NumPy (and SciPy)

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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.)

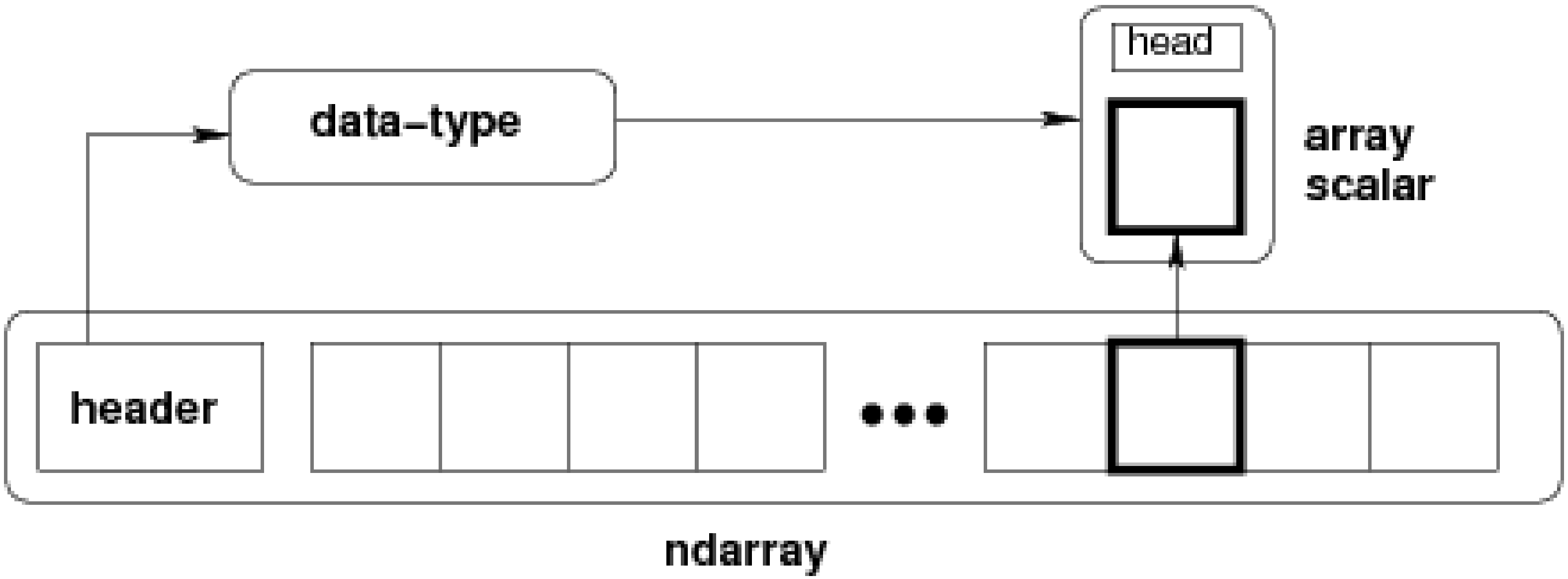
UNIVERSAL FUNCTIONS (UFUNC)

functions that operate element-by-element and return result

- fast-loops registered for each fundamental data-type
- $\sin(\mathbf{x}) = [\sin(x_i)\ i=0..N]$
- $\mathbf{x}+\mathbf{y} = [x_i + y_i\ i=0..N]$

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 into
# 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
```

column

row

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

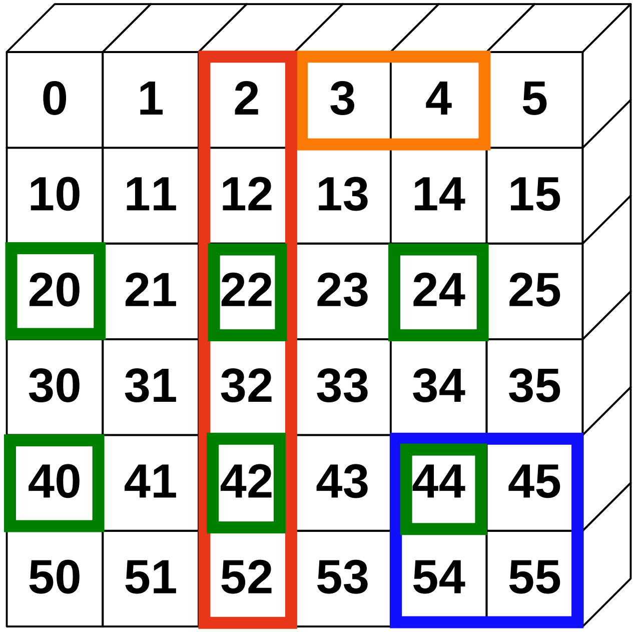
ADDRESS FIRST ROW USING SINGLE INDEX

```
>>> 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])
```

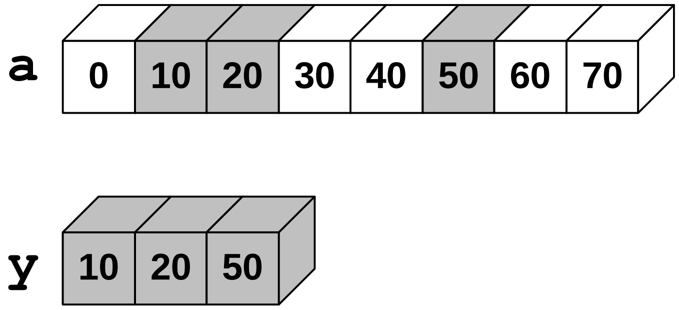
Fancy Indexing

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]
```

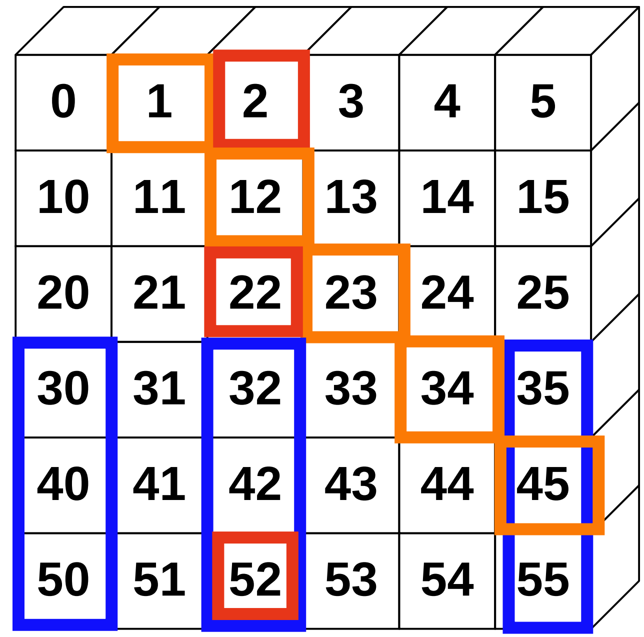
INDEXING WITH BOOLEANS

```
>>> 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.

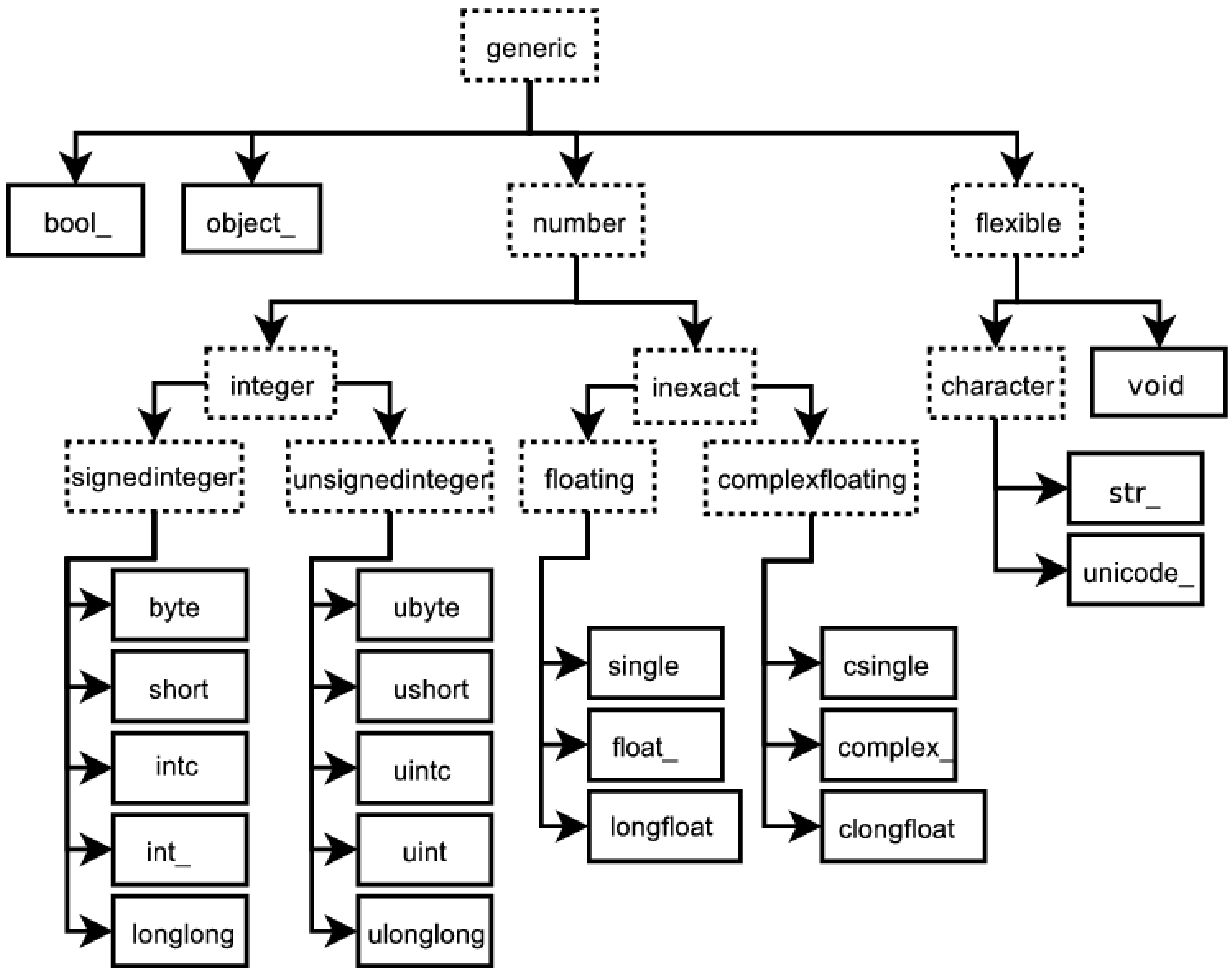
Data-types

- 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.])
```

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
0.62831853071795862
>>> 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]
[2.7182818284590451,
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.

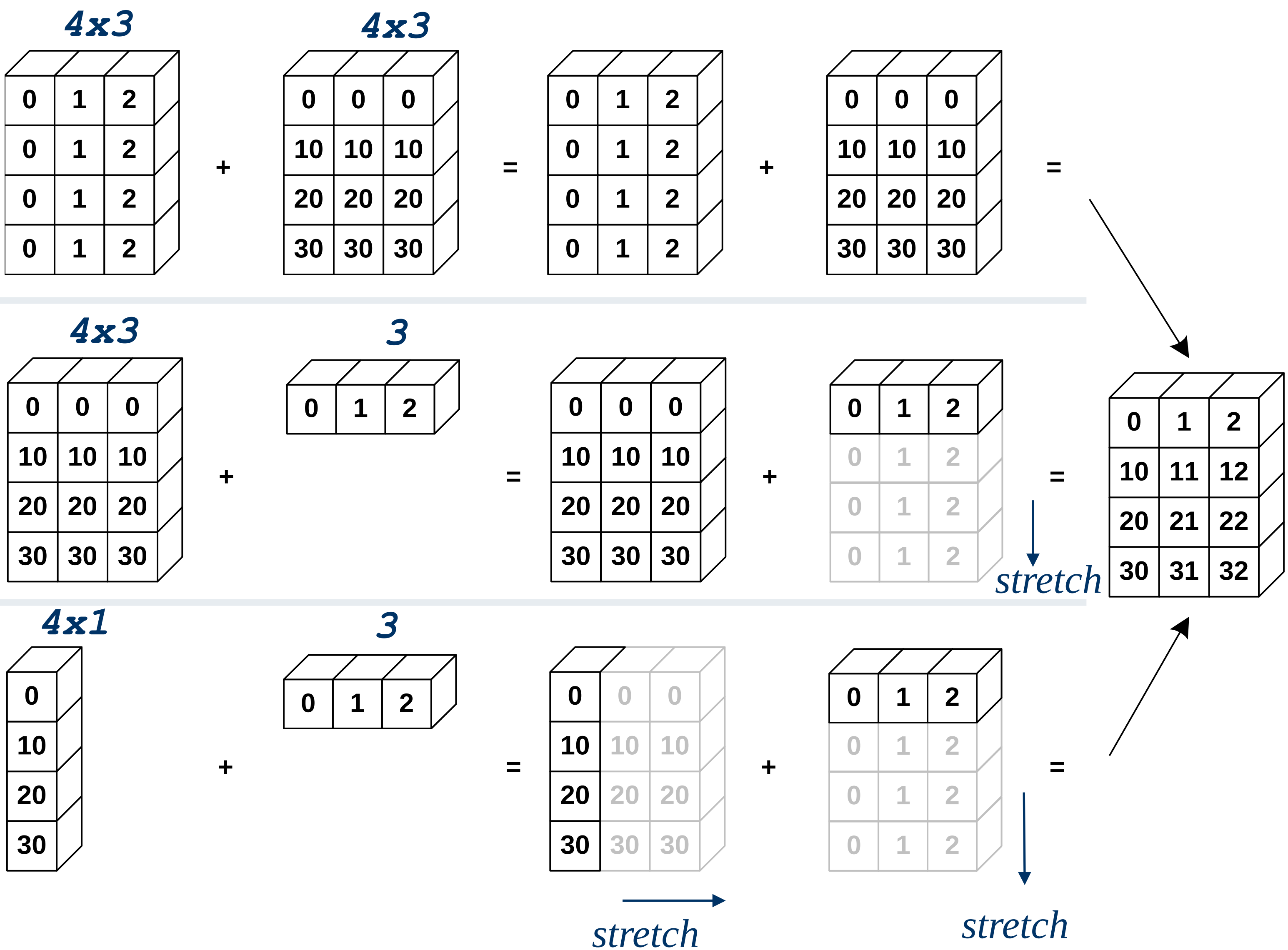
```
>>> x = [1,2,3,4];
>>> y = [[10],[20],[30]]
>>> print N.add(x,y)
[[11 12 13 14]
 [21 22 23 24]
 [31 32 33 34]]
>>> x = array(x)
>>> y = array(y)
>>> print x+y
[[11 12 13 14]
 [21 22 23 24]
 [31 32 33 34]]
```

x has shape (4,) the ufunc sees it as having shape (1,4)

y has shape (3,1)

