BTEP course

Center for Cancer Research
BTEP
Bioinformatics Training & Education Program

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Bioinformatics Training and Education Program

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Course Overview

Welcome to the Python Introductory Education Series (PIES) course. This course is composed of four lessons (see schedule below) and is meant to help those with no or limited experience in Python get started using this general purpose scripting language for data analyses. Each one-hour lesson will be followed by an optional one-hour help session. At the end of this course series, participants should

- Have obtained a broad overview of Python, including
  - Familiarity with tools used to write Python code
  - Knowledge of Python command syntax
  - Ability to find help for Python commands
  - Knowledge of where to find Python packages
  - Familiarity with self-learning resources
- Be able to describe Python data types and structures and provide examples of where some of the data structures are used
- Know how to work with and wrangle tabular data
- Be able to construct data visualizations

Lesson schedule:

- Lesson 1: Short introduction to Python, signing onto Biowulf, and starting Jupyter Lab (Tuesday, August 15, 2023) *(https://bioinformatics.ccr.cancer.gov/docs/pies-2023/pies_lesson1/)*
  - Lesson 1 recording *(https://cbiit.webex.com/cbiit/ldr.php?RCID=28b10cbe0179993cd0008f1300a1a9ed)*
- Lesson 2: Python data types and structures (Thursday, August 17, 2023) *(https://bioinformatics.ccr.cancer.gov/docs/pies-2023/pies_lesson2/)*
  - Lesson 2 recording *(https://cbiit.webex.com/cbiit/ldr.php?RCID=41f35ca8d9d251425edd765389b47c32)*
- Lesson 3: Data wrangling using Python (Tuesday, August 22, 2023) *(https://bioinformatics.ccr.cancer.gov/docs/pies-2023/pies_lesson3/)*
  - Lesson 3 recording *(https://cbiit.webex.com/cbiit/ldr.php?RCID=0749d0a1a34b9dbcc3abfbb6b34292ff)*
- Lesson 4: Data visualization using Python (Thursday, August 24, 2023) *(https://bioinformatics.ccr.cancer.gov/docs/pies-2023/pies_lesson4/)*
  - Lesson 4 recording *(https://cbiit.webex.com/cbiit/ldr.php?RCID=f6dc3393c95acb10a4ffb2a3b1be6a29)*

A Biowulf account is needed for this class. Visit the Biowulf User Dashboard *(https://hpcnihapps.cit.nih.gov/auth/dashboard/)* to unlock an inactive account. For instructions on obtaining a Biowulf account, visit https://hpc.nih.gov/docs/accounts.html *(https://hpc.nih.gov/docs/accounts.html)*.

Example data used in this course

Download data used in this course

Lesson 1 slides

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Lesson 1: Short introduction to Python, signing onto Biowulf, and starting Jupyter Lab

Learning objectives

After this lesson, participants will

- Be able to describe Python and provide rationale for using it
- Know how to start a Jupyter Lab session on Biowulf (Jupyter Lab will be used to interact with Python throughout this course)
- Be familiar with places for getting Python packages
- Become familiar with navigating the Jupyter Lab environment
- Be able to describe Python command syntax
- Know how to find help for Python commands
- Become familiar with continuing and self-learning resources

What is Python and why use it?

- Scripting language
    - Facilitates reuse and reproducibility
- Can be used to analyze large datasets
- Extensive external packages that can be used for
    - Data wrangling
    - Data visualization
    - Single cell RNA sequencing analysis
    - Working with biological sequences
    - Interfacing with bioinformatics databases
- Strong support community
- Easy to learn

Note

Python packages can be found at The Python Package Index *(https://pypi.org)*.

Signing onto Biowulf

In this course series, participants will interact with Python through Jupyter Lab on Biowulf. Thus, the first step is to sign onto Biowulf using `ssh`. Replace username with participant's own Biowulf username.

```
ssh username@biowulf.nih.gov
```

- Mac: use `ssh` through the Terminal
- Windows: use `ssh` through the command prompt

Change into Biowulf data directory

Use `cd` to change into the participant's data directory on Biowulf. Again, replace username with participant's Biowulf username.

```
cd /data/username
```

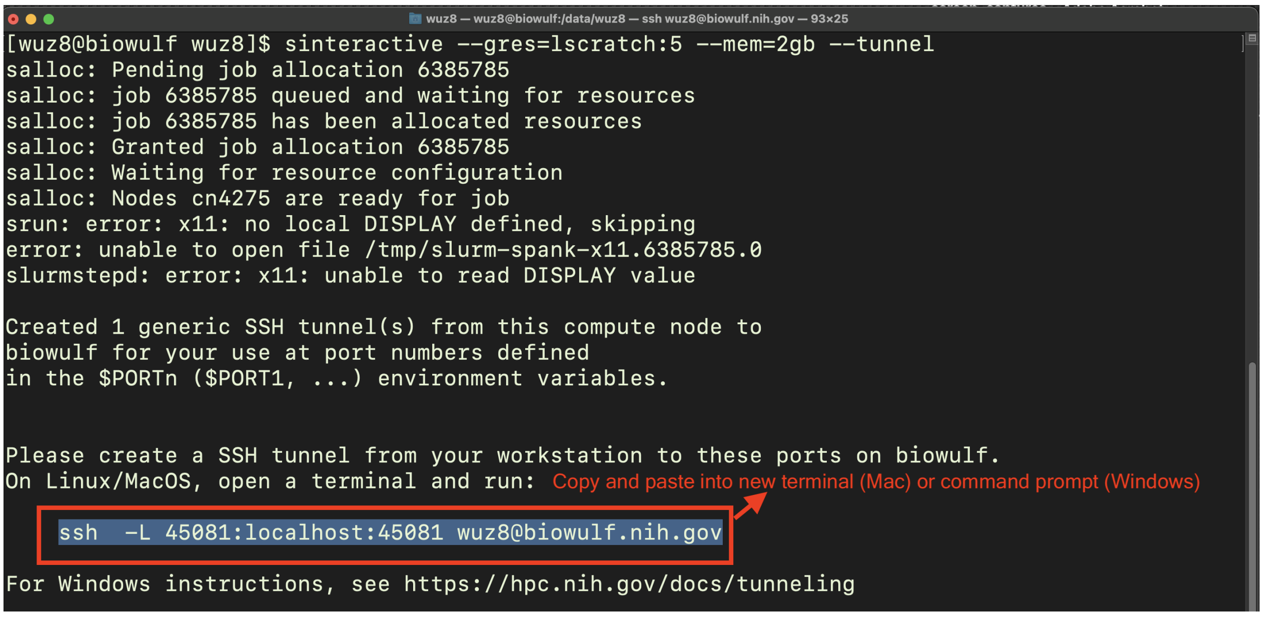
Request an interactive session

Request an interactive session using `sinteractive` with the following options.

