Numerical Analysis and Programming: Numpy Tutorial

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This tutorial is based on the the official tentative Numpy tutorial (http://www.scipy.org/Tentative_NumPy_Tutorial), and you should always consult the official Numpy reference manual for information, see http://docs.scipy.org/doc/ for more details.

1 Importing the NumPy module

There are several ways to import NumPy. The standard approach is to use a simple import statement:

```
>>> import numpy
```

However, for large amounts of calls to NumPy functions, it can become tedious to write numpy . X over and over again. Instead, it is common to import under the briefer name np:

```
>>> import numpy as np
```

This statement will allow us to access NumPy objects using np. X instead of numpy. X. It is also possible to import NumPy directly into the current namespace so that we don't have to use dot notation at all, but rather simply call the functions as if they were built-in:

```
>>> from numpy import *
```

However, this strategy is usually not recommended except for short interactive sessions because it removes some of the nice organization that modules provide. For the remainder of this tutorial, we will assume that the import numpy as np has been used. Notice ipython notebook automatically import numpy and alias it as np.

2 Basics

NumPy's main object is the homogeneous multidimensional array. It is a table of elements (usually numbers), all of the same type, indexed by a tuple of positive integers. In Numpy dimensions are called *axes* and the number of axes is *rank*. For example, the coordinates of a point in 3D space [1, 2, 1] is an array of rank 1, because it has one axis. That axis has a length of 3. In example pictured below, the array has rank 2 (it is 2-dimensional). The first dimension (axis) has a length of 2, the second dimension has a length of 3.

```
[[ 1., 0., 0.],
[ 0., 1., 2.]]
```

Numpy's array class is called ndarray. It is also known by the alias array. The more important attributes of an ndarray object are:

• **ndarray.ndim** gives the number of axes (dimensions) of the array. In the Python world, the number of dimensions is referred to as rank.

```
>>> x = np.array( ((11,12,13), (21,22,23) ))
>>> x.ndim
2
```

• ndarray. shape gives the dimensions of the array. This is a tuple of integers indicating the size of the array in each dimension. For a matrix with n rows and m columns, shape will be (n,m). The length of the shape tuple is therefore the rank, or number of dimensions, ndim.

- **ndarray.size** gives the total number of elements of the array. This is equal to the product of the elements of shape.
- ndarray.dtype gives an object describing the type of the elements in the array. One can create or specify dtype's using standard Python types. Additionally NumPy provides types of its own. numpy.int32, numpy.int16, and numpy.float6 are some examples.

- **ndarray.itemsize** gives the size in bytes of each element of the array. For example, an array of elements of type float 64 has itemsize 8 (=64/8), while one of type complex 32 has itemsize 4 (=32/8).
- ndarray.data gives the buffer containing the actual elements of the array. Normally, we won't need to use this attribute because we will access the elements in an array using indexing facilities.

3 Example

```
>>>import numpy as np
>>> a = np.arange(15).reshape(3, 5)
>>> a
array([[ 0, 1, 2, 3, 4],
      [5, 6, 7, 8, 9],
      [10, 11, 12, 13, 14]])
>>> a.shape
(3, 5)
>>> a.ndim
>>> a.dtype.name
'int32'
>>> a.itemsize
>>> a.size
15
>>> type(a)
numpy.ndarray
>>> b = np.array([6, 7, 8])
>>> b
array([6, 7, 8])
>>> type(b)
numpy.ndarray
```

4 Array Creation

There are several ways to create arrays. For example, you can create an array from a regular Python list or tuple using the array function. The type of the resulting array is deduced from the type of the elements in the sequences.

```
>>> a = np.array( [2,3,4] )
>>> a
array([2, 3, 4])
>>> a.dtype
dtype('int32')
>>> b = np.array([1.2, 3.5, 5.1])
```

```
>>> b.dtype dtype('float64')
```

A frequent error consists in calling array with multiple numeric arguments, rather than providing a *single list of numbers* as an argument.

```
>>> a = np.array(1,2,3,4)  # WRONG
>>> a = np.array([1,2,3,4])  # RIGHT
```

array transforms sequences of sequences into two-dimensional arrays, sequences of sequences of sequences into three-dimensional arrays, and so on.

