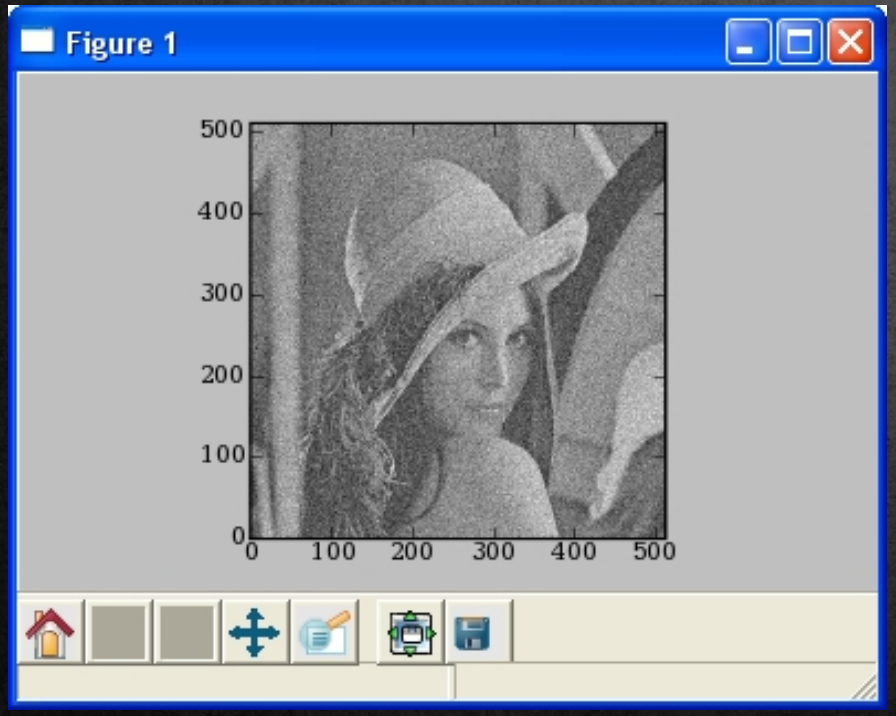


Image Processing

```
# Noise removal using wiener filter
>>> from scipy.stats import norm
>>> ln = lena + norm(0,32).rvs(lena.shape)
>>> imshow(ln)
>>> cleaned = signal.wiener(ln)
>>> imshow(cleaned)
```

NOISY IMAGE



FILTERED IMAGE

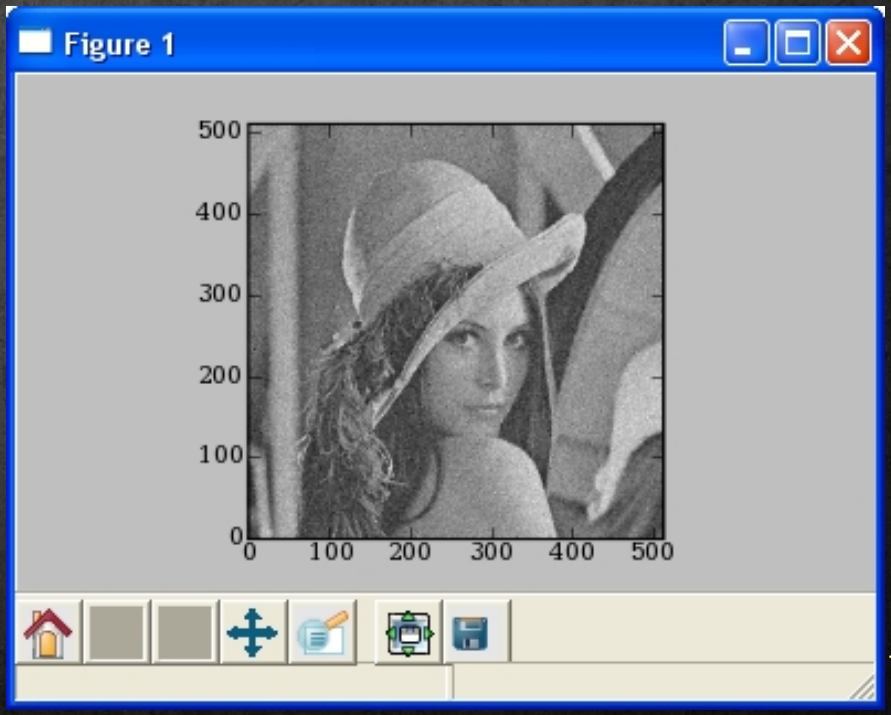
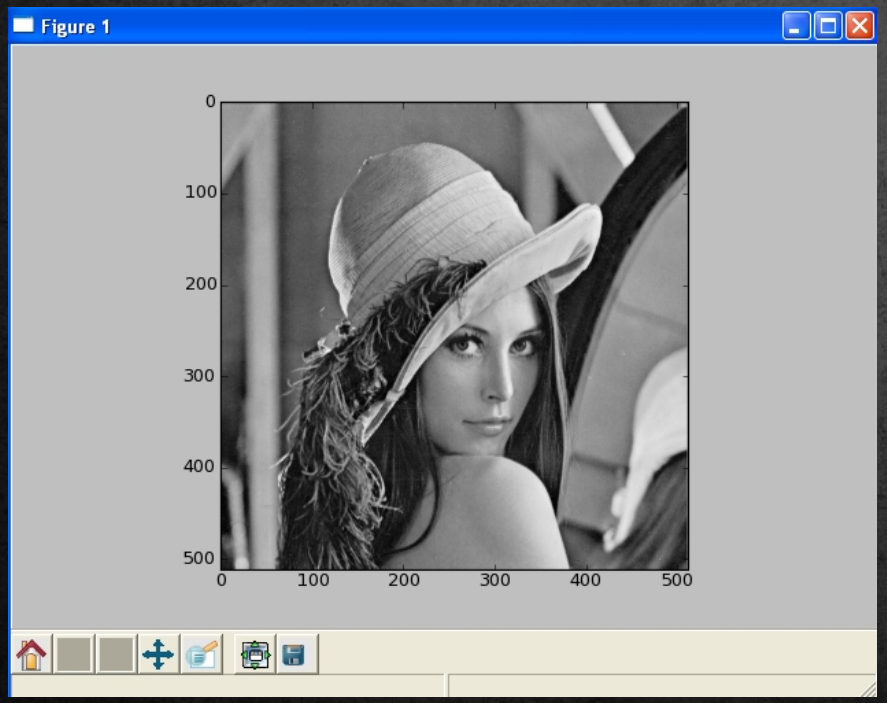


