NumPy, SciPy and Visualization

Quantitative Applications for Data Analylsis

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Today's class

Today we will discuss two packages that are often considered as the basis of many scientific and numerical computing tasks in python:

- NumPy - the fundamental package for scientific computing with Python, containing a powerful N-dimensional array object, and useful linear algebra, Fourier transform, and random number capabilities.
- SciPy - provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimization.

Multidimensional lists in Python

The element of a list in Python can be of any type, including a list, that is we can create a list of lists or multidimensional list. For example, this is how you can create a Vandermonde matrix:

```
>>> vander_matrix = [[1.0, 1.0, 1.0], [1.0, 2.0, 4.0], [1.0, 3.0, 9.0]]
```

Here we have a three-element list where each element consists of a three-element list.

```
>>> vander_matrix[0]
[1.0, 1.0, 1.0]
>>> vander_matrix[1]
[1.0, 2.0, 4.0]
>>> vander_matrix[0][0]
1.0
>>> vander_matrix[1][1]
2.0
```

Remember that list indices in Python start at 0.

NumPy arrays

The NumPy array is similar to a list but where all the elements of the list are of the same type.

NumPy has a number of functions for creating arrays. The first of these, the `array` function, converts a list to an array.

```
>>> import numpy
>>> vander_matrix
[[1.0, 1.0, 1.0], [1.0, 2.0, 4.0], [1.0, 3.0, 9.0]]
>>> vander_matrix_numpy = numpy.array(vander_matrix)
>>> vander_matrix_numpy
array([[1., 1., 1.],
       [1., 2., 4.],
       [1., 3., 9.]])
```

Remember to `import numpy` module in your script.

NumPy arrays

The second way arrays can be created is using the NumPy `linspace` function. It creates an array of `N` evenly spaced points between a starting point and an ending point. The form of the function is `linspace(start, stop, N)`. If the third argument `N` is omitted, then `N = 50`.

```
>>> numpy.linspace(0, 3, 7)
array([0. , 0.5, 1. , 1.5, 2. , 2.5, 3. ])
```

The third way arrays can be created is using the NumPy `arange` function. The form of the function is `arange(start, stop, step)`. If the third argument is omitted `step = 1`. If the first and third arguments are omitted, then `start = 0` and `step = 1`.

```
>>> numpy.arange(0,1,0.1)
array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9])
>>> numpy.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

NumPy arrays

A fourth way to create an array is with the `zeros` and `ones` functions which create arrays where all the elements are either zeros or ones.

```
>>> numpy.zeros(5)
array([0., 0., 0., 0., 0.])
>>> numpy.ones(5)
array([1., 1., 1., 1., 1.])
```

Very often you find that instead of typing the name of the module `numpy`, it is imported with a short alias `np`.

```
>>> import numpy as np
>>> np.ones(3)
array([1., 1., 1.])
```

Mathematical operations with arrays

It is very easy to perform mathematical operations on every element in the array.

```
>>> vander_matrix_numpy
array([[1., 1., 1.],
       [1., 2., 4.],
       [1., 3., 9.]])
>>> vander_matrix_numpy * 2
array([[ 2.,  2.,  2.],
       [ 2.,  4.,  8.],
       [ 2.,  6., 18.]])
```

This works not only for multiplication, but for any other mathematical operation.

```
>>> vander_matrix_numpy - 1
array([[0., 0., 0.],
       [0., 1., 3.],
       [0., 2., 8.]])
```

Mathematical operations with arrays

Multiplication of two arrays is performed element-wise.

```
>>> vander_matrix_numpy * vander_matrix_numpy
array([[ 1.,  1.,  1.],
       [ 1.,  4., 16.],
       [ 1.,  9., 81.]])
```

To calculate the dot product of two arrays use function `np.dot`.