The type of the array can also be explicitly specified at creation time:

Often, the elements of an array are originally unknown, but its size is known. Hence, NumPy offers several functions to create arrays with initial placeholder content. These minimize the necessity of growing arrays, an expensive operation. The function zeros creates an array full of zeros, the function ones creates an array full of ones, and the function empty creates an array whose initial content is random and depends on the state of the memory. By default, the dtype of the created array is float 64.

```
>>> np.zeros((3,4))
array([[0., 0., 0.,
                       0.],
             0., 0.,
                       0.],
       [0.,
       [0., 0., 0.,
                       0.]])
>>> np.ones((2,3,4), dtype=int16)
array([[[ 1, 1, 1, 1],
       [ 1, 1, 1, 1],
       [ 1, 1, 1, 1]],
       [[1, 1, 1, 1],
        [ 1, 1, 1, 1],
        [ 1, 1, 1, 1]]], dtype=int16)
>>> np.empty( (2,3) )
array([[ 3.73603959e-262, 6.02658058e-154, 6.55490914e-260],
       [ 5.30498948e-313, 3.14673309e-307, 1.00000000e+000]])
```

To create sequences of numbers, NumPy provides a function analogous to range that returns arrays instead of lists

```
>>> np.arange( 10, 30, 5 ) array([10, 15, 20, 25])
```

```
>>> np.arange( 0, 2, 0.3 ) array([ 0., 0.3, 0.6, 0.9, 1.2, 1.5, 1.8])
```

When arange is used with floating point arguments, it is generally not possible to predict the number of elements obtained, due to the finite floating point precision. For this reason, it is usually better to use the function linspace that receives as an argument the number of elements that we want, instead of the step:

```
>>> np.linspace( 0, 2, 9 ) # 9 numbers from 0 to 2
array([ 0., 0.25, 0.5, 0.75, 1., 1.25, 1.5, 1.75, 2.])
>>> x = np.linspace( 0, 2*np.pi, 100 )
>>> f = np.sin(x)
```

5 Basic Operations

Arithmetic operators on arrays apply elementwise. A new array is created and filled with the result.

```
>>> a = np.array( [20,30,40,50] )
>>> b = np.arange( 4 )
>>> b
array([0, 1, 2, 3])
>>> c = a-b
>>> c
array([20, 29, 38, 47])
>>> b**2
array([0, 1, 4, 9])
>>> 10*np.sin(a)
array([ 9.12945251, -9.88031624, 7.4511316 , -2.62374854])
>>> a<35
array([True, True, False, False], dtype=bool)
```

Unlike in many matrix languages, the product operator * operates *elementwise* in NumPy arrays. The matrix product can be performed using the dot function or creating matrix objects.

Some operations, such as += and *=, act in place to modify an existing array rather than create a new one.

When operating with arrays of different types, the type of the resulting array corresponds to the more general or precise one (a behavior known as *upcasting*).

6 Universal Functions

NumPy provides familiar mathematical functions such as sin, cos, and exp, etc. In NumPy, these are called "universal functions" (ufunc). Within NumPy, these functions operate *elementwise* on an array, producing an array as output.

```
>>> B = np.arange(3)

>>> B

array([0, 1, 2])

>>> np.exp(B)

array([1., 2.71828183, 7.3890561])

>>> np.sqrt(B)

array([0., 1., 1.41421356])

>>> C = np.array([2., -1., 4.])
```

```
>>> np.add(B, C) array([ 2., 0., 6.])
```

The items in an array can be summed or multiplied:

```
>>> a = np.array([2, 4, 3], float)
>>> a.sum()
9.0
>>> a.prod()
24.0
```

In this example, member functions of the arrays were used. Alternatively, standalone functions in the NumPy module can be accessed:

```
>>> np.sum(a)
9.0
>>> np.prod(a)
24.0
```

For most of the routines described below, both standalone and member functions are available. A number of routines enable computation of statistical quantities in array datasets, such as the mean (average), variance, and standard deviation:

```
>>> a = np.array([2, 1, 9], float)
>>> a.mean()
4.0
>>> a.var()
12.66666666666666666666
>>> a.std()
3.5590260840104371
```

It's also possible to find the minimum and maximum element values:

```
>>> a = np.array([2, 1, 9], float)
>>> a.min()
1.0
>>> a.max()
9.0
```

The argmin and argmax functions return the array indices of the minimum and maximum values:

```
>>> a = np.array([2, 1, 9], float)
>>> a.argmin()
1
>>> a.argmax()
2
```