- `--gres=lscratch:5`: to allocate 5gb of local temporary/scratch storage space
- `--mem=2gb`: to request 2gb of memory or RAM
- `--tunnel`: to open up a channel of communication between local machine and Biowulf to allow interaction with applications like Jupyter Lab

```
sinteractive --gres=lscratch:5 --mem=2g --tunnel
```

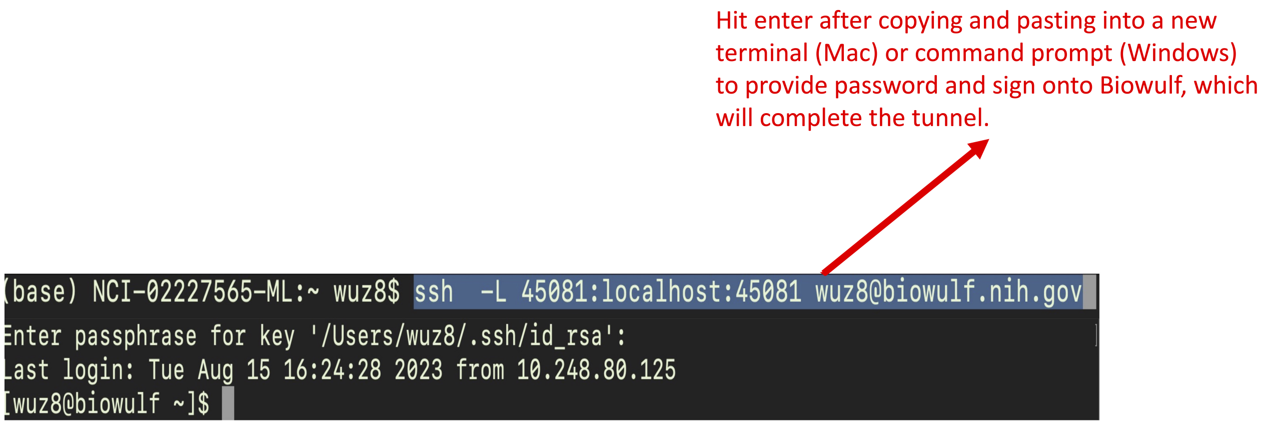
After resources for the interactive session has been granted, users will see the information similar to that shown in Figure 1.


wuz8 — wuz8@biowulf:/data/wuz8 — ssh wuz8@biowulf.nih.gov — 93×25
Copy and paste into new terminal (Mac) or command prompt (Windows)

```
[wuz8@biowulf wuz8]$ sinteractive --gres=lscratch:5 --mem=2gb --tunnel
salloc: Pending job allocation 6385785
salloc: job 6385785 queued and waiting for resources
salloc: job 6385785 has been allocated resources
salloc: Granted job allocation 6385785
salloc: Waiting for resource configuration
salloc: Nodes cn4275 are ready for job
srun: error: x11: no local DISPLAY defined, skipping
error: unable to open file /tmp/slurm-spank-x11.6385785.0
slurmstepd: error: x11: unable to read DISPLAY value

Created 1 generic SSH tunnel(s) from this compute node to
biowulf for your use at port numbers defined
in the $PORTn ($PORT1, ...) environment variables.


Please create a SSH tunnel from your workstation to these ports on biowulf.
On Linux/MacOS, open a terminal and run:

    ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov

For Windows instructions, see https://hpc.nih.gov/docs/tunneling
```

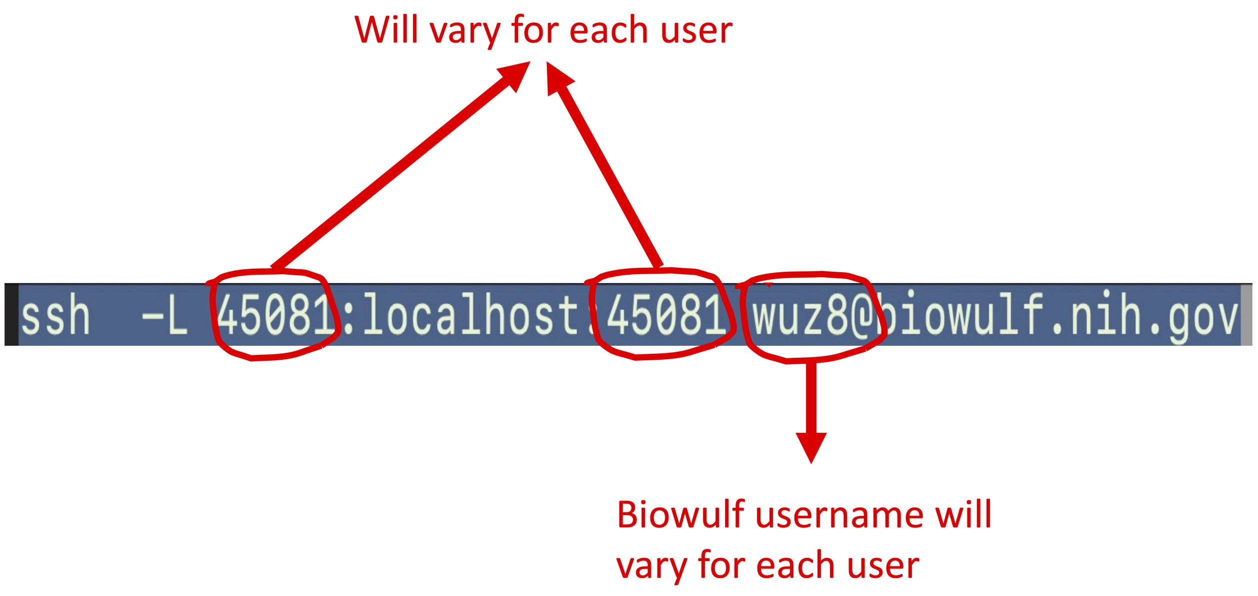
Figure 1: After interactive session resources have been allocated, users will see a `ssh` command that looks like that enclosed in the red rectangle. Open a new terminal (if working on a Mac) or command prompt (if working on a Windows computer) and then copy and paste this `ssh` command into the new terminal.

After copying and pasting the `ssh` command shown in Figure 1 to a new terminal or command prompt, hit enter to supply password and log in to Biowulf. This will complete the tunnel.


Hit enter after copying and pasting into a new terminal (Mac) or command prompt (Windows) to provide password and sign onto Biowulf, which will complete the tunnel.

```
(base) NCI-02227565-ML:~ wuz8$ ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov
Enter passphrase for key '/Users/wuz8/.ssh/id_rsa':
Last login: Tue Aug 15 16:24:28 2023 from 10.248.80.125
[wuz8@biowulf ~]$
```

Figure 2: Hit enter after copying and pasting the `ssh` command to a new terminal to provide password and log into Biowulf. This will complete the tunnel.



