Python Programming for Data Processing and Climate Analysis

Jules Kouatchou and Hamid Oloso

Jules.Kouatchou@nasa.gov and Amidu.o.Oloso@nasa.gov

Goddard Space Flight Center
Software System Support Office
Code 610.3

March 11, 2013

Training Objectives

We want to introduce:

- Basic concepts of Python programming
- Array manipulations
- Handling of files
- 2D visualization
- EOFs

Obtaining the Material

Slides for this session of the training are available from:

https://modelingguru.nasa.gov/docs/DOC-2322

You can obtain materials presented here on *discover* at

/discover/nobackup/jkouatch/pythonTrainingGSFC.tar.gz

After you untar the above file, you will obtain the directory *pythonTrainingGSFC/* that contains:

```
Examples/
Slides/
```

Settings on *discover*

We installed a Python distribution. To use it, you need to load the modules:

```
module load other/comp/gcc-4.5-sp1
module load lib/mkl-10.1.2.024
module load other/SIVO-PyD/spd_1.7.0_gcc-4.5-sp1
```

Recall from the Last Session-1

Numbers:

Integer	1234, -24, 0
Unlimited precision integers	999999999999999L
Floating	1.23, 3.14e-10, 4E210, 4.0e+210
Oct and hex	0177, 0x9ff
Complex	3+4j, 3.0+4.0j, 3j

Recall from the Last Session-2

Built-in object types:

Number	3.1415, 1234, 999L, 3+4j
Strings	'spam', "guido's"
Lists	[1, [2,'tree'], 4]
Dictionaries	'food':'spam', 'taste':'yum'
Tuples	(1,'spam', 4, 'U')
Files	text = open('eggs', 'r').read()

What Will be Covered Today

1. NumPy
   - Arrays
   - Array Indexing and Slicing
   - Loop over Array
   - Vectorization
   - Matrices
   - Matlab Users
   - Linear Algebra
2. SciPy
   - Interpolation
   - Optimization
   - Integration
   - Statistical Analysis
   - Fast Fourier Transform
   - Signal Processing

NumPy

Useful Links for NumPy

- **Tentative NumPy Tutorial**
  http://www.scipy.org/Tentative_NumPy_Tutorial
- **NumPy Reference**
  http://docs.scipy.org/doc/numpy/reference
- **NumPy for MATLAB Users**
  http://mathesaurus.sourceforge.net/matlab-numpy.html
- **NumPy for R (and S-Plus) Users**
  http://mathesaurus.sourceforge.net/r-numpy.html

What is NumPy?

- Efficient array computing in Python
- Creating arrays
- Indexing/slicing arrays
- Random numbers
- Linear algebra
- (The functionality is close to that of Matlab)

Using NumPy

- The critical thing to know is that Python **for** loops are *slow*! One should try to use array-operations as much as possible
- NumPy provides mathematical functions that operate on an entire array.

Making Arrays

```
>>> from numpy import *
>>> n = 4
>>> a = zeros(n)      # one-dim. array of length n
>>> print a           # str(a), float (C double) is default type
[ 0.  0.  0.  0.]
>>> a                               # repr(a)
array([ 0.,  0.,  0.,  0.])
>>> p = q = 2
>>> a = zeros((p,q,3))  # p*q*3 three-dim. Array
>>> print a
[[[ 0.  0.  0.]
  [ 0.  0.  0.]]

 [[ 0.  0.  0.]
  [ 0.  0.  0.]]]
>>> a.shape                 # a's dimension
(2, 2, 3)
```

Making Int, Float, Complex Arrays

```
>>> a = zeros(3)
>>> print a.dtype # a's data
Typefloat64
>>> a = zeros(3, int)
>>> print a
[0 0 0]
>>> print a.dtype
Int32
>>> a = zeros(3, float32)   # single precision
>>> print a
[ 0.  0.  0.]
>>> print a.dtype
Float32
>>> a = zeros(3, complex)
>>> a
array([ 0.+0.j,  0.+0.j,  0.+0.j])
>>> a.dtype
dtype('complex128)
```

Array with Sequence of number

- linspace(a, b, n) generates n uniformly spaced coordinates, starting with a and ending with b

```
>>> x = linspace(-5, 5, 11)
>>> print x
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- A special compact syntax is available through the syntax

```
>>> a = r_[-5:5:11j]        # same as linspace(-1, 1, 11)
>>> print a
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

- arange works like range (xrange)

```
>>> x = arange(-5, 5, 1, float)
>>> print x                # upper limit 5 is not included!!
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.]
```

Array Construct from a Python List

- array(list, [datatype]) generates an array from a list:

```
>>> pl = [0, 1.2, 4, -9.1, 5, 8]
>>> a = array(pl)
```

- The array elements are of the simplest possible type:

```
>>> z = array([1, 2, 3])
>>> print z            # int elements possible
[1 2 3]
>>> z = array([1, 2, 3], float)
>>> print z
[ 1.  2.  3.]
```

- A two-dim. array from two one-dim. lists:

```
>>> x = [0, 0.5, 1]; y = [-6.1, -2, 1.2]    # Python lists
>>> a = array([x, y])  # form array with x and y as rows
```

From "Anything" to a NumPy Array

- Given an object a,

```
a = asarray(a)
converts a to a NumPy array (if possible/necessary)
```

- Arrays can be ordered as in C (default) or Fortran:

```
a = asarray(a, order='Fortran')
isfortran(a)       # returns True of a's order is Fortran
```

- Use asarray to, e.g., allow flexible arguments in functions:

```
def myfunc(some_sequence, ...):
    a = asarray(some_sequence)
    # work with a as array

myfunc([1,2,3], ...)
myfunc((-1,1), ...)
myfunc(zeros(10), ...)
```

Changing Array Dimension

```
>>> a = array([0, 1.2, 4, -9.1, 5, 8])
>>> a.shape = (2,3) # turn a into a 2x3 matrix
>>> a.size
6
>>> a.shape = (a.size,) # turn a into a vector of length 6 aga
>>> a.shape
(6,)
>>> a = a.reshape(2,3) # same effect as setting a.shape
>>> a.shape(2, 3)
```