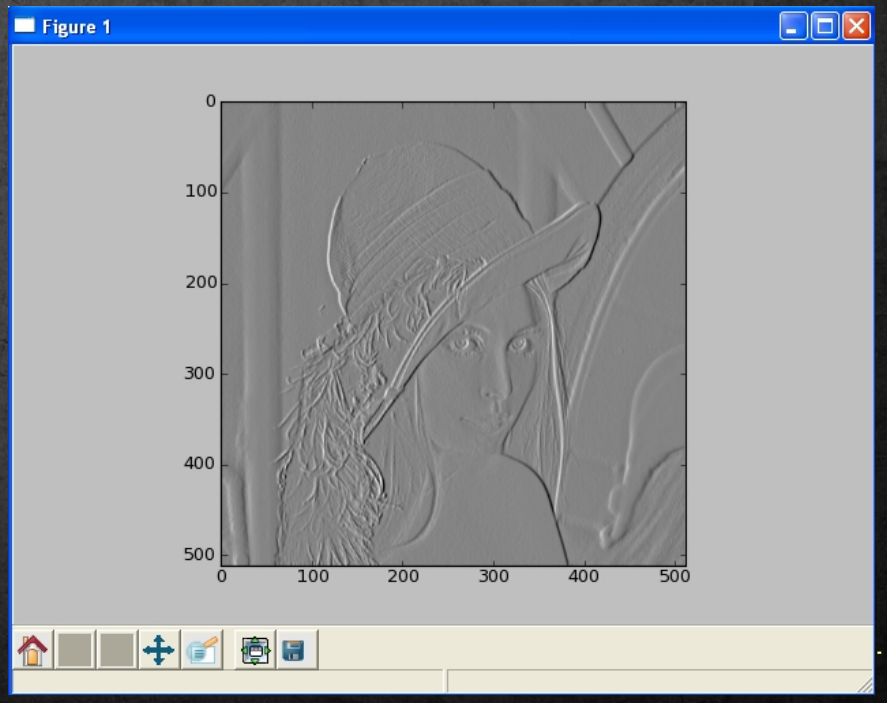
Image Processing

```
# Edge detection using Sobel filter
>>> from scipy.ndimage.filters import sobel
>>> imshow(lena)
>>> edges = sobel(lena)
>>> imshow(edges)
```

NOISY IMAGE



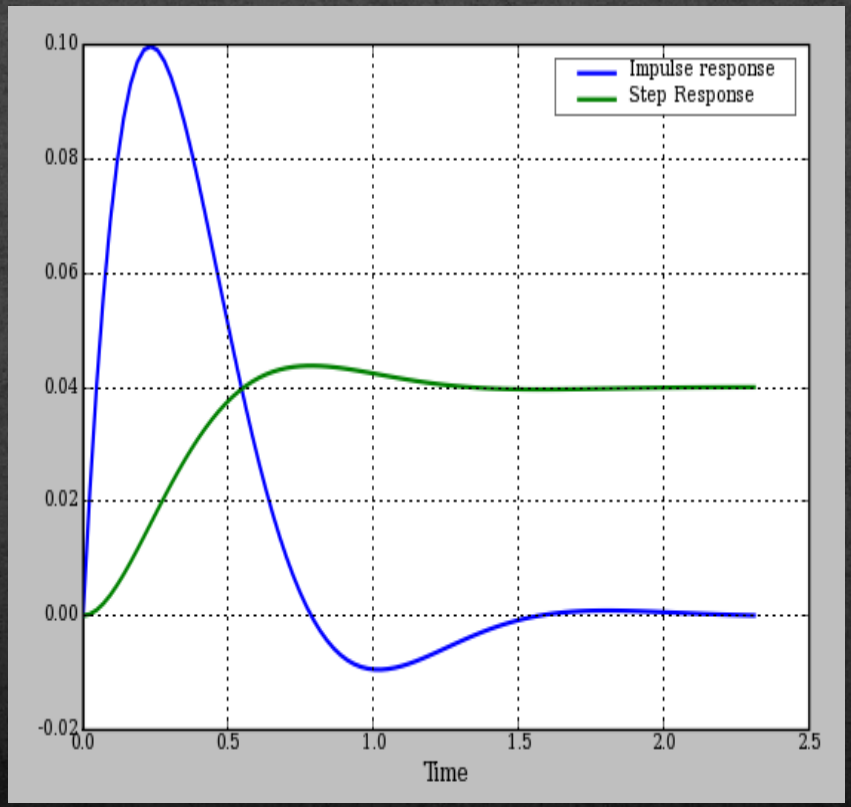
FILTERED IMAGE



LTI Systems

```
>>> b,a = [1],[1,6,25]
>>> ltisys = signal.lti(b,a)
>>> t,h = ltisys.impulse()
>>> ts,s = ltisys.step()
>>> plot(t,h,ts,s)
>>> legend(['Impulse response','Step response'])
```

$$H(s) = \frac{1}{s^2 + 6s + 25}$$



Optimization

scipy.optimize --- unconstrained minimization and root finding

- Unconstrained Optimization

  fmin (Nelder-Mead simplex), **fmin_powell** (Powell's method), **fmin_bfgs** (BFGS quasi-Newton method), **fmin_ncg** (Newton conjugate gradient), **leastsq** (Levenberg-Marquardt), **anneal** (simulated annealing global minimizer), **brute** (brute force global minimizer), **brent** (excellent 1-D minimizer), **golden**, **bracket**

- Constrained Optimization

  fmin_l_bfgs_b, fmin_tnc (truncated newton code), **fmin_cobyla** (constrained optimization by linear approximation), **fminbound** (interval constrained 1-d minimizer)

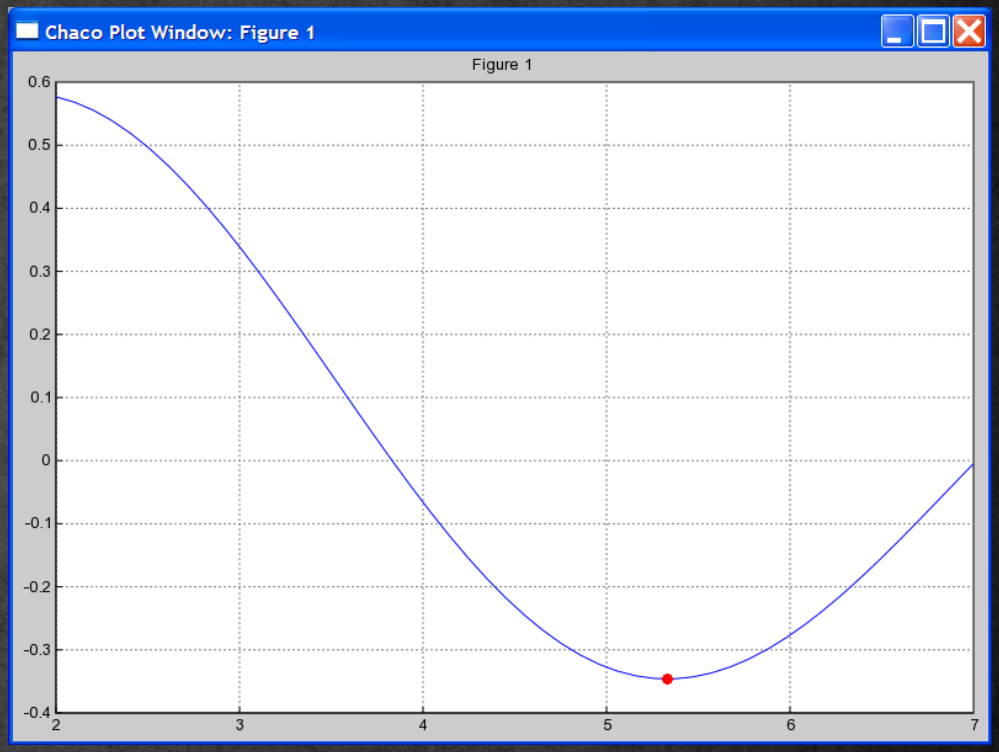
- Root finding

  fsolve (using MINPACK), **brentq**, **brenth**, **ridder**, **newton**, **bisect**, **fixed_point** (fixed point equation solver)

Optimization

EXAMPLE: MINIMIZE BESSEL FUNCTION

```
# minimize 1st order bessel
# function between 4 and 7
>>> from scipy.special import j1
>>> from scipy.optimize import \
    fminbound

>>> x = r_[2:7.1:.1]
>>> j1x = j1(x)
>>> plot(x,j1x,'-')
>>> hold(True)
>>> x_min = fminbound(j1,4,7)
>>> j1_min = j1(x_min)
>>> plot([x_min],[j1_min],'ro')
```