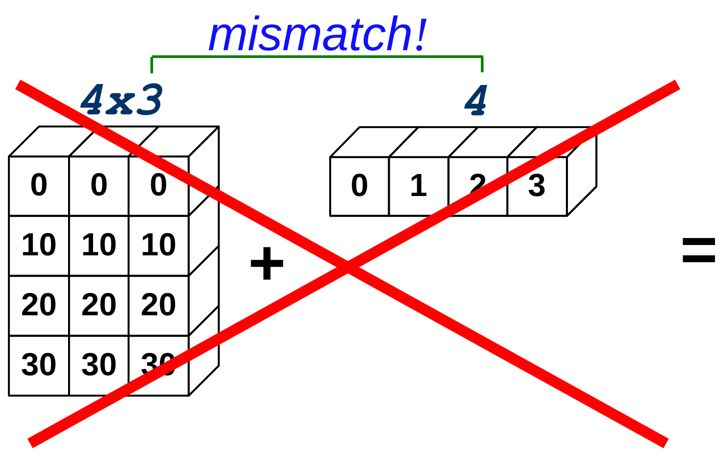
The ufunc result has shape (3,4)

Array Broadcasting



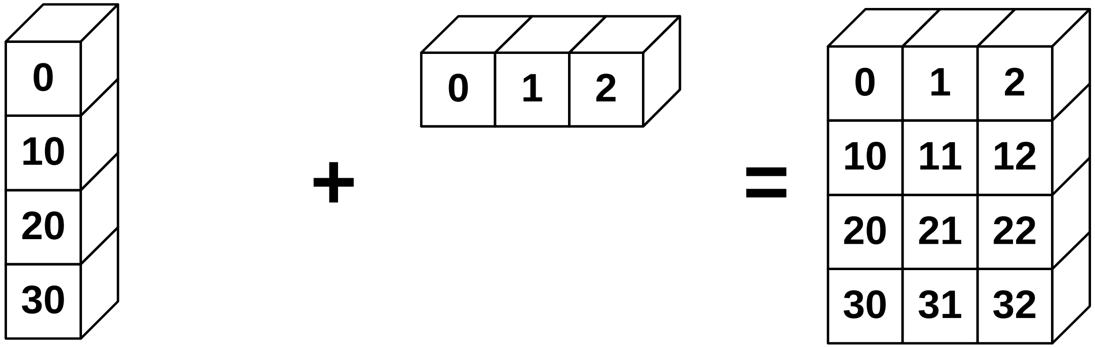
Broadcasting Rules

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)
```

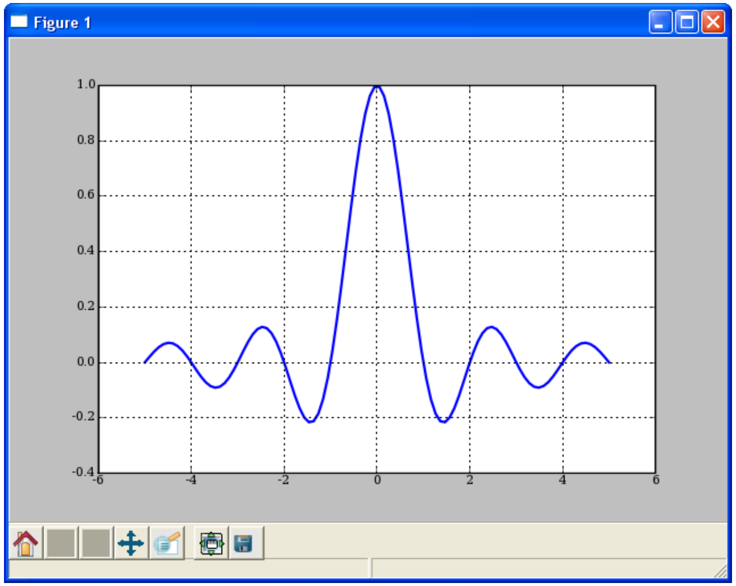
Vectorizing Functions

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

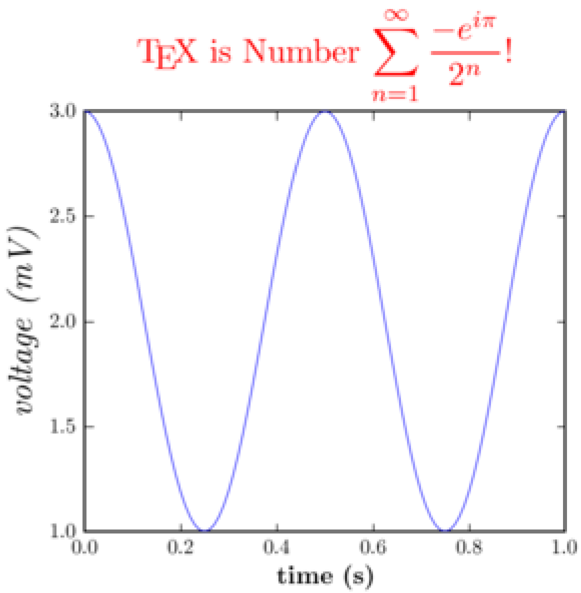
```
>>> from numpy import vectorize
>>> vsinc = vectorize(sinc)
>>> vsinc([1.3,1.5])
array([-0.1981, -0.2122])
```

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.

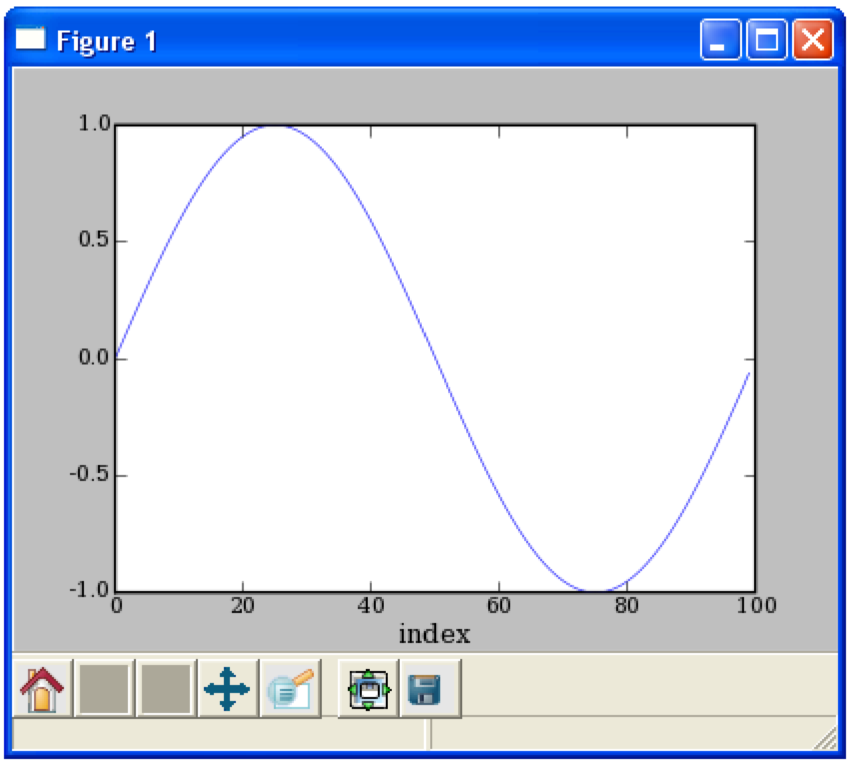
- Chaco for building interactive plotting applications

  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

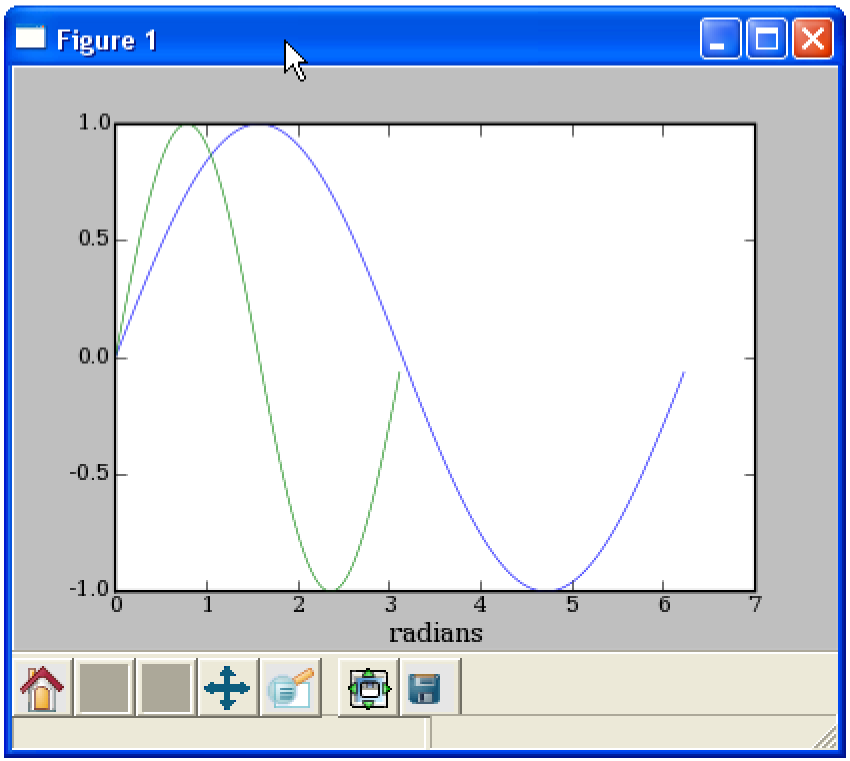
PLOT AGAINST INDICES

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



MULTIPLE DATA SETS

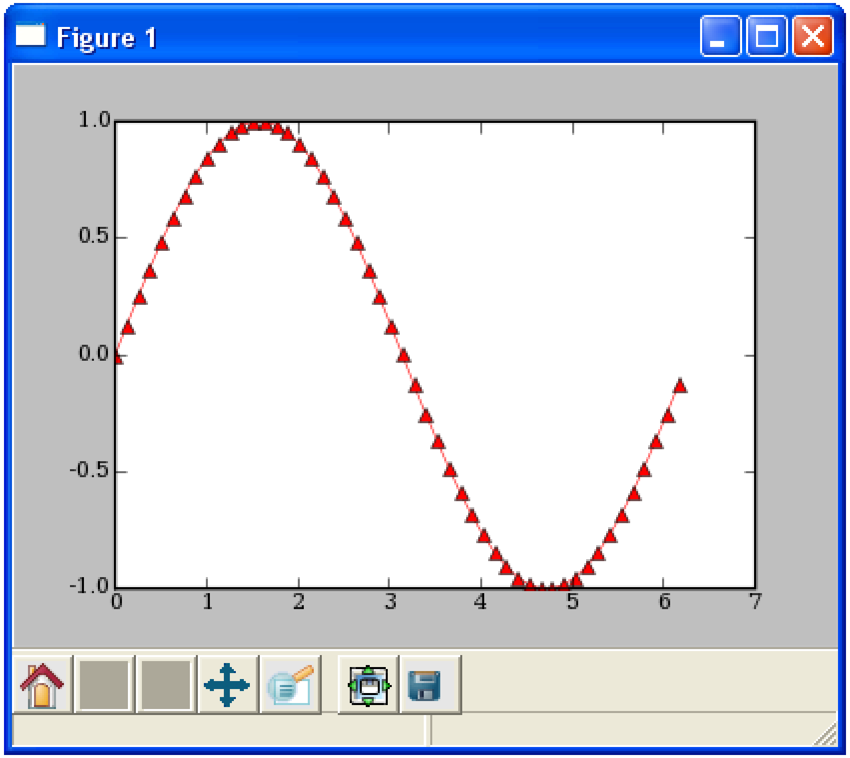
```
>>> plot(x,y,x2,y2)
>>> xlabel('radians')
```



Line Plots

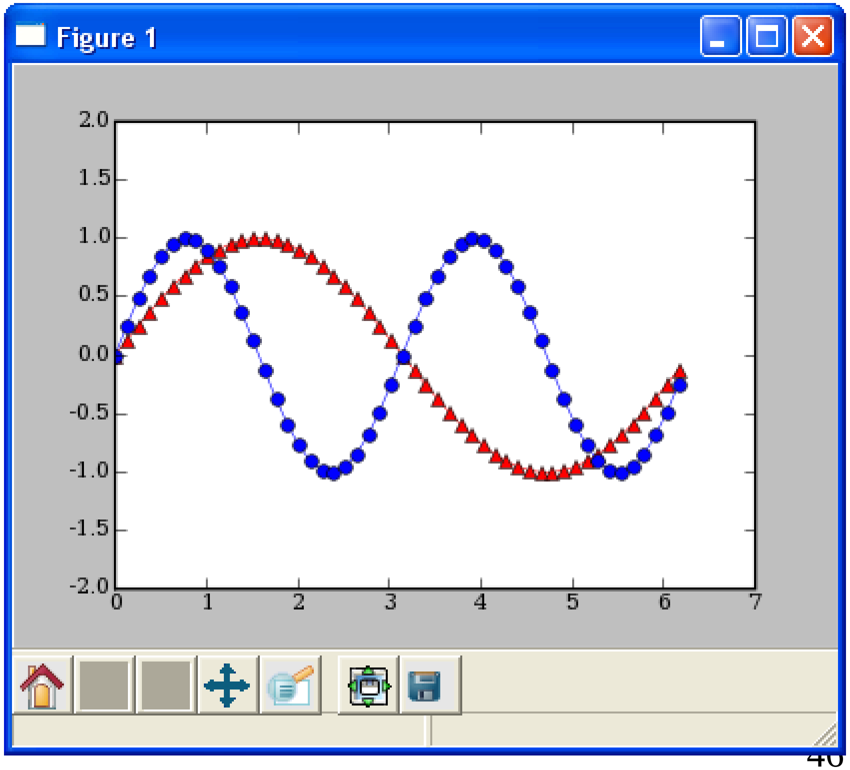