For multidimensional arrays, each of the functions thus far described can take an optional argument axis that will perform an operation along only the specified axis, placing the results in a return array:

```
>>> a = np.array([[0, 2], [3, -1], [3, 5]], float)
>>> a.mean(axis=0)
array([ 2., 2.])
>>> a.mean(axis=1)
array([ 1.,  1.,  4.])
>>> a.min(axis=1)
array([ 0., -1.,  3.])
>>> a.max(axis=0)
array([ 3., 5.])
```

7 Array mathematics

When standard mathematical operations are used with arrays, they are applied on an *element-wise* basis. This means that the arrays should be the same size during addition, subtraction, etc.:

```
>>> 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.])
```

For two-dimensional arrays, multiplication remains elementwise and does not correspond to matrix multiplication. There are special functions for matrix math that we will cover later.

```
>>> a = np.array([[1,2], [3,4]], float)
>>> b = np.array([[2,0], [1,3]], float)
>>> a * b
array([[2., 0.], [3., 12.]])
```

Errors are thrown if arrays do not match in size:

```
>>> a = np.array([1,2,3], float)
>>> b = np.array([4,5], float)
>>> a + b
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: shape mismatch:
objects cannot be broadcast to a single shape
```

8 Vector and matrix mathematics

NumPy provides many functions for performing standard vector and matrix multiplication routines. To perform a dot product,

```
>>> a = np.array([1, 2, 3], float)
>>> b = np.array([0, 1, 1], float)
>>> np.dot(a, b)
5.0
```

The dot function also generalizes to matrix multiplication:

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

It is also possible to generate inner, outer, and cross products of matrices and vectors. For vectors, note that the inner product is equivalent to the dot product:

```
>>> a = np.array([1, 4, 0], float)

>>> b = np.array([2, 2, 1], float)

>>> np.outer(a, b)

array([[ 2., 2., 1.],

  [ 8., 8., 4.],

  [ 0., 0., 0.]])

>>> np.inner(a, b)

10.0

>>> np.cross(a, b)

array([ 4., -1., -6.])
```

For a high-dimensional tensors, the function tensordot computes tensor dot product along specified axes.

```
[[ 0.95568698,
                       0.60541739, 0.657405 ],
        [ 0.21022514,
                       0.27462493, 0.32806541],
        [ 0.80856084,
                      0.06451977, 0.33994045],
        [0.46833801, 0.35243041, 0.83470196]])
>>>>> b=np.array(np.random.random((4,3,2)))
>>> b
array([[[ 0.87176381, 0.68883495],
       [ 0.16451053,
                       0.8020721 ],
                       0.15417885]],
        [ 0.82210924,
       [[ 0.01163689,
                       0.67328002],
        [ 0.61299208,
                       0.619379041,
        [ 0.91849722,
                       0.05603531]],
       [[ 0.66886977,
                       0.20655257],
       [ 0.06674962,
                       0.33113124],
        [ 0.05115619,
                       0.75813028]],
       [[0.50889226, 0.44853399],
        [ 0.30247792, 0.63194832],
        [ 0.83564744,
                       0.98830335]])
>>>np.tensordot(a,b, axes=2)
array([[ 2.65168075, 2.44608012],
       [ 3.55027721, 3.27909354]])
\Rightarrow a = np.arange(60.).reshape(3,4,5)
>>> b = np.arange(24.).reshape(4,3,2)
>>> c = np.tensordot(a,b, axes=([1,0],[0,1]))
>>> c.shape
(5, 2)
>>> c
array([[ 4400., 4730.],
       [ 4532.,
               4874.],
       [ 4664., 5018.],
       [ 4796., 5162.],
       [ 4928.,
               5306.11)
```

NumPy also provides a number of built-in routines for linear algebra calculations. These can be found in the sub-module linalg. Among these are routines for dealing with matrices and their inverses. The determinant of a matrix can be found:

```
>>> a = np.array([[4, 2, 0], [9, 3, 7], [1, 2, 1]], float)
>>> a
array([[ 4., 2., 0.],
        [ 9., 3., 7.],
        [ 1., 2., 1.]])
>>> np.linalg.det(a)
-53.9999999999999
```

One can find the eigenvalues and eigenvectors of a matrix:

```
>>> vals, vecs = np.linalg.eig(a)
>>> vals
```

```
array([ 9. , 2.44948974, -2.44948974])
>>> vecs
array([[-0.3538921 , -0.56786837, 0.27843404],
    [-0.88473024, 0.44024287, -0.89787873],
    [-0.303333608, 0.69549388, 0.34101066]])
```

