NUMPY AND SCIPY PACKAGES

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NUMPY

- The numpy package is used in almost all numerical computation using Python
- It is a package that provide high-performance vector, matrix and higher-dimensional data structures
- It is implemented in C and Fortran so when calculations are vectorized (formulated with vectors and matrices), performance is very good

To use numpy you need to import the module

```
import numpy as np
print("Numpy version {:}".format(np.__version__))
```

```
Numpy version 1.8.2
```

GETTING STARTED

- Getting Numpy
- Numpy and scipy documentation page
- Numpy tutorial
- Numpy for MATLAB Users
- Numpy functions by category

CREATING NUMPY ARRAYS

There are a number of ways to initialize new numpy arrays, for example from

- a Python list or tuples
- using functions that are dedicated to generating Numpy arrays, such as np.arange, np.linspace, etc.
- reading data from files

FROM LISTS

```python
# a vector: the argument to the function is a Python list
v = np.array([1, 2, 3, 4])
print(v)
```

```
>>> [1 2 3 4]
```

```python
# a matrix: the argument to the function is a nested Python list
M = np.array([[1, 2], [3, 4]])
print(M)
```

```
>>> [[1 2]
 [3 4]]
```

DIFFERENCE BETWEEN V AND M

```
print(type(v), type(M))
```

```
(<type 'numpy.ndarray'>, <type 'numpy.ndarray'>)
```

The difference between the v and M arrays is only their shapes. The information about the shape of an array by using the `ndarray.shape` property.

```
print(v.shape, M.shape)
```

```
((4,), (2, 2))
```

NUMPY ARRAY VS. LISTS

So far the `numpy.ndarray` looks awefully much like a Python list (or nested list). Why not simply use Python lists for computations instead of a new array type?

There are several reasons:

- Python lists are very general. Each element can be any kind of object. They are dynamically typed. They do not support mathematical functions such as matrix and dot multiplications, etc. Implementating such functions for Python lists would not be very efficient because of the dynamic typing

- Numpy arrays are statically typed and homogeneous. The type of the elements is determined when the array is created.
- Numpy arrays are memory efficient and element access is fast.
- Because of the static typing, fast implementation of mathematical functions such as multiplication and addition of numpy arrays can be implemented in a compiled language (C and Fortran is used).

TYPE OF AN ARRAY

Using the `ndarray.dtype` (data type) property, we can see the type of an array:

```
print(v.dtype, M.dtype)
```

```
(dtype('int64'), dtype('int64'))
```

We get an error if we try to assign a value of an uncastable type to an element in a Numpy array:

```
M[0, 0] = "hello"
```

```
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: invalid literal for long() with base 10: 'hello'
```

But be aware that the type is defined by the array at the initialization and won't be changed if a value from another type is assigned

```
M[0, 0] = 1.2345
print(M[0, 0], M.dtype)
```

```
(1, dtype('int64'))
```

However, the data type can be changed later if it is desired (e.g. using `numpy.ndarray.astype`).

```
x = M.astype(np.float32)
print(x, x.dtype)
```

```
(array([[ 1.,  2.],
       [ 3.,  4.]], dtype=float32), dtype('float32'))
```

If we want, we can explicitly define the data type of the array during creation, using the `dtype` keyword argument.

```
M = np.array([[1, 2], [3, 4]], dtype=np.complex)
print(M)
```

```
[[ 1.+0.j  2.+0.j]
 [ 3.+0.j  4.+0.j]]
```

Common types that can be used with `dtype` are, e.g.: `np.int8`, `np.int16`, `np.int32`, `np.int64`, `np.uint8`, `np.uint16`, `np.uint32`, `np.uint64`, `np.float32`, `np.float64`, `np.complex`, `np.bool`, `np.object`, etc.

USING ARRAY-GENERATING FUNCTIONS

For larger arrays it is unpractical to initialize the data manually, using explicit python lists. Instead we can use one of the many functions in Numpy that generate arrays of different forms. Some of the more common ones are:

Ones and Zeros

np.empty, np.zeros, np.ones

Numerical ranges

np.arange, np.linspace, np.logspace

Random numbers

np.random.rand, np.random.randn

Building matrices

np.identity, np.diag, np.tri, np.tril, p.triu

From existing data

np.fromfile, np.fromstring, np.loadtxt

ONES AND ZEROS

np.zeros

```
x = np.zeros(3, dtype=np.int)
print(x)
```

```
[0 0 0]
```

np.ones

```
x = np.ones((3, 3), dtype=np.float)
print(x)
```

```
[[ 1.  1.  1.]
 [ 1.  1.  1.]
 [ 1.  1.  1.]]
```