Array Initialization from a Python Function

```
>>> def myfunc(i, j):
...     return (i+1)*(j+4-i)
...
>>> # make 3x6 array where a[i,j] = myfunc(i,j):
>>> a = fromfunction(myfunc, (3,6))
>>> a
array([[  4.,   5.,   6.,   7.,   8.,   9.],
       [  6.,   8.,  10.,  12.,  14.,  16.],
       [  6.,   9.,  12.,  15.,  18.,  21.]])
```

Basic Array Indexing

```
a = linspace(-1, 1, 6)
a[2:4] = -1          # set a[2] and a[3] equal to -1
a[-1]  = a[0]        # set last element equal to first one
a[:]   = 0           # set all elements of a equal to 0
a.fill(0)            # set all elements of a equal to 0

a.shape = (2,3)      # turn a into a 2x3 matrix
print a[0,1]         # print element (0,1)
a[i,j] = 10          # assignment to element (i,j)
a[i][j] = 10         # equivalent syntax (slower)
print a[:,k]         # print column with index k
print a[1,:]         # print second row
a[:,:] = 0           # set all elements of a equal to 0
```

More Advanced Array Indexing

```
>>> a = linspace(0, 29, 30)
>>> a.shape = (5,6)
>>> a
array([[  0.,   1.,   2.,   3.,   4.,   5.,]
    [  6.,   7.,   8.,   9., 10., 11.,]
    [ 12., 13., 14., 15., 16., 17.,]
    [ 18., 19., 20., 21., 22., 23.,]
    [ 24., 25., 26., 27., 28., 29.,]])
>>> a[1:3,:-1:2]   # a[i,j] for i=1,2 and j=0,2,4
array([[  6.,   8.,  10.],
    [ 12.,  14.,  16.]])
>>> a[::3,2:-1:2]   # a[i,j] for i=0,3 and j=2,4
array([[  2.,   4.],
    [ 20.,  22.]])
>>> i = slice(None, None, 3);  j = slice(2, -1, 2)
>>> a[i,j]
array([[  2.,   4.],
    [ 20.,  22.]])
```

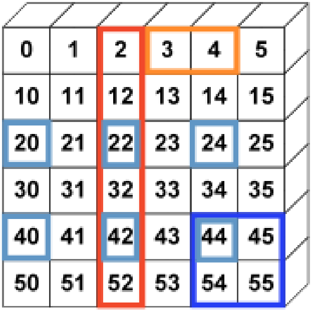
Array Slicing

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] ])
```



Slices Refer the Array Data

- With a as list, a[:] makes a copy of the data
- With a as array, a[:] is a reference to the data

```
>>> b = a[1,:]        # extract 2nd column of a
>>> print a[1,1]
12.0
>>> b[1] = 2
>>> print a[1,1]
2.0                   # change in b is reflected in a!
```

- Take a copy to avoid referencing via slices:

```
>>> b = a[1,:].copy()
>>> print a[1,1]
12.0
>>> b[1] = 2       # b and a are two different arrays now
>>> print a[1,1]
12.0               # a is not affected by change in b
```

Integer Arrays as Indices

- An integer array or list can be used as (vectorized) index

```
>>> a = linspace(1, 8, 8)
>>> aarray([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.])
>>> a[[1,6,7]] = 10
>>> a
array([  1.,  10.,   3.,   4.,   5.,   6.,  10.,  10.])
>>> a[range(2,8,3)] = -2
>>> aarray([  1.,  10.,  -2.,   4.,   5.,  -2.,  10.,  10.])
>>> a[a < 0]             # pick out the negative elements of a
array([-2., -2.])
>>> a[a < 0] = a.max()
>>> a
array([  1.,  10.,  10.,   4.,   5.,  10.,  10.,  10.])
```

- Such array indices are important for efficient vectorized code

Loop over Arrays-1

- Standard loop over each element:

```
for i in xrange(a.shape[0]):
    for j in xrange(a.shape[1]):
        a[i,j] = (i+1)*(j+1)*(j+2)
        print 'a[%d,%d]=%g ' % (i,j,a[i,j]),
    print  # newline after each row
```

- A standard for loop iterates over the first index:

```
>>> print a
[[  2.   6.  12.]
 [  4.  12.  24.]]
>>> for e in a:
...     print e
...
[  2.   6.  12.]
[  4.  12.  24.]
```

Loop over Arrays-2

- View array as one-dimensional and iterate over all elements:

```
for e in a.flat:
    print e
```

- For loop over all index tuples and values:

```
>>> for index, value in ndenumerate(a):
...     print index, value
...
(0, 0) 2.0
(0, 1) 6.0
(0, 2) 12.0
(1, 0) 4.0
(1, 1) 12.0
(1, 2) 24.0
```

Array Computations

Arithmetic operations can be used with arrays:

```
b = 3*a - 1     # a is array, b becomes array
```

The above operation generates a temporary array:

```
tb = 3*a
b  = tb - 1
```

As far as possible, we want to avoid the creation of temporary arrays to limit the memory usage and to decrease the computational time associated with with array computations.

In-Place Array Arithmetics

- With in-place modifications of arrays, we can avoid temporary arrays (to some extent) to compute b = 3a - 1

```
b = a
b *= 3  # or multiply(b, 3, b)
b -= 1  # or subtract(b, 1, b)
```

- In-place operations:

```
a *= 3.0     # multiply a's elements by 3
a -= 1.0     # subtract 1 from each element
a /= 3.0     # divide each element by 3
a += 1.0     # add 1 to each element
a **= 2.0    # square all elements
```

Timing Array Basic Operations

We want to perform the array operation

```
b = 3*a + 1
```

in three different ways: (1) looping over the entries of the array, (2) using Numpy array operation, and (3) using in-place arithmetic.

a.size	Loop	Numpy	In-Place
10^7	20.13	0.09	0.06
10^8	214.77	0.94	0.48

Math Functions and Array Arguments

```
# let b be an array
c = sin(b)
c = arcsin(c)
c = sinh(b)
# same functions for the cos and tan families
c = b**2.5  # power function
c = log(b)
c = exp(b)
c = sqrt(b)
```

Other Useful Array Operations

```
# a is an array
a.clip(min=3, max=12)   # clip elements
a.mean(); mean(a)      # mean value
a.var();  var(a)        # variance
a.std();  std(a)         # standard deviation
median(a)
cov(x,y)               # covariance
trapz(a)               # Trapezoidal integration
diff(a)                # finite differences (da/dx)

