

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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- 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

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-)

$$\hat{H}(t)\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N; t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N; t)$$

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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

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- 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**

- A relatively young language: first release by Guido van Rossum in 1991, followed by Python 2 (2000) and Python 3 (2008)
- 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

The screenshot shows the Python.org website with a dark blue header. The Python logo is on the left, and navigation links for 'About', 'Downloads', 'Documentation', 'Community', 'Success Stories', 'News', and 'Events' are in the center. On the right, there are 'Donate', 'Search', 'GO', and 'Socialize' buttons. The main content area features a code editor with Python code for list comprehensions and the enumerate function, and a 'Compound Data Types' section explaining lists. Below the code, there are five numbered buttons (1-5). At the bottom, there are four columns: 'Get Started', 'Download', 'Docs', and 'Jobs', each with a brief description and a link.

```
# Python 3: List comprehensions
>>> fruits = ['Banana', 'Apple', 'Lime']
>>> loud_fruits = [fruit.upper() for fruit in fruits]
>>> print(loud_fruits)
['BANANA', 'APPLE', 'LIME']

# List and the enumerate function
>>> list(enumerate(fruits))
[(0, 'Banana'), (1, 'Apple'), (2, 'Lime')]
```

Compound Data Types
Lists (known as arrays in other languages) are one of the compound data types that Python understands. Lists can be indexed, sliced and manipulated with other built-in functions. [More about lists in Python 3](#)

Python is a programming language that lets you work quickly and integrate systems more effectively. [>>> Learn More](#)

Get Started
Whether you're new to programming or an experienced developer, it's easy to learn and use Python.
[Start with our Beginner's Guide](#)

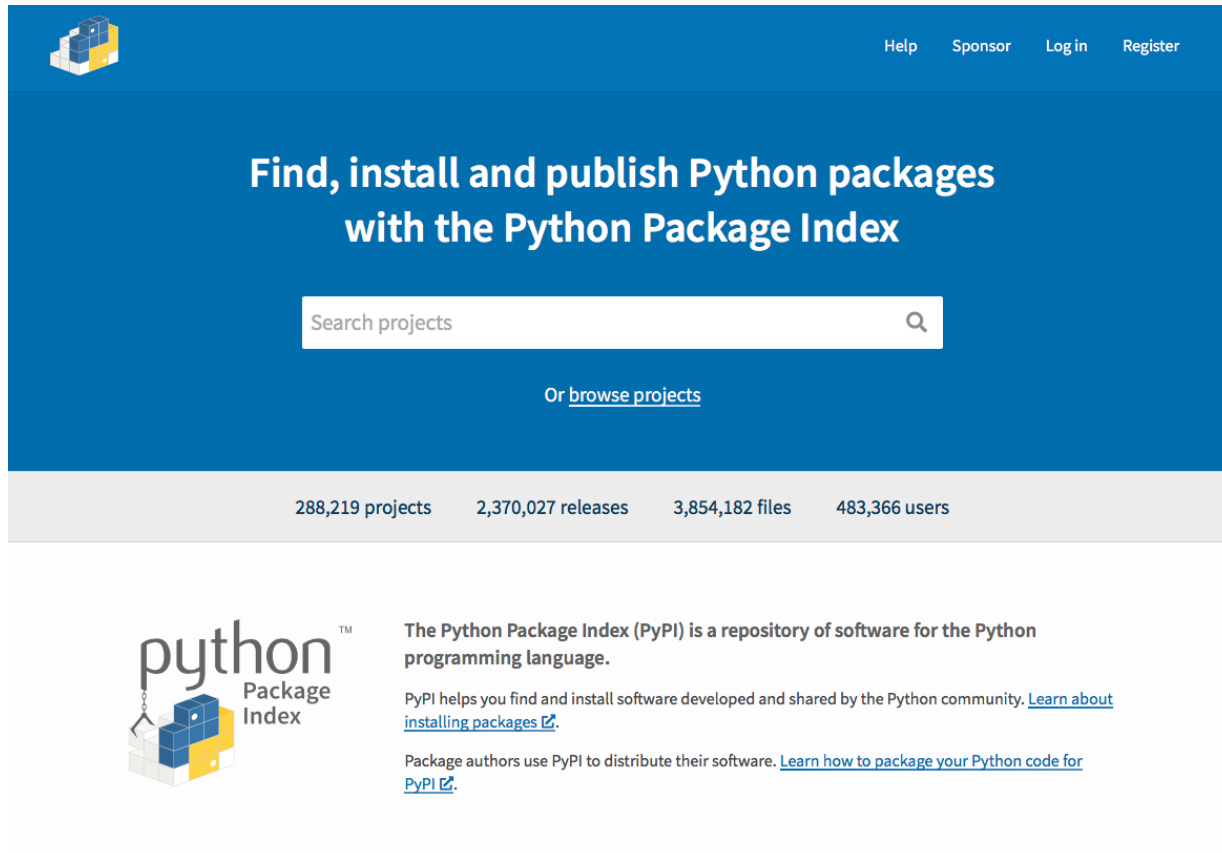
Download
Python source code and installers are available for download for all versions!
Latest: [Python 3.9.1](#)

