Introduction to Beginner-Level Python

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CRC Foundational Python Track

Part 1: Introduction to Beginner-Level Python (2/22/2023)

Part 2: Introduction to Intermediate-Level Python (2/16/2023)

Part 3: Introduction to Data Manipulation and Visualization (3/2/2023)

Industry-sponsored AI/ML Workshops
More details to come in February.

https://crc.pitt.edu/training/crc-workshops-spring-2023
Purpose of this Workshop

- Learn how to use Python for automating simple repetitive tasks
- Basic ideas on how to create and run programs in Python
- Understand how to structure a code to make it reusable and readable
- Learn how to install packages to extend Python’s capabilities
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About me

PhD in Physical and Theoretical Chemistry (Oxford, UK, 2001)
Postdoc in Theoretical Chemistry (Cambridge, UK, 2001-2004)
Postdoc in Theoretical Chemistry (Amsterdam, The Netherlands, 2004-2008)
Principal Scientist (STFC Rutherford-Appleton Lab, UK, 2008-2018)
Research Assistant Professor in Chemistry and Consultant at CRC (2018-)

\[ \hat{H}(t) \psi(r_1, \ldots, r_N; t) = i\hbar \frac{\partial}{\partial t} \psi(r_1, \ldots, r_N; t) \]
Overview

1. Introduction: What is Python
2. How to run Python
3. Python syntax
4. Examples
5. Virtual environments
6. Introduction to NumPy/Matplotlib
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Introduction
- A **general-purpose** scripting and programming language
- It is a **high-level** language: it looks more like English than machine language
- It is an **interpreted** language: the interpreter converts it line-by-line into ML

- The structure of Python helps programmers write clear and readable code
- It can be useful for **small scripts** as well as for **large software projects**

- Widely used in industry and academia
- One of the main strength of Python is the existence of a huge **standard library**: over 287,000 packages for science, machine learning, data analytics, etc.
- Python is free and open source
- It is maintained and distributed by the Python Software Foundation
- It is available on most OSs

https://www.python.org
- Python packages are distributed by their developers
- They are typically very easy to install

https://pypi.org
Main strength of Python

The ability to write clear and well-structured code, with no need to worry about low level operations (e.g., memory management)

Main disadvantage

Python code is slow compared to compiled languages (https://julialang.org/benchmarks/)

Often the best solution is to write computationally intensive parts of a code in a compiled language and use Python wrappers to orchestrate these low-level, but very efficient, parts of the code.
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How to run Python
How to run Python

1) Through an interactive session
2) Executing a script/program
3) Using Jupyter notebooks (https://jupyter.org)
4) Using Google Colab (https://colab.research.google.com)
5) Using an integrated development environment (IDE), e.g., PyCharm (https://www.jetbrains.com/pycharm/)

Jupyter notebooks on the CRC cluster through Jupyter Hub and Open Ondemand

https://crc.pitt.edu/Access-CRC-Web-Portals
Interactive sessions

1) Start Python: `python` (for Python2) or `python3`
2) Type commands line by line
3) Exit using: `Ctrl + D`
   
   or:
   
   `exit()`
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Python syntax
Data types

Numbers

12, 299792458, 0.001, 3+5j
Python as a calculator
Variable assignment (e.g., c = 299792458)

Operators

+, -, *, /, %, //, **  
==, !=, <, >, >=, <=  
Logical variables (True and False)

The `math` module:

```python
import math
dir(math)
```

*Built-in* modules: help('modules')
Data types

Lists

$l = [1, 2, 13.3, \text{“today”}, 6+5j]$  

List index (always integer; can be negative)  
Length of a list: $\text{len}(l)$

Sublists: note **slicing** is from an index to a given element position

List manipulation:  
`insert(pos, element), append(), remove(), pop(), extend()`  
`list1 + list2`

Membership operators: `in / not in`

Nested lists
Data types

Strings

```python
string1 = "today"
string2 = 'tomorrow'
string3 = ""yesterday"
```

String indices
Substrings, slicing

Concatenation: `string1 + string2 + string3`
Repetition: `string1 * 3`

Membership operators: `in` / `not in`
Data types

Tuples
Similar to strings, but their elements are immutable

t1 = (1, 2, 3)