LINE FORMATTING

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



MULTIPLE PLOT GROUPS

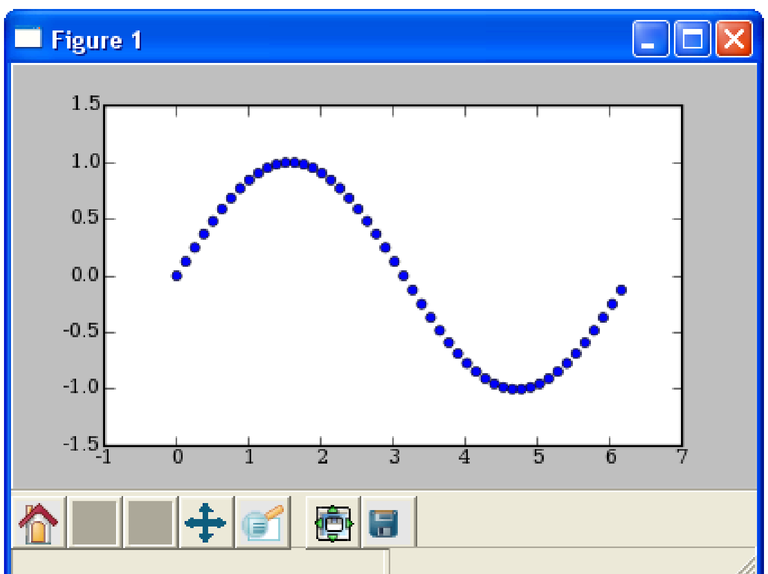
```
>>> plot(x,y1,'b-o', x,y2), r-^')
>>> axis([0,7,-2,2])
```



Scatter Plots

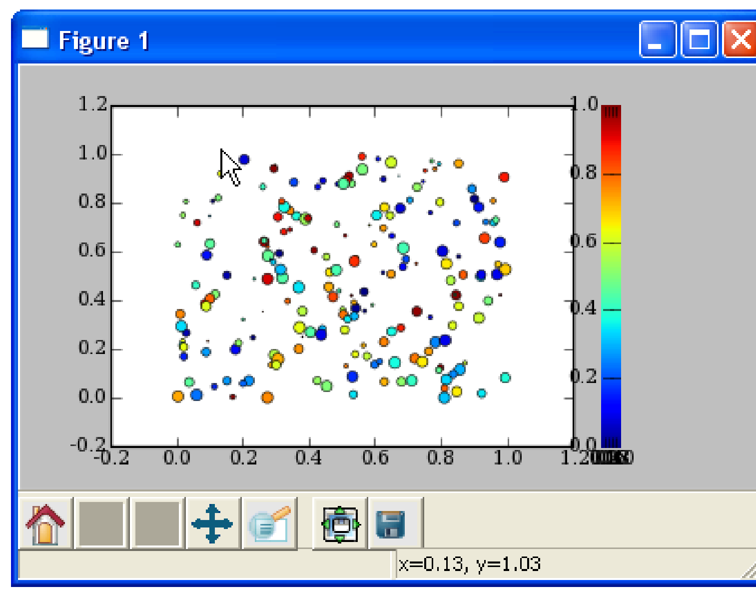
SIMPLE SCATTER PLOT

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



COLORMAPPED SCATTER

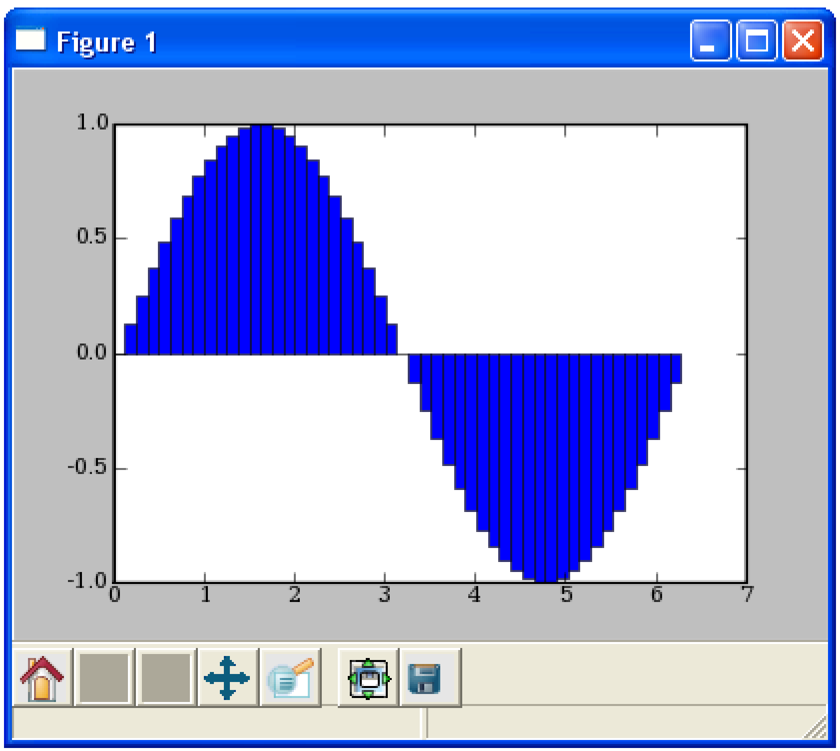
```
# marker size/color set with data
>>> x = rand(200)
>>> y = rand(200)
>>> size = rand(200)*30
>>> color = rand(200)
>>> scatter(x, y, size, color)
>>> colorbar()
```



Bar Plots

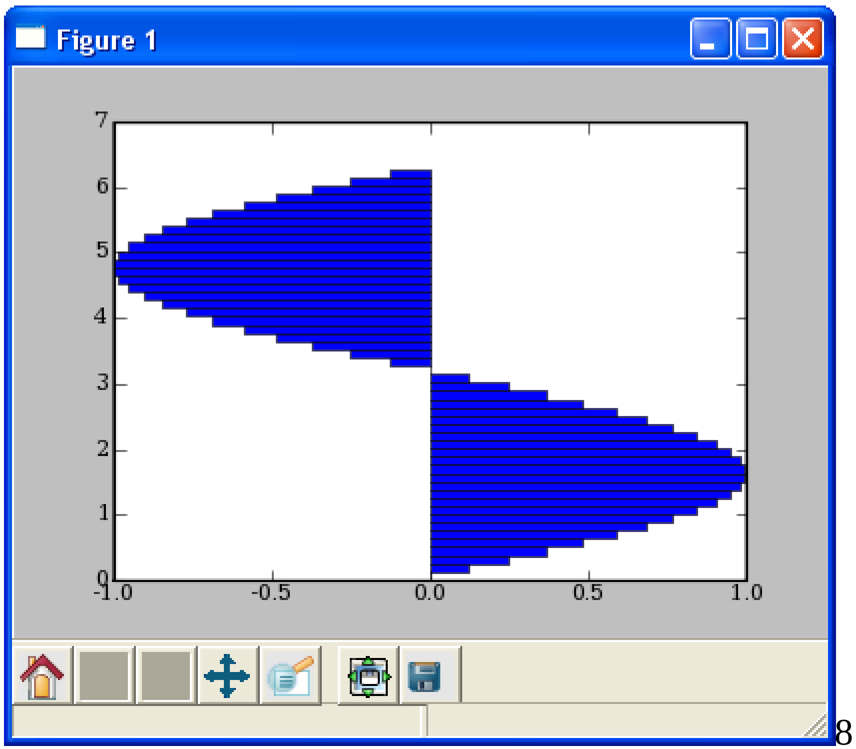
BAR PLOT

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



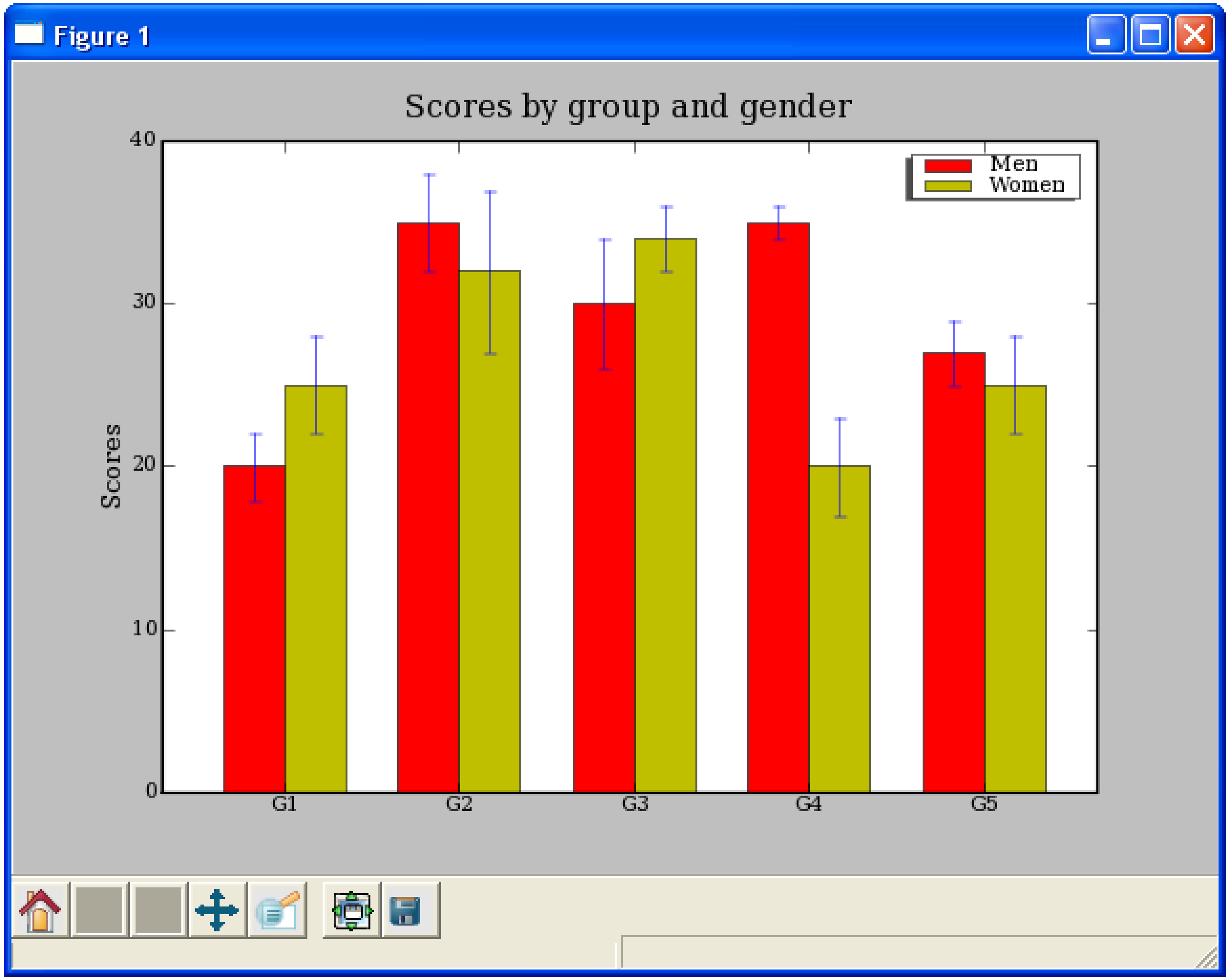
HORIZONTAL BAR PLOT

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



Bar Plots

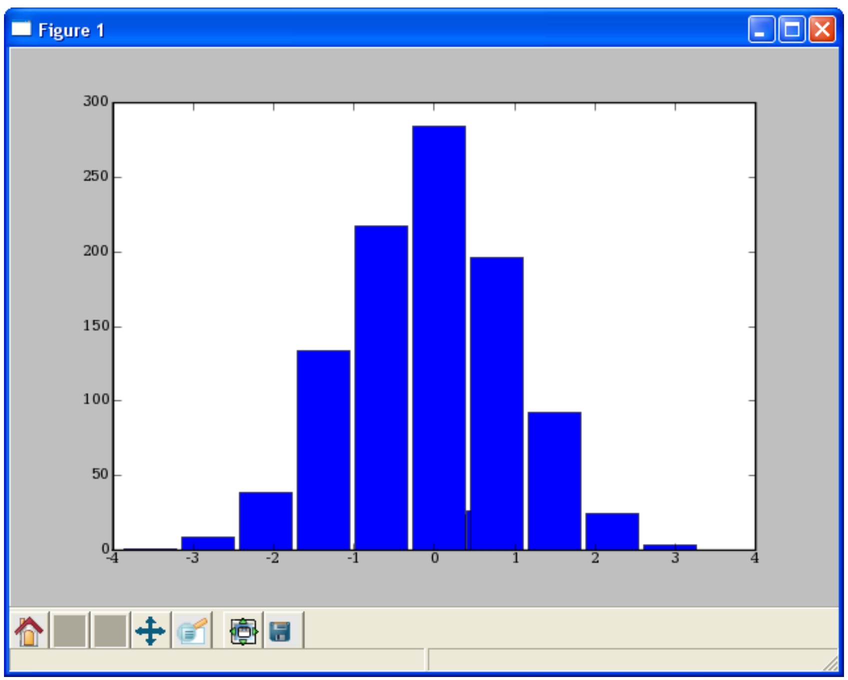
DEMO/MATPLOTLIB_PLOTTING/BARCHART_DEMO.PY



HISTOGRAMS

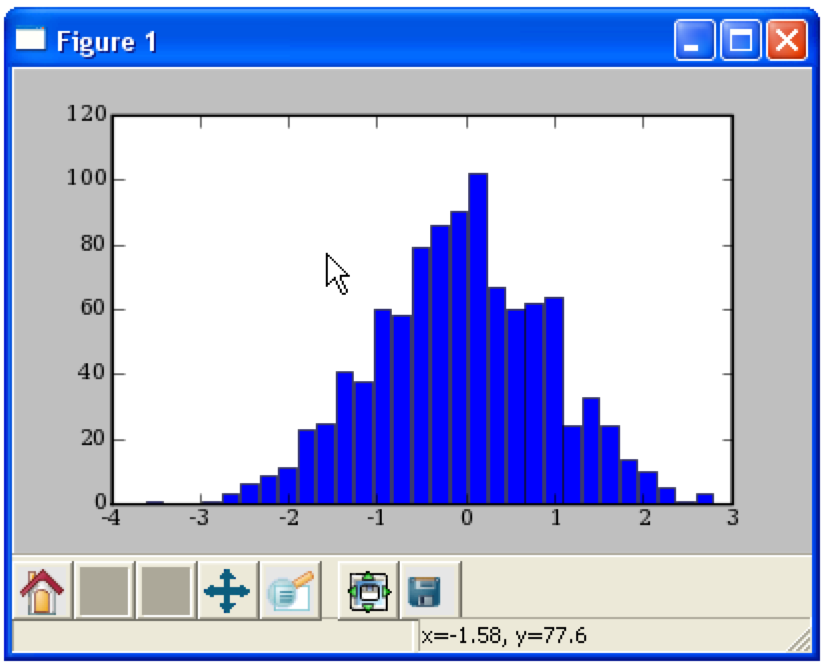
HISTOGRAM