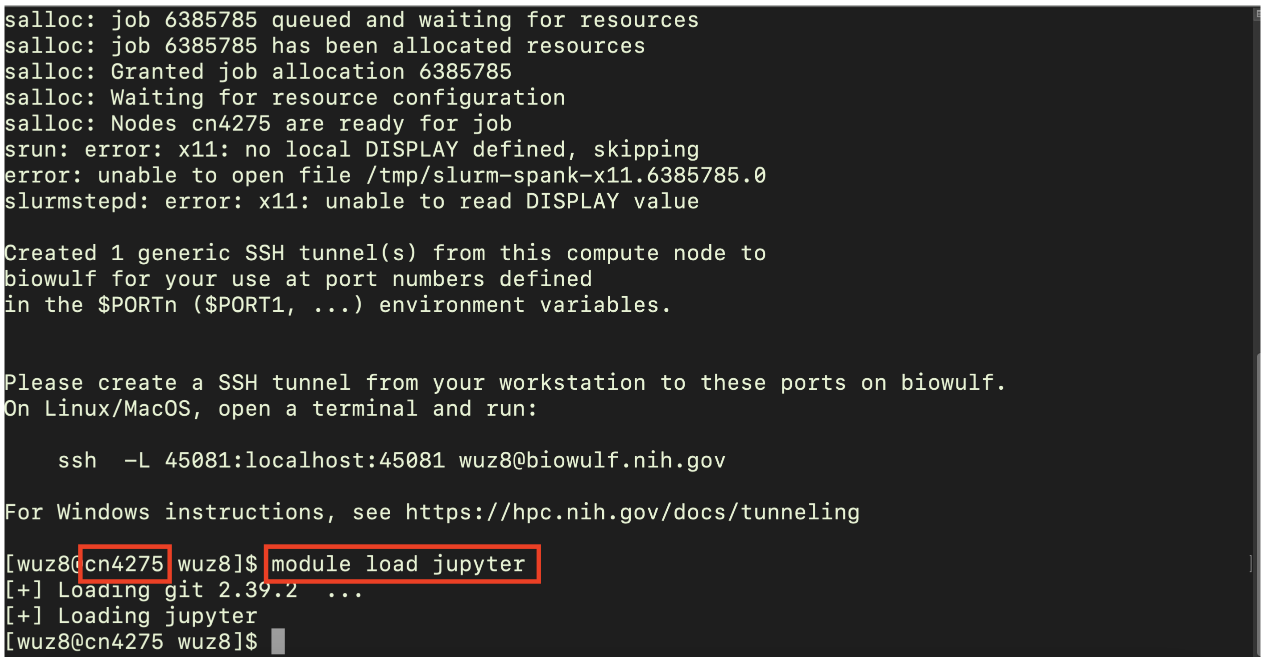
```
ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov
```

Figure 3: In the `ssh` command shown in Figure 1 and Figure 2, the numbers preceding and following "localhost" will differ depending on user. Also, the Biowulf username will differ for each user (wuz8 is the instructor's Biowulf username).

Load Jupyter

After the tunnel has been created, go back terminal (Mac) or command prompt (Windows) with the Biowulf interactive session and activate Jupyter (see Figure 4).

```
module load jupyter
```



```
salloc: job 6385785 queued and waiting for resources
salloc: job 6385785 has been allocated resources
salloc: Granted job allocation 6385785
salloc: Waiting for resource configuration
salloc: Nodes cn4275 are ready for job
srun: error: x11: no local DISPLAY defined, skipping
error: unable to open file /tmp/slurm-spank-x11.6385785.0
slurmstepd: error: x11: unable to read DISPLAY value

Created 1 generic SSH tunnel(s) from this compute node to
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Please create a SSH tunnel from your workstation to these ports on biowulf.
On Linux/MacOS, open a terminal and run:

    ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov

For Windows instructions, see https://hpc.nih.gov/docs/tunneling

[wuz8@cn4275 wuz8]$ module load jupyter
[+] Loading git 2.39.2  ...
[+] Loading jupyter
[wuz8@cn4275 wuz8]$
```
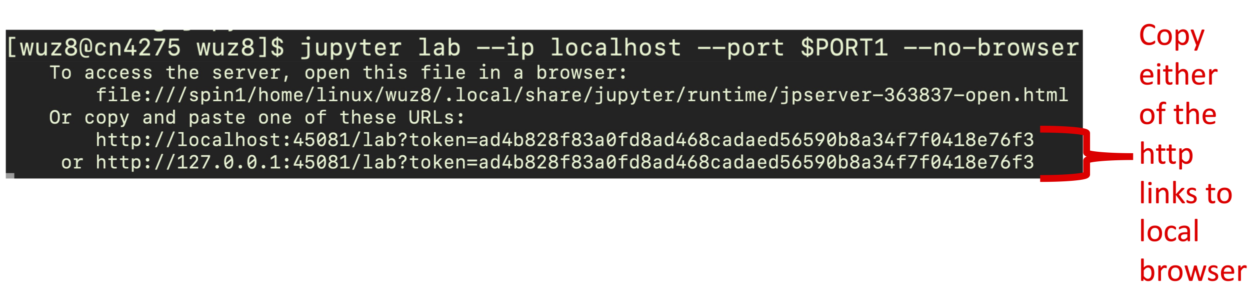

Figure 4: Go back to the terminal (Mac) or command prompt (Windows) with the interactive session (look for cn#### at the prompt). Do `module load jupyter` from here.

Start Jupyter Lab

Use the command below to start a Jupyter Lab session. Copy and paste either of the http links to a local browser to interact with Jupyter (see Figure 5).

```
jupyter lab --ip localhost --port $PORT1 --no-browser
```



```
[wuz8@cn4275 wuz8]$ jupyter lab --ip localhost --port $PORT1 --no-browser
    To access the server, open this file in a browser:
        file:///spin1/home/linux/wuz8/.local/share/jupyter/runtime/jpserver-363837-open.html
    Or copy and paste one of these URLs:
        http://localhost:45081/lab?token=ad4b828f83a0fd8ad468cadaed56590b8a34f7f0418e76f3
     or http://127.0.0.1:45081/lab?token=ad4b828f83a0fd8ad468cadaed56590b8a34f7f0418e76f3
```

