Computational Analysis of Physical Systems (Lecture 6)

Matrix Operations

Matrix operations

- Use NumPy (or SciPy)

```
>>> import numpy
```

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

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

Matrix operations

```
>>> a = np.array([1, 4, 5, 8], float)
>>> a
array([ 1.,  4.,  5.,  8.])
>>> type(a)
<type 'numpy.ndarray'>
```

```
>>> a[:2]
array([ 1.,  4.])
>>> a[3]
8.0
>>> a[0] = 5.
>>> a
array([ 5.,  4.,  5.,  8.])
```

Matrix operations

```
>>> a = np.array([[1, 2, 3], [4, 5, 6]], float)
>>> a
array([[ 1.,  2.,  3.],
       [ 4.,  5.,  6.]])
>>> a[0,0]
1.0
>>> a[0,1]
2.0
```

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

Matrix operations

```
>>> a.shape
(2, 3)
```

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

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

Matrix operations

The `in` statement can be used to test if values are present in an array:

```
>>> a = np.array([[1, 2, 3], [4, 5, 6]], float)
>>> 2 in a
True
>>> 0 in a
False
```

```
>>> a = np.array(range(10), float)
>>> a
array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9.])
>>> a = a.reshape((5, 2))
>>> a
array([[ 0.,  1.],
       [ 2.,  3.],
       [ 4.,  5.],
       [ 6.,  7.],
       [ 8.,  9.]])
>>> a.shape
(5, 2)
```

Matrix operations

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

Lists can also be created from arrays:

```
>>> a = np.array([1, 2, 3], float)
>>> a.tolist()
[1.0, 2.0, 3.0]
>>> list(a)
[1.0, 2.0, 3.0]
```

Matrix operations

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

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

Matrix operations

One-dimensional versions of multi-dimensional arrays can be generated with `flatten`:

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

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

Matrix operations

the dimensionality of an array can be increased using the `newaxis` constant in bracket notation:

```
>>> a = np.array([1, 2, 3], float)
>>> a
array([1., 2., 3.])
>>> a[:,np.newaxis]
array([[ 1.],
       [ 2.],
       [ 3.]])
>>> a[:,np.newaxis].shape
(3,1)
>>> b[np.newaxis,:]
array([[ 1.,  2.,  3.]])
>>> b[np.newaxis,:].shape
(1,3)
```

Matrix operations

```
>>> np.arange(5, dtype=float)
array([ 0.,  1.,  2.,  3.,  4.])
>>> np.arange(1, 6, 2, dtype=int)
array([1, 3, 5])
```

```
>>> np.ones((2,3), dtype=float)
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
>>> np.zeros(7, dtype=int)
array([0, 0, 0, 0, 0, 0, 0])
```

Matrix operations

The `zeros_like` and `ones_like` functions create a new array with the same dimensions and type of an existing one:

```
>>> a = np.array([[1, 2, 3], [4, 5, 6]], float)
>>> np.zeros_like(a)
array([[ 0.,  0.,  0.],
       [ 0.,  0.,  0.]])
>>> np.ones_like(a)
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

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

```
>>> np.eye(4, k=1, dtype=float)
array([[ 0.,  1.,  0.,  0.],
       [ 0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.],
       [ 0.,  0.,  0.,  0.]])
```

Matrix operations

When standard mathematical operations are used with arrays, they are applied on an element-by-element 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.])
```

Matrix operations

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
```

Matrix operations

However, arrays that do not match in the number of dimensions will be *broadcasted* by Python to perform mathematical operations. This often means that the smaller array will be repeated as necessary to perform the operation indicated. Consider the following:

```
>>> a = np.array([[1, 2], [3, 4], [5, 6]], float)
>>> b = np.array([-1, 3], float)
>>> a
array([[ 1.,  2.],
       [ 3.,  4.],
       [ 5.,  6.]])
>>> b
array([-1.,  3.])
>>> a + b
array([[ 0.,  5.],
       [ 2.,  7.],
       [ 4.,  9.]])
```

Matrix operations

```
>>> a = np.array([1, 4, 9], float)
>>> np.sqrt(a)
array([ 1.,  2.,  3.])
```

```
>>> a = np.array([1.1, 1.5, 1.9], float)
>>> np.floor(a)
array([ 1.,  1.,  1.])
>>> np.ceil(a)
array([ 2.,  2.,  2.])
>>> np.rint(a)
array([ 1.,  2.,  2.])
```

```
>>> np.pi
3.1415926535897931
>>> np.e
2.7182818284590451
```

Matrix operations

It is possible to iterate over arrays in a manner similar to that of lists:

```
>>> a = np.array([1, 4, 5], int)
>>> for x in a:
...   print x
... <hit return>
1
4
5
```

```
>>> a = np.array([[1, 2], [3, 4], [5, 6]], float)
>>> for x in a:
...   print x
... <hit return>
[ 1.  2.]
[ 3.  4.]
[ 5.  6.]
```

Matrix operations

```
>>> a = np.array([[1, 2], [3, 4], [5, 6]], float)
>>> for (x, y) in a:
...   print x * y
...  <hit return>
2.0
12.0
30.0
```

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

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

Matrix operations

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()
12.666666666666666
>>> 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
```

Matrix operations

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
```

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

Matrix operations

```
>>> a = np.array([6, 2, 5, -1, 0], float)
>>> sorted(a)
[-1.0, 0.0, 2.0, 5.0, 6.0]
>>> a.sort()
>>> a
array([-1.,  0.,  2.,  5.,  6.])
```

Unique elements can be extracted from an array:

```
>>> a = np.array([1, 1, 4, 5, 5, 5, 7], float)
>>> np.unique(a)
array([ 1.,  4.,  5.,  7.])
```

For two dimensional arrays, the diagonal can be extracted:

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

Matrix operations

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

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

Matrix operations

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

```
>>> 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)
-53.999999999999993
```

Matrix operations

```
>>> 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],
       [-0.30333608,  0.69549388,  0.34101066]])
```

```
>>> b = np.linalg.inv(a)
>>> b
array([[ 0.14814815,  0.07407407, -0.25925926],
       [ 0.2037037 , -0.14814815,  0.51851852],
       [-0.27777778,  0.11111111,  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]])
```

Matrix operations

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]])
```

Matrix operations

```
>>> np.random.rand(2,3)
array([[ 0.50431753,  0.48272463,  0.45811345],
       [ 0.18209476,  0.48631022,  0.49590404]])
>>> np.random.rand(6).reshape((2,3))
array([[ 0.72915152,  0.59423848,  0.25644881],
       [ 0.75965311,  0.52151819,  0.60084796]])
```

```
>>> l = range(10)
>>> l
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
>>> np.random.shuffle(l)
>>> l
[4, 9, 5, 0, 2, 7, 6, 8, 1, 3]
```