Tuple indices

Substrings, slicing

Nested tuples and their indices
Membership operators: in / not in
Data types

Dictionaries

\[
d1 = {}
d1[1] = 1; \; d1[2] = 4; \; \text{etc.}
\]

Keys: \(d1\text{.keys()}
\)
Values: \(d1\text{.values()}
\)
Clear: \(d1\text{.clear()}
\)

Nested dictionaries
Data types

Files
Read from file and write to file

Read from file:
input_file = open('input.file', 'r')
input_file.read()
input_file.close()

Write to file:
output_file = open('output.file', 'w')
output_file.write()
output_file.close()

We can read/write a file as a single string or as a sequence of lines
Control statements and loops

Conditional

if \textit{condition1}:
    \begin{tabular}{l}
    \hspace{1cm}(execute some instructions)
    \end{tabular}

elif \textit{condition2}:
    \begin{tabular}{l}
    \hspace{1cm}(execute some other instructions)
    \end{tabular}

elif \textit{condition3}:
    \begin{tabular}{l}
    \hspace{1cm}(execute some other instructions)
    \end{tabular}

else:
    \begin{tabular}{l}
    \hspace{1cm}(execute some other instructions)
    \end{tabular}

\textbf{Indentation (four blank spaces) is very important in Python!!!}

Switch to running scripts.

/ihome/sam/leb140/IntroToPython/example1.py
a = 15

if a == 10:
    print(a)
    print("... It is Monday")
elif a == 15:
    print(a)
    print("... It is Tuesday")
else:
    print("... I do not know what day it is")
Control statements and loops

for loop

for variable in sequence:
    (execute some instructions)

The function range():

    range(n)
    range(start, stop)
    range(start, stop, step)

Nested loops

Loops with if/else blocks:
for variable in sequence:
    if Condition:
        (execute some instructions)
    else:
        (execute some other instructions)

Loops and conditionals: example2.py
#mylist = [1, 2, 3]
#
# for element in mylist:
#     print(element)
#
# I am going to ignore the lines above

# for i in range(0, 50, 2):
#     print(i)

mylist = [1, 2, 3, 4, 5, 6]

for element in mylist:
    if element % 2 == 0:
        print(element)
        print("Even number")
    else:
        print(element)
        print("Odd number")

"example2.py" 19L, 340C
Control statements and loops

Reading files line-by-line

```python
open_file = open("some_file", "r")

for line in open_file:
    (execute some instructions on the line)

open_file.close()
```

Example: read a file with multiple values per line and store the values in lists

The `strip()` and `split()` methods

`example3.py`
myfile = open("file.txt", "r")

for line in myfile:
    mylist = line.strip("\n").split("\","
    print(int(mylist[0]) + int(mylist[1]))
    #print(line.strip("\n"))
    print(mylist)

myfile.close()
Control statements and loops

while loop

while *condition*:  
    (execute some instructions)

Nested loops

Loops with else blocks:
while *condition*:  
    (execute some instructions)
else:
    (execute some other instructions)

example4.py
i = 0

while i <= 10:
    if i <= 5:
        print(i)
    else:
        print("i is larger than 5")
    i += 1

"example4.py" 8L, 111C
Control statements and loops

The **break** statement
It is used to terminate a for/while loop when a given condition is met

```python
for variable in sequence:
    (execute some instructions)
    if condition:
        break
        <- Will exit the loop
    (execute some other instructions)
```

The **continue** statement
It is used to skip instructions within a for/while loop

```python
for variable in sequence:
    (execute some instructions)
    if condition:
        continue
        <- Will be skipped, but will not exit the loop
    (execute some other instructions)
```
Control statements and loops

The **pass statement**
It tells the Python interpreter to *do nothing*. It works as a placeholder.

```
for variable in sequence:
    (execute some instructions)
    if condition:
        pass
    else:
        (do something else)
```
Functions

Functions are blocks of code that carry out specific tasks. They are useful if a given set of operations must be repeated more than once in a code.

