Scientific Computing in Python – NumPy, SciPy, Matplotlib

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Based on Lecture Material by
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Python for Scientific Computing?

• Pro:
  • Programming in Python is convenient
  • Development is fast (no compilation, no linking)

• Con:
  • Interpreted language is slower than compiled code
  • Lists are wasteful and inefficient for large data sets

=> NumPy to the rescue

• NumPy is also a great example for using OO-programming to hide implementation details
NumPy and SciPy

- NumPy provides functionality to create, delete, manage and operate on large arrays of typed “raw” data (like Fortran and C/C++ arrays)
- SciPy extends NumPy with a collection of useful algorithms like minimization, Fourier transform, regression and many other applied mathematical techniques
- Both packages are add-on packages (not part of the Python standard library) containing Python code and compiled code (fftpack, BLAS)
Installation of NumPy / SciPy

- Package manager of your Linux distribution
- Listed on PyPi
  - Installation via “pip install numpy scipy”
- See http://www.scipy.org/install.html for other alternatives, suitable for your platform
- After successful installation, “numpy” and “scipy” can be imported like other packages:

  ```python
  import numpy as np
  import scipy as sp
  ```
The Basic Data Structure in NumPy

• The essential component of NumPy is the "array", which is a container similar to the C++ std::array, but more powerful and flexible.

• Data is stored "raw" and all elements of one array have to have the same type (efficient!)

• Data access similar to Python list:

```python
>>> a = np.array([1, 4, 9, 16], np.float32)
>>> print(a[0], a[-1])
(1.0, 16.0)
>>> a
array([ 1.,  4.,  9., 16.], dtype=float32)
```
NumPy Data Types

- Numpy supports a larger number of data types, and similar to compiled languages, you can specify how many bits are used, e.g.: bool, int, int8, int16, uint32, uint64, float32, float64, complex64, complex128

```python
>>> a = np.array([0,2,3,4],np.complex128)
>>> a
array([ 0.+0.j,  2.+0.j,  3.+0.j,  4.+0.j])
>>> a = np.array([0,2,3,4],dtype=np.int8)
>>> a[1] += 128
>>> print (a[1])
-126
```
Multi-dimensional Arrays

• Multi-dimensional arrays are like lists of lists:

```python
>>> b = np.array([[0,1,-1],[2,3,4]],np.int8)
>>> b
array([[ 0,  1, -1],
       [ 2,  3,  4]], dtype=int8)
>>> b.shape
(2, 3)
>>> b[1][0]
2
>>> b[0,1]
1
```
Reshaping Arrays

- Same as in Fortran, arrays can be recast into different shapes, while data remains in place:

```python
>>> a = np.array(range(10),np.float64)
>>> a
Array([0., 1., 2., 3., 4., 5., 6., 7., 8., 9.])
>>> b = a.reshape(2,5)
>>> a
array([0., 1., 2., 3., 4., 5., 6., 7., 8., 9.])
>>> b
array([[ 0.,  1.,  2.,  3.,  4.],
       [ 5.,  6.,  7.,  8.,  9.]])
```
Array Assignments are Shallow

- Plain assignments creates a new “view” of the same data. Array copies must be explicit:

```python
>>> a = np.array(range(10), np.float64)
>>> b = a.reshape(2,5)
>>> c = a.copy()
>>> a[0] = 1
>>> a
Array([1., 1., 2., 3., 4., 5., 6., 7., 8., 9.])
>>> b
array([[ 1.,  1.,  2.,  3.,  4.],
       [ 5.,  6.,  7.,  8.,  9.]])
>>> c
Array([0., 1., 2., 3., 4., 5., 6., 7., 8., 9.])
```
More Array operations

- Arrays can be filled with a single value
- Arrays can be resized (if only one reference)

```python
>>> a = np.array(range(6),float)
>>> a
array([ 0.,  1.,  2.,  3.,  4.,  5.])
>>> a.fill(1)
>>> a
Array([ 1.,  1.,  1.,  1.,  1.,  1.])

>>> a = np.array(range(6),float)
>>> a.resize(9)
>>> a
array([ 0.,  1.,  2.,  3.,  4.,  5.,  0.,  0.,  0.])
```
More Array operations

- Multi-dimensional arrays can be transposed

```python
>>> a = np.array(range(6),float).reshape(2,3)
>>> b = a.transpose()
>>> a
array([[ 0.,  1.,  2.],
       [ 3.,  4.,  5.]])
>>> b
array([[ 0.,  3.],
       [ 1.,  4.],
       [ 2.,  5.]])
```
More Array operations

• Combine multiple arrays through concatenate

```python
>>> a = np.array([1,2], np.float)
>>> b = np.array([3,4,5,6], np.float)
>>> c = np.array([7,8,9], np.float)
>>> np.concatenate((a, b, c))
array([1., 2., 3., 4., 5., 6., 7., 8., 9.])
```
More Array operations