```
# 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()
```

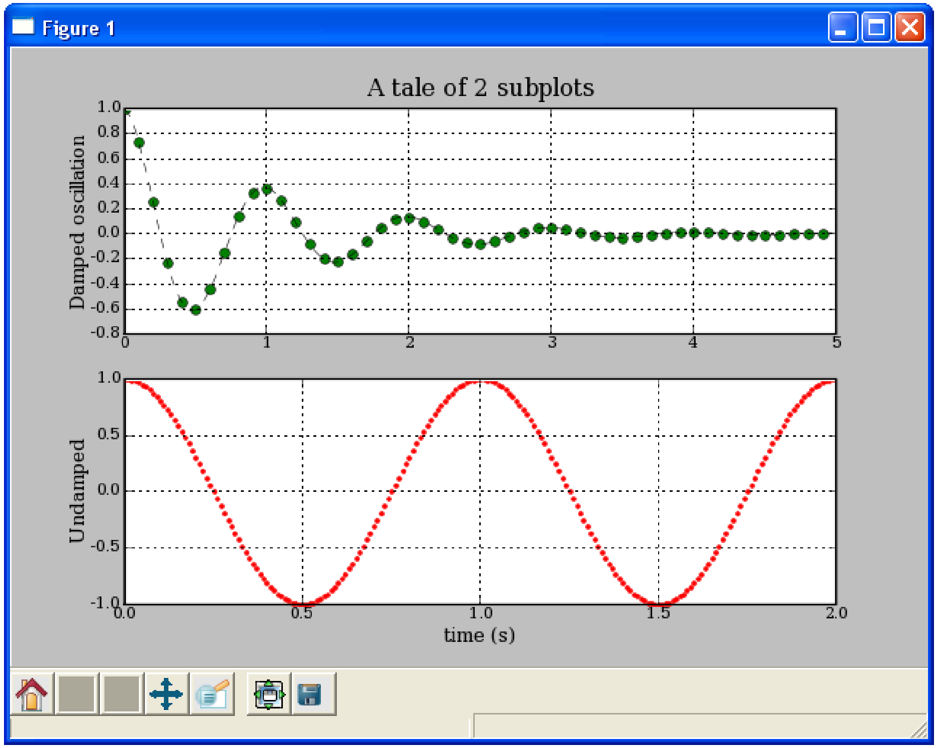
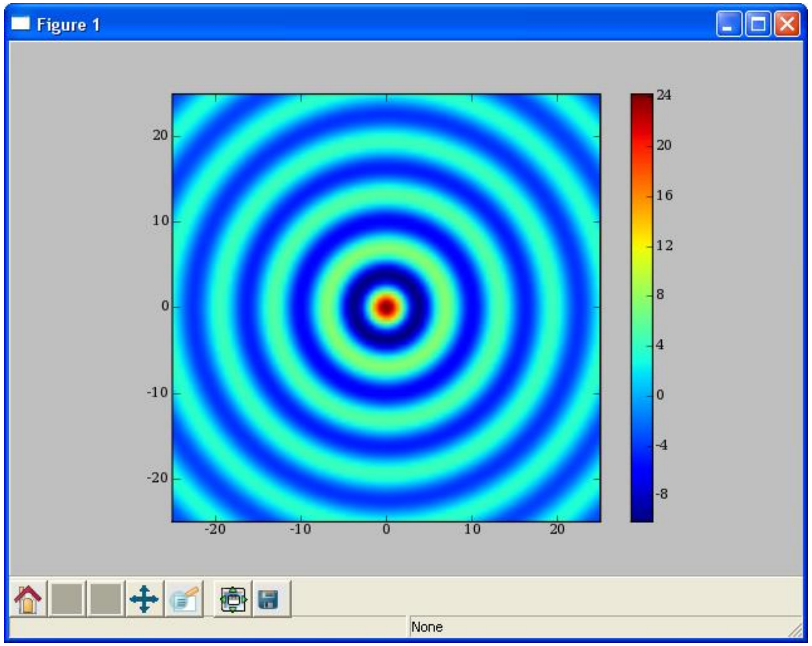


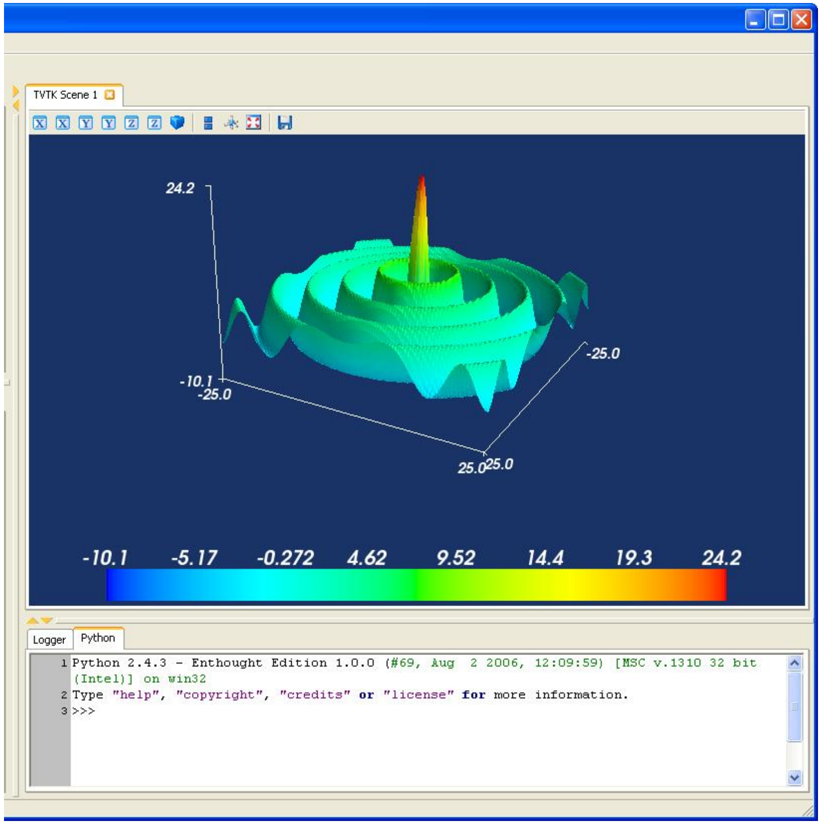
Image Display

```
# 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

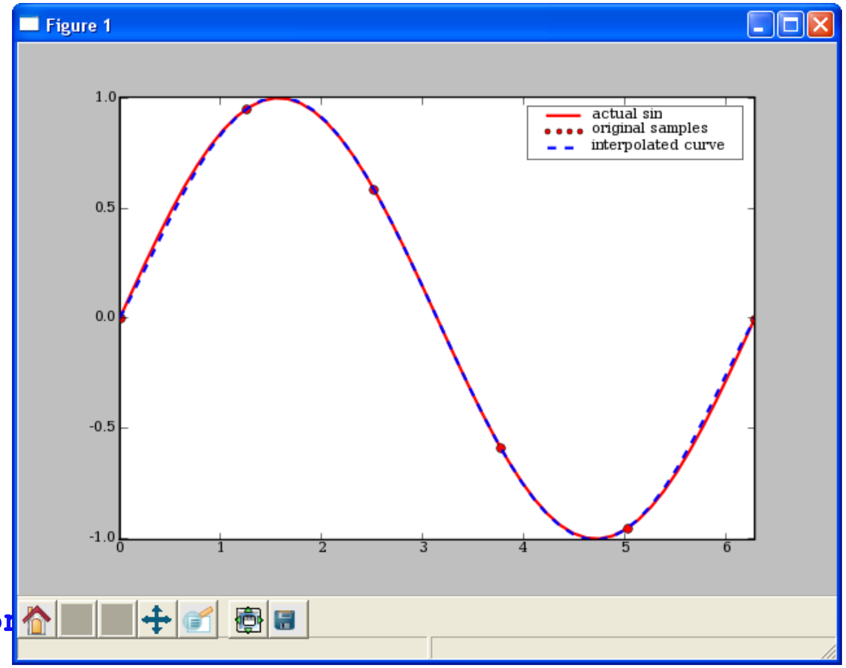
- Available at www.scipy.org
- Open Source BSD Style License
- Over 30 svn “committers” to the project

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

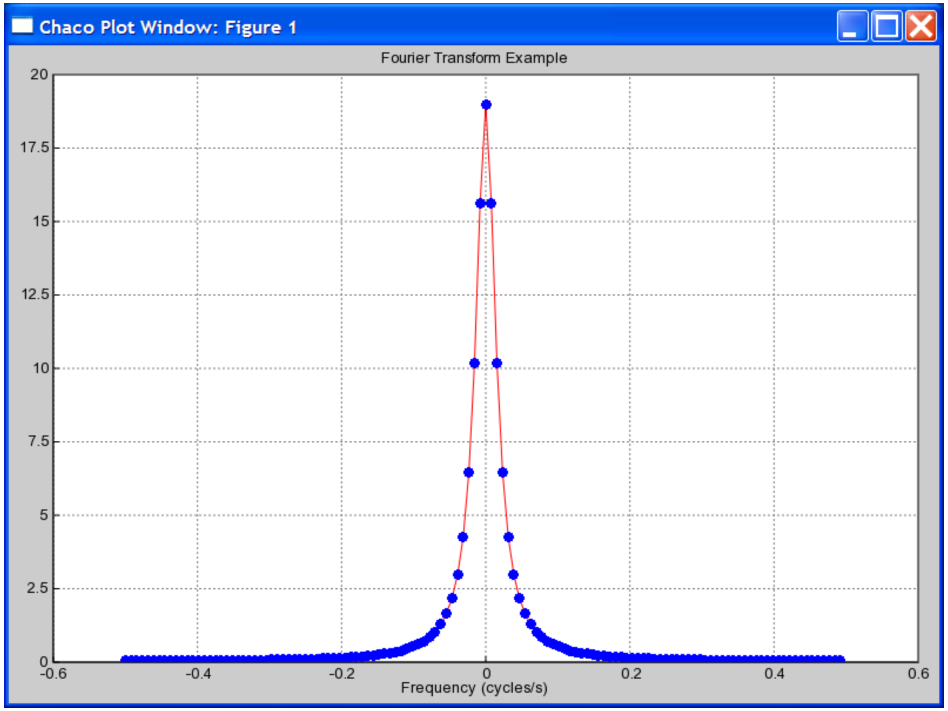
```
# demo/interpolate/spline.py
from scipy.interpolate import interp1d
from pylab import plot, axis, legend
from numpy import linspace

# 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 interpolatio
# kind=2 or
spline_fit = interp1d(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

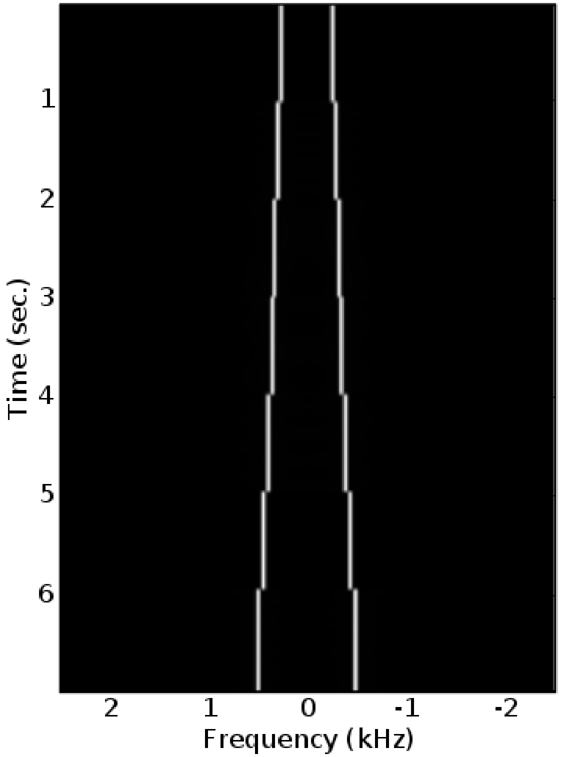
```
>>> n = fftfreq(128)*128
>>> f = fftfreq(128)
>>> ome = 2*pi*f
>>> x = (0.9)**abs(n)
>>> X = fft(x)
>>> z = exp(1j*ome)
>>> Xexact = (0.9**2 - 1)/0.9*z /    \
...             (z-0.9) / (z-1/0.9)
>>> f = fftshift(f)
>>> plot(f, fftshift(X.real),'r-',
...       f, fftshift(Xexact.real),'bo')
>>> title('Fourier 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