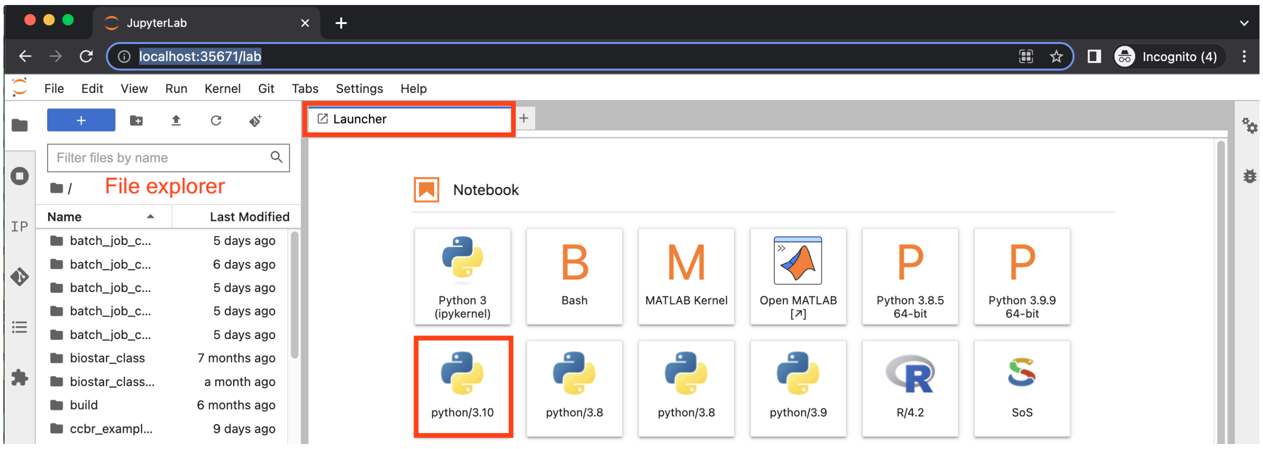
Figure 5: Start a Jupyter lab session using `jupyter lab --ip localhost --port $PORT1 --no-browser` and copy and paste either one of the http links to a local browser.

Warning

The URLs change with each Jupyter Lab session, so please do not copy from the examples shown below. Copy from the URLs provided in the Biowulf interactive session terminal instead.

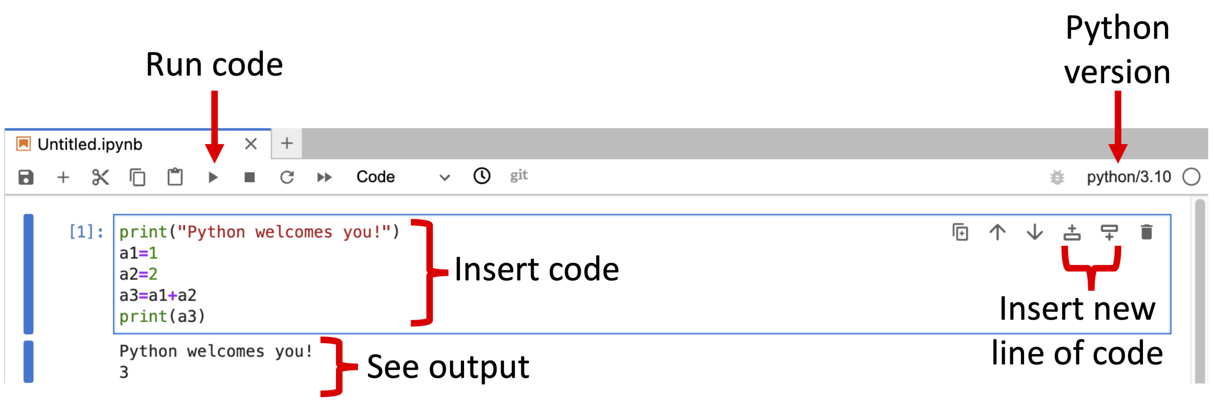
Jupyter Lab - file explorer and launcher

- File explorer
- Launcher for starting language specific notebooks (for this course series, choose the python/3.10 notebook)



Name	Last Modified
batch_job_c...	5 days ago
batch_job_c...	6 days ago
batch_job_c...	5 days ago
batch_job_c...	5 days ago
batch_job_c...	5 days ago
biostar_class	7 months ago
biostar_class...	a month ago
build	6 months ago
ccbr_exampl...	9 days ago

Jupyter Notebook - cells



```
[1]: print("Python welcomes you!")
     a1=1
     a2=2
     a3=a1+a2
     print(a3)

     Python welcomes you!
     3
```

Python education resources

- Coursera
  - Programming for Everybody (Getting Started with Python)
    - Instructor: Charles Severance, PhD (University of Michigan)
  - Data Analysis with Python
    - Instructor: IBM staff
    - Includes data wrangling and regression analysis
  - Data Visualization with Python
    - Intructor: IBM staff
    - Introduces data visualization using packages such as Matplotlib and Seaborn
- Dataquest
  - https://www.dataquest.io/course/introduction-to-python/ *(https://www.dataquest.io/course/introduction-to-python/)*
  - https://www.dataquest.io/path/data-scientist/ *(https://www.dataquest.io/path/data-scientist/)*
  - https://www.dataquest.io/path/data-analyst/ *(https://www.dataquest.io/path/data-analyst/)*

Visit the self learning resources page *(https://bioinformatics.ccr.cancer.gov/btep/self-learning/)* to request a Dataquest or Coursera license.

Python command syntax

The command syntax for Python is composed of the

- Command
- Argument, which is enclosed in the parentheses and what the command will act on
- Options, which is enclosed in parentheses and alters the way the command runs

```
command(argument, options)
```

Example of a Python command with and without options

```
print("Hello", "welcome to Python")
```

```
Hello welcome to Python
```

Include option `sep` to place a comma between "Hello" and "welcome to Python".

```
print("Hello", "welcome to Python", sep=", ")
```

```
Hello, welcome to Python
```

Finding help for Python commands

The `help` command can be used to view documentations for Python commands. It follows the Python command syntax. Insert the command in which help is needed into the parentheses.

```
help()
```

Example of using help

```
help(print)
```

```
Help on built-in function print in module builtins:

print(...)
    print(value, ..., sep=' ', end='\n', file=sys.stdout, flush=Fals

    Prints the values to a stream, or to sys.stdout by default.
    Optional keyword arguments:
    file:  a file-like object (stream); defaults to the current sys.
    sep:   string inserted between values, default a space.
    end:   string appended after the last value, default a newline.
    flush: whether to forcibly flush the stream.
```

Copy class data to data directory

The example datasets used for this course series reside in `/data/classes/BTEP/pies_2023_data`. Make a copy in your `data` directory.

```
cp -r /data/classes/BTEP/pies_2023_data ./pies_2023
```

Lesson 2: Python data types and structures

Learning objectives

After this class, participants will

- Be able to describe some common Python data types and structures
- Be able to identify Python data types
- Become familiar with variable assignment
- Be able to use conditional operators and if-else statements
- Be able to load packages
- Know how to import tabular data
- Know how to view tabular data
- Become familiar with constructing a `for` loop in Python

Signing onto Biowulf

Sign onto Biowulf using the `ssh` command. Replace username with user's Biowulf ID.

```
ssh username@biowul.nih.gov
```