# more Matlab-like functions:
corrcoeff, cumprod, diag, eig, eye, fliplr,
flipud, max, min,prod, ptp, rot90, squeeze, sum,
svd, tri, tril, triu
```

More Useful Array Methods and Attributes

```
>>> a = zeros(4) + 3
>>> a
array([ 3.,  3.,  3.,  3.])    # float data
>>> a.item(2)           # more efficient than a[2]
3.0
>>> a.itemset(3,-4.5)   # more efficient than a[3]=-4.5
>>> a
array([ 3. ,  3. ,  3. , -4.5])
>>> a.shape = (2,2)
>>> a
array([[ 3. ,  3. ],       [ 3. , -4.5]])
>>> a.ravel()  # from multi-dim to one-dim
array([ 3. ,  3. ,  3. , -4.5])
>>> a.ndim  # no of dimensions
2
>>> len(a.shape)   # no of dimensions
2
>>> rank(a)  # no of dimensions
2
>>> a.size  # total no of elements
4
>>> b = a.astype(int)   # change data type
>>> b
array([3, 3, 3, 3])
```

Complex Number Computing

```
>>> from math import sqrt
>>> sqrt(-1)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: math domain error

>>> from numpy import sqrt
>>> sqrt(-1)
Warning: invalid value encountered in sqrt
nan
>>> from cmath import sqrt   # complex math functions
>>> sqrt(-1)
1j
>>> sqrt(4)   # cmath functions always return complex...
(2+0j)
>>> from numpy.lib.scimath import sqrt
>>> sqrt(4)
2.0                # real when possible
>>> sqrt(-1)
1j                 # otherwise complex
```

A Root Function

```
# Goal: compute roots of a parabola, return real when possible,
        otherwise complex
def roots(a, b, c):
    # compute roots of a*x^2 + b*x + c = 0
    from numpy.lib.scimath import sqrt
    q = sqrt(b**2 - 4*a*c)  # q is real or complex
    r1 = (-b + q)/(2*a)
    r2 = (-b - q)/(2*a)
    return r1, r2>

>> a = 1; b = 2; c = 100
>>> roots(a, b, c)                              # complex roots
((-1+9.94987437107j), (-1-9.94987437107j))

>>> a = 1; b = 4; c = 1
>>> roots(a, b, c)                              # real roots
(-0.267949192431, -3.73205080757)
```

Array Type and Data Type

```
>>> import numpy
>>> a = numpy.zeros(5)
>>> type(a)
<type 'numpy.ndarray
>>>> isinstance(a, ndarray)    # is a of type ndarray?
True
>>> a.dtype                    # data (element) type object
dtype('float64')
>>> a.dtype.name
'float64
>>> a.dtype.char               # character code
'd
>>> a.dtype.itemsize           # no of bytes per array element
8
>>> b = zeros(6, float32)
>>> a.dtype == b.dtype  # do a and b have the same data type?
False
>>> c = zeros(2, float)
>>> a.dtype == c.dtype
True
```

Concept of Vectorization

- Loops over an array run slowly
- Vectorization = replace explicit loops by functions calls such that the whole loop is implemented in C (or Fortran)
- Explicit loops:

```
r = zeros(x.shape, x.dtype)
for i in xrange(x.size):
    r[i] = sin(x[i])
```

- Vectorized version:

```
r = sin(x)
```

- Arithmetic expressions work for both scalars and arrays
- Many fundamental functions work for scalars and arrays
- Ex: x**2 + abs(x) works for x scalar or array

Vectorization using Functions

A mathematical function written for scalar arguments can (normally) take a array arguments:

```
>>> def f(x):
...     return x**2 + sinh(x)*exp(-x) + 1
...
>>> # scalar argument:
>>> x = 2
>>> f(x)
5.4908421805556333

>>> # array argument:
>>> y = array([2, -1, 0, 1.5])
>>> f(y)
array([ 5.49084218, -1.19452805,  1.,  3.72510647])
```

Vectorization of Functions with if-tests

- Consider a function with an if test:

```
def somefunc(x):
    if x < 0:
       return 0
    else:
       return sin(x)
# or
def somefunc(x): return 0 if x < 0 else sin(x)
```

- This function works with a scalar x but not an array
- Problem: $x < 0$ results in a boolean array, not a boolean value that can be used in the if test

```
>>> x = linspace(-1, 1, 3); print x[-1.  0.  1.]
>>> y = x < 0
>>> y
array([ True, False, False], dtype=bool)
>>> 'ok' if y else 'not ok'  # test of y in scalar boolean context
...
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

Vectorization of Functions with if-tests

- Simplest remedy: call NumPy's vectorize function to allow array arguments to a function:

```
>>> somefuncv = vectorize(somefunc, otypes='d')
>>> # test:
>>> x = linspace(-1, 1, 3); print x[-1.  0.  1.]
>>> somefuncv(x)
array([ 0.        ,  0.        ,  0.84147098])
```

  Note: The data type must be specified as a character
- The speed of somefuncv is unfortunately quite slow
- A better solution, using where:

```
def somefunc_NumPy2(x):
    x1 = zeros(x.size, float)
    x2 = sin(x)
    return where(x < 0, x1, x2)
```

Genenal Vectorization with if-else Tests

```
def f(x):                      # scalar x
    if condition:
        x = <expression1>
    else:
        x = <expression2>
    return x

def f_vectorized(x):           # scalar or array x
    x1 = <expression1>
    x2 = <expression2>
    return where(condition, x1, x2)
```

Vectorization via Slicing

- Consider for instance a recursion scheme which arises from a one-dimensional diffusion equation
- Straightforward (slow) Python implementation:

```
n = size(u)-1
for i in xrange(1,n,1):
    u_new[i] = beta*u[i-1] + (1-2*beta)*u[i] + beta*u[i+1]
```

- Slices enable us to vectorize the expression:

```
u[1:n] = beta*u[0:n-1] + (1-2*beta)*u[1:n] + beta*u[2:n+1]
```

Matrix Objects-1

- NumPy has an array type, matrix, much like Matlab's array type

```
>>> x1 = array([1, 2, 3], float)
>>> x2 = matrix(x)                    # or just mat(x)
>>> x2                                # row vector
matrix([[ 1.,  2.,  3.]])
>>> x3 = mat(x).transpose()           # column vector
>>> x3
matrix([[ 1.],
 [ 2.],
 [ 3.]])
>>> type(x3)
<class 'numpy.core.defmatrix.matrix>
>>> isinstance(x3, matrix)
True
```