Optimization

EXAMPLE: SOLVING NONLINEAR EQUATIONS

Solve the non-linear equations

$$\begin{aligned} 3x_0 - \cos(x_1 x_2) + a &= 0 \\ x_0^2 - 81(x_1 + 0.1)^2 + \sin(x_2) + b &= 0 \\ e^{-x_0 x_1} + 20x_2 + c &= 0 \end{aligned}$$

```
>>> def nonlin(x,a,b,c):
>>>     x0,x1,x2 = x
>>>     return [3*x0-cos(x1*x2)+ a,
>>>             x0*x0-81*(x1+0.1)**2                    +
sin(x2)+b,
>>>             exp(-x0*x1)+20*x2+c]
>>> a,b,c = -0.5,1.06,(10*pi-3.0)/3
>>> root = optimize.fsolve(nonlin,  [0.1,0.1,-
0.1],args=(a,b,c))
>>> print root
[ 0.5     0.     -0.5236]
>>> print nonlin(root,a,b,c)
[0.0, -2.231104190e-12, 7.46069872e-14]
```

starting location for search

Optimization

EXAMPLE: MINIMIZING ROSENBROCK FUNCTION

Rosenbrock function

$$f(\mathbf{x}) = \sum_{i=1}^{N-1} 100\left(x_i - x_{i-1}^2\right)^2 + (1 - x_{i-1})^2 .$$

WITHOUT DERIVATIVE

```
>>> rosen = optimize.rosen
>>> import time
>>> x0 = [1.3,0.7,0.8,1.9,1.2]
>>> start = time.time()
>>> xopt = optimize.fmin(rosen,
x0, avegtol=1e-7)
>>> stop = time.time()
>>> print_stats(start, stop, xopt)
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 316
         Function evaluations: 533
Found in 0.08052992820744 seconds
Solution: [ 1.  1.  1.  1.  1.]
Function value: 2.67775760157e-15
Avg. Error: 1.5323906899e-08
```

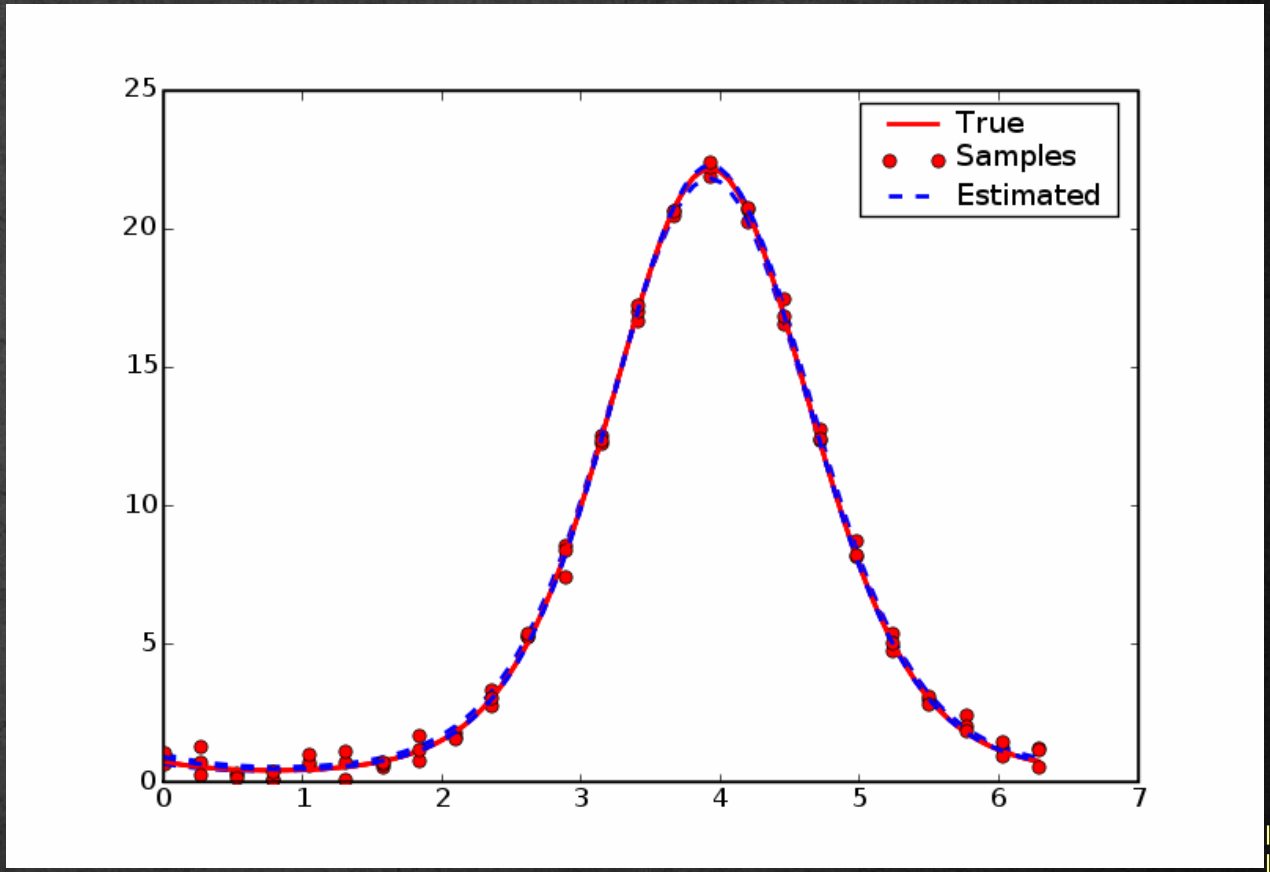
USING DERIVATIVE

```
>>> rosen_der = optimize.rosen_der
>>> x0 = [1.3,0.7,0.8,1.9,1.2]
>>> start = time.time()
>>> xopt = optimize.fmin_bfgs(rosen,
x0, fprime=rosen_der, avegtol=1e-7)
>>> stop = time.time()
>>> print_stats(start, stop, xopt)
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 111
         Function evaluations: 266
         Gradient evaluations: 112
Found in 0.0521121025085 seconds
Solution: [ 1.  1.  1.  1.  1.]
Function value: 1.37391034754e-18
Avg. Error: 1.13246034772e-10
```