NUMERICAL RANGES

np.arange

```
# creates a range, arguments: [start=0], stop, [step=1]
x = np.arange(10)
print(x)
```

```
>>> [0 1 2 3 4 5 6 7 8 9]
```

```
x = np.arange(2, -1, -0.5)
print(x)
```

```
[ 2.   1.5  1.   0.5  0.  -0.5]
```

np.linspace

```python
# using linspace, both end points ARE included
x = np.linspace(0, 10, 11)
print(x)
```

```
>>> [  0.    1.    2.    3.    4.    5.    6.    7.    8.    9.   10.]
```

np.logspace

```python
x = np.logspace(0, 10, 11, base=10)
print(x)
```

```
[  1.00000000e+00   1.00000000e+01   1.00000000e+02   1.00000000e+03
   1.00000000e+04   1.00000000e+05   1.00000000e+06   1.00000000e+07
   1.00000000e+08   1.00000000e+09   1.00000000e+10]
```

RANDOM NUMBERS

np.random.rand

```python
# each element is from the uniform random distribution [0,1]
x = np.random.rand(5, 5)
print(x)
```

```
>>> [[ 0.90984918  0.12546073  0.88846987  0.34910774  0.6464333 ]
 [ 0.14500223  0.75083761  0.33004131  0.68755833  0.24862768]
 [ 0.55080022  0.31571509  0.27164927  0.75086213  0.57095151]
 [ 0.14697981  0.01430727  0.51664101  0.13387468  0.61572481]
 [ 0.08381196  0.98350014  0.09873363  0.32011414  0.41068317]]
```

The standard normal distribution is available as

np.random.randn

BUILDING MATRICES

np.diag

```
x = np.diag([1, 2, 3]) # the diagonal of an otherwise zero matrix
print(x)
```

```
[[1 0 0]
 [0 2 0]
 [0 0 3]]
```

```
y = np.diag(x)
print(y)
```

```
[1 2 3]
```

np.tri

```
# ones at and below the given diagonal and zeros elsewhere
x = np.tri(3)
print(x)
```

```
>>> [[ 1.  0.  0.]
 [ 1.  1.  0.]
 [ 1.  1.  1.]]
```

np.triu

```
# Upper triangle of an array.
x = np.triu(np.ones((3, 3))*2)
print(x)
```

```
>>> [[ 2.  2.  2.]
 [ 0.  2.  2.]
 [ 0.  0.  2.]]
```

MORE PROPERTIES OF THE NUMPY ARRAYS

```
M = np.ones((3, 3), dtype=np.uint8) * 21
print(M.dtype)
M.itemsize # bytes per element
```

```
uint8
1
```

```
M.nbytes # number of bytes
```

```
9
```

```
M.ndim # number of dimensions
```

```
2
```

MANIPULATING ARRAYS

- Basic indexing and slicing
- Advanced indexing
  - Index arrays
  - Boolean index arrays

BASIC INDEXING

Array indexing refers to any use of the square brackets `[ ]` to index array values. There are many options to indexing, which give Numpy indexing great power, but with power comes some complexity and the potential for confusion.

We can index elements in an array using the square bracket and indices:

```
# v is a vector, and has only one dimension, taking one index
v = np.arange(10)
print(v[0], v[-2])
```

```
>>> (0, 8)
```

BASIC INDEXING

Unlike lists and tuples, Numpy arrays support multidimensional indexing for multidimensional arrays. That means that it is not necessary to separate each dimension's index into its own set of square brackets.

```
v.shape = (2, 5)
print(v)
# v is now a 2 dimensional array, taking two indices
print(v[1, 1]) # same as v[1][1]
```

```
[[0 1 2 3 4]
 [5 6 7 8 9]]
... 6
```

BASIC INDEXING

Note that if one indexes a multidimensional array with fewer indices than dimensions, one gets a subdimensional array. For example:

```
print(v[0])
```

```
[0 1 2 3 4]
```

The same thing can be achieved with using `:`

```
print(v[0, :])
```

```
[0 1 2 3 4]
```

BASIC INDEXING

It must be noted that the returned array is not a copy of the original, but points **to the same values in memory** as does the original array. In the next example, the 1-D array at the first position (0) is returned.

```
print(v[0])
```

```
[0 1 2 3 4]
```

So using a single index on the returned array, results in a single element being returned. That is:

```
print(v[0][2])
```

```
2
```

BASIC INDEXING

Note that `v[0, 2] = v[0][2]` though the second case is more inefficient a new temporary array is created after the first index that is subsequently indexed by 2.