Change into data directory and copy course data

Replace username with user's Biowulf ID.

```
cd /data/username
```

The `cp` command below will copy pies_2023_data in /data/classes/ to the user's data directory (denoted as "." as this should be present working directory) and save it as a folder called pies_2023.

```
cp -r /data/classes/BTEP/pies_2023_data ./pies_2023
```

Change into pies_2023.

```
cd pies_2023
```

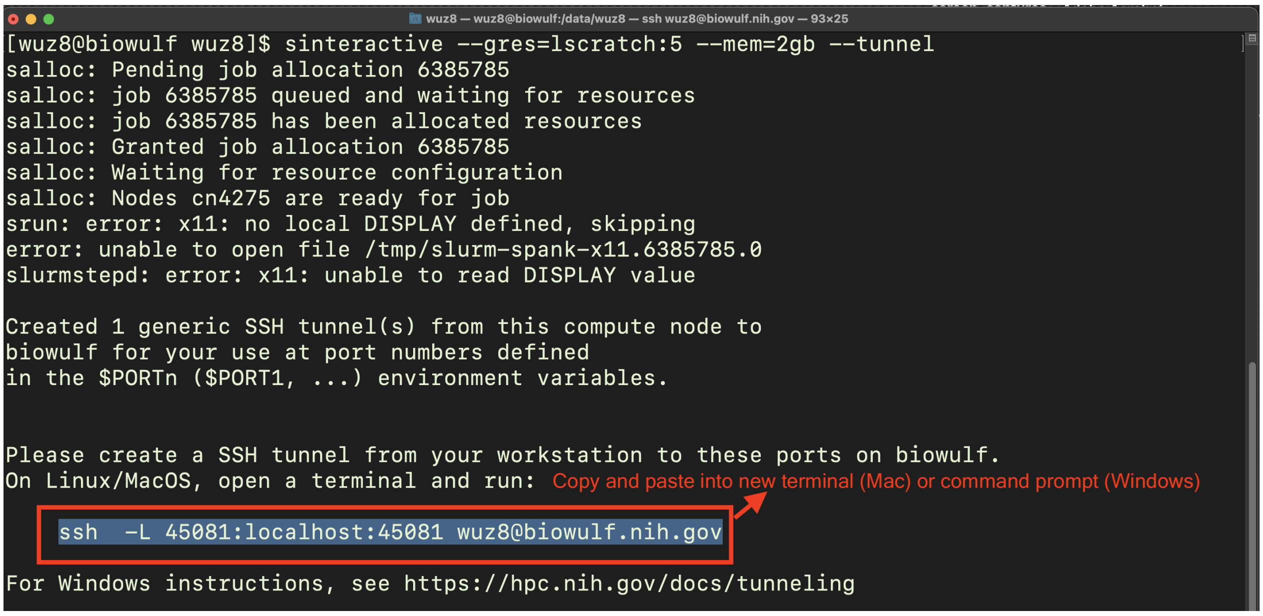
Request interactive session

Stay in the /data/username/pies_2023 folder and request an interactive session using `sinteractive` with the following options.

- `--gres=lscratch:5`: to allocate 5gb of local temporary/scratch storage space
- `--mem=2gb`: to request 2gb of memory or RAM
- `--tunnel`: to open up a channel of communication between local machine and Biowulf to allow interaction with applications like Jupyter Lab

```
sinteractive --gres=lscratch:5 --mem=2g --tunnel
```

After resources for the interactive session has been granted, users will see the information similar to that shown in Figure 1.


wuz8 — wuz8@biowulf:/data/wuz8 — ssh wuz8@biowulf.nih.gov — 93×25
Copy and paste into new terminal (Mac) or command prompt (Windows)

```
[wuz8@biowulf wuz8]$ sinteractive --gres=lscratch:5 --mem=2gb --tunnel
salloc: Pending job allocation 6385785
salloc: job 6385785 queued and waiting for resources
salloc: job 6385785 has been allocated resources
salloc: Granted job allocation 6385785
salloc: Waiting for resource configuration
salloc: Nodes cn4275 are ready for job
srun: error: x11: no local DISPLAY defined, skipping
error: unable to open file /tmp/slurm-spank-x11.6385785.0
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On Linux/MacOS, open a terminal and run:

    ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov

For Windows instructions, see https://hpc.nih.gov/docs/tunneling
```
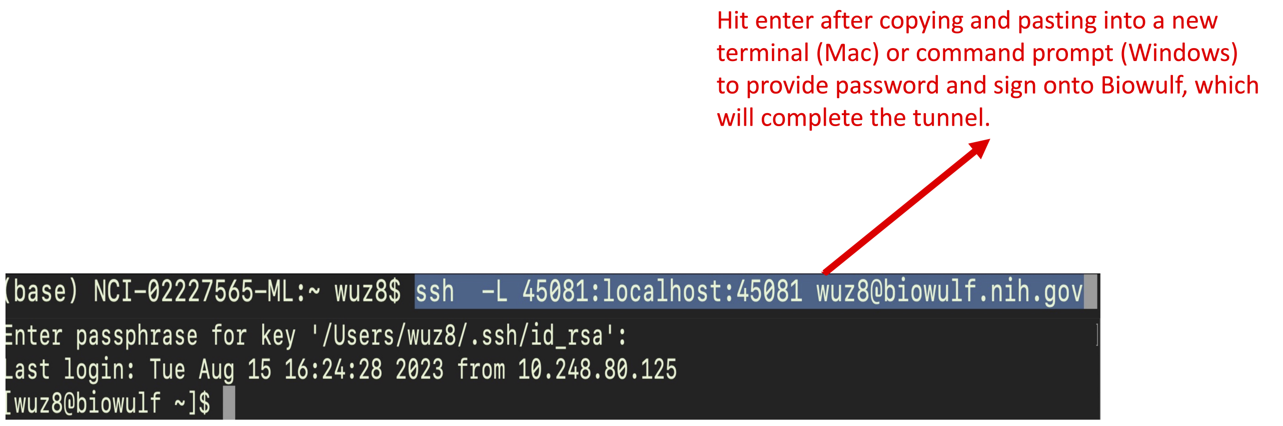
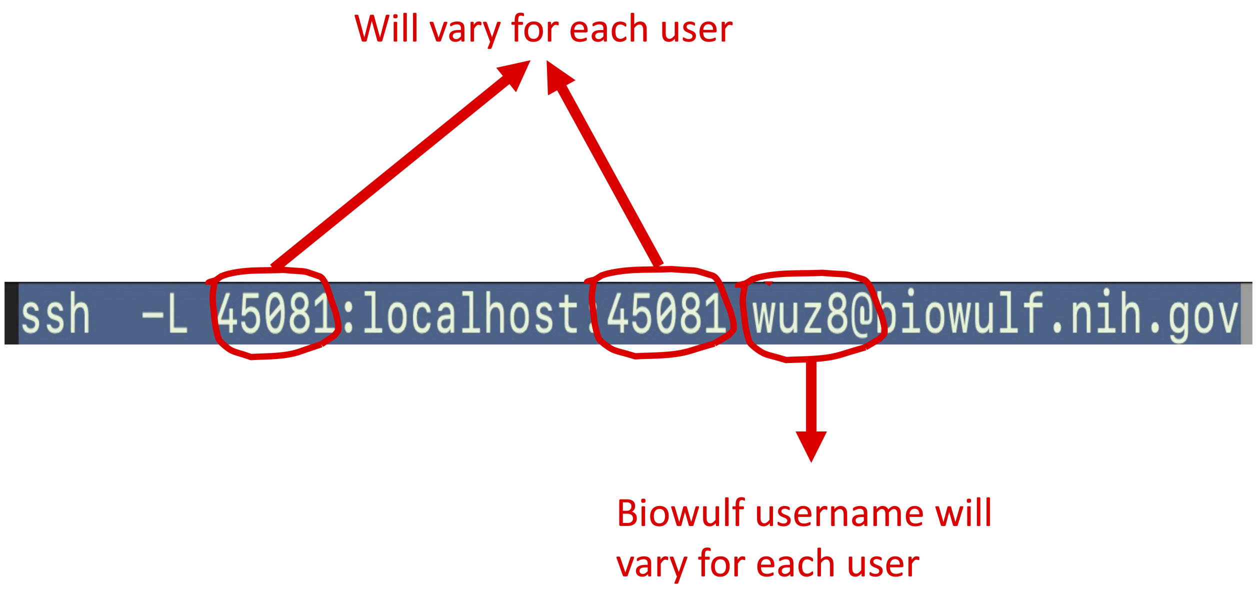