- Only 1- and 2-dimensional arrays can be matrix

Matrix Objects

For matrix objects, the * operator means matrix-matrix or matrix-vector multiplication (not elementwise multiplication)

```
>>> A = eye(3)                  # identity matrix
>>> A = mat(A)                  # turn array to matrix
>>> A
matrix([[ 1.,  0.,  0.],
 [ 0.,  1.,  0.],
 [ 0.,  0.,  1.]])
>>> y2 = x2*A                   # vector-matrix product
>>> y2
matrix([[ 1.,  2.,  3.]])
>>> y3 = A*x3                   # matrix-vector product
>>> y3
matrix([[ 1.],
[ 2.],
[ 3.]])
```

Example 1

```
a = array([[1,2],[3,4]])
a
m = mat(a)
m
a[0]
m[0]
a*a
m*m
dot(a, a)
```

Example 2

```
x = array([1,0,2,-1,0,0,8])
indices = x.nonzero()
indices
x[indices]
indices = (x >-1).nonzero()
x[indices]
```

Example 3

```
a = array([1,2,3])
a.prod()
prod(a)

b = array([[1,2,3],[4,5,6]])
b.prod(dtype=float)
b.prod(axis=0)
b.prod(axis=1)
```

Overview

- In NumPy, operation are elementwise by default
- There is a matrix type for linear algebra (subclass of array)
- Indexing start at 0 in NumPy
- Using Python with NumPy gives more programming power
- Function definition in Matlab have many restriction
- NumPy/SciPy is free but still widely used
- Matlab have lots of 'toolboxes' for specific task (lot less in NumPy/SciPy)
- There are many packages for plotting in Python that are as good as Matlab

Matlab/NumPy Equivalence-1

Matlab	NumPy
a = [1 2 3; 4 5 6]	a = array([[1.,2.,3.],[4.,5.,6.]])
a(end)	a[-1]
a(2,5)	a[1,4]
a(2,:)	a[1] or a[1,:]
a(1:5,:)	a[0:5] or a[:5] or a[0:5,:]
a(end-4:end,:)	a[-5:]
a(1:3,5:9)	a[0:3][:,4:9]
a(1:2:end,:)	a[::2,:]
a(end:-1:1,:) or flipud(a)	a[::-1,:]
a.'	a.transpose() or a.T
a'	a.conj().transpose() or a.conj().T
a * b	dot(a,b)
a .* b	a * b
a./b	a/b

Matlab/NumPy Equivalence-2

Matlab	NumPy
diag(a)	g(a) or a.diagonal()
diag(a,0)	diag(a,0) or a.diagonal(0)
rand(3,4)	random.rand(3,4)
linspace(1,3,4)	inspace(1,3,4)
$[x, y] = meshgrid(0:8, 0:5)$	$grid[0:9., 0:6.]$
repmat(a, m, n)	tile(a, (m, n))
$[a\ \ b]$	concatenate((a,b),1) or hstack((a,b))
	or c $[a, b[a; b]]$
$[a; b]$	concatenate((a,b)) or vstack((a,b)) or r $[a, b]$
max(max(a))	a.max()
max(a)	a.max(0)
max(a,[],2)	a.max(1)
max(a,b)	re(a>b, a, b)
norm(v)	sqrt(dot(v,v)) or linalg.norm(v)

Matlab/NumPy Equivalence-3

Matlab	**NumPy**
inv(a)	linalg.inv(a)
pinv(a)	linalg.pinv(a)
$a\backslash b$	linalg.solve(a,b)
b/a	Solve a.T x.T = b.T instead
$[U, S, V]$=svd(a)	(U, S, V) = linalg.svd(a)
chol(a)	linalg.cholesky(a)
$[V, D]$=eig(a)	linalg.eig(a)
$[Q, R, P]$=qr(a,0)	Q,R)=Sci.linalg.qr(a)
$[L, U, P]$=lu(a)	(L,U)=linalg.lu(a) or (LU,P)=linalg.lu factor(a)
conjgrad	Sci.linalg.cg
fft(a)	fft(a)
ifft(a)	ifft(a)
sort(a)	sort(a) or a.sort()
sortrows(a,i)	a$[argsort(a[:, 0], i)]$

Matlab/NumPy Equivalence-4

Matlab	NumPy
a.^3	$a * *3$
find(a>0.5)	where(a>0.5)
a(a<0.5)=0	a[a<0.5]=0
a(:) = 3	a[:] = 3
y=x	y = x.copy()
y=x(2,:)	y = x[2, :].copy()
y=x(:)	y = x.flatten(1)
1:10	arange(1.,11.) or r [1. : 11.]
0:9	arange(10.) or r [: 10.]
zeros(3,4)	zeros((3,4))
zeros(3,4,5)	eros((3,4,5))
ones(3,4)	ones((3,4))
eye(3)	eye(3)

Sample Matrix Multiplication

Given two $n \times n$ matrices A and B, we want to compute:

$$C = A \times B$$

A and B have randomly generated entries.

Check the files:

```
matMultiPython.py # Multiply two matrices using do loops
matMultiNumpy.py  # Multiply two matrices using NumPy functio
```

Timing Results of the Matrix Multiplication

	n = 1000	n = 1200	n = 1500
Python			
NumPy	8.14	14.04	28.15
Matlab	0.023	0.048	0.057
gfortran (matmult)	0.604	1.212	3.000
gfortran with Blas	0.180	0.300	0.596
gcc	0.60	1.110	2.940
g++	1.351	2.382	4.928

For additional information, go to:

Comparing Python, NumPy, Matlab, Fortran, etc.

https://modelingguru.nasa.gov/docs/DOC-1762

Random Numbers

- Drawing scalar random numbers:

```
import random
random.seed(2198)  # control the seed
print 'uniform random number on (0,1):',  random.random()
print 'uniform random number on (-1,1):', random.uniform(-1,1)
print 'Normal(0,1) random number:',       random.gauss(0,1)
```

- Vectorized drawing of random numbers (arrays):

```
from numpy import random
random.seed(12)                # set seed
u = random.random(n)           # n uniform numbers on (0,1)
u = random.uniform(-1, 1, n)   # n uniform numbers on (-1,1)
u = random.normal(m, s, n)     # n numbers from N(m,s)
```