SLICING

It is possible to slice and stride arrays to extract arrays of the same number of dimensions, but of different sizes than the original. The slicing and striding works exactly the same way it does for lists and tuples except that they can be applied to multiple dimensions as well.

```
x = np.arange(10)
print(x[2:5])
print(x[:-7])
print(x[1:7:2])
```

```
[2 3 4]
[0 1 2]
[1 3 5]
```

VIEWS

Note that slices of arrays do not copy the internal array data but also produce new **views** of the original data.

```python
x = np.arange(5)
y = x[::2]
print(x)
print(y)
y[0] = 3
print(x)
print(y)
```

```
>>> [0 1 2 3 4]
[0 2 4]
>>> [3 1 2 3 4]
[3 2 4]
```

Making changes to the view changes the underlying array!

VIEWS

np.ndarray.view

New view of array with the same data and is used two different ways:

1. `a.view(some_dtype)` or `a.view(dtype=some_dtype)` constructs a view of the array's memory with a different data-type. This can cause a reinterpretation of the bytes of memory.
2. `a.view(ndarray_subclass)` or `a.view(type=ndarray_subclass)` just returns an instance of ndarray_subclass that looks at the same array (same shape, dtype, etc.) This does not cause a reinterpretation of the memory.

ADVANCED INDEXING

It is possible to index arrays with other arrays for the purposes of selecting lists of values out of arrays into new arrays. There are two different ways of accomplishing this.

- One uses one or more arrays of index values.
- The other involves giving a boolean array of the proper shape to indicate the values to be selected.

Index arrays are a very powerful tool that allow one to avoid looping over individual elements in arrays and thus greatly improve performance.

INDEX ARRAYS

The use of index arrays ranges from simple, straightforward cases to complex, hard-to-understand cases. For all cases of index arrays, what is returned is a **copy** of the original data, not a view as one gets for slices.

```
x = np.arange(10, 1, -1)
y = x[np.arange(0, 8, 2)]
print(x)
print(y)
y[0] = 55
print(x)
print(y)
```

```
>>> [10  9  8  7  6  5  4  3  2]
[10  8  6  4]
>>> [10  9  8  7  6  5  4  3  2]
[55  8  6  4]
```

BOOLEAN INDEX ARRAYS

Boolean arrays used as indices are treated in a different manner entirely than index arrays. Boolean arrays must be of the same shape as the initial dimensions of the array being indexed.

```
y = np.arange(10)
b = y > 5
print(b, y[b])
```

```
>>> (array([False, False, False, False, False, False,  True,  True,
 True,  True], dtype=bool), array([6, 7, 8, 9]))
```

COMBINING INDEX ARRAYS WITH SLICES

Index arrays may be combined with slices. For example:

```
y = np.arange(64).reshape(8, 8)
print(y[np.array([0,2,4]),1:3])
```

```
[[ 1  2]
 [17 18]
 [33 34]]
```

Likewise, slicing can be combined with broadcasted boolean indices:

```
b = y < 10
print(y[b[:, 1], 1:3])
```

```
[[ 1  2]
 [ 9 10]]
```

STRUCTURAL INDEXING TOOLS

To facilitate easy matching of array shapes with expressions and in assignments, the `np.newaxis` object can be used within array indices to add new dimensions with a size of 1. For example:

```
y = np.ones((3, 3))
print(y.shape)
print(y[:,np.newaxis,:].shape)
```

```
(3, 3)
(3, 1, 3)
```

LINEAR ALGEBRA

Vectorizing code is the key to writing efficient numerical calculation with Python/Numpy. That means that as much as possible of a program should be formulated in terms of matrix and vector operations, like matrix-matrix multiplication.