Figure 1: After interactive session resources have been allocated, users will see a `ssh` command that looks like that enclosed in the red rectangle. Open a new terminal (if working on a Mac) or command prompt (if working on a Windows computer) and then copy and paste this `ssh` command into the new terminal.

After copying and pasting the `ssh` command shown in Figure 1 to a new terminal or command prompt, hit enter to supply password and log in to Biowulf. This will complete the tunnel.


Hit enter after copying and pasting into a new terminal (Mac) or command prompt (Windows) to provide password and sign onto Biowulf, which will complete the tunnel.

```
(base) NCI-02227565-ML:~ wuz8$ ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov
Enter passphrase for key '/Users/wuz8/.ssh/id_rsa':
Last login: Tue Aug 15 16:24:28 2023 from 10.248.80.125
[wuz8@biowulf ~]$
```

Figure 2: Hit enter after copying and pasting the `ssh` command to a new terminal to provide password and log into Biowulf. This will complete the tunnel.



```
ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov
```

Figure 3: In the `ssh` command shown in Figure 1 and Figure 2, the numbers preceding and following "localhost" will differ depending on user. Also, the Biowulf username will differ for each user (wuz8 is the instructor's Biowulf username).

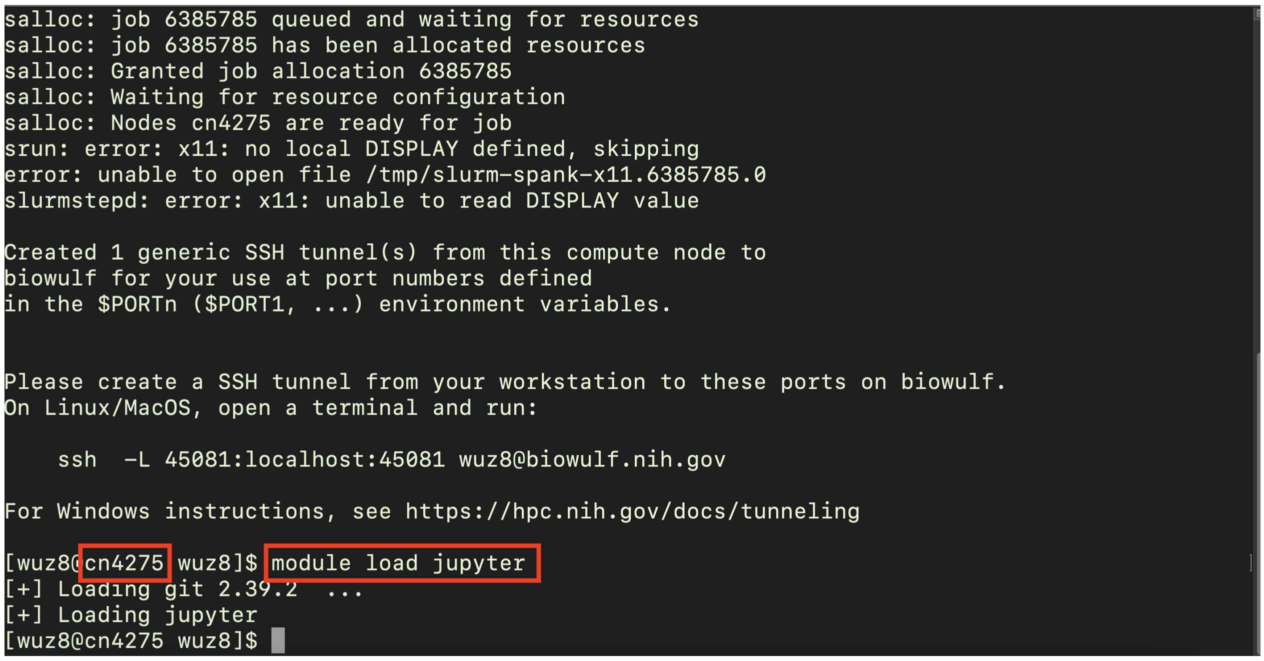
Load Jupyter

Warning

Make sure to stay in the /data/username/pies_2023 folder for this step.

After the tunnel has been created, go back terminal (Mac) or command prompt (Windows) with the Biowulf interactive session and activate Jupyter (see Figure 4).

```
module load jupyter
```



```
salloc: job 6385785 queued and waiting for resources
salloc: job 6385785 has been allocated resources
salloc: Granted job allocation 6385785
salloc: Waiting for resource configuration
salloc: Nodes cn4275 are ready for job
srun: error: x11: no local DISPLAY defined, skipping
error: unable to open file /tmp/slurm-spank-x11.6385785.0
slurmstepd: error: x11: unable to read DISPLAY value

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    ssh  -L 45081:localhost:45081 wuz8@biowulf.nih.gov

For Windows instructions, see https://hpc.nih.gov/docs/tunneling

[wuz8@cn4275 wuz8]$ module load jupyter
[+] Loading git 2.39.2  ...
[+] Loading jupyter
[wuz8@cn4275 wuz8]$
```

Figure 4: Go back to the terminal (Mac) or command prompt (Windows) with the interactive session (look for cn#### at the prompt). Do `module load jupyter` from here.