- Note that both modules have the name random! A remedy:

```
import random as random_number   # rename random for scalars
from numpy import *              # random is now numpy.random
```

Basic Linear Algebra

NumPy contains the **linalg** module for:

- Solving linear systems
- Computing the determinant of a matrix
- Computing the inverse of a matrix
- Computing eigenvalues and eigenvectors of a matrix
- Solving least-squares problems
- Computing the singular value decomposition of a matrix
- Computing the Cholesky decomposition of a matrix

numpy.linalg

```
cholesky(A)        # Cholesky decomposition
qr(a[,mode])       # Compute the qr factorization of a matrix
svd(a[,full_matrices,compute_uv]) # Singular Value Decomposition
eig(A)             # Compute the eigenvalues and right
                   # eigenvectors of a square array
eigvals(A)         # Compute the eigenvalues of a general matrix.
det(A)             # Compute the determinant of a matrix
matrix_power(M,n) # Raise a square matrix to the (integer) power n
solve(A,b)      # Solve a linear matrix equation,
                # or system of linear scalar equations.
inv(A)          # Compute the (multiplicative) inverse of a matrix
```

Sample Linear Algebra Session

```
b = dot(A, x)           # matrix vector product
y = linalg.solve(A, b)     # solve A*y = b
if allclose(x, y, atol=1.0E-12, rtol=1.0E-12):
   print 'correct solution!'

d = linalg.det(A)
B = linalg.inv(A)

R = dot(A, B) - eye(n)   # residual
R_norm = linalg.norm(R)  # Frobenius norm of matrix R
print 'Residual R = A*A-inv - I:', R_norm

A_eigenvalues = linalg.eigvals(A)  # eigenvalues only
A_eigenvalues, A_eigenvectors = linalg.eig(A)

for e, v in zip(A_eigenvalues, A_eigenvectors):
    print 'eigenvalue %g has corresponding vector\n%s'
```

Jacobi Iterations

We want to find the numerical solution of the 2D Laplace equation:

$$u_{xx} + u_{yy} = 0.$$

We use the Jacobi iterative solver.

Finite Difference Schemes

We use two schemes:

$$u_{i,j} = \frac{1}{4}(u_{i-1,j} + u_{i,j-1} + u_{i+1,j} + u_{i,j+1}) \tag{1}$$

$$\begin{aligned} u_{i,j} = {} & \frac{1}{20}(4(u_{i-1,j} + u_{i,j-1} + u_{i+1,j} + u_{i,j+1}) + \\ & u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1}) \end{aligned} \tag{2}$$

Timing Results with Scheme 1

	n = 50	n = 100
Python	22.818	350.912
NumPy	0.2706	2.61626
Matlab	0.5016	1.88999
f2py	0.0327	0.50701
Fortran	0.0280	0.34800

Timing Results with Scheme 2

	n = 50	n = 100
Python	32.771	547.349
NumPy	0.4109	4.24026
Matlab	0.4021	3.06696
f2py	0.0842	1.34566
Fortran	0.0400	0.58000

SciPy

Useful Links for SciPy

- **How to Think Like a Computer Scientist: Learning with Python**, 2nd Edition, Jeffrey Elkner, Allen B. Downey, and Chris Meyers
  http://openbookproject.net//thinkCSpy
- **Dive Into Python: Python from Novice to Pro**, Mark Pilgrim
  http://diveintopython.org

What is SciPy?

- Collection of mathematical algorithms and convenience functions built on the Numeric extension for Python
- Adds significant power to the interactive Python session
- Can become a data-processing and system-prototyping environment

What SciPy Can Do

stats	:	Statistical Functions
signal	:	Signal Processing Tools
linalg	:	Linear Algebra Tools
linsolve	:	Linear Solvers
sparse	:	Sparse Matrix
fftpack	:	Discrete Fourier Transform Algorithms
ndimage	:	n-dimensional Image Package
io	:	Data Input and Output
integrate	:	Integration Routines
interpolate	:	Interpolation Tools

SciPy and NumPy

- The SciPy library is built to work with NumPy arrays
- Depends on NumPy for array manipulations

Loading SciPy

- Loading the SciPy module:

```
import scipy
```

- The following command will import all SciPy functions:

```
from scipy import *
```

- Help on SciPy:

```
scipy.info(scipy)
help(scipy)
```

scipy.interpolate

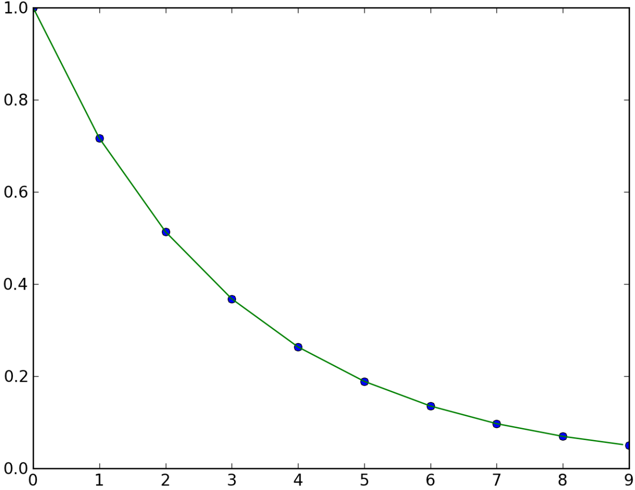
Two general interpolation facilities:

1. One class that performs 1D linear interpolation (interp1d)
2. Another (based on FITPACK) which provides 1D and 2D cubic-spline interpolations (splrep, splev, bisplrep, bisplev)