- Some more ways to create arrays

```python
>>> np.linspace(30, 40, 5)
Array([30. , 32.5, 35. , 37.5, 40. ])
>>> np.ones((2, 3), dtype=float32)
Array([[ 1., 1., 1.],
      [ 1., 1., 1.]], dtype=float32)
>>> np.zeros(7, dtype=int)
array([0, 0, 0, 0, 0, 0, 0])
>>> a = np.array([[1, 2, 3], [4, 5, 6]])
>>> np.zeros_like(a)
array([[ 0, 0, 0],
      [ 0, 0, 0]])
```
Element-by-Element Operations

```python
>>> a = np.array([1,2,3],float)
>>> b = np.array([5,2,6],float)
>>> a + b
array([ 6.,  4.,  9.])
>>> a - b
array([-4.,  0., -3.])
>>> a * b
array([  5.,   4.,  18.])
>>> b / a
array([ 5.,  1.,  2.])
>>> a % b
array([ 1.,  0.,  3.])
>>> b ** a
array([  5.,   4.,  216.])
```
Mathematical Operations

- NumPy has a large set of mathematical functions that can be applied to arrays, e.g.:
  - `abs`, `sign`, `sqrt`, `log`, `log10`, `exp`, `sin`, `cos`, `tan`, ...

```python
>>> a = np.linspace(0.3, 0.6, 4)
>>> print(a)
[ 0.3  0.4  0.5  0.6]
>>> np.sin(a)
array([ 0.29552021,  0.38941834,  0.47942554,  0.56464247])
>>> np.exp(a)
array([ 1.34985881,  1.4918247 ,  1.64872127,  1.82211884])
```
Reduction Operations

```python
>>> a = np.array([2,4,3], dtype=np.float64)
>>> a.sum()
9.0
>>> a.prod()
24.0
>>> np.sum(a)
9.0
>>> a.mean()
3.0
>>> a.var()
0.6666666666666666
>>> a.std()
0.81649658092772603
```
Boolean Operations

- Boolean operators can be used on whole arrays and then produces an array of booleans.

- Comparisons can be used as “filters”.

```python
>>> a = np.array([[6,4],[5,9]])
>>> print (a >= 6)
[[ True False]
 [False  True]]
>>> print (a[ a >= 6])
[6 9]
>>> b = a < 6
>>> print (a[b])
[4 5]
```
Linear Algebra Operations

- Operations on matrices and vectors in NumPy are very efficient because they are linked to compiled in BLAS/LAPACK code (can use MKL, OpenBLAS, ACML, ATLAS, etc.)
- => vector-vector, vector-matrix, matrix-matrix multiplication are supported with dot()
- Also available inner(), outer(), cross()
Linear Algebra Operations

```python
>>> a = np.array([[0, 1], [2, 3]], float)
>>> b = np.array([2, 3], float)
>>> c = np.array([[1, 1], [4, 0]], float)
>>> np.dot(b, a)
array([  6.,  11.])
>>> np.dot(a, b)
array([  3.,  13.])
>>> np.dot(a, c)
array([[  4.,   0.],
       [ 14.,   2.]])
>>> np.outer(b, b)
array([[ 4.,  6.],
       [ 6.,  9.]])
```
Linear Algebra Operations

• Several built-in linear algebra operations are located in the linalg submodule

```python
>>> a = np.array([[4,2,0],[9,3,7],[1,2,1]],float)
>>> np.linalg.det(a)
-48.000000000000028
>>> vals,vecs = np.linalg.eig(a)
>>> vals
array([ 8.85591316,  1.9391628 , -2.79507597])
>>> vecs
array([[ 0.3663565 , -0.54736745,  0.25928158],
       [ 0.88949768,  0.5640176 , -0.88091903],
       [ 0.27308752,  0.61828231,  0.39592263]])
```
This is Only the Beginning

- NumPy has much more functionality:
  - Polynomial mathematics
  - Statistical computations
  - Pseudo random number generators
  - Discrete Fourier transforms
  - Size / shape / type testing of arrays
- To learn more, check out the NumPy docs at: http://docs.scipy.org/doc/
SciPy

- SciPy is built on top of NumPy and implements many specialized scientific computation tools:
  - Clustering, Fourier transforms, numerical integration, interpolations, data I/O, LAPACK, sparse matrices, linear solvers, optimization, signal processing, statistical functions, sparse eigenvalue solvers, ...
Matplotlib

- Powerful library for 2D (and some 3D) plotting
- Well designed, interactive use and scripted, common tasks easy, complex tasks possible
Matplotlib

- Example workflow for plotting with matplotlib.
- Check out: http://matplotlib.org/gallery.html

```python
>>> import pylab as pl
>>> xs = pl.linspace(0,100,101)
>>> ys = pl.sin(xs)
>>> cols = pl.random(101)
>>> sizes = 100.0 * pl.random(101)
>>> pl.scatter(xs,ys,c=cols,s=sizes)
<matplotlib.collections.PathCollection object at 0x7fa0b4430ba8>
>>> pl.savefig('scatter-test.png')
```
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