```
>>> np.dot(vander_matrix_numpy, vander_matrix_numpy)
array([[ 3.,  6., 14.],
       [ 7., 17., 45.],
       [13., 34., 94.]])
```

These kinds of operations with arrays are called vectorized operations because the entire array, or "vector", is processed as a unit. Vectorized operations are much faster than processing each element of arrays one by one.

Multidimensional arrays

We can create a multidimensional array by applying `array` function to the multidimensional list

```
>>> numpy.array([[1,2,3,4,5],[6,7,8,9,10]])
array([[ 1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10]])
```

To create a multidimensional array using the `zeros` and `ones` functions we need to specify number of rows and number of columns. In NumPy rows are always specified first.

```
>>> numpy.ones((3, 4))
array([[1., 1., 1., 1.],
       [1., 1., 1., 1.],
       [1., 1., 1., 1.]])
```

Notice the way we specified the number of rows and columns: `(3, 4)`. This structure is called tuple. Tuples are very similar to lists, but the main difference between them is that the tuples cannot be changed unlike lists.

Array indexing

NumPy offers several ways to index arrays.

```
>>> all_data = numpy.arange(10, 0, -1)
>>> all_data
array([10,  9,  8,  7,  6,  5,  4,  3,  2,  1])
>>> all_data[0]
10
>>> all_data[-1] # supports negative indices
1
>>> all_data[2:]
array([8, 7, 6, 5, 4, 3, 2, 1])
>>> all_data[:2]
array([10,  9])
>>> all_data[0:2] # slice items between indexes
array([10,  9])
```

While slicing between indices, the `start` index is included and the `stop` index is not included.

Boolean indexing

Frequently we want to select or modify only the elements of an array satisfying some condition (fancy indexing).

```
>>> all_data
array([10,  9,  8,  7,  6,  5,  4,  3,  2,  1])
>>> (all_data <= 7) & (all_data >= 5)
array([False, False, False,  True,  True,  True, False, False, False, False])
>>> all_data[(all_data <= 7) & (all_data >= 5)]
array([7, 6, 5])
>>> even_nums = all_data[(all_data % 2) == 0]
>>> even_nums
array([10,  8,  6,  4,  2])
```

The "%" symbol is the modulo operator.

Multidimensional slices

You can slice multidimensional arrays in a similar way.

```
>>> vander_matrix_numpy
array([[1., 1., 1.],
       [1., 2., 4.],
       [1., 3., 9.]])
>>> vander_matrix_numpy[1,1]
2.0
>>> vander_matrix_numpy[2,:]
array([1., 3., 9.])
>>> vander_matrix_numpy[1:,1:]
array([[2., 4.],
       [3., 9.]])
```

Shape and reshape

The `shape` property returns a tuple of array's dimensions and can be used to change the dimensions of an array.

```
>>> seq_array = numpy.arange(1,11)
>>> seq_array
array([ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10])
>>> seq_array.shape
(10,)
```

Here the shape (10,) means the array is indexed by a single index which runs from 0 to 9.

NumPy allows you to modify the shape of an array once it already exists. The `reshape` function gives a new shape to an array without changing the data.

```
>>> seq_array2d = seq_array.reshape((2,5))
>>> seq_array2d
array([[ 1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10]])
```

Shape and reshape

Reshaping array doesn't change the data in the memory. Instead, it creates a new view that describes a different way to interpret the data.

The `shape` of an multidimensional array is a tuple of its dimensions where first element of the tuple represents the number of rows and the second is the number of columns.

```
>>> seq_array2d
array([[ 1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10]])
>>> seq_array2d.shape
(2, 5)
```

Shape and reshape

Specifying −1 as one of the dimensions while reshaping, forces NumPy to calculate this dimension based on the total amount of elements in the array and already specified dimensions.