SCALAR-ARRAY OPERATIONS

We can use the usual arithmetic operators to multiply, add, subtract, and divide arrays with scalar numbers.

```python
v = np.arange(5)
print(v * 2, v + 3, v / 2., v - 5)
```

```
(array([0, 2, 4, 6, 8]), array([3, 4, 5, 6, 7]), array([ 0. ,  0.5,
 1. ,  1.5,  2. ]), array([-5, -4, -3, -2, -1]))
```

ELEMENT-WISE ARRAY-ARRAY OPERATIONS

When we add, subtract, multiply and divide arrays with each other, the default behaviour is element-wise operations:

```python
m = np.arange(9).reshape(3, 3)
v = np.arange(3)
print(m * m)
print(m ** 2)
print(m * v)
```

```
>>> [[ 0  1  4]
 [ 9 16 25]
 [36 49 64]]
[[ 0  1  4]
 [ 9 16 25]
 [36 49 64]]
[[ 0  1  4]
 [ 0  4 10]
 [ 0  7 16]]
```

MATRIX ALGEBRA

We can either use the np.dot function, which applies a matrix-matrix, matrix-vector, or inner vector multiplication to its two arguments:

```
print(np.dot(m, v))
```

```
[ 5 14 23]
```

For 2-D arrays it is equivalent to matrix multiplication, and for 1-D arrays to inner product of vectors.

MATRIX ALGEBRA

Alternatively, we can cast the array objects to the type np.matrix. This changes the behavior of the standard arithmetic operators +, -, * to use matrix algebra.

```
M = np.matrix(m)
vec = np.matrix(v).T # make it a column vector
print(M * vec)
```

```
>>> [[ 5]
 [14]
 [23]]
```

MATRIX ALGEBRA

More examples

```
# inner product
print(np.dot(v, v))
print(vec.T * vec)
```

```
5
[[5]]
```

```
# with matrix objects, standard matrix algebra applies
print(vec + M * vec)
```

```
[[ 5]
 [15]
 [25]]
```

MATRIX COMPUTATIONS

Inverse: np.linalg.inv

```
M = np.matrix([[4, 2, 9], [11, 2, 3], [9, 3, 1]])
print(np.linalg.inv(M))
```

```
[[-0.05035971  0.17985612 -0.08633094]
 [ 0.11510791 -0.55395683  0.62589928]
 [ 0.10791367  0.04316547 -0.10071942]]
```

Determinant: np.linalg.det

```
print(np.linalg.det(M))
```

```
139.0
```

MATHEMATICAL FUNCTIONS

Exponents and logarithms, trigonometric functions

- np.exp, np.log, np.cos, np.sin, np.tan, np.arcsin, …

Linear algebra

- linalg.svd, linalg.eig, linalg.qr, …

Handling complex numbers

- np.real, np.imag, np.conj, …

Floating functions, and miscellaneous

- np.floor, np.ceil, np.isnan, np.sqrt, np.convolve, …

DATA PROCESSING

Often it is useful to store datasets in Numpy arrays. Numpy provides a number of functions to calculate statistics of datasets in arrays.

- np.mean, np.std, np.var
- np.amin, np.amax
- np.sum, np.prod, np.cumsum, np.cumprod

SOME EXAMPLES

```python
x = np.arange(10)
print(np.sum(x))
```

```
45
```

```python
print(np.mean(x))
```

```
4.5
```

```python
print(np.var(x))
```

```
8.25
```

RESHAPING, RESIZING AND STACKING ARRAYS

The shape of an Numpy array can be modified without copying the underlaying data, which makes it a fast operation even for large arrays.

RESHAPING

```
x = np.arange(24)
print(x)
```

```
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 2
2 23]
```

```
v = np.reshape(x, (4, 6))
print(v)
```

```
[[ 0  1  2  3  4  5]
 [ 6  7  8  9 10 11]
 [12 13 14 15 16 17]
 [18 19 20 21 22 23]]
```

RESIZING

```
v = np.array([[0, 1], [2, 3]])
x = np.resize(v, (1,4))
print(x)
```

```
>>> [[0 1 2 3]]
```

REPEATING AND STACKING

Using function np.repeat, np.tile, np.vstack, np.hstack, and np.concatenate we can create larger vectors and matrices from smaller ones:

```
v = np.array([[1, 2], [3, 4]])
# repeat each element 3 times
print(np.repeat(v, 3))
```

```
... [1 1 1 2 2 2 3 3 3 4 4 4]
```

```
# tile the matrix 3 times
print(np.tile(v, 3))
```

```
[[1 2 1 2 1 2]
 [3 4 3 4 3 4]]
```

STACKING

```python
v = np.array([[0, 1], [2, 3]])
w = np.array([[5, 6]])
print(np.concatenate((v, w), axis=0))
```

```
>>> [[0 1]
 [2 3]
 [5 6]]
```

```python
print(np.concatenate((v, w.T), axis=1))
```

```
[[0 1 5]
 [2 3 6]]
```

STACKING

```
v = np.array([[0, 1], [2, 3]])
w = np.array([[5, 6]])
x = np.vstack((v, w))
print(x)
```

```
>>> >>> [[0 1]
 [2 3]
 [5 6]]
```

```
x = np.hstack((v, w.T))
print(x)
```

```
[[0 1 5]
 [2 3 6]]
```

COPY AND "DEEP COPY"

To achieve high performance, assignments in Python usually do not copy the underlaying objects. This is important for example when objects are passed between functions, to avoid an excessive amount of memory copying when it is not necessary (technical term: pass by reference).