Docs
Documentation for Python's standard library, along with tutorials and guides, are available online.
[docs.python.org](#)

Jobs
Looking for work or have a Python related position that you're trying to hire for? Our **relaunched community-run job board** is the place to go.
[jobs.python.org](#)

<https://www.python.org>

- Python packages are distributed by their developers
- They are typically very easy to install



The screenshot shows the Python Package Index (PyPI) homepage. At the top left is the PyPI logo, a stack of blue and yellow cubes. In the top right corner, there are links for "Help", "Sponsor", "Log in", and "Register". The main heading reads "Find, install and publish Python packages with the Python Package Index". Below this is a search bar with the placeholder text "Search projects" and a magnifying glass icon. Underneath the search bar is a link that says "Or [browse projects](#)". A statistics bar displays: "288,219 projects", "2,370,027 releases", "3,854,182 files", and "483,366 users". The bottom section features the "python Package Index" logo on the left and a descriptive paragraph on the right: "The Python Package Index (PyPI) is a repository of software for the Python programming language. PyPI helps you find and install software developed and shared by the Python community. [Learn about installing packages](#). Package authors use PyPI to distribute their software. [Learn how to package your Python code for PyPI](#)."

<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.

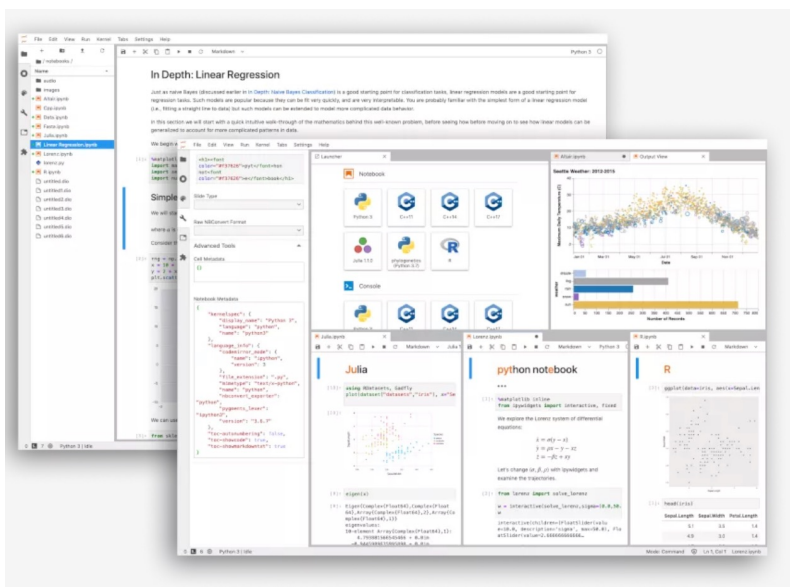


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How to run Python