```
>>> seq_array2d.reshape((5,-1))
array([[ 1,  2],
       [ 3,  4],
       [ 5,  6],
       [ 7,  8],
       [ 9, 10]])
>>> seq_array2d.reshape((3,-1))
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: cannot reshape array of size 10 into shape (3,newaxis)
>>> numpy.arange(9).reshape((-1,3))
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]])
```

The `linalg` submodule

The `linalg` submodule of SciPy contains useful functions for matrix algebra.

- Typical matrix functions: `inv`, `det`, `norm`, etc.
- More advanced functions: `eig`, `SVD`, `cholesky`, etc.
- Both NumPy and SciPy have a `linalg` module. Use SciPy, because it is compiled with optimized BLAS/LAPACK support.

```
>>> import numpy
>>> import scipy
>>> from scipy import linalg
>>> A = numpy.array([[1,2,3], [3,4,5], [1,1,2]])
>>> linalg.det(A)
-2.0
>>> scipy.dot(A, linalg.inv(A))
array([[ 1.00000000e+00,  2.22044605e-16, -2.22044605e-16],
       [ 1.66533454e-16,  1.00000000e+00, -6.66133815e-16],
       [ 0.00000000e+00,  0.00000000e+00,  1.00000000e+00]])
```

Solving systems of equations

The `solve` function in the `linalg` module is used to solve the system of equations $Ax = b$.

```
>>> A
array([[1, 2, 3],
       [3, 4, 5],
       [1, 1, 2]])
>>> b = numpy.array([3, 4, 2])
>>> b
array([3, 4, 2])
>>> x = linalg.solve(A, b)
>>> x
array([-0.5, -0.5,  1.5])
```

$$\begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 1 & 1 & 2 \end{bmatrix} \cdot \begin{bmatrix} -0.5 \\ -0.5 \\ 1.5 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ 2 \end{bmatrix}$$

Statistics

SciPy contains all of the statistical functions that you'll probably ever need.

- The scipy.stats module is based around the idea of the random variable type.
- A whole variety of standard distributions are available:
  - Continuous distributions: Normal, Maxwell, Cauchy, Chi-squared, Gumbel Left-scewed, Gilbrat, Nakagami, etc.
  - Discrete distributions: Poisson, Binomial, Geometric, Bernoulli, etc.
- The random variables have all of the statistical properties of the distributions built into them already: cdf, pdf, mean, variance, moments, etc.

Statistics

Let us create a normally distributed random variable with the mean of 1.0 and the standard deviation of 0.5.

```
>>> from scipy import stats
>>> x = stats.norm(1, 0.5)
>>> x.mean()
1.0
>>> x.median()
1.0
>>> x.std()
0.5
>>> x.var()
0.25
```

Statistics

We can evaluate the probability distribution function, the cumulative distribution function, etc., using the pdf, cdf, etc. These functions could take a value, or an array of values, where the function will be evaluated.

```
>>> x.pdf([0, 1, 2])
array([0.10798193, 0.79788456, 0.10798193])
>>> x.cdf([0, 1 ,2])
array([0.02275013, 0.5       , 0.97724987])
```

The `interval` method can be used to compute the lower and upper values of `x` such that a given percentage of the probability distribution falls within the interval (lower, upper). This method is useful for computing confidence intervals

```
>>> x.interval(0.95)
(0.020018007729972975, 1.979981992270027)
```

Visualization

There are a number of high-quality visualization packages available in Python

- `matplotlib` focuses on generating publication-quality plots
- `seaborn` targets statistical data analysis
- `ggplot` is based on the famous `R` package
- `Plotly` and `Bokeh` focus on interactivity
- and others

Installing Matplotlib

To install `matplotlib` package run the following command in your terminal

```
$ pip install matplotlib
```

Anaconda base environment comes with pre-installed `matplotlib` package. If you need to install it in a new environment, you can run this command