WITHOUT COPY

```
A = np.array([[1, 2], [3, 4]])
# now B is referring to the same array data as A
B = A
# changing B affects A
B[0, 0] = 10
print(A)
```

```
... >>> ... >>> [[10  2]
 [ 3  4]]
```

```
print(B)
```

```
[[10  2]
 [ 3  4]]
```

COPY

If we want to avoid this behavior, so that when we get a new completely independent object B copied from A, then we need to do a so-called "deep copy" using the function copy:

```
A = np.array([[1, 2], [3, 4]])
B = A.copy()
# now, if we modify B, A is not affected
B[0, 0] = -5
print(A)
```

```
>>> ... >>> [[1 2]
 [3 4]]
```

```
print(B)
```

```
[[-5  2]
 [ 3  4]]
```

ITERATING OVER ARRAY ELEMENTS

Generally, we want to avoid iterating over the elements of arrays whenever we can (at all costs). The reason is that in a interpreted language like Python (or MATLAB), iterations are really slow compared to vectorized operations.

```
v = np.array([1,2,3,4])
for element in v:
    print(element)
```

```
... ... 1
2
3
4
```

SOME NUMPY FUNCTIONS

NP.WHERE

The position index can be found using the np.where function

```
x = np.arange(10) + 20
indices = np.where((x >= 20) & (x < 25))
print(indices)
```

```
>>> (array([0, 1, 2, 3, 4]),)
```

```
print(x)
```

```
[20 21 22 23 24 25 26 27 28 29]
```

NP.CHOOSE

Constructs an array by picking elements form several arrays using np.choose

```
which = [1, 0, 1, 0]
choices = [[-2, -2, -2, -2], [5, 5, 5, 5]]
x = np.choose(which, choices)
print(x)
```

```
>>> >>> [ 5 -2  5 -2]
```

NP.TAKE

Take elements from an array along an axis (for completeness, the function np.take does the same thing as "fancy" indexing (i.e. indexing arrays using arrays); however it can be easier to use if you need elements along a given axis.

```python
v = np.array([4, 3, 5, 7, 6, 8])
indices = np.array([0, 1, 4])
x = np.take(v, indices)
print(x)
print(v[indices])
```

```
>>> >>> [4 3 6]
[4 3 6]
```

NP.SELECT

Return an array drawn from elements in choicelist, depending on conditions using np.select.

```
x = np.arange(10)
condlist = [x<3, x>5]
choicelist = [x, x**2]
v = np.select(condlist, choicelist)
print(v)
```

```
>>> >>> >>> [ 0  1  2  0  0  0 36 49 64 81]
```

NP.PLACE

Change elements of an array based on conditional and input values using np.place.

```
m = np.arange(6).reshape(2, 3)
print(m)
np.place(m, m>2, [44, 55])
print(m)
```

```
[[0 1 2]
 [3 4 5]]
[[ 0  1  2]
 [44 55 44]]
```

AND MANY MORE ...

The Numpy reference manual gives details on functions, modules, and objects included in Numpy, describing what they are and what they do.

FURTHER NUMPY TOPICS

- Masked arrays
- Numpy IO (will be covered in another session)
- Datetime and timedeltas
- Numpy polynomials functions
- Sorting, searching, counting
- Logic functions
- More on statistics
- Structured arrays (aka "Record arrays")
- Byte-swapping
- Subclassing ndarray
- and many more …

SCIPY

Scipy (Scientific Computing Tools for Python) is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:

- Python (2.x >= 2.6 or 3.x >= 3.2)
- NumPy (>= 1.6)
- Scipy library (>= 0.10)
- Matplotlib (>= 1.1)
- dateutil
- pytz

SCIPY LIBRARY

The Scipy library is one of the core packages that make up the Scipy stack. It provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimization.

