lab0_1-Introduction-to-Python-for-Scientific-Computing

August 25, 2016

Lab 0 - Tutorials Part 1 - Python for Scientific Computing

In [7]: %matplotlib inline

NOTE: This tutorial (and the class in general) assume that you've had at least some exposure to programming, no matter the language. If you haven't, you need to run through the Codecademy Python course as soon as you can. Your goal is to learn the material on neural computation, not get bogged down in implementation details that depend on the programming language, and it'd be super lame if those problems prevented you from learning as much as you could in this course!

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these links only work in the interactive version of the document

0.2 Why Python?

Python is, as of August 2016, one of the top five most popular programming languages according to the TIOBE Index. Of the five most popular languages, it is universally acclaimed as the easiest to use, as it operates at a higher level of abstraction than the other top contenders. This has lead to Python becoming the language of choice for teaching introductory computer science (data as of 2014) and the second-most popular language for data science (data as of 2015).

Python emphasizes the human side of coding: it is considered more important in Python for a human programmer to be able to easily and quickly understand what a piece of code does and why than it is for that code to run quickly when implemented by a machine. This is especially important in an educational setting where understanding is paramount and speed is secondary.

0.2.1 Why Not MATLAB?

This blog post introduces MATLAB users to Python and states two reasons not to use MATLAB:

- 1. Python is free and MATLAB is not.
- 2. Python is a general-purpose programming language and MATLAB is not.

Let me expand on those two points:

- 1. The fact that Python is free means that there is a larger community contributing software that you can use (like Jupyter Notebooks, which are developed at Berkeley!) and which determines the direction of the language in a relatively democratic and open manner. It also means that your code is more portable.
- 2. MATLAB is an almost-unbeatably efficient matrix-manipulation scripting language. It struggles, however, to deal with any data structure that isn't "like" a matrix. This includes strings, data frames, and even functions. This means that Python can be used in a whole variety of situations in which MATLAB isn't a great choice: building graphical user interfaces, providing web services, processing text corpora, scraping data from the web, and so on.

0.2.2 Why Python 3?

Some people may be coming in using Python 2.7, even though the current (as of August 19, 2016) release version of Python is 3.5. This is due to the non-backwards-compatibility of Python 3, which meant that many scientific computing libraries were slow to update. As recently as two years ago, there were still many packages that were only available in 2.7, but there has been a sea change, and almost all packages are 3-compatible, and soon some of them will only support Python 3.

A notable benefit of using a general-purpose open-source language like Python is that you won't be forced to uninstall any version of Python that you currently have. Many of you probably have the Anaconda distribution of Python, and so have a built-in system for managing multiple Python versions. We'll be using virtual environments, which achieve the same thing but are more lightweight.

One big benefit of Python 3.5 for this course is something that appears quite small: matrix/vector multiplication in Python now has its own operator: @. In past versions of Python, taking a dot product involved using the function np.dot. This may seem small, but it means that instead of having to write and read expressions like:

```
dw = np.dot((dataset-np.dot(weights,output)),output.T)
you'll find:
  dw = (dataset - weights @ output) @ output.T
which looks a lot more like the math:
```

$$\Delta w = (D - W \cdot O) \cdot O^T$$

and is hopefully easier to read (or at least, it will be a few weeks into the course!).

0.3 How Python?

The following is based on a tutorial from Jess Hamrick, a Berkeley PhD student in Tom Griffiths' Lab who is also one of the heads of the Jupyter project.

As in most programming languages, in Python we assign names to variables and apply functions to variables in order to transform them – to perform computations.

We'll briefly review some of the major syntax you need to work in Python.

0.3.1 from __future__ import jetpack

When you start up a Python environment (e.g. when you open a Jupyter notebook), there is only a small set of data structures and functions, called the "standard library".

In order to do most things we're doing in this course, we need the following libraries:

- NumPy is a numerical computing library that adds support for vector and matrix math to Python. It's a big and powerful library, so it can be a bit intimidating. If you have experience with a different language, check out one of these specific guides:
 - NumPy for Matlab Users
 - NumPy for R/S+ Users
- matplotlib is a plotting library that uses a MATLAB-esque syntax. Plotting and visualizing data is a key skill for any scientist, so I strongly recommend following the link above and checking out some of the tutorials so that you can become a master plotter!

We load up these libraries with import statements. We additionally give the library a shorter nickname using the as keyword:

Now, we can access all of the functions inside the module numpy, like numpy.zeros and numpy.multiply by typing np.zeros and so on. The . symbol in Python means that we're looking for a thing, like a variable or a function, inside another thing. This means we can have a function dot that does something different from np.dot and Python won't get confused about which dot we're looking for. Radical!

