

Introductory Scientific Computing with Python

Numpy arrays

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Outline

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numpy arrays

- Slicing arrays
- Array creation
- Example: plotting data from file

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The numpy module

- Efficient, powerful array type
- Abstracts out standard operations on arrays
- Convenience functions
- **ipython --pylab** imports part of numpy

Without Pylab

```
In []: from numpy import *
In []: x = linspace(0, 1)
```

Note that we had done this “import” earlier!

Can also do this:

```
In []: import numpy
In []: x = numpy.linspace(0, 1)
```

or

```
In []: import numpy as np
In []: x = np.linspace(0, 1)
```

Note the use of **numpy.linspace**

numpy arrays

- Fixed size (`arr.size`)
- Same type (`arr.dtype`)
- Arbitrary dimensionality: `arr.shape`
- `shape`: extent (size) along each dimension
- `arr.itemsize`: number of bytes per element
- **Note:** `shape` can change so long as the `size` is constant
- Indices start from 0
- Negative indices work like lists

numpy arrays

```
In []: a = array([1,2,3,4])  
In []: b = array([2,3,4,5])
```

```
In []: print(a[0], a[-1])  
(1, 4)
```

```
In []: a[0] = -1  
In []: a[0] = 1
```

Operations are elementwise

Simple operations

```
In []: a + b
```

```
Out[]: array([3, 5, 7, 9])
```

```
In []: a*b
```

```
Out[]: array([2, 6, 12, 20])
```

```
In []: a/b
```

```
Out[]: array([0, 0, 0, 0])
```

- Operations are **element-wise**
- Types matter

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Data type matters

Try again with this:

```
In []: a = array([1.,2,3,4])  
In []: a/b
```

Examples

`pi` and `e` are defined.

```
In []: x = linspace(0.0, 10.0, 200)
```

```
In []: x *= 2*pi/10
```

apply functions to array.

```
In []: y = sin(x)
```

```
In []: y = cos(x)
```

```
In []: x[0] = -1
```

```
In []: print(x[0], x[-1])
```

```
(-1.0, 10.0)
```

size, shape, rank etc.

```
In []: x = array([1., 2, 3, 4])
In []: size(x)
Out[]: 4
In []: x.dtype
dtype('float64')
In []: x.shape
Out[]: (4,)
In []: rank(x)
Out[]: 1
In []: x.itemsize
Out[]: 8
```

Multi-dimensional arrays

```
In []: a = array([[ 0,  1,  2,  3],  
...:                 [10,11,12,13]])
```

```
In []: a.shape # (rows, columns)
```

```
Out[]: (2, 4)
```

```
In []: a[1,3]
```

```
Out[]: 13
```

```
In []: a[1,3] = -1
```

```
In []: a[1] # The second row  
array([10,11,12,-1])
```

```
In []: a[1] = 0 # Entire row to zero.
```

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Slicing arrays

```
In []: a = array([[1,2,3], [4,5,6],  
...:                 [7,8,9]])
```

```
In []: a[0,1:3]
```

```
Out[]: array([2, 3])
```

```
In []: a[1:,1:]
```

```
Out[]: array([[5, 6],  
...:                 [8, 9]])
```

```
In []: a[:,2]
```

```
Out[]: array([3, 6, 9])
```

Slicing arrays

```
In []: a = array([[1,2,3], [4,5,6],  
...: [7,8,9]])
```

```
In []: a[0,1:3]
```

```
Out[]: array([2, 3])
```

```
In []: a[1:,1:]
```

```
Out[]: array([[5, 6],  
[8, 9]])
```

```
In []: a[:,2]
```

```
Out[]: array([3, 6, 9])
```

Slicing arrays

```
In []: a = array([[1,2,3], [4,5,6],  
...: [7,8,9]])
```

```
In []: a[0,1:3]
```

```
Out[]: array([2, 3])
```

```
In []: a[1:,1:]
```

```
Out[]: array([[5, 6],  
[8, 9]])
```

```
In []: a[:,2]
```

```
Out[]: array([3, 6, 9])
```

Slicing arrays

```
In []: a = array([[1,2,3], [4,5,6],  
...: [7,8,9]])
```

```
In []: a[0,1:3]
```

```
Out[]: array([2, 3])
```

```
In []: a[1:,1:]
```

```
Out[]: array([[5, 6],  
[8, 9]])
```

```
In []: a[:,2]
```

```
Out[]: array([3, 6, 9])
```

Slicing arrays ...

```
In []: a = array([[1,2,3], [4,5,6],  
...:                 [7,8,9]])
```

```
In []: a[0::2,0::2] # Striding...
```

```
Out[]: array([[1, 3],  
              [7, 9]])
```

Slices refer to the same memory!

Slicing arrays ...

```
In []: a = array([[1,2,3], [4,5,6],  
...:                 [7,8,9]])
```

```
In []: a[0::2,0::2] # Striding...
```

```
Out[]: array([[1, 3],  
              [7, 9]])
```

Slices refer to the same memory!