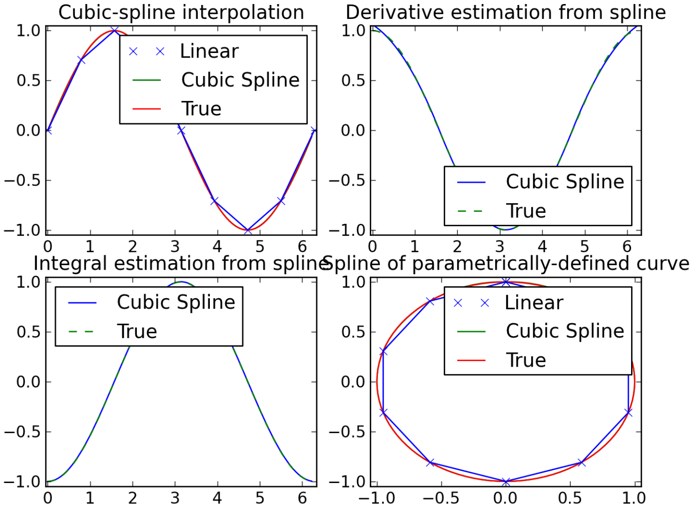
scipy.interpolate Syntax

```
f = interp1d(x,y)        # 1D linear interpolation

tck = splrep(x,y, k=n) # B-spline representation of 1-D
ynew = splev(xnew,tck,der=n) # evaluate the value of the
                             # polynomial and it s der

tck = bisplrep(x,y,z)          # compute a B-spline repre
                               # of the surface
znew = bisplev(xnew,ynew,tck) # spline function values
```

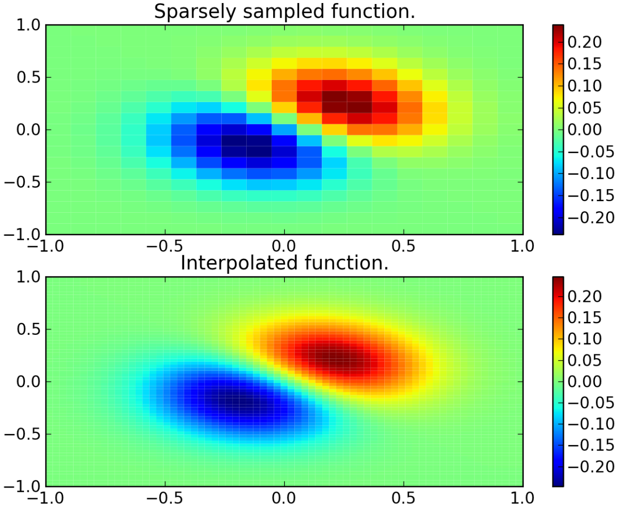
1D Linear Interpolation



1D Cubic Spline Interpolation



2D Cubic Spline Interpolation



scipy.optimize

A collection of general-purpose optimization routines. We can mention:

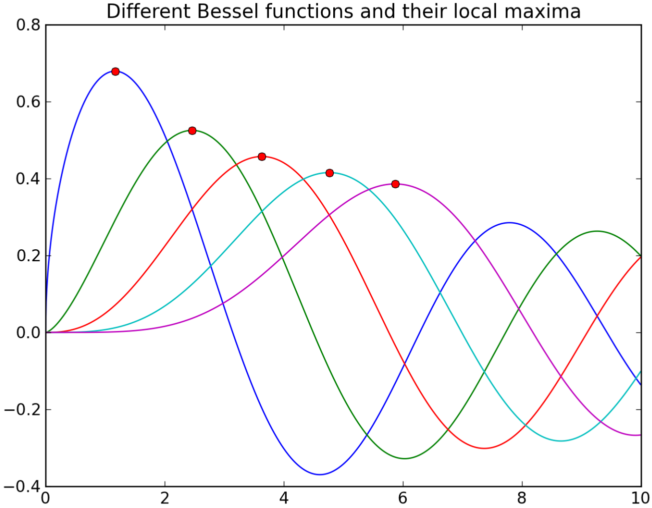
- fminbound : Bounded minimization for scalar functions
- fsolve : Find the roots of a function
- fmin : Minimize a function using the downhill simplex algorithm
- fixed_point : Find the point where func(x) = x
- leastsq : Minimize the sum of squares of a set of equations

Bessell Functions and their Max

We want to plot a set of Bessell functions together with their maximum values.

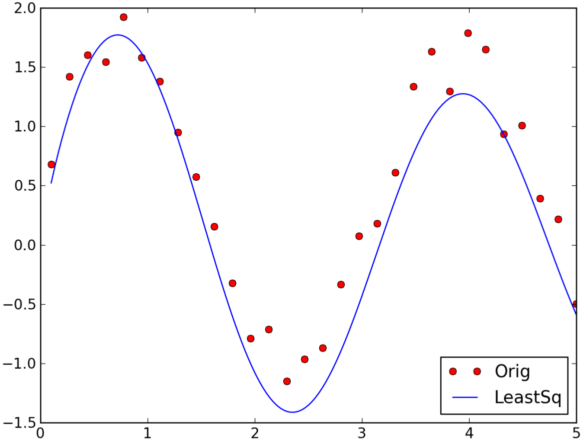
```
x = arange(0,10,0.01)

for k in arange(0.5,5.5):
     y = special.jv(k,x)
     plt.plot(x,y)
     f = lambda x: -special.jv(k,x)
     x_max = optimize.fminbound(f,0,6)
     plt.plot([x_max], [special.jv(k,x_max)],'ro')
```

Plots of Bessell Functions



Least Square Approximation

leastsq(efunc, x0, args=(x,y))



Root Finding with fsolve

Assume that we want to solve the equations:

$$x + 2\cos(x) = 0$$

$$\left\{ \begin{array}{rcl} x_0 \cos(x_1) & = & 4 \\ x_0 x_1 - x_1 & = & 5 \end{array} \right.$$

Code with fsolve

```
from scipy.optimize import fsolve

def func(x):
    return x + 2*scipy.cos(x)

def func2(x):
    out = [x[0]*scipy.cos(x[1]) - 4]
    out.append(x[1]*x[0] - x[1] -5)
    return out

x0 = fsolve(func, 0.3)
print x0

x02 = fsolve(func2, [1, 1])
print x02
```

Minimization Problem

Assume that we want to minimize the function:

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

Code with fmin

```python
from scipy.optimize import fmin
def rosen(x):
    """The Rosenbrock function"""
    return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + \
           (1-x[:-1])**2.0)

x0 = [1.3, 0.7, 0.8, 1.9, 1.2]
xopt = fmin(rosen, x0, xtol=1e-8)
```

Code with fixed_point

```
from scipy.optimize import fixed_point

def func(x, c1, c2):
    return sqrt(c1/(x+c2))

c1 = array([10,12.])
c2 = array([3, 5.])
print fixed_point(func, [1.2, 1.3], args=(c1,c2))
```

scipy.integrate

- quad : General purpose integration.
- dblquad : General purpose double integration.
- tplquad : General purpose triple integration.
- fixed_quad : Integrate using Gaussian quadrature of order n.
- quadrature : Integrate with given tolerance using Gaussian quadrature.
- romberg : Integrate func using Romberg integration.
- trapz : Use trapezoidal rule to compute integral from samples.
- cumtrapz : Use trapezoidal rule to cumulatively compute integral.
- simps : Use Simpson's rule to compute integral from samples.
- romb : Use Romberg Integration to compute integral from (2**k + 1) evenly-spaced samples.
- odeint : General integration of ordinary differential equations.
- ode : Integrate ODE using VODE and ZVODE routines.