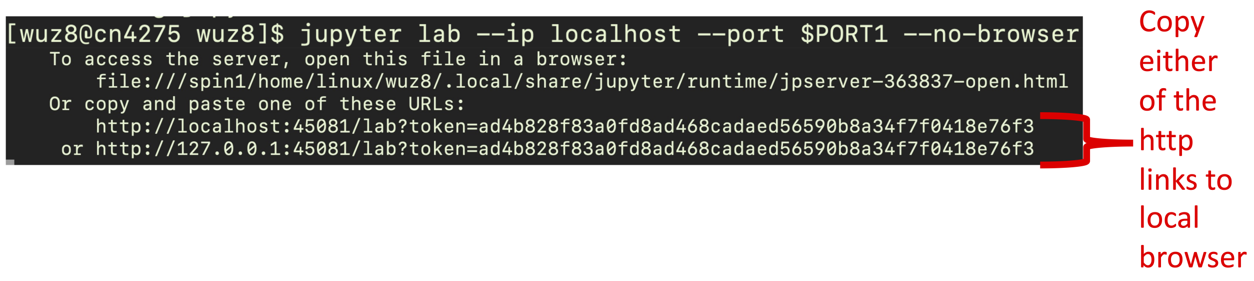
Start Jupyter Lab

Warning

Make sure to stay in the /data/username/pies_2023 folder for this step.

Use the command below to start a Jupyter Lab session. Copy and paste either of the http links to a local browser to interact with Jupyter (see Figure 5).

```
jupyter lab --ip localhost --port $PORT1 --no-browser
```



```
[wuz8@cn4275 wuz8]$ jupyter lab --ip localhost --port $PORT1 --no-browser
    To access the server, open this file in a browser:
        file:///spin1/home/linux/wuz8/.local/share/jupyter/runtime/jpserver-363837-open.html
    Or copy and paste one of these URLs:
        http://localhost:45081/lab?token=ad4b828f83a0fd8ad468cadaed56590b8a34f7f0418e76f3
     or http://127.0.0.1:45081/lab?token=ad4b828f83a0fd8ad468cadaed56590b8a34f7f0418e76f3
```

Figure 5: Start a Jupyter lab session using `jupyter lab --ip localhost --port $PORT1 --no-browser` and copy and paste either one of the http links to a local browser.

Python data types and data structures

An important step to learning any new programming language and data analysis is to understand its data types and data structures. Common data types and structures that will be encountered include the following.

- Text (str)
- Numeric
    - int (ie. integers)
    - float (ie. decimals)
- Boolean (True or False)
    - conditionals
    - filtering criteria
    - command options
- Data frames
- Lists
- Arrays
- Tuples
- Range
- Dictionaries

Identifying data type and structure in Python

The command `type` can be used to identify data types and structures in Python.

```
type(100)
```

```
int
```

```
type(3.1415926)
```

```
float
```

```
type("bioinformatics")
```

```
str
```

Variable assignments

In Python, variables are assigned to values using "=". Users can assign variables to integers, float, or string.

```
perfect=100
perfect
```

```
100
```

```
mole=6.02e23
mole
```

```
6.02e+23
```

```
btep_class="Python Introductory Education Series"
btep_class
```

```
'Python Introductory Education Series'
```

The command `type(btep_class)` will return `str` because the variable btep_class is text.

```
type(btep_class)
```

```
str
```

Conditionals

Conditionals evaluate the validity of certain conditions and operators include:

- ==: is equal to?
- >: is greater than?
- >=: is greater than or equal to?
- <: is less than?
- <=: is less than or equal to?

- `!=`: is not equal to?
- `and`
- `or`

The command below will evaluate if the variable perfect is equal to the variable mole and returns the Boolean value, False.

```
perfect==mole
```

```
False
```

If statements are also conditionals and are used to instruct the computer to do something if a condition is met. To have the computer do something when the condition is not met, use `elif` (else if) or `else`.

The command below will accomplish the following:

- Use `if` to evaluate if perfect==mole, if yes then indicate using `print` that the two variables are equal
- In the case that perfect does not equal mole, use `elif` (which stands for else if) to evaluate if perfect>mole, if yes then use the `print` statement to indicate that perfect is greater than mole
- `else` when the previous two conditions are not met, use `print` to indicate that perfect is less than mole

```
if perfect==mole:
    print(perfect, "is equal to", mole)
elif perfect>mole:
    print(perfect, "is greater than", mole)
else:
    print(perfect, "is less than", mole)
```

```
100 is less than 6.02e+23
```

Note

The `print` command can be used to print variables by not enclosing in quotes.

A ":" is required after `if`, `elif`, and `else`. The command(s) to execute when conditions are met are placed on a separate line but tab indented.

Data frames

Often, in bioinformatics and data science, data comes in the form of rectangular tables, which are referred to as data frames. Data frames have the following property.

- Study variable(s) form the columns
- Observation(s) form rows
- Can have a mix of data types (strings and numeric) but **each column/study variable can contain only one data type**
- Limited to one value per cell

A popular package for working with data frames in Python is Pandas *(https://pandas.pydata.org)*.

To load a Python package use the `import` command followed by the package name (ie. pandas).

```
import pandas
```

Sometimes the name of the package is long, so users might want to shorten it by creating an alias. The alias "pd" is often used for the Pandas package. To add an alias, just append `as` followed by the user defined alias to the package import command.

```
import pandas as pd
```

Importing tabular data with Pandas

This exercise will use the `read_csv` function of Pandas to import a comma separated value (csv) file called hbr_uhr_chr22_rna_seq_counts.csv, which contains RNA sequencing gene expression counts from the Human Brain Reference (hbr) and Universal Human Reference (uhr) study *(https://rnabio.org/module-01-inputs/0001/05/01/RNAseq_Data/)*.

```
hbr_uhr_chr22_counts=pandas.read_csv("./hbr_uhr_chr22_rna_seq_counts
```

Note

If a Python package was imported using an alias (ie. pd for Pandas) then use the alias to call the package. For instance, `pd.read_csv` rather than `pandas.read_csv` when the pd alias is used for Pandas.

Take note of the way the csv import command is constructed. First the user specifies the name of package (ie. pandas) and then the function within the package (ie. read_csv). The package name and function name is separated by a period.