EXAMPLE I - INTERPOLATION (SCIPY.INTERPOLATE)

There are several general interpolation facilities available in Scipy, for data in 1, 2, and higher dimension

```
from scipy.interpolate import interp1d
x = np.linspace(0, 10, 10)
y = np.cos(-x**2 / 8.0)
f = interp1d(x, y, kind='cubic')
print(y[:4])
```

```
>>> >>> >>> [ 1.          0.98811613  0.81545357  0.18090587]
```

```
print(f(x)[:4])
```

```
[ 1.          0.98811613  0.81545357  0.18090587]
```

EXAMPLE II - STATISTICS (SCIPY.STATS)

This module contains a large number of probability distributions as well as a growing library of statistical functions. There are several general

```
from scipy.stats import norm

# The probability density function for norm is:
# norm.pdf(x) = exp(-x**2/2)/sqrt(2*pi)

# Calculate a few first moments
mean, var, skew, kurt = norm.stats(moments='mvsk')
print(mean, var, skew, kurt)
```

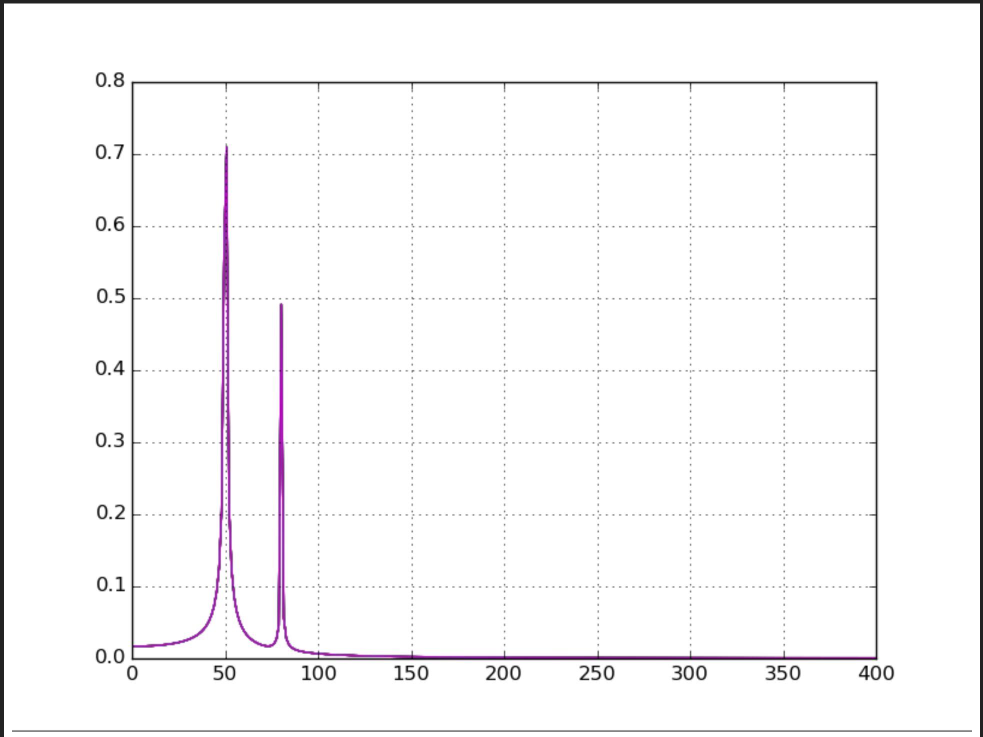
```
>>> ... ... >>> ... >>> (array(0.0), array(1.0), array(0.0), array(0
.0))
```

EXAMPLE II - STATISTICS (SCIPY.STATS)

```
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(norm.ppf(0.01), norm.ppf(0.99), 100)

plt.plot(x, norm.pdf(x), 'r-', lw=2)
plt.savefig('./graphics/norm_pdf.png')
```



NUMPY EXERCISE

1. Show that A * A^-1 = I
2. Find indices of non-zero elements from [1, 2, 0, 0, 4, 0].
3. Declare a 3x3 identity matrix.
4. Create 1000 random values from a normal distribution.
5. Calculate mean, std, var from a vector of your choice.

SCIPY EXERCISE

1. Define a function of your choice (e.g. x^2 + 10 * sin(x)) and find the roots (HINT: optimize.root)
2. Calculate the Fourier Transform of the signal = sin(50 * 2 * pi * x) + sin(80 * 2 * pi * x), with x defined between 0 and N=1200, and a temporal sampling of T=1.0/1200.0