The inverse of a matrix can be found:

```
>>> b = np.linalg.inv(a)

>>> b

array([[ 0.14814815, 0.07407407, -0.25925926],

[ 0.2037037 , -0.14814815, 0.51851852],

[-0.27777778, 0.111111111, 0.11111111]])

>>> np.dot(a, b)

array([[ 1.00000000e+00, 5.55111512e-17, 2.22044605e-16],

[ 0.00000000e+00, 1.00000000e+00, 5.55111512e-16],

[ 1.11022302e-16, 0.00000000e+00, 1.00000000e+00]])
```

Singular value decomposition (analogous to diagonalization of a nonsquare matrix) can also be performed:

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

>>> U, s, Vh = np.linalg.svd(a)

>>> U

array([[-0.6113829 , -0.79133492],

  [-0.79133492, 0.6113829 ]])

>>> s

array([ 7.46791327, 2.86884495])

>>> Vh

array([[-0.61169129, -0.45753324, -0.64536587],

  [ 0.78971838, -0.40129005, -0.46401635],

  [-0.046676 , -0.79349205, 0.60678804]])
```

9 Indexing, Slicing and Iterating

One-dimensional arrays can be indexed, sliced and iterated over, much like lists and other Python sequences.

```
>>> a = np.arange(10) **3
>>> a
array([ 0,  1,  8,  27,  64, 125, 216, 343, 512, 729])
>>> a[2]
8
>>> a[2:5]
array([ 8,  27,  64])
>>> a[:6:2] = -1000
>>> a
array([-1000, 1, -1000, 27, -1000, 125, 216, 343, 512, 729])
>>> a[::-1]
array([ 729, 512, 343, 216, 125, -1000, 27, -1000, 1, -1000])
```

```
>>> for i in a:
... print i**(1/3.),
...
nan 1.0 nan 3.0 nan 5.0 6.0 7.0 8.0 9.0
```

Multidimensional arrays can have one index per axis. These indices are given in a tuple separated by commas:

```
>>> def f(x,y):
            return 10*x+y
. . .
>>> b = fromfunction(f,(5,4),dtype=int)
>>> b
array([[ 0, 1, 2, 3],
       [10, 11, 12, 13],
       [20, 21, 22, 23],
       [30, 31, 32, 33],
       [40, 41, 42, 43]])
>>> b[2,3]
23
>>> b[0:5, 1]
array([ 1, 11, 21, 31, 41])
>>> b[ : ,1]
array([ 1, 11, 21, 31, 41])
>>> b[1:3, : ]
array([[10, 11, 12, 13],
       [20, 21, 22, 23]])
```

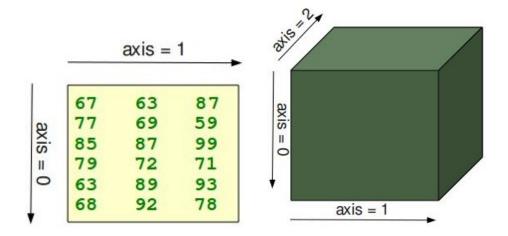


Figure 1: Examples of rank-2 and -3 arrays.

When fewer indices are provided than the number of axes, the missing indices are considered complete slices:

```
>>> b[-1]
array([40, 41, 42, 43])
```

The expression within brackets in b[i] is treated as an i followed by as many instances of: as needed to represent the remaining axes. NumPy also allows you to write this using dots as b[i,...]. The dots (...) represent as many colons as needed to produce a complete indexing tuple. For example, if x is a rank 5 array (i.e., it has 5 axes), then x[1,2,...] is equivalent to x[1,2,:,:,:], x[...,3] to x[:,:,:,:,:] and x[4,...,5,:] to x[4,:,:,5,:].

Iterating over multidimensional arrays is done with respect to the first axis:

```
>>> for row in b:
... print row
...
[0 1 2 3]
[10 11 12 13]
[20 21 22 23]
[30 31 32 33]
[40 41 42 43]
```

However, if one wants to perform an operation on each element in the array, one can use the flat attribute which is an iterator over all the elements of the array:

```
>>> for element in b.flat:
... print element,
...
0 1 2 3 10 11 12 13 20 21 22 23 30 31 32 33 40 41 42 43
```

10 Shape Manipulation

10.1 Changing the shape of an array

An array has a shape given by the number of elements along each axis:

```
>>> a.shape (3, 4)
```

The shape of an array can be changed with various commands:

The order of the elements in the array resulting from ravel() is normally "C-style", that is, the rightmost index "changes the fastest", so the element after a[0,0] is a[0,1]. If the array is reshaped to some other shape, again the array is treated as "C-style". The functions ravel() and reshape() can also be instructed, using an optional argument, to use FORTRAN-style arrays, in which the leftmost index changes the fastest.

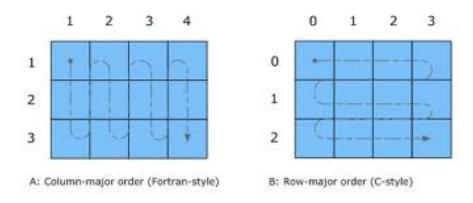


Figure 2: Memory layout of a FORTRAN-style and a C-style array.

The reshape function returns its argument with a modified shape, whereas the resize method modifies the array itself:

If a dimension is given as -1 in a reshaping operation, the other dimensions are automatically calculated:

10.2 Stacking together different arrays

Several arrays can be stacked together along different axes:

```
>>> a = np.floor(10*np.random.random((2,2)))
>>> a
array([[ 1., 1.],
      [ 5., 8.]])
>>> b = np.floor(10*np.random.random((2,2)))
>>> b
array([[ 3., 3.],
       [ 6., 0.]])
>>> np.vstack((a,b))
array([[ 1., 1.],
       [ 5., 8.],
       [ 3., 3.],
       [ 6., 0.]])
>>> np.hstack((a,b))
array([[ 1., 1., 3., 3.],
       [5., 8., 6., 0.]])
```

The function column_stack stacks 1D arrays as columns into a 2D array. It is equivalent to vstack only for 1D arrays:

```
>>> column_stack((a,b))
                           # With 2D arrays
array([[ 1., 1., 3., 3.],
       [ 5., 8., 6., 0.]])
>>> a=np.array([4.,2.])
>>> b=np.array([2.,8.])
>>> a[:,np.newaxis]
array([[ 4.],
       [ 2.]])
>>> column_stack((a[:,np.newaxis],b[:,np.newaxis]))
array([[ 4., 2.],
       [ 2., 8.]])
>>> vstack((a[:,np.newaxis],b[:,np.newaxis]))
array([[ 4.],
       [ 2.],
       [ 2.],
       [ 8.]])
```

10.3 Splitting one array into several smaller ones

Using hsplit, you can split an array along its horizontal axis, either by specifying the number of equally shaped arrays to return, or by specifying the columns after which the division should occur:

vsplit splits along the vertical axis, and array split allows one to specify along which axis to split.

11 Copies and Views

When operating and manipulating arrays, their data is sometimes copied into a new array and sometimes not. This is often a source of confusion for beginners. There are three cases:

11.1 No Copy at All

Simple assignments make no copy of array objects or of their data.

```
>>> a = np.arange(12)
>>> b = a  # no new object is created
>>> b is a
True
>>> b.shape = 3,4
>>> a.shape
(3, 4)
```

Python passes mutable objects as references, so function calls make no copy.

```
>>> def f(x):
... print id(x)
...
>>> id(a)  # id is a unique identifier of an object
148293216
```

```
>>> f(a)
148293216
```

11.2 View or Shallow Copy

Different array objects can share the same data. The view method creates a new array object that looks at the same data.

```
>>> c = a.view()
>>> c is a
False
>>> c.base is a
True
>>> c.flags.owndata
False
>>>
>>> c.shape = 2,6
>>> a.shape
(3, 4)
>>> c[0,4] = 1234
>>> a
                        2,
                               3],
array([[
          Ο,
                  1,
       [1234,
                  5,
                              7],
                       6,
           8,
                  9,
                       10,
                             11]])
```

Slicing an array returns a view of it:

```
>>> s = a[:, 1:3]
>>> s[:] = 10
>>> a
          0,
                       10,
                               3],
array([[
                 10,
                               7],
       [1234,
                       10,
                 10,
       [
           8,
                 10,
                       10,
                              11]])
```

11.3 Deep Copy

The copy method makes a complete copy of the array and its data.

```
>>> d = a.copy()
>>> d is a
False
>>> d.base is a
False
>>> d[0,0] = 9999
>>> a
          Ο,
                       10,
array([[
                 10,
                               3],
       [1234,
                       10,
                 10,
                               7],
                 10,
                       10,
                              11]])
           8,
```