Optimization

EXAMPLE: Non-linear least-squares data fitting

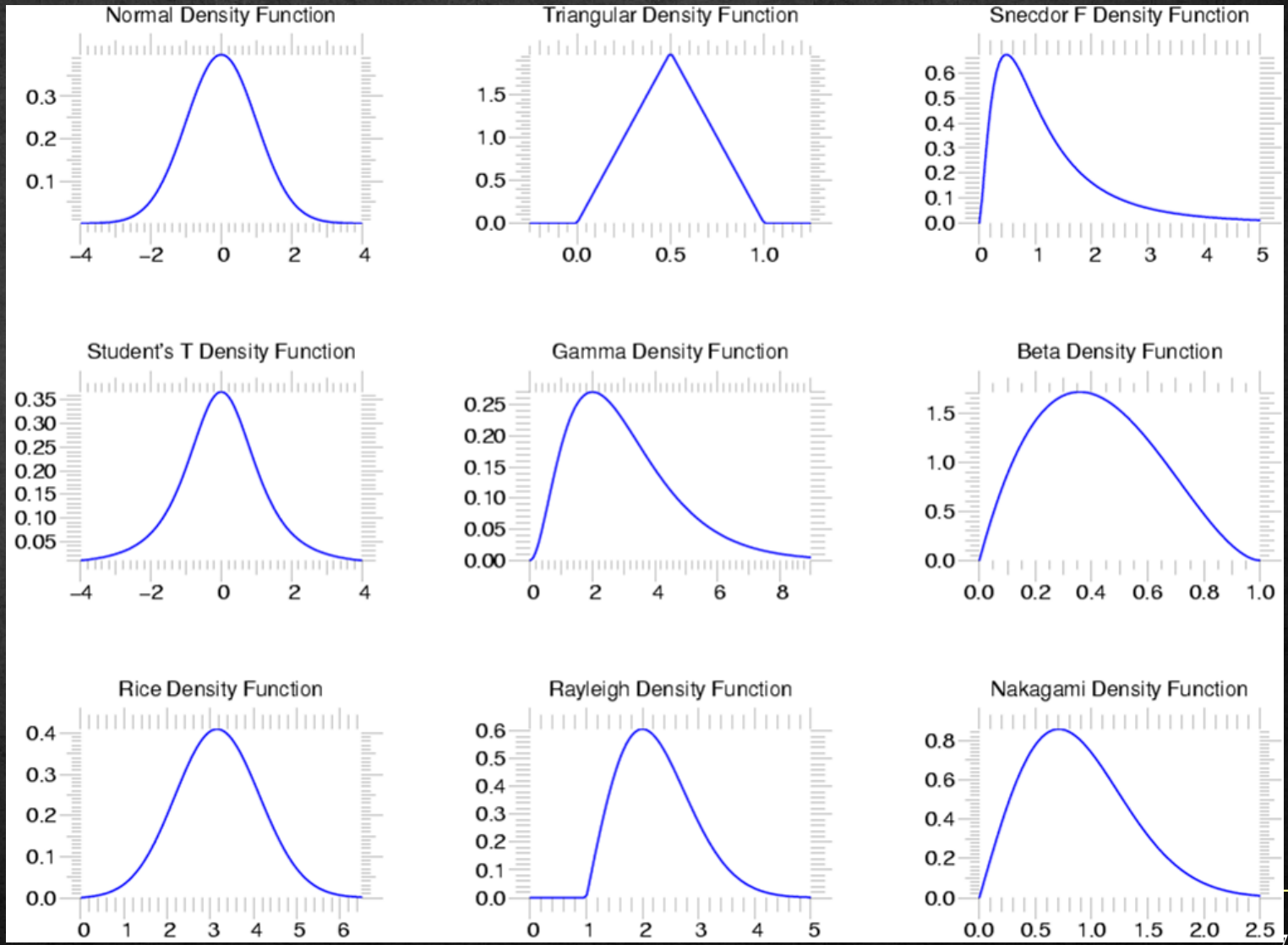
```
# fit data-points to a curve
# demo/data_fitting/datafit.py
>>> from numpy.random import randn
>>> from numpy import exp, sin, pi
>>> from numpy import linspace
>>> from scipy.optimize import leastsq
>>> def func(x,A,a,f,phi):
    return A*exp(-a*sin(f*x+pi/4))
>>> def errfunc(params, x, data):
    return func(x, *params) - data
>>> ptrue = [3,2,1,pi/4]
>>> x = linspace(0,2*pi,25)
>>> true = func(x, *ptrue)
>>> noisy = true + 0.3*randn(len(x))
>>> p0 = [1,1,1,1]
>>> pmin, ier = leastsq(errfunc, p0,
                        args=(x, noisy))
>>> pmin
array([3.1705, 1.9501, 1.0206, 0.7034])
```



Statistics

scipy.stats --- CONTINUOUS DISTRIBUTIONS

over 80 continuous distributions!



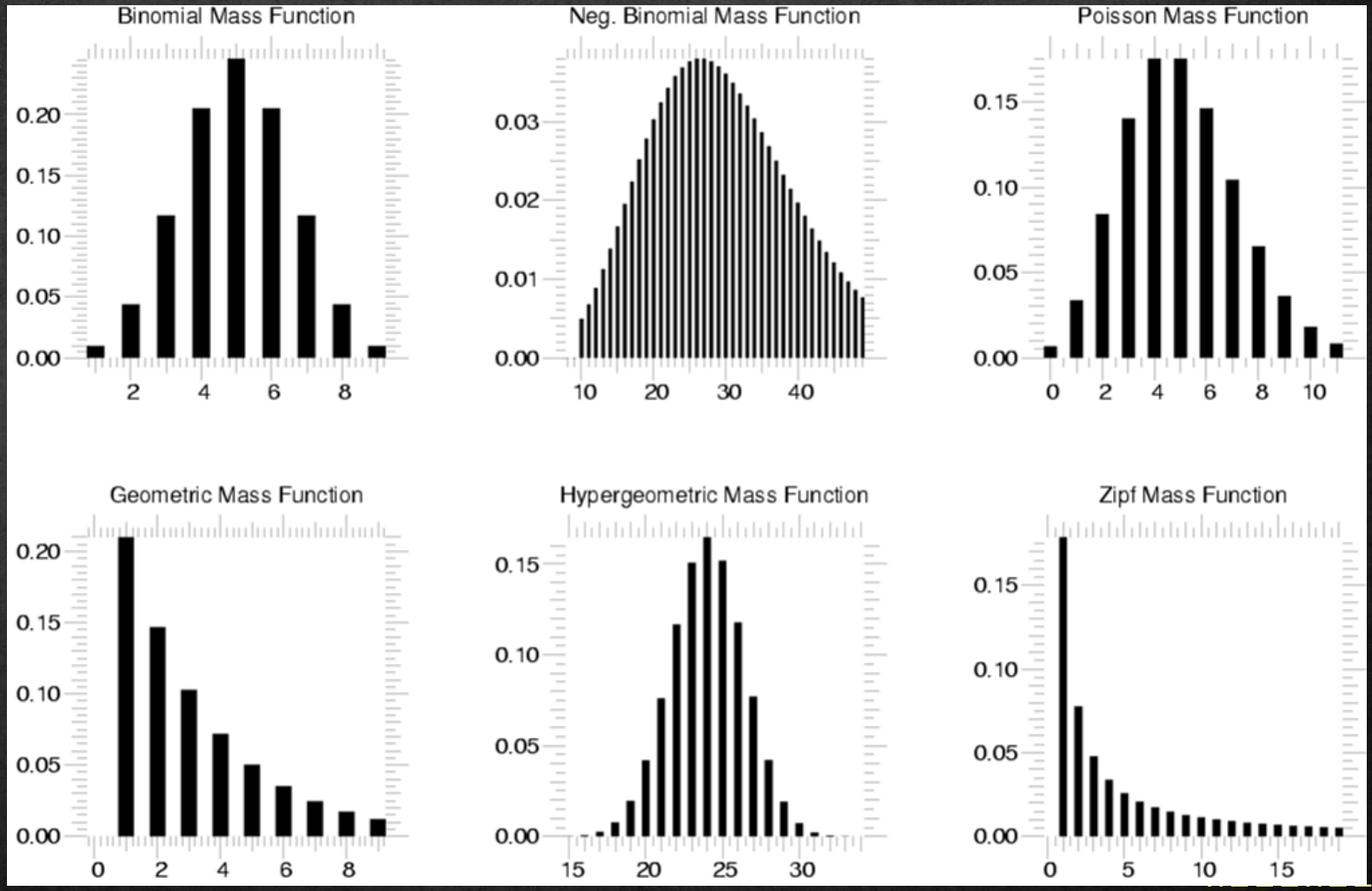
METHODS

- pdf
- cdf
- rvs
- ppf
- stats

Statistics

scipy.stats --- Discrete Distributions

10 standard discrete distributions (plus any arbitrary finite RV)