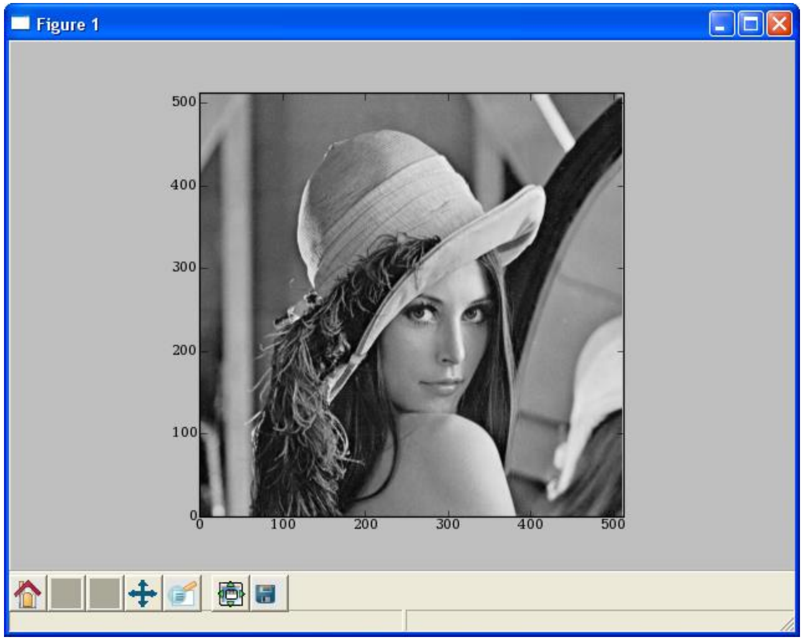
Impulse and step responses

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

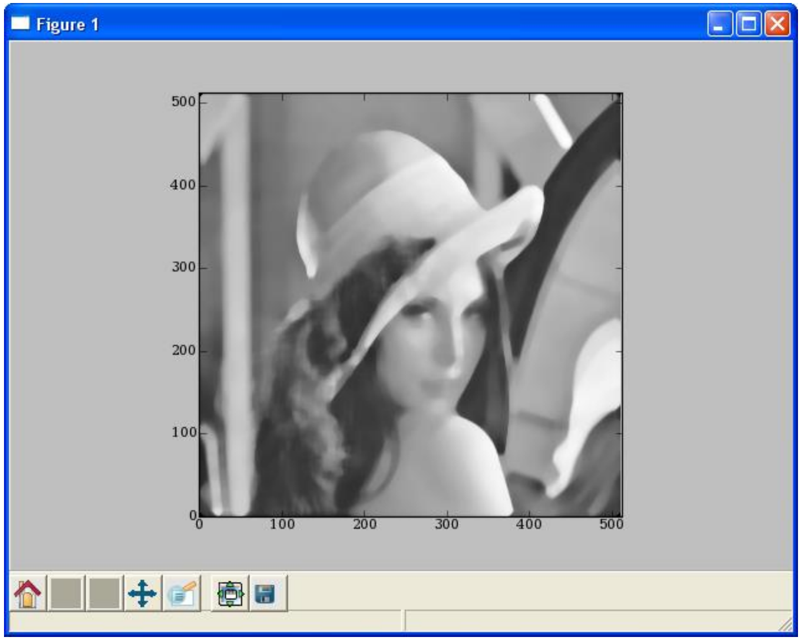
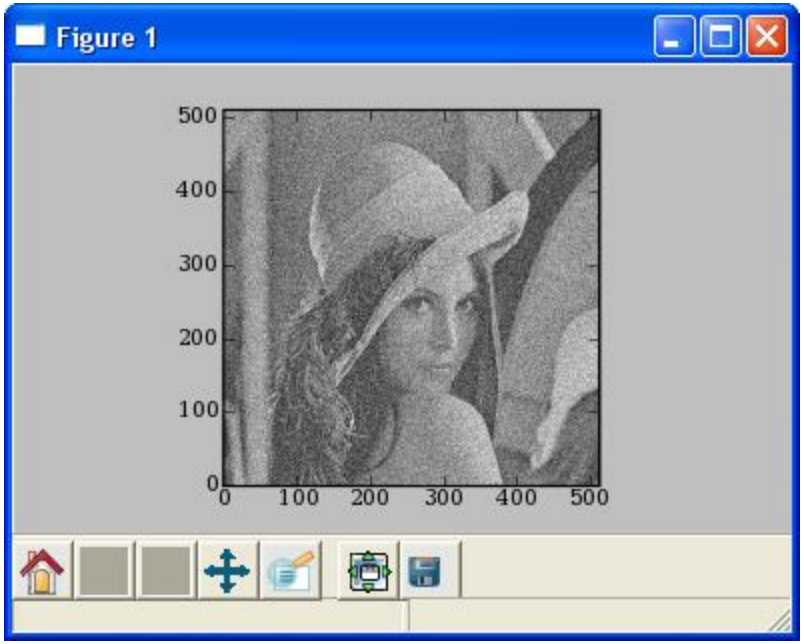


Image Processing

```
# 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

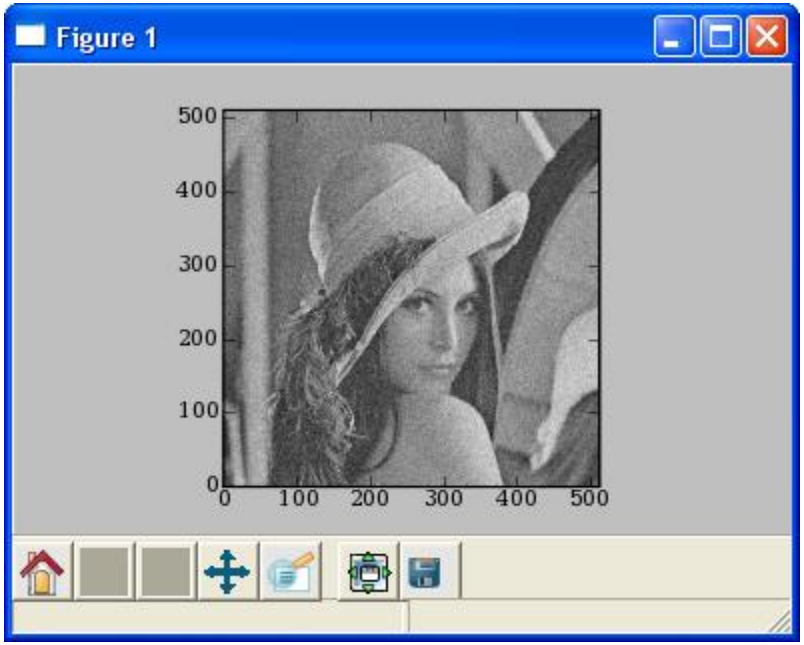
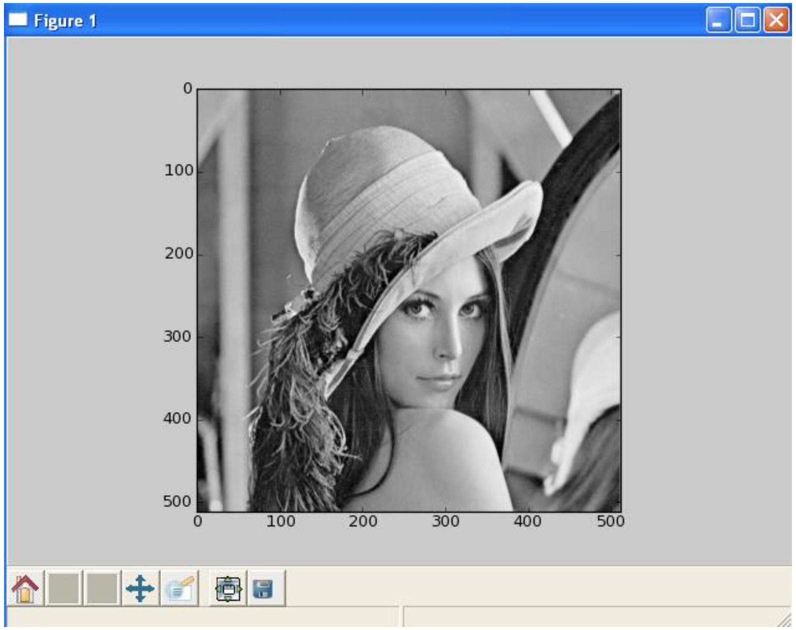


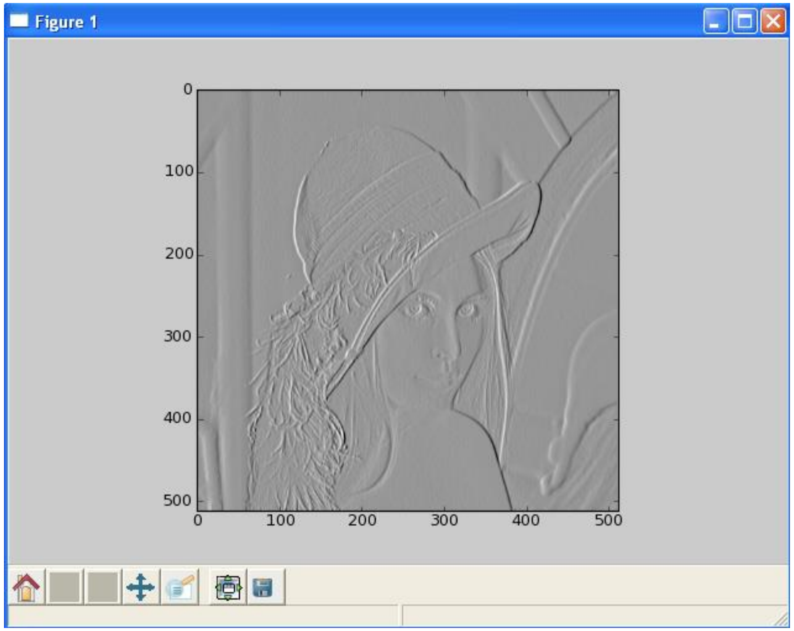
Image Processing

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

NOISY IMAGE



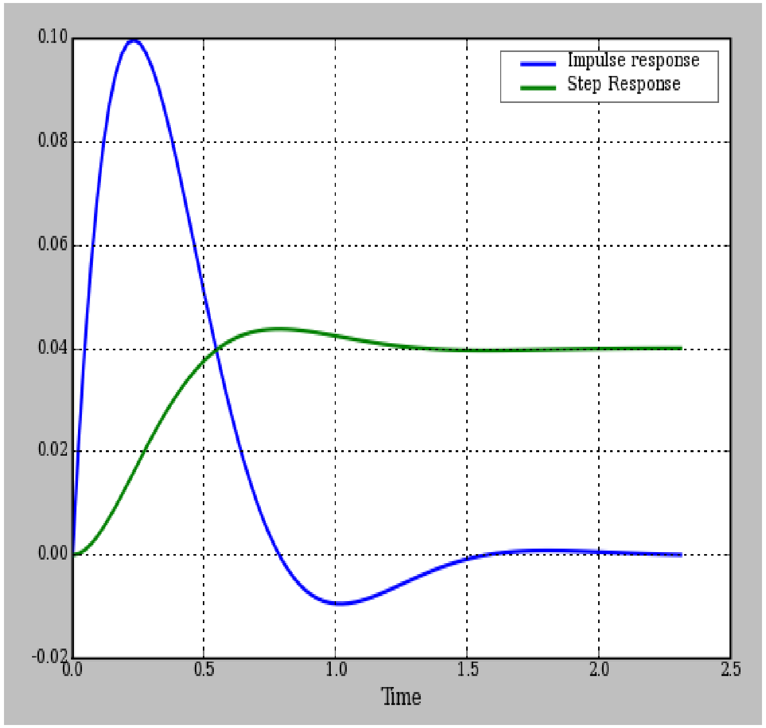
FILTERED IMAGE



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)

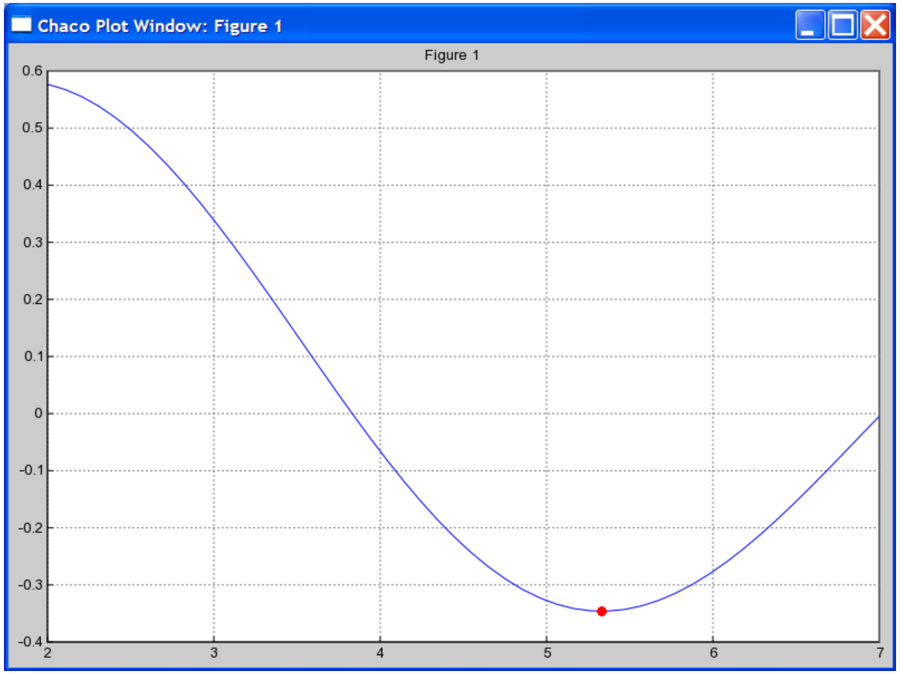
- **Root finding**

  `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

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