They give the code re-usability, i.e., the ability to use a given set of instructions at different stages of the computation without having to modify the code.

They help with code readability, especially if they are well documented. All the instructions required by a given task are grouped together.

They also avoid redundancy, helping with code maintainability and greatly improving extendibility.

Functions (and their equivalents in other programming languages) are essential ingredients in good programming practice.
Functions

def function_name(function_arguments):
    (do something)
    return

(return is optional)

Default arguments can be used to avoid errors when calling a function

def function_name(arg1, arg2=something):
    (do something)
    return

Functions always appear before the main code.

User defined functions and built-in functions

See  function1.py
A function that takes two numbers as input, squares the first number and adds the second number and returns the result.

```python
def myfunction(a_number, another_number):
    """This function does what I wrote above.""
    return a_number * a_number + another_number

def anotherfunction(a_number):
    """This function computed the square of a_number.""
    return a_number * a_number

# Main code
for a in range(10):
    b = a + 4
    print(myfunction(a, b))
    print(anotherfunction(a))
```

"function1.py" 21L, 498C
Invoking external commands in Python

List files using `ls` command:

```python
from subprocess import call
call('ls')
```

Return date using the Unix ‘date’ command:

```python
import subprocess
time = subprocess.check_output('date')
print("It is", time)
```
PEP8: Style Guide for Python code

Guidelines that improve the readability and consistency of Python code

https://peps.python.org/pep-0008/

Python syntax checkers can be installed, which parse Python code and report any PEP8 violations, e.g., pip8 and pycodestyle.

They can be installed in a virtual environment (see below) using

```
python3 -m pip install pep8
```

or

```
python3 -m pip install pycodestyle
```
4 Examples
Functions

Exercise 1
Write a function that returns all *prime numbers* up to a given maximum.

A prime number is an integer greater than 1 that cannot be written as the product of any lower natural number: 2 is prime, 3 is prime, 4=2*2 is not prime, *etc.*

Questions:
1) What should the input parameter(s) of the function be?
2) How do we use loops to find out if a given number is the product of two lower numbers?
3) What should the function return?
def primes(maxnumber):

    """This function returns a list of prime numbers within the range (2, maxnumber).

    Input:
        maxnumber = maximum number in the range to consider;
    Output:
        A list of prime numbers up to maxnumber.""

    # Define the list of prime numbers
    prime_numbers = []

    # Loop over all integers from 2 to maxnumber
    for i in range(2, maxnumber+1):

        # I assume that i is prime
        i_is_prime = True

        # Loop over integers lower than i
        for j in range(2, i):

            if i%j == 0:
                i_is_prime = False
                break

        if i_is_prime:
            prime_numbers.append(i)

    return(prime_numbers)
Functions

Exercise 2
Write a code (containing at least one function) that computes the difference between a series of numbers read from two different files (number from file1 minus number from file 2) and saves these differences to an output file file3.

Note: each of the two input files contains one number per line, but the two files need not have the same number of lines. We will only compute differences for numbers that can be read from both files.

Questions:
1) How many files do we need to open at a given time?
2) How do we deal with the fact that the number of lines in the two input files can be different?
Possible solution to Exercise 2.

Can we improve this code?
Possible solution to Exercise 2.

Can we improve this code?

Unnecessary code duplication
def subtract(a, b):
    """This function computes an element-by-element difference between the two lists a and b
    and returns is as a list c."""

    # Initialize return list c (an empty list)
    c = []

    # Find the number of elements for which the difference can be computed:
    # We use the intrinsic function min
    maxel = min(len(a), len(b))

    # Index for elements of a and b
    index = 0

    # Loop on the elements of a
    while index < maxel:
        c.append(a[index] - b[index])
        index += 1

    return c

# Exception handling
try:
    c.append(a[index] - b[index])
    index += 1
except:
    break
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Virtual environments
Virtual environments

A virtual environment is a complete Python installation which is isolated from the system Python and from other virtual environments.

The Python interpreter, scripts, libraries and packages installed in the virtual environment are independent and may differ from the system Python.

Virtual environments are useful for maintaining specific sets of packages or different versions of the same package.