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Array creation functions

- `array(object)`
- `linspace(start, stop, num=50)`
- `ones(shape)`
- `zeros((d1, ..., dn))`
- `empty((d1, ..., dn))`
- `identity(n)`
- `ones_like(x), zeros_like(x),
empty_like(x)`

May pass an optional `dtype=` keyword argument
For more dtypes see: `numpy.typeDict`

Creation examples

```
In []: a = array([1,2,3], dtype=float)
```

```
In []: ones_like(a)
```

```
Out[]: array([ 1.,  1.,  1.])
```

```
In []: ones( (2, 3) )
```

```
Out[]: array([[ 1.,  1.,  1.],
              [ 1.,  1.,  1.]])
```

```
In []: identity(3)
```

```
Out[]: array([[ 1.,  0.,  0.],
              [ 0.,  1.,  0.],
              [ 0.,  0.,  1.]])
```

Array math

- Basic **elementwise** math (given two arrays **a**, **b**):
 - **a + b** → **add(a, b)**
 - **a - b**, → **subtract(a, b)**
 - **a * b**, → **multiply(a, b)**
 - **a / b**, → **divide(a, b)**
 - **a % b**, → **remainder(a, b)**
 - **a ** b**, → **power(a, b)**
- Inplace operators: **a += b**, or **add(a, b, a)**
What happens if **a is **int** and **b** is **float**?**

Array math

- Logical operations: `==`, `!=`, `<`, `>`, etc.
- `sin(x)`, `arcsin(x)`, `sinh(x)`,
`exp(x)`, `sqrt(x)` etc.
- `sum(x, axis=0)`, `product(x, axis=0)`
- `dot(a, b)`

Convenience functions: `loadtxt`

- `loadtxt(file_name)`: loads a text file
- `loadtxt(file_name, unpack=True)`:
loads a text file and unpacks columns

```
In []: x = loadtxt('pendulum.txt')
```

```
In []: x.shape
```

```
Out[]: (90, 2)
```

```
In []: x, y = loadtxt('pendulum.txt',  
...:                      unpack=True)
```

```
In []: x.shape
```

```
Out[]: (90, )
```

Advanced

- Only scratched the surface of numpy
- **reduce**, **outer**
- Typecasting
- More functions: **take**, **choose**, **where**,
compress, **concatenate**
- Array broadcasting and **None**
- Record arrays

Learn more

- <https://docs.scipy.org/doc/numpy-dev/user/quickstart.html>
- <http://numpy.org>

Recap

- Basic concepts: creation, access, operations
- 1D, multi-dimensional
- Slicing
- Array creation, dtypes
- Math
- `loadtxt`

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Example: plotting data from file

Data is usually present in a file!

Lets look at the `pendulum.txt` file.

```
In []: cat pendulum.txt
```

```
1.0000e-01 6.9004e-01
```

```
1.1000e-01 6.9497e-01
```

```
1.2000e-01 7.4252e-01
```

```
1.3000e-01 7.5360e-01
```

```
...
```

Reading pendulum.txt

- File contains L vs. T values
- First Column - L values
- Second Column - T values
- Let us generate a plot from the data file

Gotcha and an aside

Ensure you are in the same directory as

pendulum.txt

if not, do the following on IPython:

```
In []: %cd directory_containing_file  
# Check if pendulum.txt is there.
```

```
In []: ls
```

```
# Also try
```

```
In []: !ls
```

Note: `%cd` is an IPython magic command. For more information do:

```
In []: ?
```

```
In []: %cd?
```

Exercise

- Plot L versus T square with dots
- No line connecting points

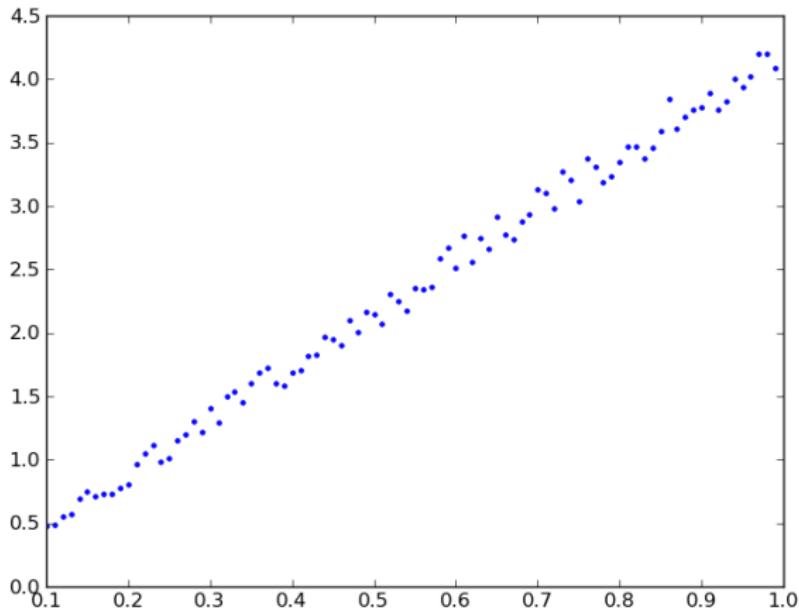
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Solution

```
In []: L, t = loadtxt('pendulum.txt',
....:                      unpack=True)
In []: plot(L, t*t, '.'')
```

or

```
In []: x = loadtxt('pendulum.txt')
In []: L, t = x[:,0], x[:,1]
In []: plot(L, t*t, '.'')
```



Odds and ends

```
In []: mean(L)
```

```
Out []: 0.5449999999999993
```

```
In []: std(L)
```

```
Out []: 0.25979158313283879
```

Summary

- Introduction to numpy arrays
- Slicing arrays
- Multi-dimensional arrays
- Array operations
- Creating arrays
- Loading data from file

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