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**

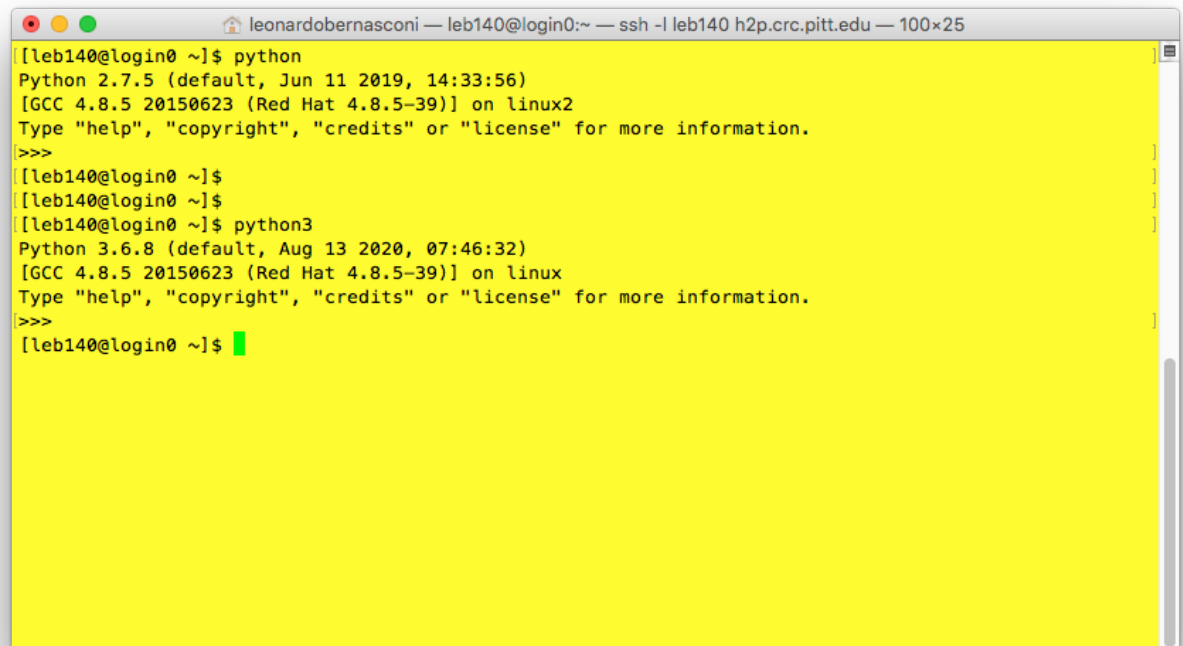
<https://crc.pitt.edu/Access-CRC-Web-Portals>

Interactive sessions

- 1) Start Python: **python** (for Python2) or **python3**
- 2) Type commands line by line
- 3) Exit using: 

or:

exit()



```
leonardobernasconi — leb140@login0:~ — ssh -l leb140 h2p.crc.pitt.edu — 100x25
[[leb140@login0 ~]$ python
Python 2.7.5 (default, Jun 11 2019, 14:33:56)
[GCC 4.8.5 20150623 (Red Hat 4.8.5-39)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
[>>>
[[leb140@login0 ~]$
[[leb140@login0 ~]$
[[leb140@login0 ~]$ python3
Python 3.6.8 (default, Aug 13 2020, 07:46:32)
[GCC 4.8.5 20150623 (Red Hat 4.8.5-39)] on linux
Type "help", "copyright", "credits" or "license" for more information.
[>>>
[[leb140@login0 ~]$ █
```

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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:

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

Built-in modules: `help('modules')`

Data types

Lists

```
l = [1, 2, 13.3, "today", 6+5j]
```

List index (always integer; can be negative)

Length of a list: `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

```
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; etc.
```

Keys: `d1.keys()`

Values: `d1.values()`

Clear: `d1.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 condition1:
    (execute some instructions)
elif condition2:
    (execute some other instructions)
elif condition3:
    (execute some other instructions)
else:
    (execute some other instructions)
```

Indentation (four blank spaces) is very important in Python!!!

Switch to running scripts.