```
>>> 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 0.0805299282074 seconds
Solution: [ 1.  1.  1.  1.  1.]
Function value: 2.67775760157e-15
Avg. Error: 1.5323906899e-08
```

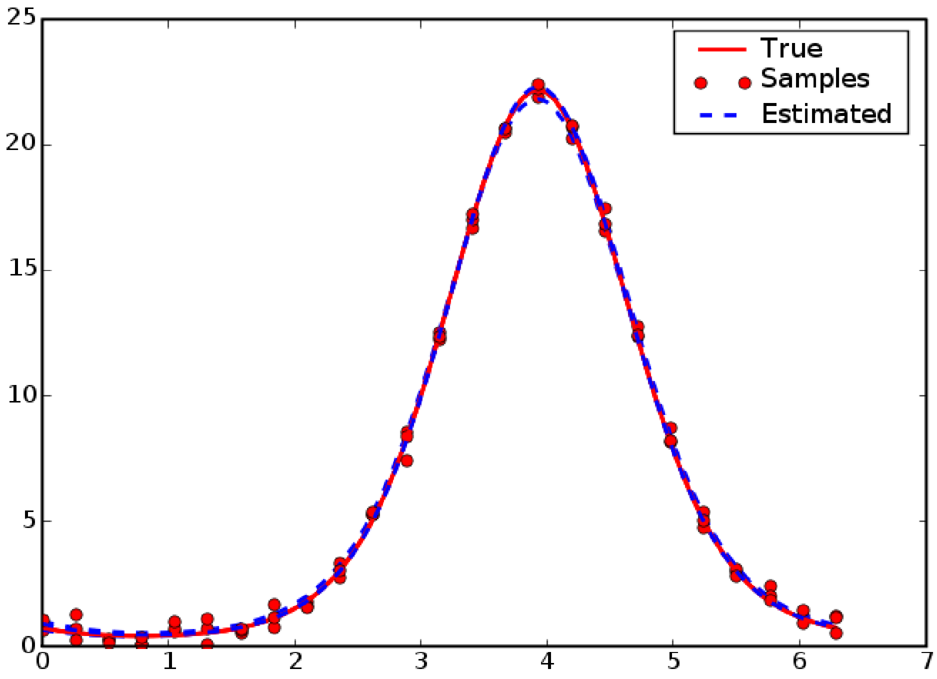
USING DERIVATIVE

```
>>> 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: 1.3739103475e-18
Avg. Error: 1.13246034772e-10
```

Optimization

EXAMPLE: Non-linear least-squares data fitting

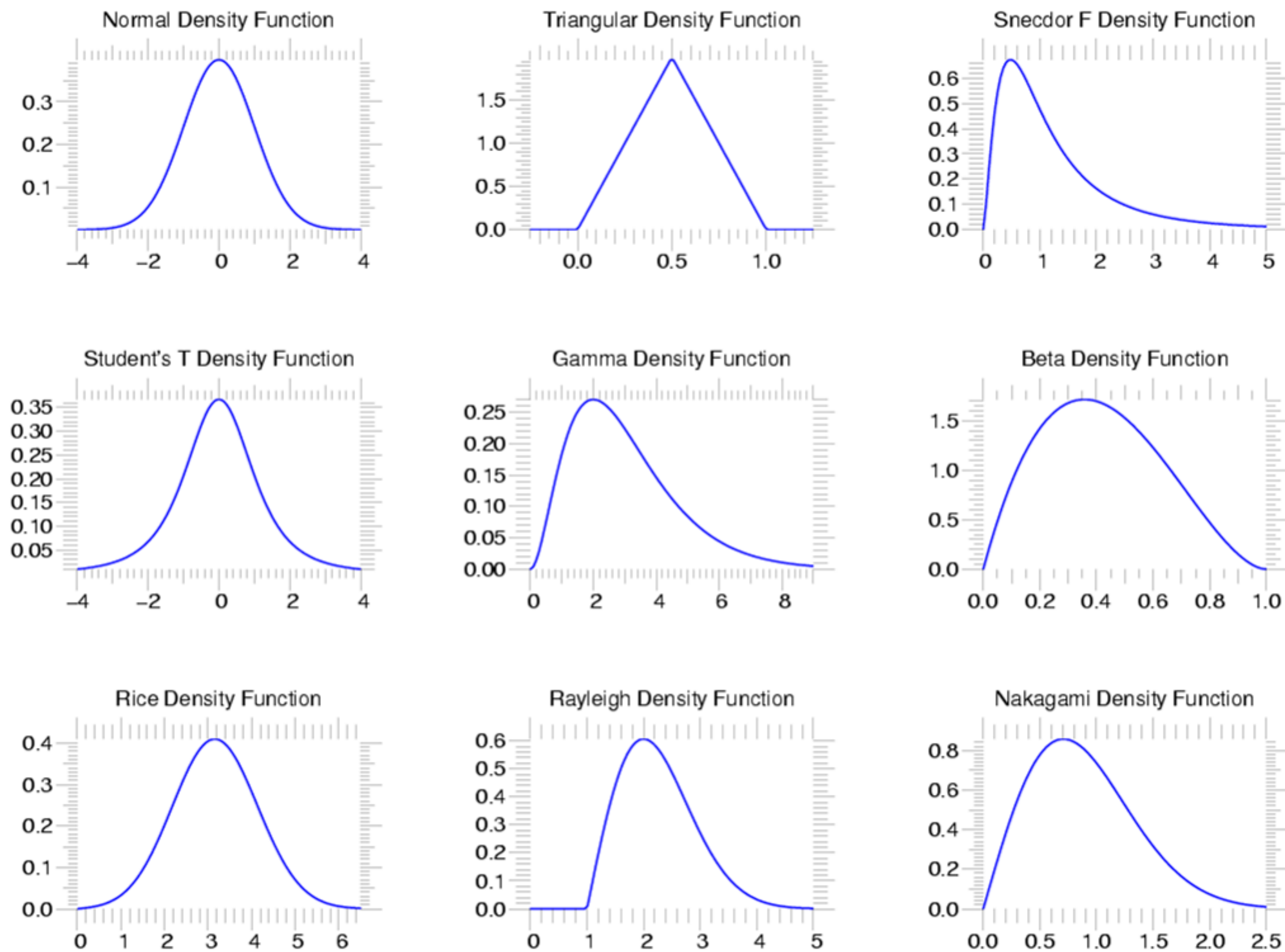
```
# fit data-points to a curve
# demo/data_fitting/datafit.py
>>> from numpy.random import randn
>>> from numpy import exp, sin, pi
>>> from numpy import linspace
>>> from scipy.optimize import leastsq
>>> def func(x,A,a,f,phi):
        return A*exp(-a*sin(f*x+pi/4))
>>> def errfunc(params, x, data):
        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`

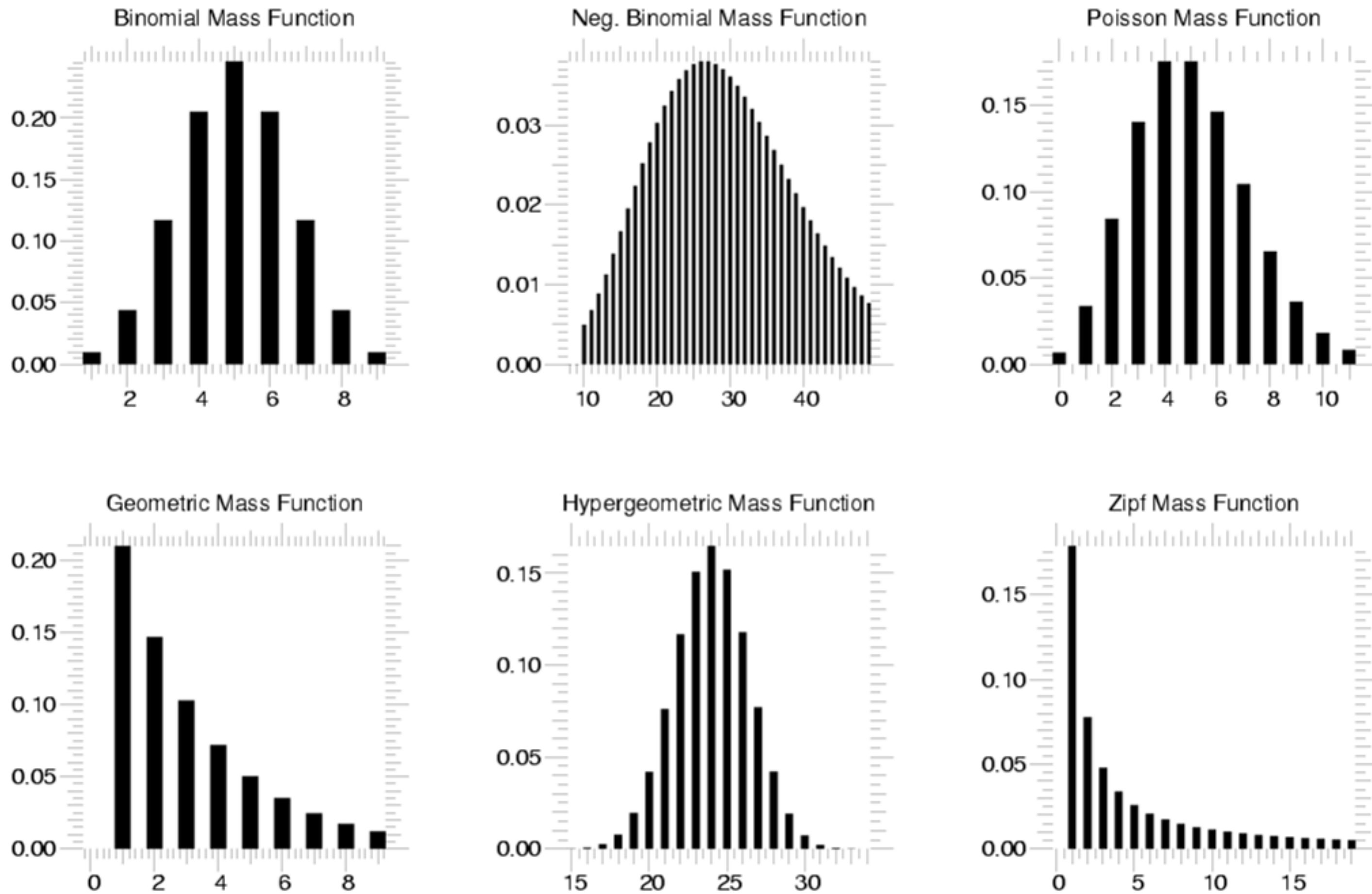
`ppf`

`stats`

Statistics

scipy.stats --- Discrete Distributions

10 standard discrete distributions (plus any arbitrary finite RV)



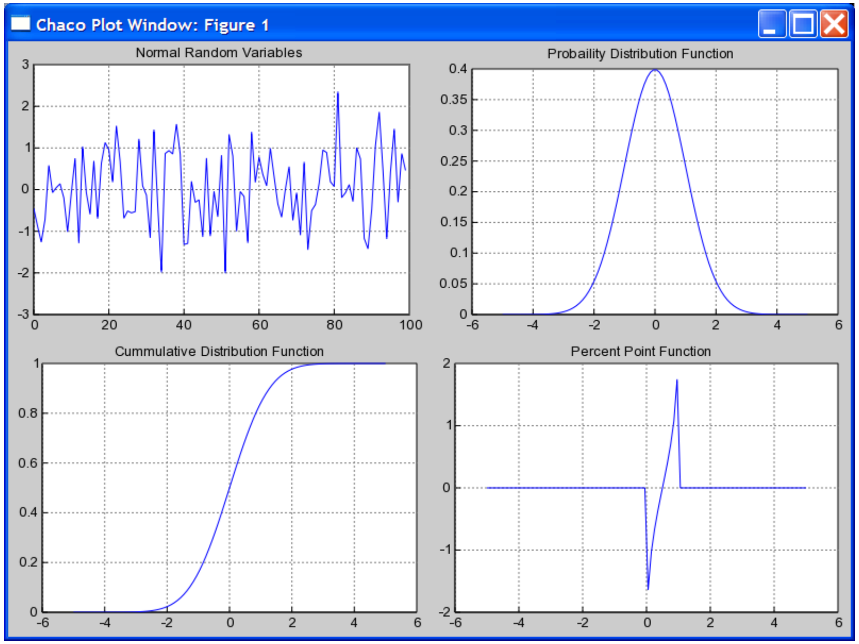
METHODS

```
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`

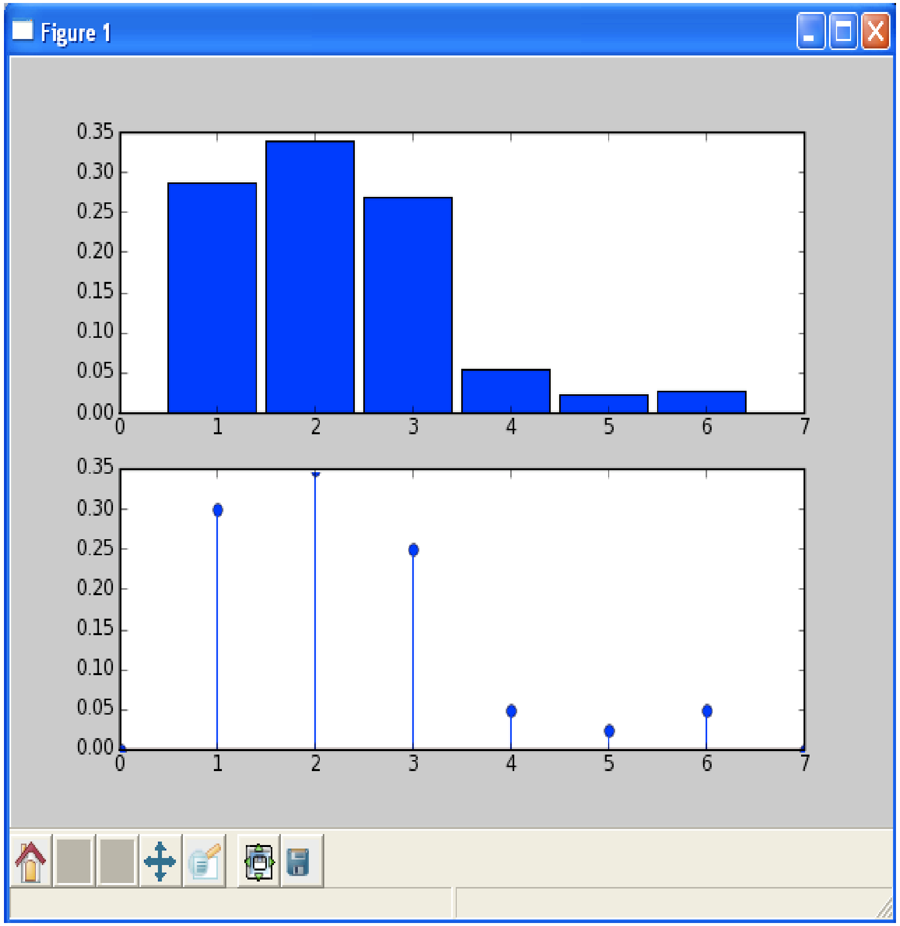
scipy.stats.bayes_mvs --- Bayesian mean, variance, and std.