```
$ conda install matplotlib
```

`matplotlib` is imported using the following command

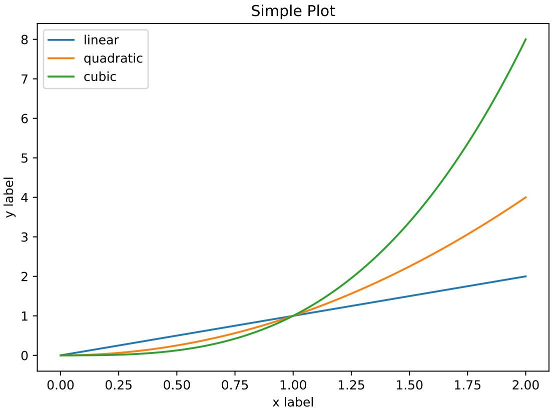
```
>>> import matplotlib.pyplot as plt
```

Also import `numpy` as it is frequently used together with `matplotlib`

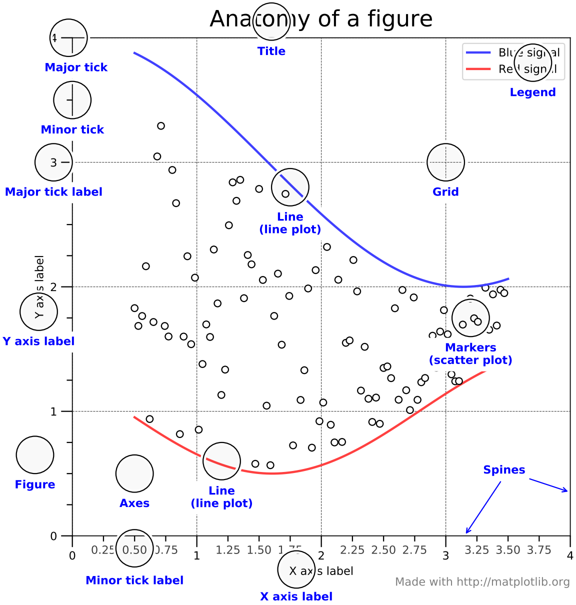
```
>>> import numpy as np
```

Simple plot in matplotlib

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

x = np.linspace(0, 2, 100)

plt.plot(x, x, label='linear')
plt.plot(x, x**2, label='quadratic')
plt.plot(x, x**3, label='cubic')
plt.xlabel('x label')
plt.ylabel('y label')
plt.title("Simple Plot")
plt.legend()

plt.show()
```



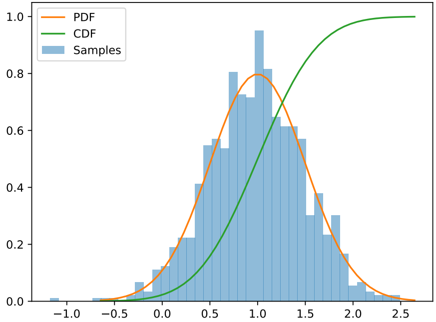
To save your plot use the command:
`plt.savefig(filename)`


Anatomy of a figure
Title
Major tick
Minor tick
Major tick label
Y axis label
Figure
Axes
Line
(line plot)
Line
(line plot)
Grid
Legend
Blue signal
Red signal
Markers
(scatter plot)
Spines
Minor tick label
X axis label
Made with http://matplotlib.org

Statistics

We can use `matplotlib` to visualize the distributions. In the histogram we use `density=True` to display a probability density, i.e., the area (or integral) under the histogram will sum to 1.

```
import numpy
from scipy import stats
import matplotlib.pyplot as plt
x = stats.norm(1, 0.5)
conf_interval = x.interval(0.999)
x_conf = numpy.linspace(
    conf_interval[0], conf_interval[1])
plt.hist(x.rvs(size=1000), density=True,
    bins=41, alpha=0.5, label="Samples")
plt.plot(x_conf,x.pdf(x_conf),label="PDF")
plt.plot(x_conf,x.cdf(x_conf),label="CDF")
plt.legend()
plt.show()
```



References

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