```
/ihome/sam/1eb140/IntroToPython/example1.py
```


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](#)

```
leo — leb140@login0:~/IntroToPython — ssh -Y -l leb140 h2p.crc.pitt.edu — 90x26
#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

```
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](#)

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](#)

Control statements and loops

The `break` statement

It is used to terminate a for/while loop when a given condition is met

```
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

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

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 extensibility.

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](#)


```
leo — leb140@login0:~/IntroToPython — ssh -Y -l leb140 h2p.crc.pitt.edu — 90x26
# A function that takes two numbers as input, squares the first number and adds
# the second number and returns the result.

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:

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

Return date using the Unix 'date' command:

```
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
```

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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?

```
leonardobernasconi — leb140@login0:~/IntroToPython — ssh -Y -l leb140 h2p.crc.pitt.edu — 113x31
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)
```

prime_numbers.py

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?

```

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

# Main program

# Read lines of file1 and store them in list aread
finput = open("file1", 'r')
aread = finput.readlines()
finput.close()

# Read lines of file2 and store them in list bread
finput = open("file2", 'r')
bread = finput.readlines()
finput.close()

# Convert aread into a list of integers (a)
a = []
for item in aread:
    a.append(int(item))
# Convert bread into a list of integers (a)
b = []
for item in bread:
    b.append(int(item))

# Compute the element-by-element difference between a and b
aminb = subtract(a, b)

# Convert aminb into a list of strings (aminbs)
aminbs = []
for item in aminb:
    aminbs.append(str(item) + "\n") # We need to add "\n" to indicate new lines

# Print aminb to a file file3
fout = open("file3", 'w')
fout.writelines(aminbs)

```

Possible solution to
Exercise 2.

Can we improve this
code?


```
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

# Main program

# Read lines of file1 and store them in list aread
finput = open("file1", 'r')
aread = finput.readlines()
finput.close()

# Read lines of file2 and store them in list bread
finput = open("file2", 'r')
bread = finput.readlines()
finput.close()

# Convert aread into a list of integers (a)
a = []
for item in aread:
    a.append(int(item))
# Convert bread into a list of integers (a)
b = []
for item in bread:
    b.append(int(item))

# Compute the element-by-element difference between a and b
aminb = subtract(a, b)

# Convert aminb into a list of strings (aminbs)
aminbs = []
for item in aminb:
    aminbs.append(str(item) + "\n") # We need to add "\n" to indicate new lines

# Print aminb to a file file3
fout = open("file3", 'w')
fout.writelines(aminbs)
```

**Unnecessary
code duplication**

Possible solution to
Exercise 2.

Can we improve this
code?

```
leonardobernasconi — leb140@login0:~/Python — ssh -Y -l leb140 h2p.crc.pitt.edu — 120x52
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
    maxlen = min(len(a), len(b))
    # Index for elements of a and b
    index = 0
    # Loop on the elements of a
    while index < maxlen:
        c.append(a[index]-b[index])
        index += 1
    return c
~
~
~
s0.py 1,1 All
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 = []
    # Index for elements of a and b
    index = 0
    # Loop on the elements of a
    for elementa in a:
        # Exception handling
        try:
            c.append(elementa-b[index])
            index += 1
        except:
            break
    return c
~
s1.py 1,1 All
```

Exception handling

Exception handling

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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:

```
python3 -m venv myenv
```

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

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

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

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

```
deactivate
```

(For Windows, see <https://docs.python.org/3/library/venv.html> or <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:

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

Install numpy:

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

Now launch the python interpreter:

```
python3
```

and check if the new package has been installed:

```
import numpy
```

To list all installed packages: `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
```

<https://uoa-eresearch.github.io/eresearch-cookbook/recipe/2014/11/20/conda/>

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:

```
module purge
module load python/3.7.0
python3 -m venv myenv
source myenv/bin/activate
python3 -m pip install ipykernel
python3 -m ipykernel 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:

```
[ ]: import sys
      print(sys.executable)
```

which should return something like

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

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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`

```
leo -- leb140@login0:~/IntroToPython -- ssh -Y -l leb140 h2p.crc.pitt.edu -- 111x42
-----
python:
-----
Description:
  Anaconda is the leading open data science platform powered by Python.