They are very useful when we work on HPC systems, like the CRC cluster, which do not allow users to modify the system Python. With virtual environments we have complete control on package installation, uninstallation, etc.

Official man page: https://docs.python.org/3/library/venv.html
Virtual environments

The command **venv** is used to create a new virtual environment:

```bash
python3 -m venv myenv
```

This will create a directory `myenv` containing the new Python installation.

We now need to **activate** the environment:

```bash
source myenv/bin/activate
```

We can ”exit” the virtual environment and return to the system Python using:

```bash
deactivate
```

(For Windows, see [https://docs.python.org/3/library/venv.html](https://docs.python.org/3/library/venv.html) or [https://realpython.com/python-virtual-environments-a-primer/](https://realpython.com/python-virtual-environments-a-primer/).)
Virtual environments: install Python packages

After activating a virtual environment, we will be using the specific version of Python built in the environment.

To install new packages, use:

```
python3 -m pip install <package_name>
```

If a given virtual environment is no longer needed, we can delete it simply by removing its directory:

```
rm -rf myenv/
```
Example: install numpy in a virtual environment myenv

Create and activate the virtual environment:

```bash
python3 -m venv myenv
source myenv/bin/activate
```

Install numpy:

```bash
python3 -m pip install numpy
```

Now launch the python interpreter:

```bash
python3
```

and check if the new package has been installed:

```python
import numpy
```

To list all installed packages:

```bash
python3 -m pip list
```
Virtual environments: Anaconda (https://anaconda.org)

Create a conda environment:

conda create -n yourenvname python=x.x anaconda

Activate the virtual environment:

source activate yourenvname

Install packages:

conda install -n yourenvname [package]

Deactivate the environment:

source deactivate

Using virtual environments with CRC JupyterHub

As an example, we will create a virtual environment called *myenv* to be used with Jupyter Hub in notebooks.

In a terminal (either on h2p or on Jupyter Hub) use the following commands:

```bash
module purge
module load python/3.7.0
python3 -m venv myenv
source myenv/bin/activate
python3 -m pip install ipyk kernel
python3 -m ipyk kernel install --user --name=myenv
```

On Jupyter Hub open a new notebook and select *myenv* from the notebook kernels available. To check that the version of Python running is the one from the virtual environment, and not the system Python, use:

```python
import sys
print(sys.executable)
```

which should return something like

```bash
[...]/.virtualenvs/myenv/bin/python
```

https://crc.pitt.edu/user-support/installed-software/python
Python on the CRC cluster

H2P access: https://crc.pitt.edu/user-support/cluster-access

To see the versions of python installed: module spider python

To use a specific version of Python: module load python/3.7.0
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NumPy/Matplotlib
SciPy (pronounced “Sigh Pie”) is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:

- **NumPy**: Base N-dimensional array package
- **SciPy library**: Fundamental library for scientific computing
- **Matplotlib**: Comprehensive 2-D plotting
- **IPython**: Enhanced interactive console
- **SymPy**: Symbolic mathematics
- **pandas**: Data structures & analysis

Large parts of the SciPy ecosystem (including all six projects above) are fiscally sponsored by NumFOCUS.

https://scipy.org
A few words on NumPy

NumPy is a Python library used for working with arrays. It also functions for working in domain of linear algebra, Fourier transform and matrices.

You can see what NumPy makes available using the dir() function

```python
import numpy as np
dir(numpy)
```

NumPy provides an array object that is up to 50x faster than traditional Python lists.

```python
arr = numpy.array([1, 2, 3, 4, 5])
print(arr)
```

```python
arr = np.array([[1, 2, 3], [4, 5, 6]])
print(arr)
```

Arrays can have 1, 2, 3 or more dimensions.
Arrays

Accessing array elements:

```python
arr = np.array([[1,2,3,4,5], [6,7,8,9,10]])
print(arr[0, 1])
```

Negative indices can be used as in standard Python lists. Slicing also works like in lists:

```python
print(arr[1, 1:4])
```

Copy and view arrays:

```python
arr = np.array([1, 2, 3, 4, 5])
x = arr.copy()
arr[0] = 0
print(arr); print(x)
```

```python
arr = np.array([1, 2, 3, 4, 5])
y = arr.view()
y[0] = 0
print(arr); print(y)
```
Shape, reshape and iteration