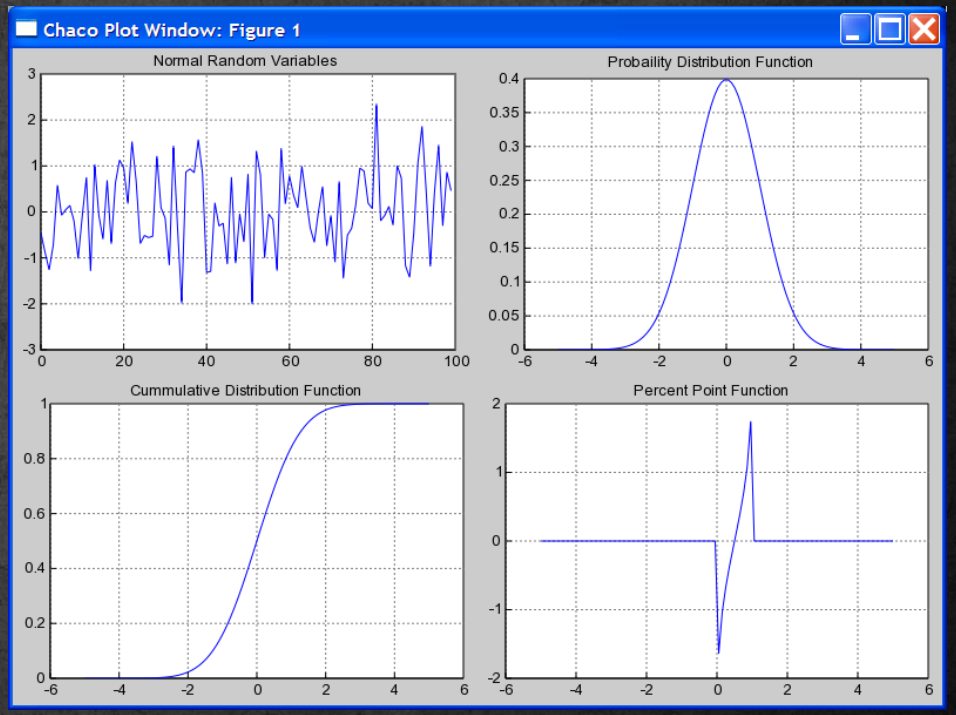
METHODS

- pdf
- cdf
- rvs
- ppf
- stats

Using stats objects

DISTRIBUTIONS

```
# Sample normal dist. 100 times.
>>> samp = stats.norm.rvs(size=100)

>>> x = r_[-5:5:100j]
# Calculate probability dist.
>>> pdf = stats.norm.pdf(x)
# Calculate cummulative Dist.
>>> cdf = stats.norm.cdf(x)
# Calculate Percent Point Function
>>> ppf = stats.norm.ppf(x)
```



Statistics

scipy.stats --- Basic Statistical Calculations on Data

numpy.mean, numpy.std, numpy.var, numpy.cov

stats.skew, stats.kurtosis, stats.moment

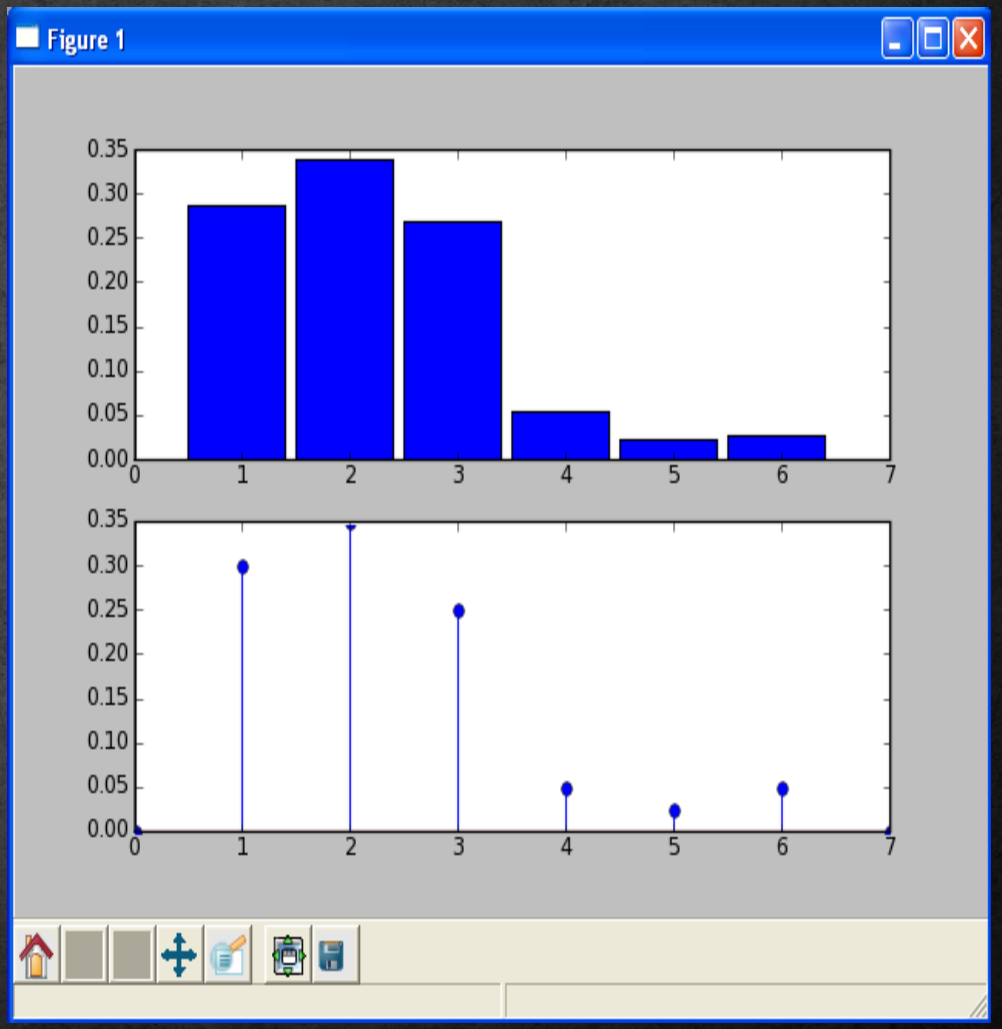
scipy.stats.bayes_mvs --- Bayesian mean, variance, and std.

```
# Create "frozen" Gamma distribution with a=2.5
>>> grv = stats.gamma(2.5)
>>> grv.stats()     # Theoretical mean and variance
(array(2.5), array(2.5))
# Estimate mean, variance, and std with 95% confidence
>>> vals = grv.rvs(size=100)
>>> stats.bayes_mvs(vals, alpha=0.95)
((2.52887906081, (2.19560839724, 2.86214972438)),
 (2.87924964268, (2.17476164549, 3.8070215789)),
 (1.69246760584, (1.47470730841, 1.95115903475)))
# (expected value and confidence interval for each of
# mean, variance, and standard-deviation)
```

