

Intro to Python

PHYS 355

Madeline Galbraith

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Why to use Python?

- Not compiled
- Easy to install and download additional packages
- Syntax is very simple compared to others
- Python has very robust capabilities in it's packages

Goal at end of today's lecture

Use python to solve HW#2 problem 1d.

Consider a two-state folder in a stop-flow experiment. Changing urea concentration [Urea], the rate of change of the unfolded protein fraction $\frac{dU}{dt} = -f_f U + k_u N$, whereas the rate of change of the folded protein fraction $\frac{dN}{dt} = k_f U - k_u N$. The experiment measures the overall signal associated to the state of the system as a function of time. Show that the decay towards equilibrium is governed by the rate $k_f + k_u$, whereas the equilibrium state is given by $\frac{k_f}{k_u}$. (Hint use the Euler method)

- Assignment

```
x=2          # This will set x to 2
x=2*y        # This won't work because we haven't defined y
a = 1        # sets a to 1
print(a)     # need parentheses because this is a function
```

- Checking inequalities

```
x > 3        # True if x>3, false otherwise
x >= 2       # This checks if x is greater than or equal to 2
a== 3        # Checks if a is equal to 3
```

- There is a package/module for everything
- NumPy - does linear algebra efficiently and is useful in scientific computing
- SciPy - useful for integration, interpolation, optimization, statistics, and solving ODEs
- Matplotlib - Python's plotting library
- Pandas - a data analysis library. Useful for parsing many different file formats quickly and efficiently

NumPy basics

```
import numpy as np
np.sin(1.4)          # np is a shortcut for the full name numpy
numpy.sqrt(9)        # but you can also use the full name
np.pi               # not a function so no parentheses

from numpy import tan
tan(3.14/4)          # can directly import functions
```

Lists vs arrays

- Creating a list

```
a = [0.1,40,3] # this is a list
```

- Getting elements from the list (aka indexing the list)

```
print(a[0])    # Indices start at 0 in computer science!  
print(a[1])    # This will print 40
```

- Creating a matrix

```
b = [[1,2,3],[4,5,6]] # A list of lists (aka a matrix)
```

- Indexing a matrix is matrix[row][column]

```
# print the row 1, column 2
```

```
print(b[1][2]) # Should print 6
```

```
#remember we start counting from 0
```

```
print(b[0]) #prints the first row
```

Lists vs arrays, cont

- Creating a numpy array from a list

```
b_array = np.array(b)    # converts the list to a numpy array
```

- NumPy arrays have similar ways of indexing

```
print(b[0])    # prints row 0  
print(b_array[0]) #prints row 0
```

- Numpy has a shortcut for indexing

- Note that Loops and indexes actually end one before the last number so if you want the first 10 numbers in a list of 100 you have to do *list[0:10+1]* not *list[0:10]*

```
# print the first 2 elements in both rows  
print(b[:][0:2])  
print(b_array[:,0:2])
```


Variable names vs objects

- In computer science an object is an abstraction that refers to the underlying structure (An object can be a list, array, plot, etc)
- We sometimes must be careful that a single list is not given two names (this is more important when you start using functions)

```
a=b    # this is a variable assignment
a==b   # Check if they have same elements
a is b # Check if they are the same object
# proof that a and b are the same object
print(b)
a[0][0] = 5
print(b)
# Make a copy that won't change the original
c = b.copy()
c[0][0] = 100
print(b)
print(c)
```

Graphs and vectorization

- NumPy is useful because you can act on all elements in the array at once instead of having to loop over it
- Matplotlib is an extremely powerful plot generator with similar syntax to Matlab

```
import matplotlib.pyplot as plt

# plot as simple scatter plot first
x=[1,2]; y=[1,2]
plt.plot(x,y)

# now plot a sine wave
x_vals = np.arange(0,10,0.1)
y_vals = np.sin(x_vals)
plt.plot(x_vals,y_vals)
```

Putting it all together: Numerical simulation of an ODE

Now we are going to use the Euler method to numerically solve the homework problem from last week.