```
# 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

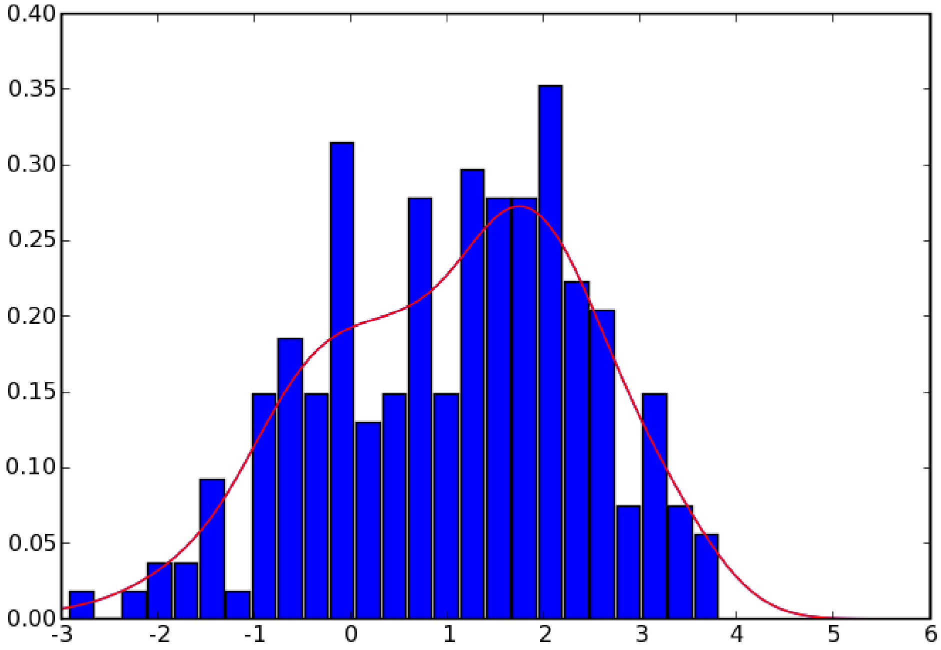
```
# Create a loaded dice.
>>> from scipy.stats import rv_discrete
>>> xk = [1,2,3,4,5,6]
>>> pk = [0.3,0.35,0.25,0.05,
          0.025,0.025]
>>> new = rv_discrete(name='loaded',
                      values=(xk,pk))

# 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))
```



Statistics

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)

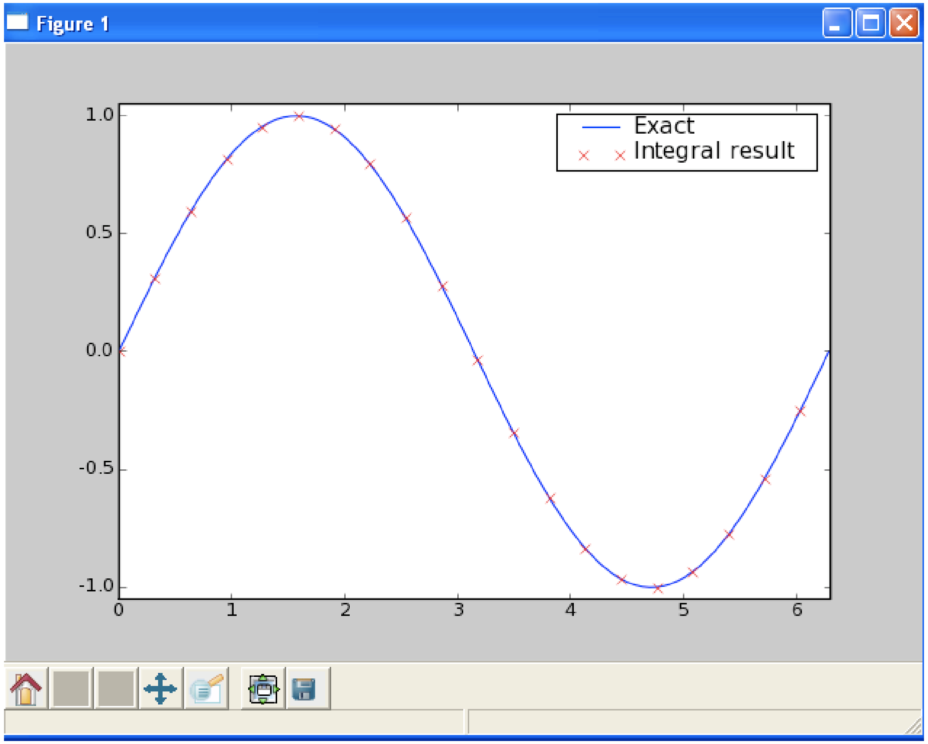
- **Arbitrary callable function**

  `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), `integrate.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