Example of ODE

Assume that we want to solve the equation:

$$x''(t) + \mu x'(t)(x^2(t) - 1) + x(t) = 0$$

It can be transformed into:

$$\begin{cases} x' & = & y \\ y' & = & -x + \mu y(1 - x^2) \end{cases}$$

Sample Code for ODE

```
import matplotlib.pyplot as plt
import scipy
from scipy import integrate

def f_1(y,t):
    return[y[1],-y[0]-10*y[1]*(y[0]**2-1)]

def j_1(y,t):
    return [ [0, 1.0],[-2.0*10*y[0]*y[1]-1.0,-10*(y[0]*y[

x= scipy.arange(0,100,.1)

y=integrate.odeint(f_1,[1,0],x,Dfun=j_1)

p=[((x[i],y[i][0])) for i in range(len(x))]
plt.plot(p)
plt.show()
```

scipy.stats

Provides tools for statistical analysis:

- More than 84 continuous distributions.
- More than 12 discrete distributions
- Tools for manipulating them:
  - Statistical functions
  - Statistical tests
  - Statistical models

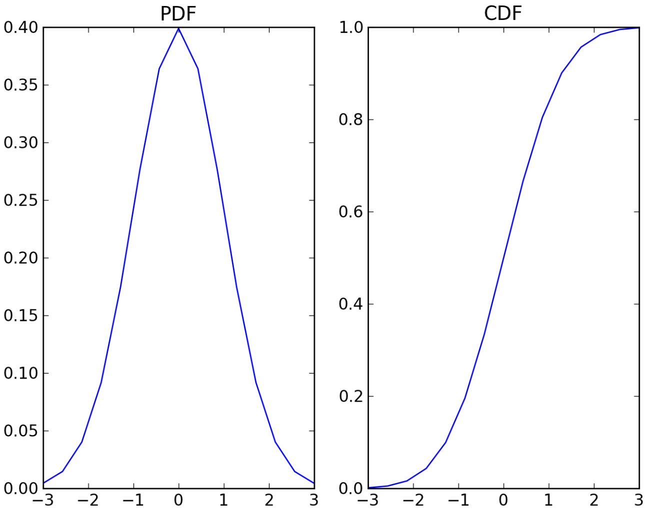
Syntax

```
probability density function
    generic.pdf(x,<shape(s)>,loc=0,scale=1)

cumulative density function
    generic.cdf(x,<shape(s)>,loc=0,scale=1)

percent point function (inverse of cdf --- percentiles)
    generic.ppf(q,<shape(s)>,loc=0,scale=1)

random variates
    generic.rvs(<shape(s)>,loc=0,scale=1,size=1)

mean('m'), variance('v'), skew('s'), and/or kurtosis('k')
    generic.stats(<shape(s)>,loc=0,scale=1,moments='mv')
```

Sample Code: Distribution

```
from scipy import stats

x = np.linspace(-3.0, 3.0, 15)
q = np.linspace(0.0, 1.0, 15)

stats.norm.pdf(x, loc=0.0, scale=1.0)
stats.norm.cdf(x, loc=0.0, scale=1.0)
stats.norm.ppf(q, loc=0.0, scale=1.0)
stats.norm.stats(loc=0.0, scale=1.0)
stats.norm.rvs(loc=0.0, scale=1.0, size=15)
```

Plots of Distributions



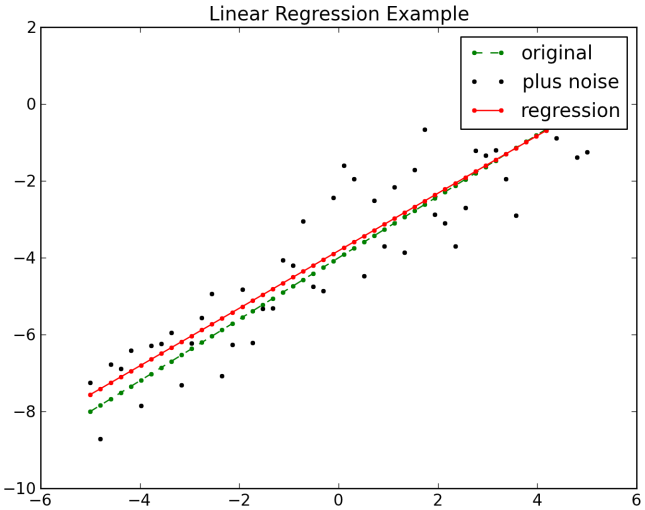
Summary Statistics

```
x = stats.norm.rvs(size=1000)

x.mean(); np.mean(x)

x.std(); np.std(x)

x.var(); np.var(x)

np.median(x)

stats.mode(stats.geom.rvs(0.1, size=1000))
```

Examples with scipy.stats

- Linear Regression: `linearRegression.py`
- Example of distribution: `distributionExample.py`
- Computation of mean, std: `statEstimatorsSample.py`