Versions:
  python/anaconda2.7-4.2.0_westpa
  python/anaconda2.7-4.2.0
  python/anaconda2.7-4.4.0_genomics
  python/anaconda2.7-5.2.0_westpa
  python/anaconda2.7-5.2.0
  python/anaconda2.7-2018.12_westpa
  python/anaconda3.5-4.2.0-dev
  python/anaconda3.5-4.2.0
  python/anaconda3.6-5.2.0_deepabcut
  python/anaconda3.6-5.2.0_leap
  python/anaconda3.6-5.2.0
  python/anaconda3.7-5.3.1_genomics
  python/anaconda3.7-2018.12_westpa
  python/anaconda3.7-2019.03_astro_bagpipes-0.8.2
  python/anaconda3.7-2019.03_astro_bagpipes-0.8.8
  python/anaconda3.7-2019.03_astro
  python/anaconda3.7-2019.03_deformetrica
  python/anaconda3.7-2019.03
  python/anaconda3.8-2020.11
  python/anaconda3.9-2021.11
  python/bioconda-2.7-5.2.0
  python/bioconda-3.6-5.2.0
  python/bioconda-3.7-2019.03
  python/intel-3.5
  python/intel-3.6_2018.3.039
  python/intel-3.6_2019.2.066
  python/intel-3.6
  python/ondemand-jupyter-python3.8
  python/3.7.0-dev
  python/3.7.0-fastx
  python/3.7.0

Other possible modules matches:
lines 1-41
```

6

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 li-
brary for scientific
computing



Matplotlib
Comprehensive 2-D
plotting

IP[y]:
IPython

IPython
Enhanced interac-
tive console







SymPy
Symbolic mathe-
matics









pandas
Data structures &
analysis



Large parts of the SciPy ecosystem (including all six projects above) are fiscally sponsored by **NumFOCUS**.
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- [About SciPy](#)
- [Getting started](#)
- [Documentation](#)
- [Install](#)
- [Bug reports](#)
- [Codes of Conduct](#)
- [SciPy conferences](#) 
- [Topical software](#)
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CORE PACKAGES:

- [NumPy](#) 
- [SciPy library](#) 
- [Matplotlib](#) 
- [IPython](#) 
- [SymPy](#) 
- [pandas](#) 

News

<https://scipy.org>

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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

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

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

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

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

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

Arrays

Accessing array elements:

```
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:

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

Copy and **view** arrays:

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

```
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:

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

Answer: (2, 4)

Reshape an array:

```
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:

```
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:

```
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:

```
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:

```
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]))
```

`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.

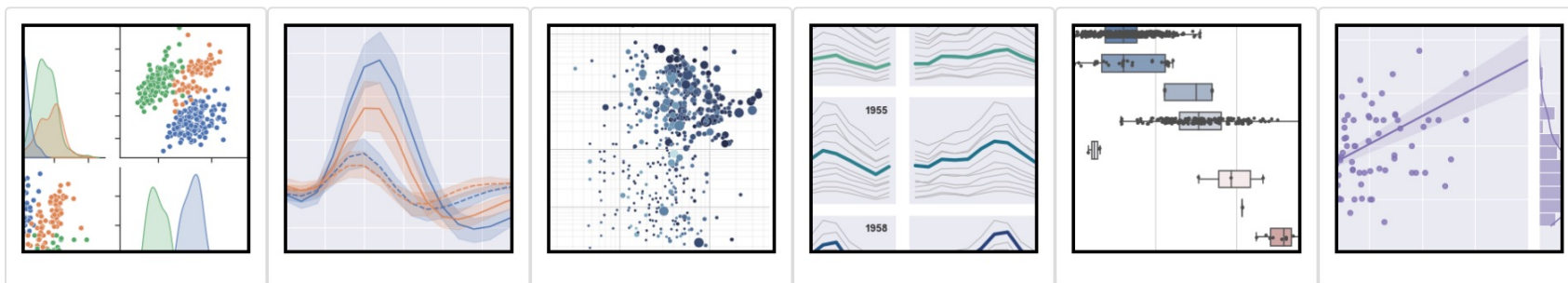
More info:

https://www.w3schools.com/python/numpy/numpy_ufunc.asp

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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>

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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>

<https://seaborn.pydata.org>

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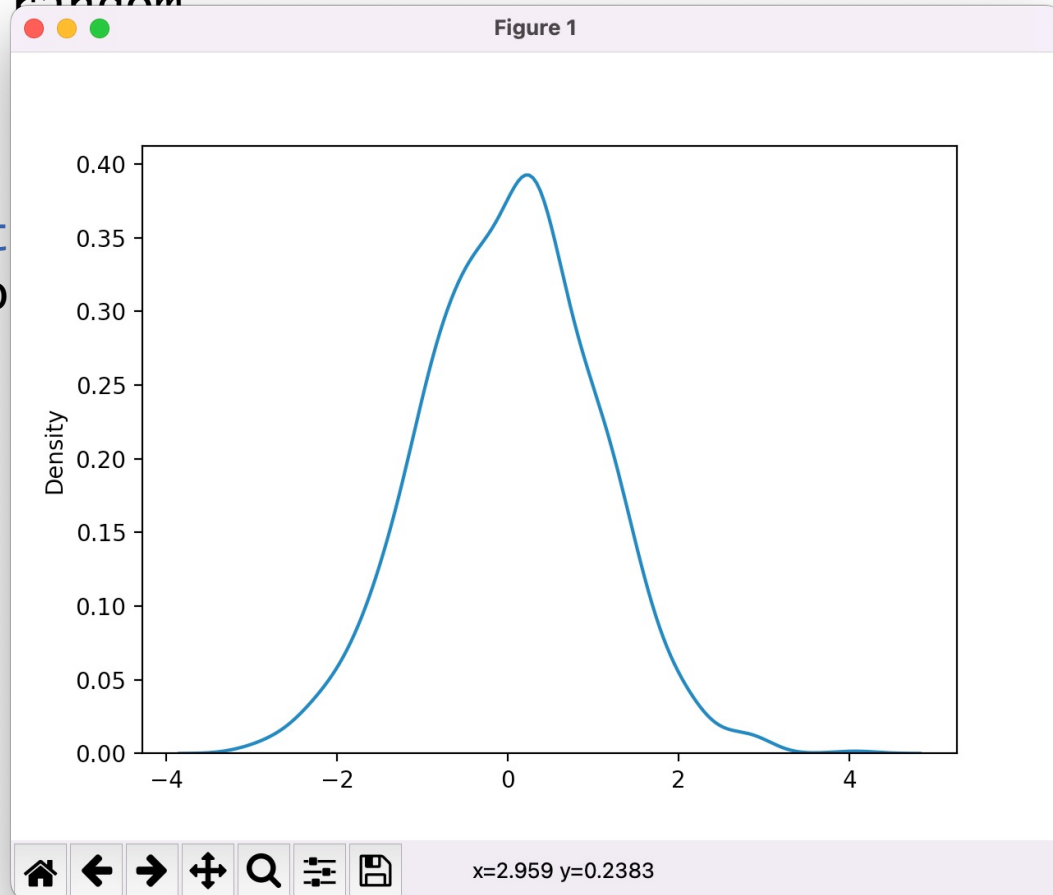
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Example: visualizing a normal distribution

```
from numpy import random
import matplotlib
import seaborn as
```

```
# Create distributed
sample = random.no
```

```
# Plot graph
sns.distplot(sample)
plt.show()
```



More info:

<https://matplotlib.org>

<https://seaborn.pydata.org>

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Example: visualizing a normal distribution

```
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>

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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>