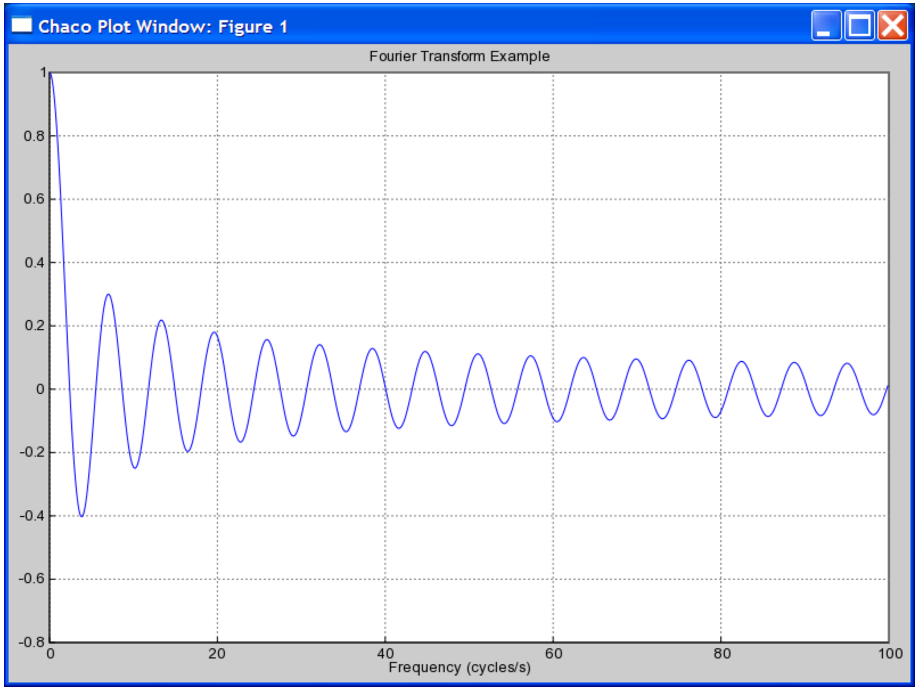
scipy.special

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)
```

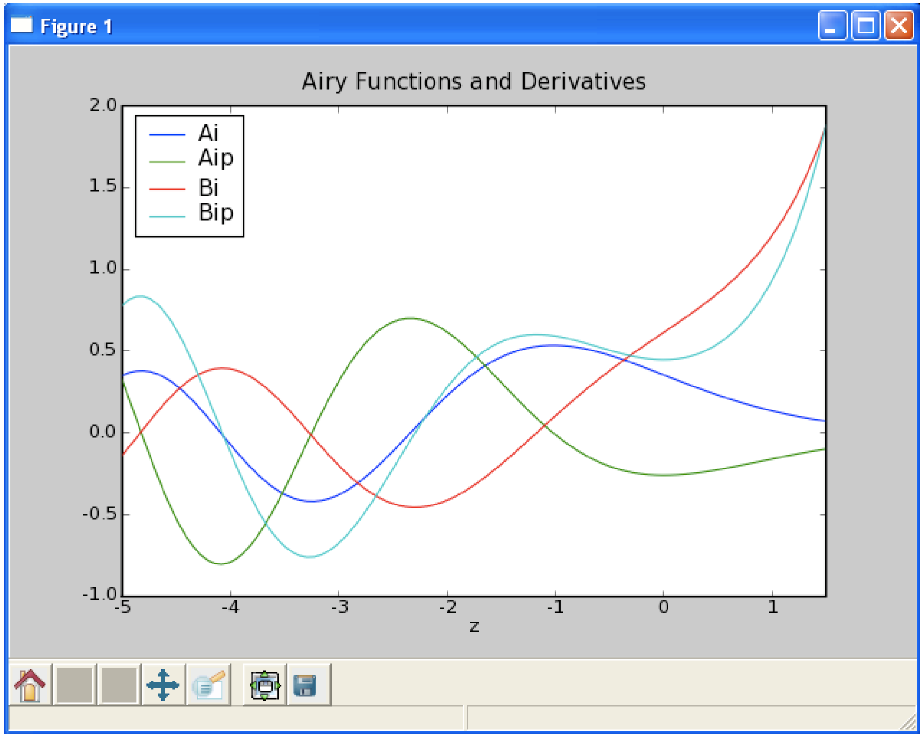


Special Functions

scipy.special

AIRY FUNCTIONS EXAMPLE

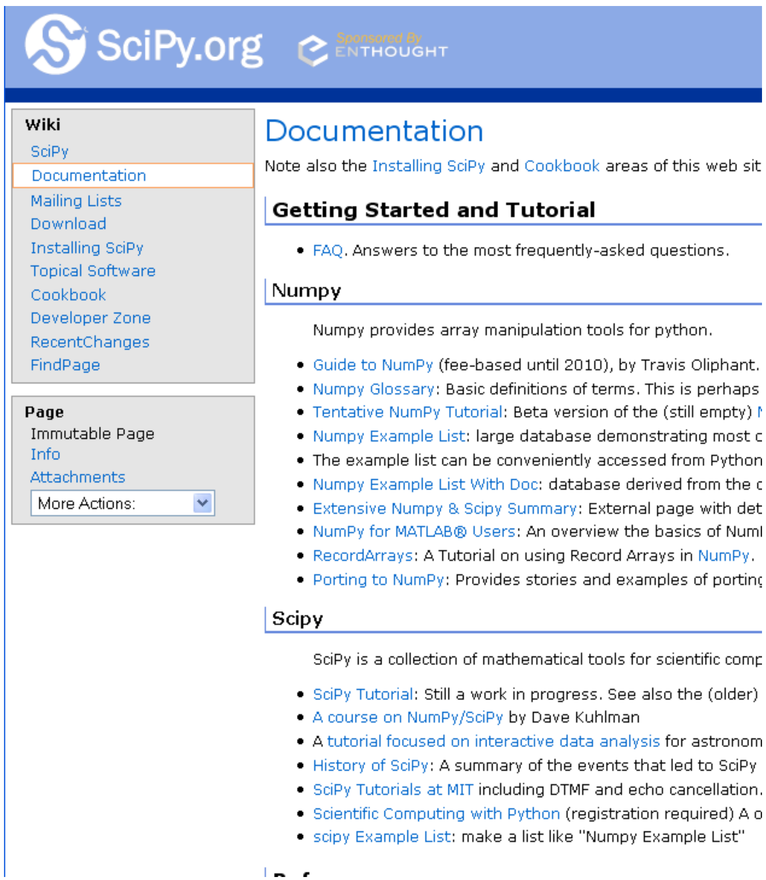
```
>>> z = r_[-5:1.5:100j]
>>> vals = special.airy(z)
>>> plot(z,array(vals).T)
>>> legend(['Ai', 'Aip',
            'Bi','Bip'])
>>> xlabel('z')
>>> title('Airy Functions and
  Derivatives')
```



Helpful Sites

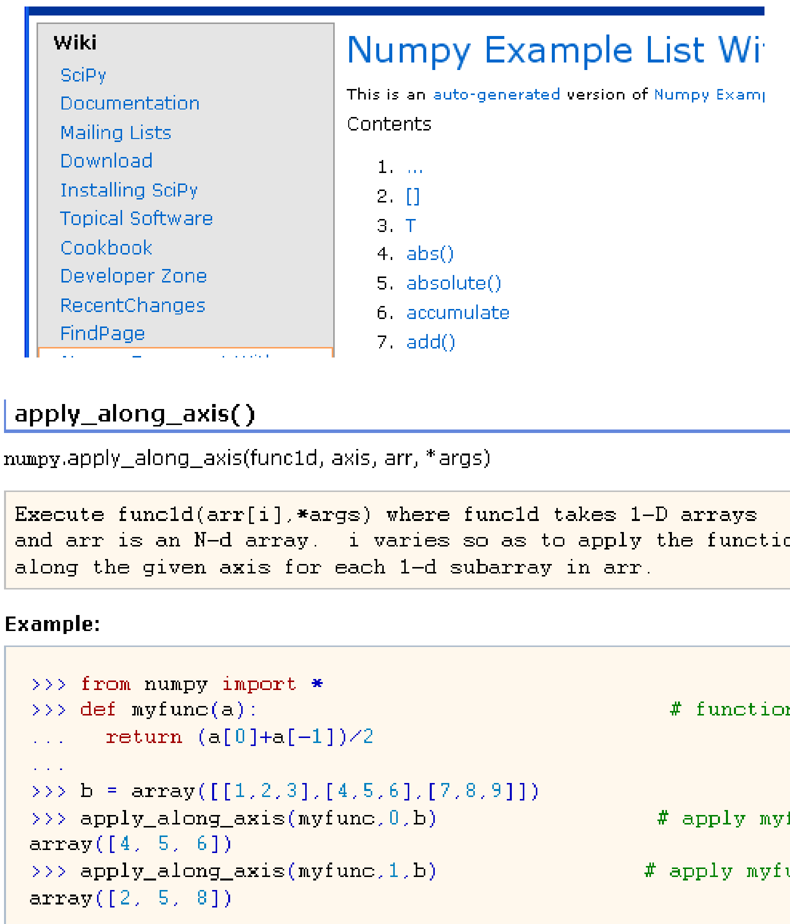
SCIPY DOCUMENTATION PAGE

http://www.scipy.org/Documentation



NUMPY EXAMPLES

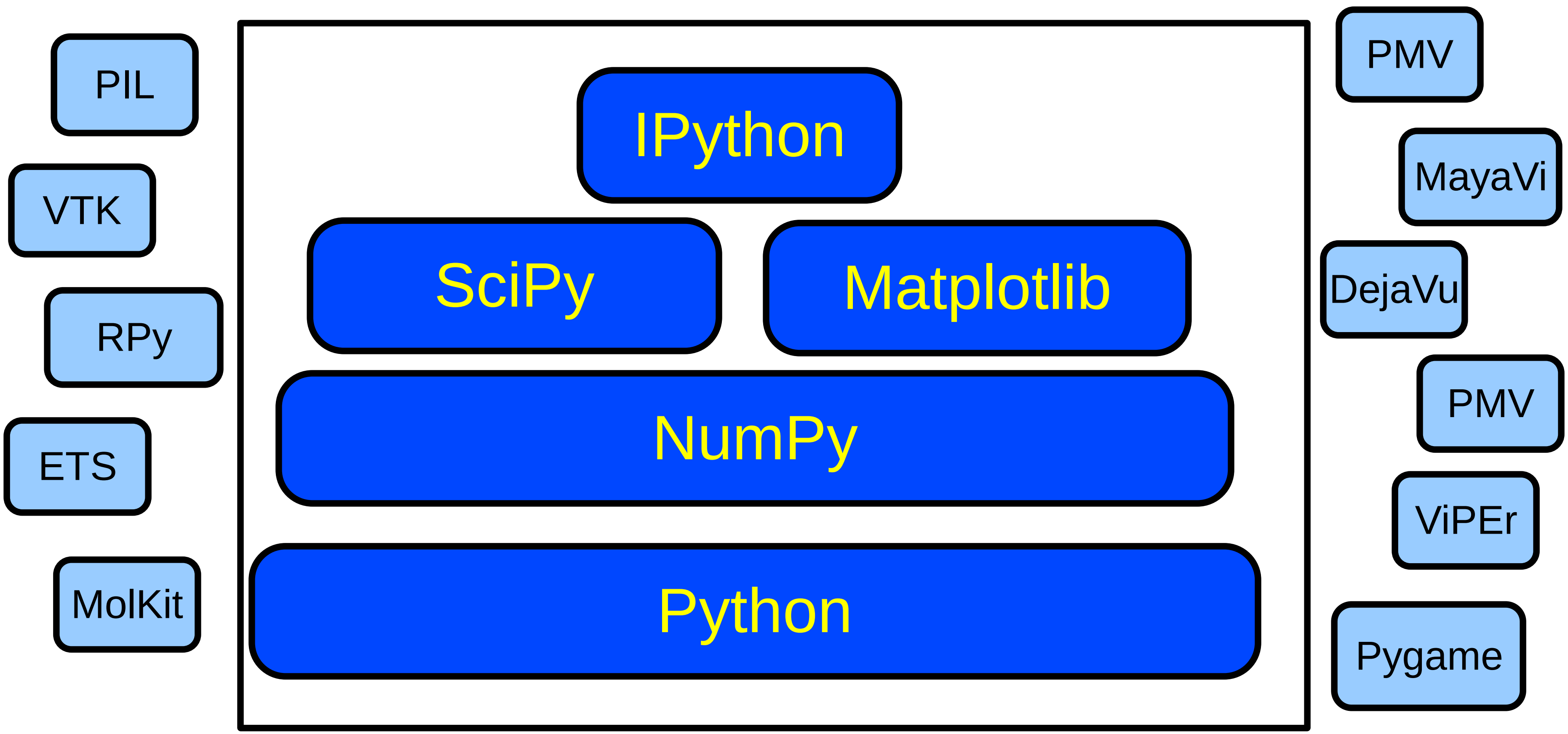
http://www.scipy.org/Numpy_Example_List_With_Doc



PyLab

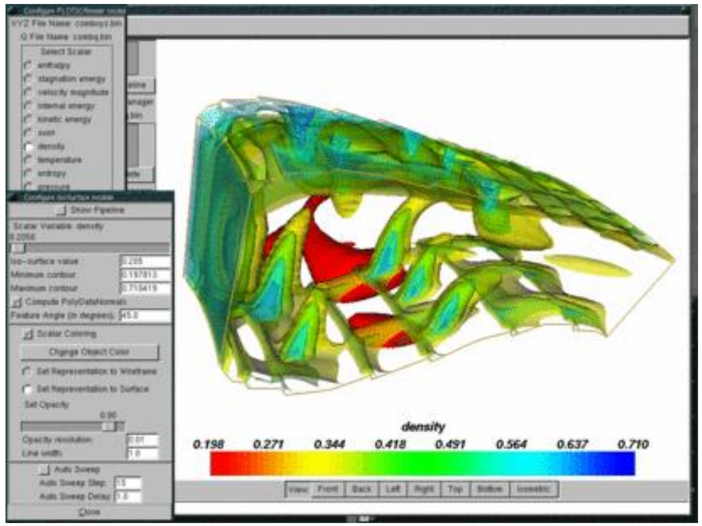
Sometimes the union of the 5 packages is called pylab: ipython -pylab.

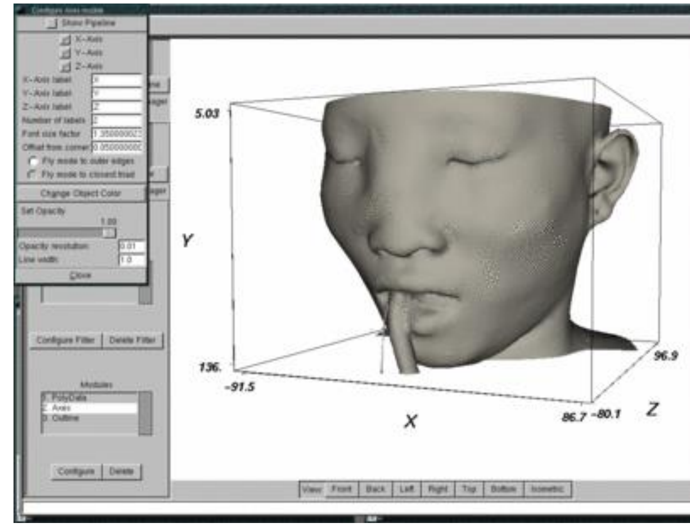
Literally 1000's more modules/packages for Python

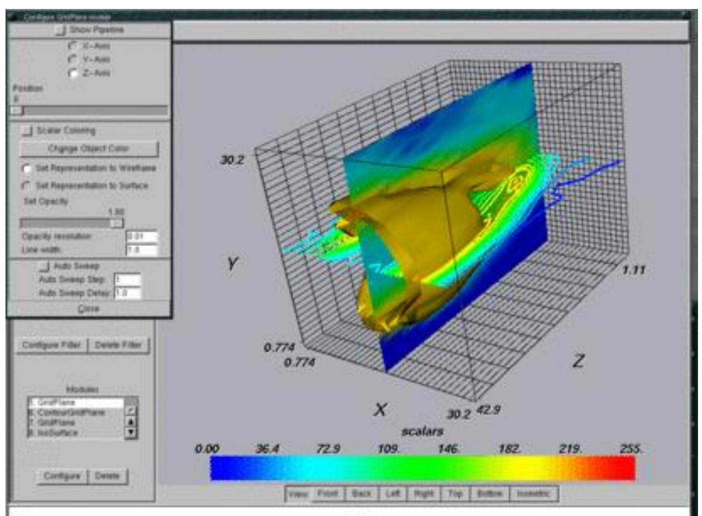


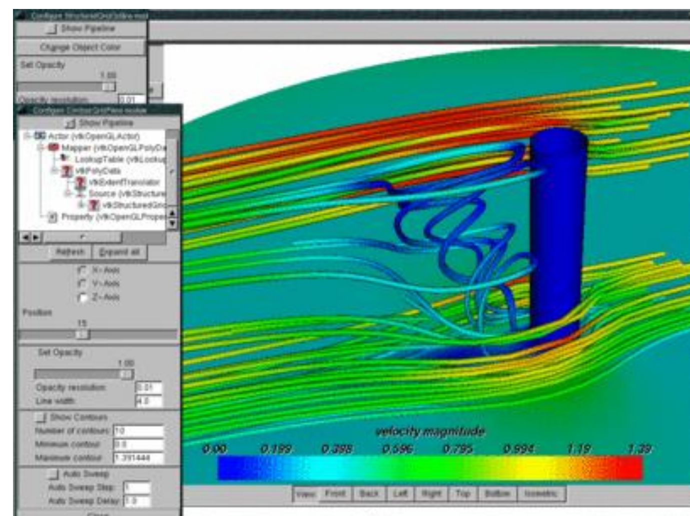
Extras: MayaVi

Prabu Ramanchandran



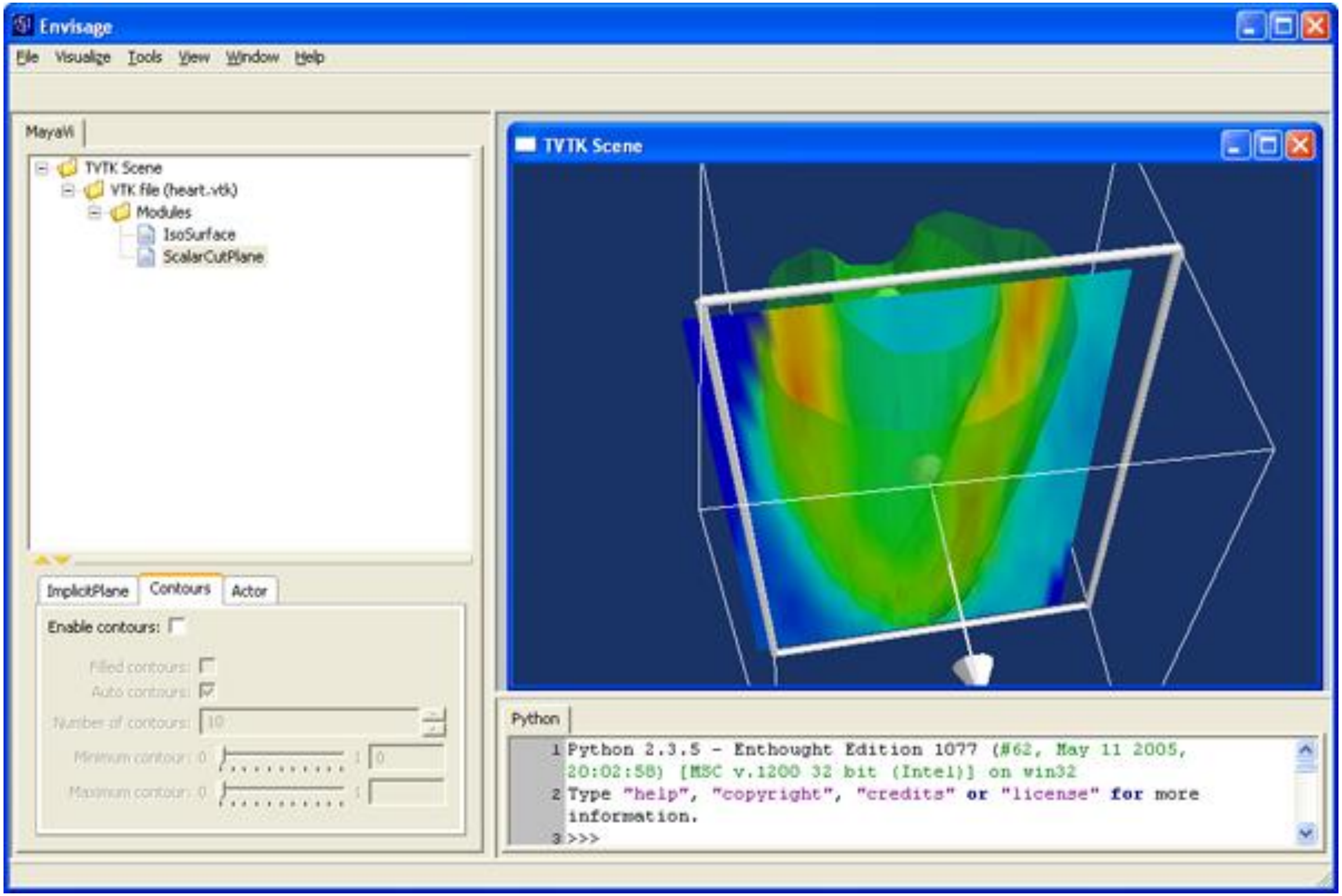






Extras: Enthought Tool Suite

http://www.enthought.com http://code.enthought.com



You can get involved

- New algorithms in SciPy
- Documentation improvements
- Community interaction (mailing lists and bug tracker)
- SciPy conference 2008 at Caltech in Pasadena, CA (August 19-24)
- http://www.scipy.org