Using stats objects

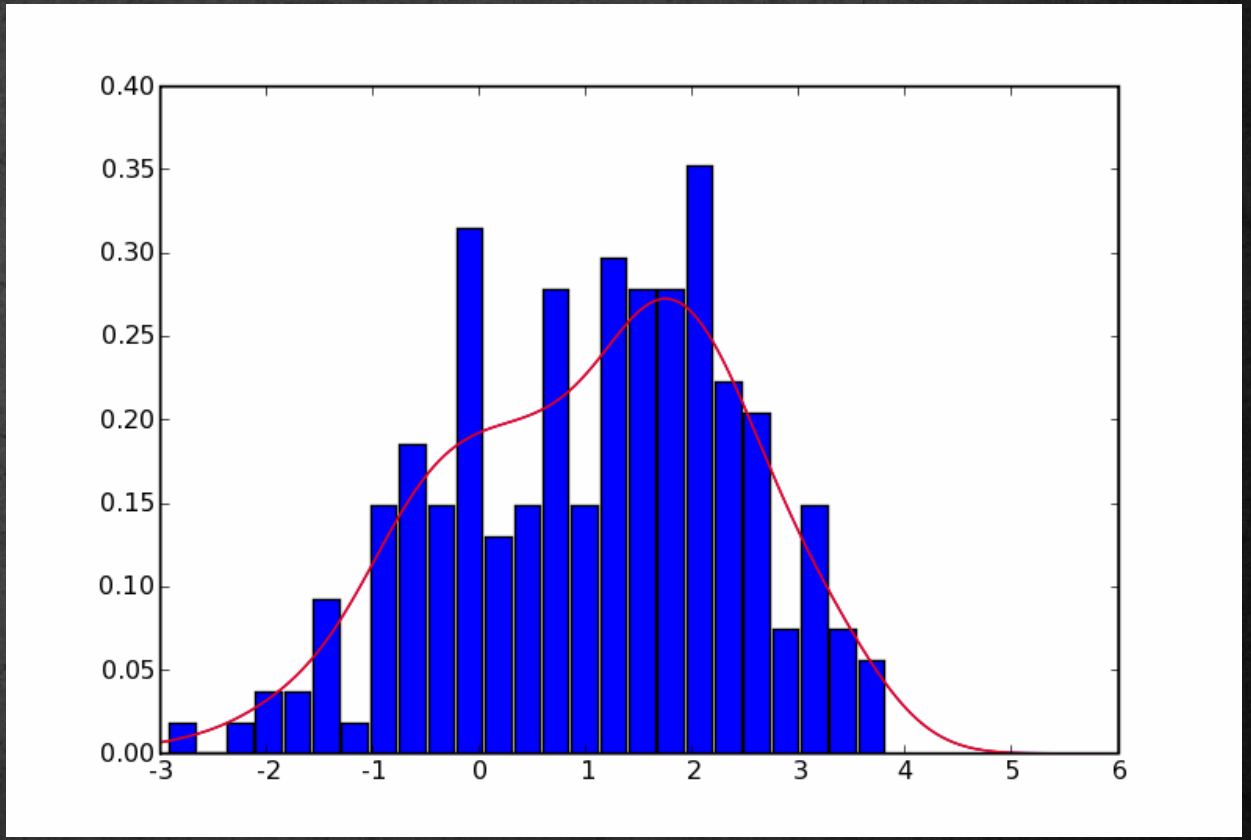
CREATING NEW DISCRETE DISTRIBUTIONS

```
# Create a loaded dice.
>>> from scipy.stats import rv_discrete
>>> xk = [1,2,3,4,5,6]
>>> pk = [0.3,0.35,0.25,0.05,
          0.025,0.025]
>>> new = rv_discrete(name='loaded',
                      values=(xk,pk))

# Calculate histogram
>>> samples = new.rvs(size=1000)
>>> bins=linspace(0.5,5.5,6)
>>> subplot(211)
>>> hist(samples,bins=bins,normed=True)
# Calculate pmf
>>> x = range(0,8)
>>> subplot(212)
>>> stem(x,new.pmf(x))
```



Continuous PDF Estimation using Gaussian Kernel Density Estimation

```
# Sample normal dist. 100 times.
>>> rv1 = stats.norm()
>>> rv2 = stats.norm(2.0,0.8)
>>> samp = r_[rv1.rvs(size=100),
              rv2.rvs(size=100)]
# Kernel estimate (smoothed histogram)
>>> apdf = stats.kde.gaussian_kde(samp)
>>> x = linspace(-3,6,200)
>>> plot(x, apdf(x),'r')

# Histogram
>>> hist(x, bins=25, normed=True)
```



Linear Algebra

scipy.linalg --- FAST LINEAR ALGEBRA

- Uses ATLAS if available --- very fast
- Low-level access to BLAS and LAPACK routines in modules linalg.fblas, and linalg.flapack (FORTRAN order)
- High level matrix routines
  - Linear Algebra Basics: inv, solve, det, norm, lstsq, pinv
  - Decompositions: eig, lu, svd, orth, cholesky, qr, schur
  - Matrix Functions: expm, logm, sqrtm, cosm, coshm, funm (general matrix functions)

Linear Algebra

LU FACTORIZATION

```
>>> from scipy import linalg
>>> a = array([[1,3,5],
...            [2,5,1],
...            [2,3,6]])
# time consuming factorization
>>> lu, piv = linalg.lu_factor(a)

# fast solve for 1 or more
# right hand sides.
>>> b = array([10,8,3])
>>> linalg.lu_solve((lu, piv), b)
array([-7.82608696,  4.56521739,
        0.82608696])
```

EIGEN VALUES AND VECTORS

```
>>> from scipy import linalg
>>> a = array([[1,3,5],
...            [2,5,1],
...            [2,3,6]])
# compute eigen values/vectors
>>> vals, vecs = linalg.eig(a)
# print eigen values
>>> vals
array([ 9.39895873+0.j,
       -0.73379338+0.j,
        3.33483465+0.j])
# eigen vectors are in columns
# print first eigen vector
>>> vecs[:,0]
array([-0.57028326,
       -0.41979215,
       -0.70608183])
# norm of vector should be 1.0
>>> linalg.norm(vecs[:,0])
1.0
```

Matrix Objects

STRING CONSTRUCTION

```
>>> from numpy import mat
>>> a = mat('[1,3,5;2,5,1;2,3,6]')
>>> a
matrix([[1, 3, 5],
        [2, 5, 1],
        [2, 3, 6]])
```

TRANSPOSE ATTRIBUTE

```
>>> a.T
matrix([[1, 2, 2],
        [3, 5, 3],
        [5, 1, 6]])
```

INVERTED ATTRIBUTE

```
>>> a.I
matrix([[-1.1739, 0.1304,  0.956],
        [ 0.4347, 0.1739, -0.391],
        [ 0.1739, -0.130,  0.0434]
       ])
# note: reformatted to fit slide
```

DIAGONAL

```
>>> a.diagonal()
matrix([[1, 5, 6]])
>>> a.diagonal(-1)
matrix([[3, 1]])
```

SOLVE

```
>>> b = mat('10;8;3')
>>> a.I*b
matrix([[-7.82608696],
        [ 4.56521739],
        [ 0.82608696]])

>>> from scipy import linalg
>>> linalg.solve(a,b)
matrix([[-7.82608696],
        [ 4.56521739],
        [ 0.82608696]])
```

Integration

scipy.integrate --- General purpose Integration

Ordinary Differential Equations (ODE)

integrate.odeint, **integrate.ode**

Samples of a 1-d function

integrate.trapz (trapezoidal Method), **integrate.simps** (Simpson Method), **integrate.romb** (Romberg Method)