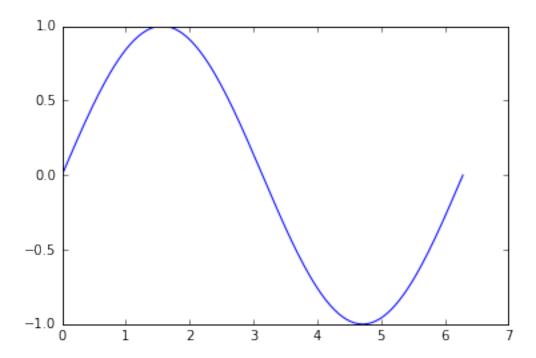
We can also have things that are inside things. In fact, there's no reasonable limit on the number of times we can "go meta" here. It's .turtles all the way down!

Let's make use of that to bring in a very important sub-component of matplotlib that has its own sub-components:

```
In [9]: import matplotlib.pyplot as plt
```

We'll be using all of the matplotlib functionality from within pyplot – or, as far as we're concerned, plt. Let's use some numpy functions to generate a basic plot.

```
In [10]: x = np.linspace(0,2*np.pi,200) #evenly-spaced numbers from 0 to 2\pi y = np.sin(x) plt.plot(x,y); plt.show()
```



Thanks to the power of Jupyter notebooks, the plot is displayed inline! This is thanks to the first cell in this notebook, which contains the magic command (yes, really) %matplotlib inline.

0.3.2 for loops and lists

In Python as in many other languages, we use for loops to tell the computer to do the same thing over and over. For example, the following prints the numbers from 0 to 9:

Much easier than writing print (1), then print (2), etc. Boring stuff like repeating yourself is the job of computers, not people!

One thing that surprises new Python programmers is that the blank spaces are important to make the code above work. Any time you do a for loop, you need to indent all of the code that's

supposed to be repeated. This includes when you're doing a for loop inside a for loop! Jupyter does a good job of handling the blank spaces for you, but it's something to watch out for.

for loops are so important that Python let's you do them over things that aren't just arrays of numbers!

```
In [18]: friends = ['joey', 'rachel', 'phoebe', 'avocado']
    #this is how you specify a list of things,
    # like a list of your friends: [friend0, friend1, friend2]

for person in friends:
    print('i love my friend '+person)

i love my friend joey
i love my friend rachel
i love my friend phoebe
i love my friend avocado
```

Of course, that takes up a lot of space. Python also offers an even more compact way of writing for loops:

```
In [19]: [print('i love my friend '+person) for person in friends];
i love my friend joey
i love my friend rachel
i love my friend phoebe
i love my friend avocado
```

This is called a "list comprehension" and it turns one list of values into another. List comprehensions are a nice way to save space, but they can be hard to read, especially when the list at the end is also made from a list comprehension!

0.3.3 Arrays

Instead of directly using lists, we'll mostly be using arrays in this class. Arrays come from numpy, and they are very similar to lists: they're containers for big collections of objects. In fact, we can turn a list into an array by using np.asarray(list). However, they act more like matrices and vectors than like lists of objects. For example, we can multiply them:

```
In [14]: vector = np.asarray([1,2,3]) # the vector [1,2,3]
    matrix = np.zeros((3,3)) # a matrix of all zeros

vectorVectorProduct = vector @ vector #vector multiplication
    vectorMatrixProduct = matrix @ vector #matrix multiplication

print('vector: {0}'.format(vector))
    print('matrix: \n {0}'.format(matrix))
    print('vec-mat product: {0}'.format(vectorMatrixProduct))
    print('vec-vec product: {0}'.format(vectorVectorProduct))
```

```
vector: [1 2 3]
matrix:
  [[ 0.  0.  0.]
  [ 0.  0.  0.]
  [ 0.  0.  0.]]
vec-mat product: [ 0.  0.  0.]
vec-vec product: 14
```

We'll be multiplying a lot of matrices in this class. One thing that often trips people up is making sure that their matrices are aligned: an M by N matrix can only multiply an N vector or and N by K matrix. We can track these very important numbers by using <code>array.shape</code>:

Note that shape is a property of every array, just like pyplot was a property of matplotlib, so it shows up after a .

Note also that I didn't use a print function on matrix.shape. That's because, by default, Jupyter notebooks show you the result of running the final line (and only the final line). MATLAB does something similar for every line, except those that end with semicolons (;). You can similarly prevent the notebook from printing the results of the last line by including a semicolon:

```
In [16]: matrix.shape; #nothing shows up!
```

0.4 More Python!

There's a ton more Python to learn!

The blog post linked all the way back at the start is written to help MATLAB users learn to use Python. It has lots of nice links to the official Python tutorial and the SciPy cookbook, which has lots of recipes specialized for the problems scientists need to solve with Python.

0.5 Moving On

To check out the next tutorial, make sure you are navigated to the folder containing this file and the rest of Lab 0 and please type the following into your terminal:

```
jupyter notebook
```

This will launch a Jupyter notebook instance in your browser. From the file menu in Jupyter, open lab0_2 so you can learn more about how Jupyter notebooks work.