Shape of an array:

```python
arr = np.array([[1, 2, 3, 4], [5, 6, 7, 8]])
print(arr.shape)
```

Answer: (2, 4)

Reshape an array:

```python
arr = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12])
newarr = arr.reshape(4, 3)
print(newarr)
```

Iterating through array elements:

```python
arr = np.array([1, 2, 3])
for x in arr:
    print(x)
```
Join, split and search arrays

Join arrays:

arr1 = np.array([[1, 2], [3, 4]])
arr2 = np.array([[5, 6], [7, 8]])
arr = np.concatenate((arr1, arr2), axis=1)

Split arrays:

arr = np.array([1, 2, 3, 4, 5, 6])
newarr = np.array_split(arr, 4)

Search arrays:

arr = np.array([1, 2, 3, 4, 5, 4, 4])
x = np.where(arr == 4)

Answer: (array([3, 5, 6]),)
Sort and filter arrays

Sort arrays:

```python
arr = np.array([3, 2, 0, 1])
print(np.sort(arr))
```

Answer: [0 1 2 3]

It can be used with higher-dimensional arrays and with arrays of strings or booleans.

Filter arrays: use a *boolean index* list to select values from an array:

```python
arr = np.array([41, 42, 43, 44])
x = [True, False, True, False]
newarr = arr[x]
print(newarr)
```

Answer: [41 43]
Universal functions (ufunc)

In addition to built-in functions, user-defined functions can be defined, which perform faster than standard Python functions on lists and operate on NumPy arrays.

Example:

```python
import numpy as np

def myadd(x, y):
    return x+y

myadd = np.frompyfunc(myadd, 2, 1)

print(myadd([[1, 2, 3, 4], [5, 6, 7, 8]]))
```

`np.frompyfunc` adds the new function `myadd` to the NumPy ufunc library. ufunc uses vectorization, which is a faster way to operate on elements of arrays.

More info:
https://www.w3schools.com/python/numpy/numpy_ufunc.asp
Plotting data

We will need to install two additional packages in our virtual environment:

```
python3 -m pip install matplotlib
python3 -m pip install seaborn
```

More info:
https://matplotlib.org
https://seaborn.pydata.org
Example: visualizing a normal distribution

The normal (or Gaussian) distribution represents the distribution of many events around a maximum. In NumPy, we can build this distribution using the `random` module:

from numpy import random

The method `random.normal` creates the distribution:

`random.normal(loc, scale, size)`

- `loc`: center of the distribution (mean)
- `scale`: width of the distribution (standard deviation)
- `size`: shape of the NumPy array containing the distribution
Example: visualizing a normal distribution

from numpy import random
import matplotlib.pyplot as plt
import seaborn as sns

# Create distribution
sample = random.normal(loc=0.0, scale=1.0, size=1000)

# Plot graph
sns.distplot(sample, hist=False)
plt.show()

# We can also save the plot to a file
plt.savefig("plot.png")

More info:
https://matplotlib.org
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Example: visualizing a normal distribution

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sns.distplot(sample, hist=False)
plt.show()
```

More info:
https://matplotlib.org
https://seaborn.pydata.org
Example: visualizing a normal distribution

```python
from numpy import random
import matplotlib.pyplot as plt
import seaborn as sns

# Make the example reproducible
np.random.seed(0)

# Create distribution
sample = random.normal(loc=0.0, scale=1.0, size=1000)

# Plot graph
sns.distplot(sample, hist=False)
plt.show()
```

More info:
https://matplotlib.org
https://seaborn.pydata.org
Summary

- Python is a powerful all-purpose programming and scripting language
- It has a huge standard library of packages
- It is easy and fun to learn
- It can be used to write wrappers for low-level code
- (It has object-oriented capabilities)

Where to go from here:
- Develop your own software project
- Test Jupyter and Colab notebooks
- Play with virtual environments; test Python packages

Questions and suggestions: leb140@pitt.edu

CRC web site: https://crc.pitt.edu