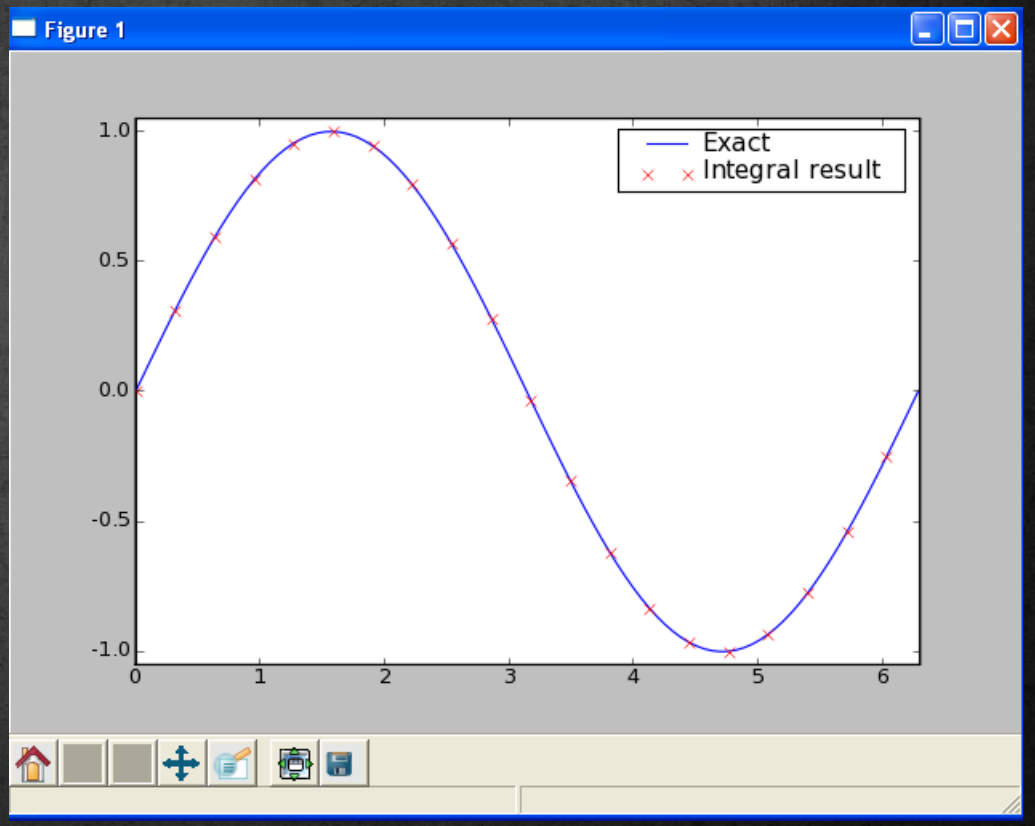
Arbitrary callable function

integrate.quad (general purpose), **integrate.dblquad** (double integration), **integrate.tplquad** (triple integration), **integrate.fixed_quad** (fixed order Gaussian integration), **integrate.quadrature** (Gaussian quadrature to tolerance), i**ntegrate.romberg** (Romberg)

Integration

scipy.integrate --- Example

```
# Compare sin to integral(cos)
>>> def func(x):
    return integrate.quad(cos,0,x)[0]
>>> vecfunc = vectorize(func)

>>> x = r_[0:2*pi:100j]
>>> x2 = x[::5]
>>> y = sin(x)
>>> y2 = vecfunc(x2)
>>> plot(x,y,x2,y2,'rx')
>>> legend(['Exact',
...         'Integral Result'])
```



Special Functions

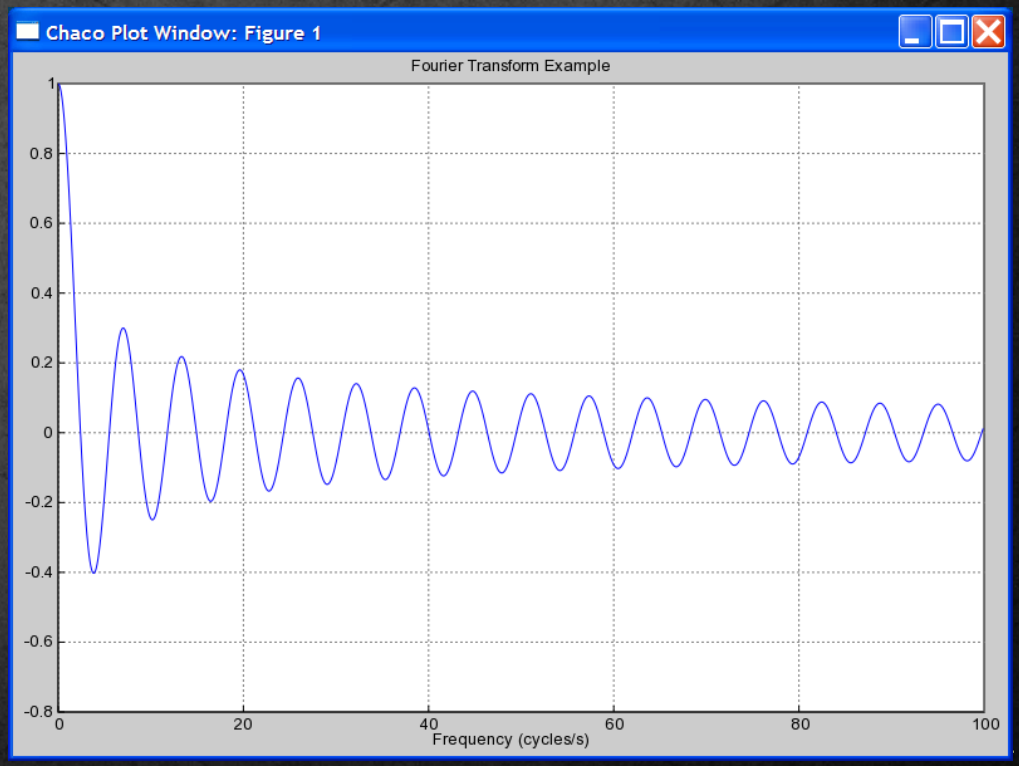
scipy.special

Includes over 200 functions:

Airy, Elliptic, Bessel, Gamma, HyperGeometric, Struve, Error, Orthogonal Polynomials, Parabolic Cylinder, Mathieu, Spheroidal Wave, Kelvin

FIRST ORDER BESSEL EXAMPLE

```
>>> from scipy import special
>>> x = r_[0:100:0.1]
>>> j0x = special.j0(x)
>>> plot(x,j0x)
```