Sample Linear Regression Plot



scipy.fftpack

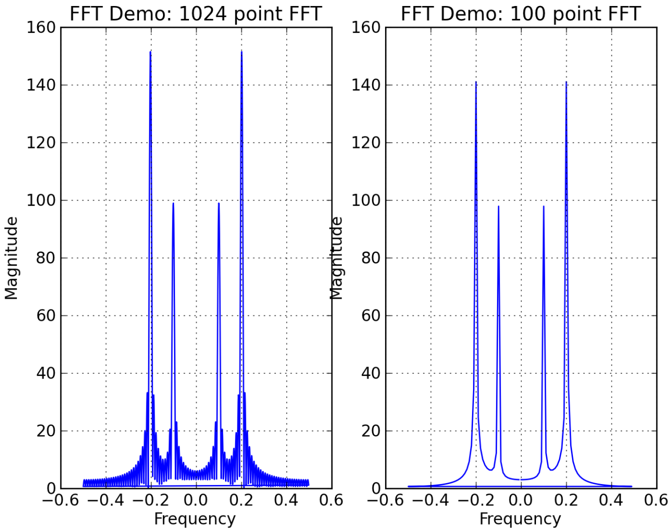
Discrete Fourier Transform Algorithms

- fft, ifft, fft2, ifft2, fftn, ifftn
- fftshift, ifftshift, fftfreq

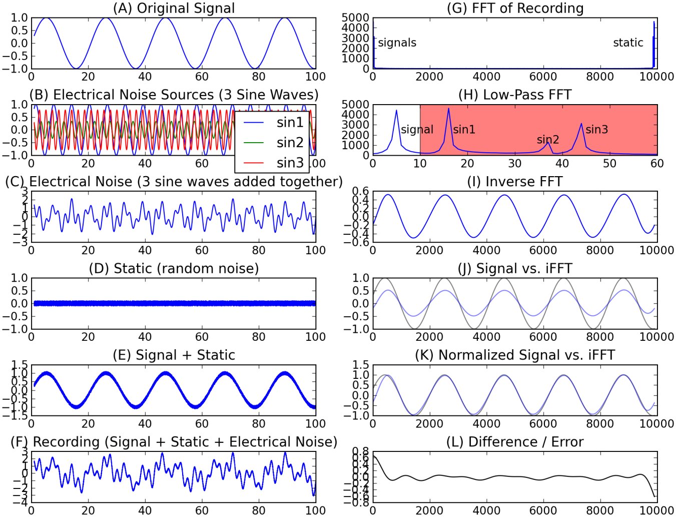
Sample FFT Session

```python
import matplotlib.pyplot as plt
from scipy import *
from scipy import *
from scipy.fftpack import fftshift, fftfreq

x = r_[0:1:100j]
y = 2*sin(2*pi*10*x) + 3*cos(2*pi*20*x)

Y02 = fft(y, 1024)
w = fftfreq(1024)
plt.plot(w,abs(Y02))
```

Sample FFT


FFT Demo: 1024 point FFT
FFT Demo: 100 point FFT
Magnitude
Frequency
0
20
40
60
80
100
120
140
160
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6

Sample Band-Pass Filtering



scipy.signal

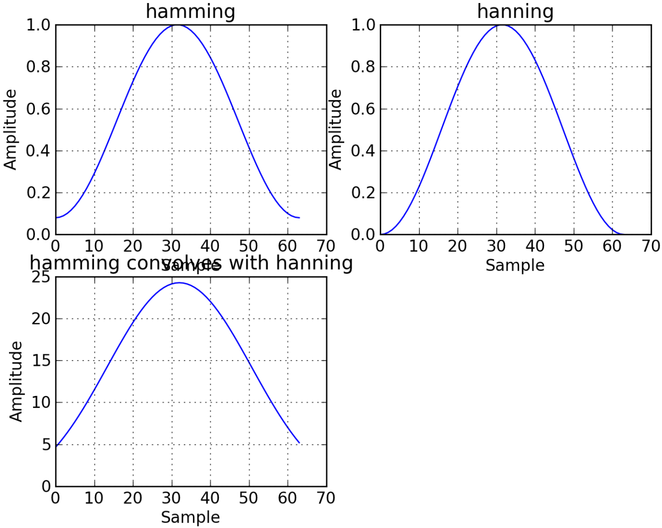
Provides functions for:

- Convolution
- B-Splines
- Filtering & Filter Design
- Linear Systems
- Window Functions
- Wavelets

Sample Convolution Code

```python
from scipy import *
from scipy import signal

n = 64
x = linspace(0,n-1,n)

y01 = hamming(n)
y02 = hanning(n)

z01 = signal.convolve(y01, y02, mode='same')
```

Sample Convolution Plot

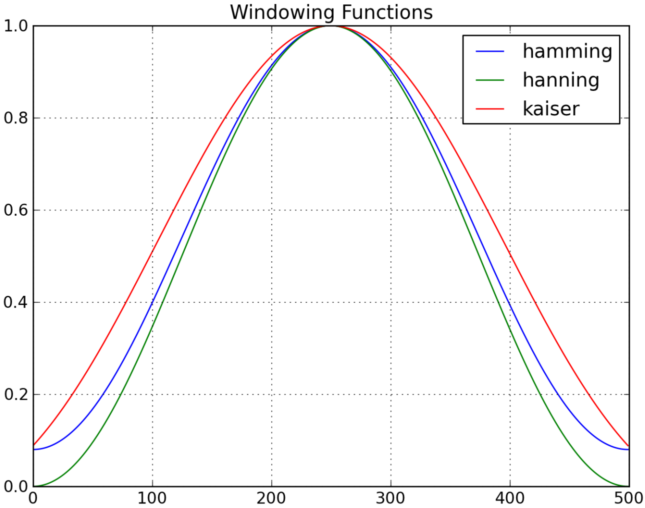


Windowing Function

Functions to generate the following types of windows:

```
boxcar(M, sym = 1)        # M-point boxcar window
triang(M, sym = 1)
blackman(M, sym = 1)
hamming(M, sym = 1)
kaiser(M, beta, sym = 1)  # Return a Kaiser window of length M
                          # with shape parameter beta
gaussian(M, std, sym = 1) # Return a Gaussian window of length M
                          # with standard-deviation std
```

Sample Convolution Plot



References I

- Johnny Wei-Bing Lin, *A Hands-On Introduction to Using Python in the Atmospheric and Oceanic Sciences*, `http://www.johnny-lin.com/pyintro`, 2012.
- Hans Petter Langtangen, *A Primer on Scientific Programming with Python*, Springer, 2009.
- Drew McCormack, *Scientific Scripting with Python*, 2009.
- Sandro Tosi, *Matplotlib for Python Developers*, 2009.
- S. van der Walt, S. C. Colbert and G. Varoquaux, The NumPy array: a structure for efficient numerical computation, *IEEE Computing in Science and Engineering*, 13(2): 22–30, 2011.