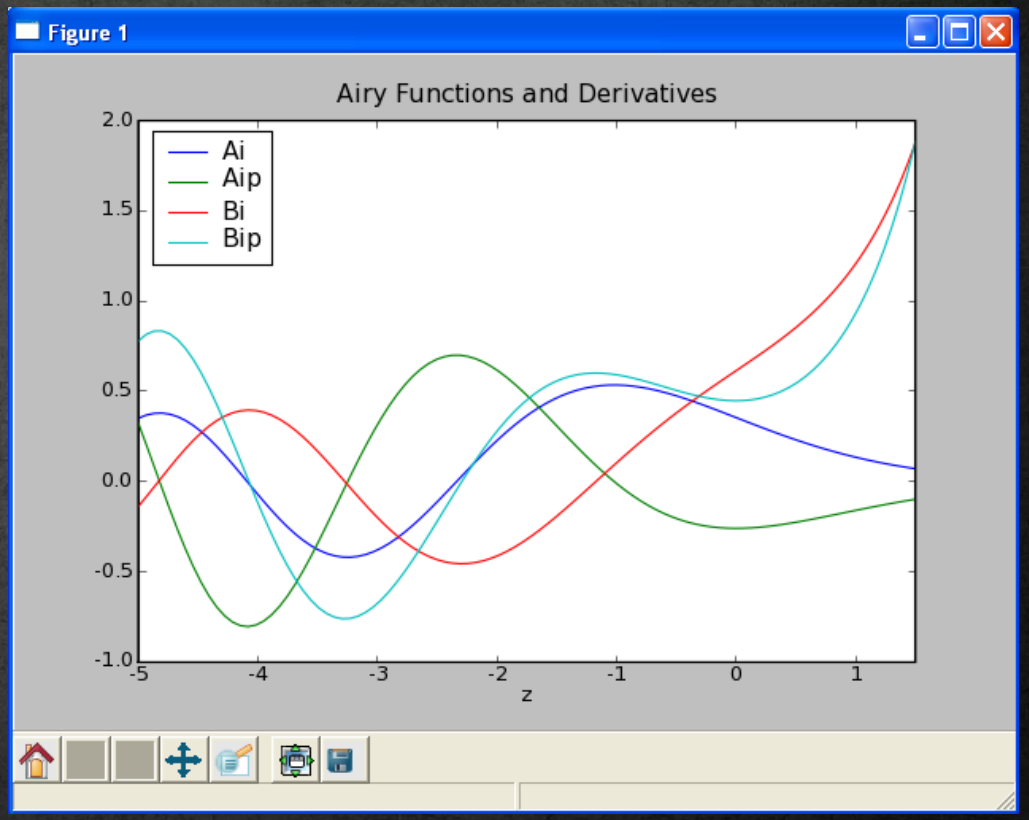


Special Functions

scipy.special

AIRY FUNCTIONS EXAMPLE

```
>>> z = r_[-5:1.5:100j]
>>> vals = special.airy(z)
>>> plot(z,array(vals).T)
>>> legend(['Ai', 'Aip', 'Bi','Bip'])
>>> xlabel('z')
>>> title('Airy Functions and Derivatives')
```



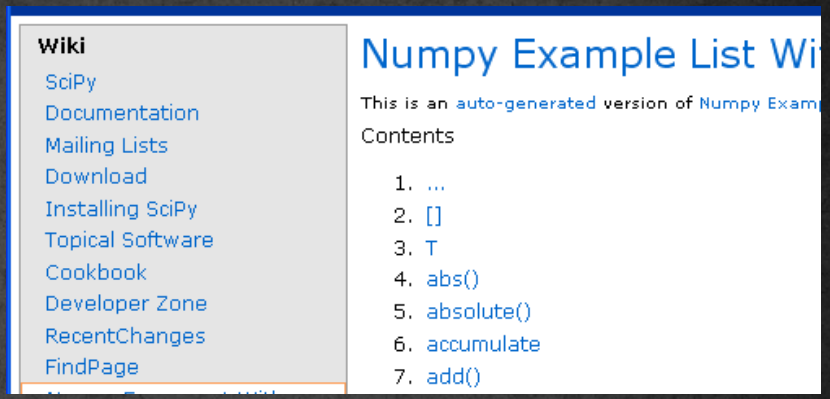
Helpful Sites

SCIPY DOCUMENTATION PAGE

http://www.scipy.org/Documentation

NUMPY EXAMPLES

http://www.scipy.org/Numpy_Example_List_With_Doc



apply_along_axis()

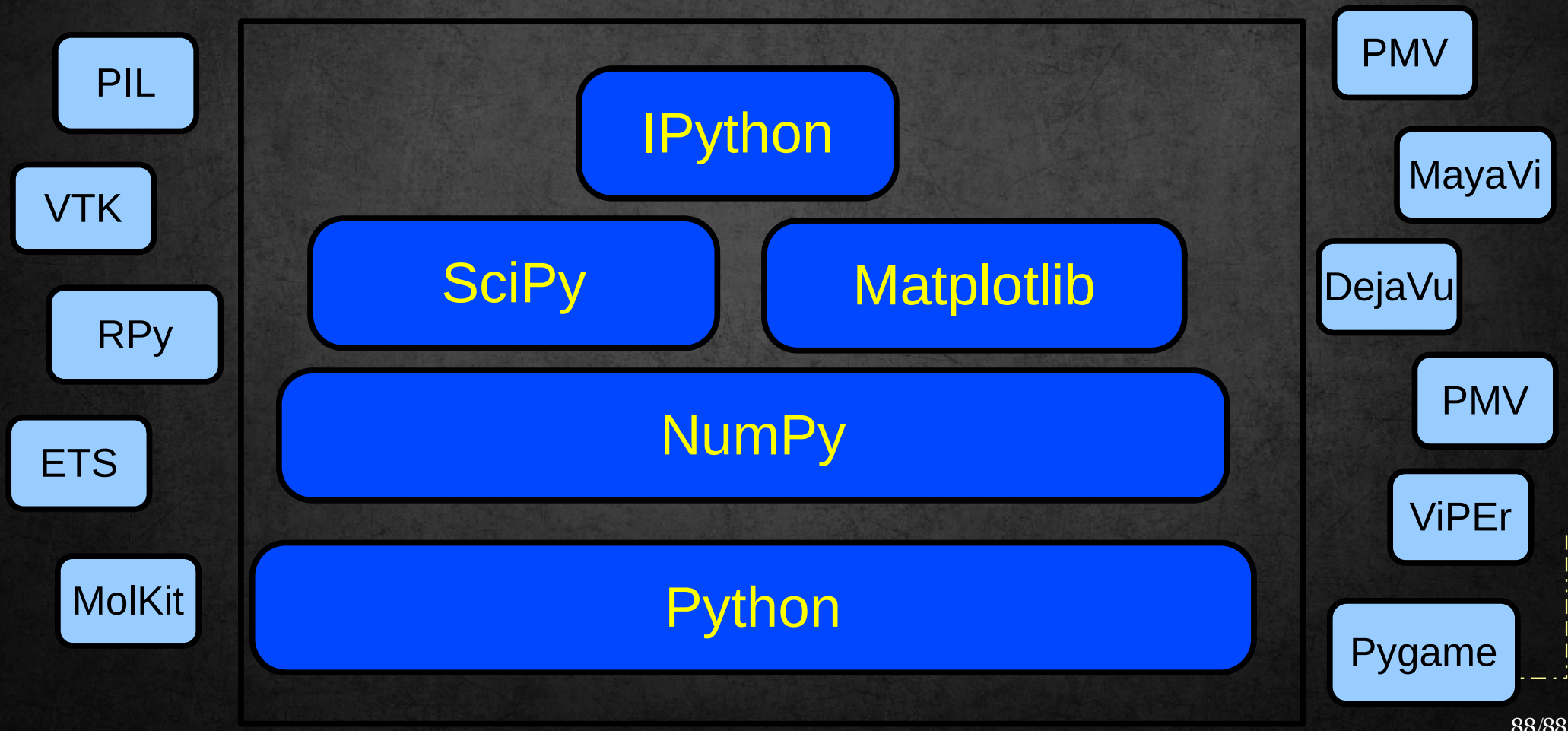
numpy.apply_along_axis(func1d, axis, arr, *args)

```
Execute func1d(arr[i],*args) where func1d takes 1-D arrays
and arr is an N-d array.  i varies so as to apply the functio
along the given axis for each 1-d subarray in arr.
```

Example:

```
>>> from numpy import *
>>> def myfunc(a):                                  # function
...     return (a[0]+a[-1])/2
...
>>> b = array([[1,2,3],[4,5,6],[7,8,9]])
>>> apply_along_axis(myfunc,0,b)                    # apply myfu
array([4, 5, 6])
>>> apply_along_axis(myfunc,1,b)                    # apply myfu
array([2, 5, 8])
```

PyLab

Sometimes the union of the 5 packages is called pylab: ipython -pylab.

Literally 1000's more modules/packages for Python