Next, use `type` to find out the data type or structure for hbr_uhr_chr22_counts.

```
type(hbr_uhr_chr22_counts)
```

```
pandas.core.frame.DataFrame
```

Take a look a the first few rows of hbr_uhr_chr22_counts.

```
hbr_uhr_chr22_counts.head()
```

	Geneid	HBR_1.bam	HBR_2.bam	HBR_3.bam	UHR_1.bam	UHR_2.bam	UHR_3.bam
0	U2	0	0	0	0	0	0
1	CU459211.1	0	0	0	0	0	0
2	CU104787.1	0	0	0	0	0	0
3	BAGE5	0	0	0	0	0	0
4	ACTR3BP6	0	0	0	0	0	0

Figure 1: Example of a data frame.

Because hbr_uhr_chr22_counts is a Pandas data frame, it is possible to append one of the many Pandas commands to it. For instance, the `head` function was appended to display the first five rows of hbr_uhr_chr22_counts. The data frame name and function is separated by a period. This is perhaps one of the most appealing aspects of Python syntax. Note that the `head` function was followed by `()`. If the parentheses is blank, then by default the first five lines will be shown. There will be more examples of the Pandas `head` function in a subsequent lesson.

Lists and tuples

Lists and tuples are one dimensional collections of data. The tuple is an immutable list, in which the elements cannot be modified.

To create a list, enclose the contents in square brackets.

```
sequencing_list=["whole genome", "rna", "whole exome"]
```

To create a tuple, enclose the contents in parentheses.

```
sequencing_tuple=("whole genome", "rna", "whole exome")
```

Lists and tuples are indexed and can contain duplicates. The first item in a list or tuple has an index of 0, the second item has an index of 1, and the last item has an index of n-1 where n is the number of items. Indices can be used to recall items in a list or tuple.

```
sequencing_list[1]
```

```
'rna'
```

List versus tuples (mutable versus immutable)

```
sequencing_list[1]="single cell RNA"
```

```
sequencing_list
```

```
['whole genome', 'single cell RNA', 'whole exome']
```

```
sequencing_tuple[1]="single cell RNA"
```

```
TypeError                                 Traceback (most recent cal
Cell In[48], line 1
----> 1 sequencing_tuple[1]="single cell RNA"

TypeError: 'tuple' object does not support item assignment
```

Instructions for modifying Python lists can be found at the W3 school *(https://www.w3schools.com/python/python_lists.asp)*

Arrays

Given a list of numbers, it is difficult to perform mathematical operations. For instance

```
list_of_numbers=[1,2,3,4,5]
```

Multiplying list_of_numbers by 2 will duplicate this list. However, multiplying a list of numbers by two should double every number in that list. Thus, the expected result is [2,4,6,8,10]. To resolve this, convert the list to an array using the package numpy *(https://numpy.org)*.

```
list_of_numbers*2
```

```
[1, 2, 3, 4, 5, 1, 2, 3, 4, 5]
```

Use the `array` function of numpy to convert list_of_numbers to an array called array_of_numbers.

```
array_of_numbers=numpy.array(list_of_numbers)
```

```
array_of_numbers*2
```

```
array([ 2,  4,  6,  8, 10])
```

The array of numbers shown here is a one dimensional array. A special case of arrays is the matrix, which is two dimensional. Like data frames, matrices store values in columns and rows. Matrices are encountered in computation and are used to store numeric values (see here for more on matrices *(https://youtu.be/IZcyZHomFQc)*).

Range

Ranges can be used to for subsetting data (ie. extract data in rows 5 thru 10 of a data frame) or applied to iterate over a task in things like a `for` loop.

For instance, a `for` loop can be used to iterate over sequencing_list_new and print the 3rd to 5th entries.

```
sequencing_list_new=["whole genome", "rna", "whole exome","single ce
```

```
for i in range(2,5):
    print(sequencing_list_new[i])
```

```
whole exome
single cell rna
chip
```

Dictionaries

Dictionaries are key-value pairs and these are encountered as ways to specify options in some Python packages.

```
my_dictionary={"apples":"red","oranges":"orange","bananas":"yellow"}
```

Lesson 3: Data wrangling using Python

Learning objectives

After this lesson, participants will

- Be able to import tabular data into Python using Pandas
- Be able to explore and modify tabular data through various data wrangling approaches, including
    - retrieving dimensions
    - subsetting
    - obtaining column statistics
    - replacing column names
    - performing mathematical operations
    - filtering
    - removing and adding columns

Importing tabular data using Pandas

Pandas *(https://pandas.pydata.org)* is a popular Python package used to work with tabular data.

To work with Pandas, first activate it using the `import` command.

```
import pandas
```

Sometimes the name of the package is long, so users might want to shorten it by creating an alias. The alias "pd" is often used for the Pandas package. To add an alias, just append `as` followed by the user defined alias to the package import command. If importing a package using an alias, then the package needes to be called using the assigned alias. For instance, if `pd` was used to import pandas, then use `pd.read_csv` to import a csv file.

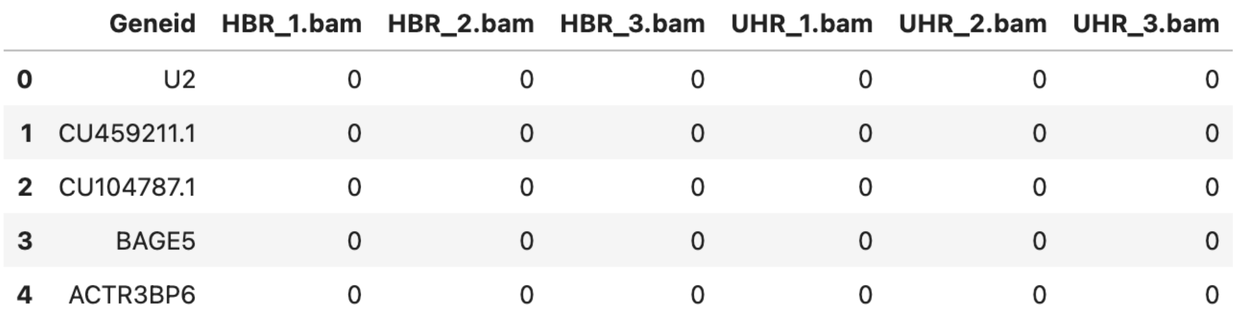
```
import pandas as pd
```

This exercise will use the `read_csv` function of Pandas to import a comma separated value (csv) file called hbr_uhr_chr22_rna_seq_counts.csv, which contains RNA sequencing gene expression counts from the Human Brain Reference (hbr) and Universal Human Reference (uhr) study *(https://rnabio.org/module-01-inputs/0001/05/01/RNAseq_Data/)*. This data will be stored as the variable hbr_uhr_chr22_counts.

```
hbr_uhr_chr22_counts=pandas.read_csv("./hbr_uhr_chr22_rna_seq_counts
```

Take a look at the first few rows of hbr_uhr_chr22_counts by appending the `head` attribute to hbr_uhr_chr22_counts.

```
hbr_uhr_chr22_counts.head()
```

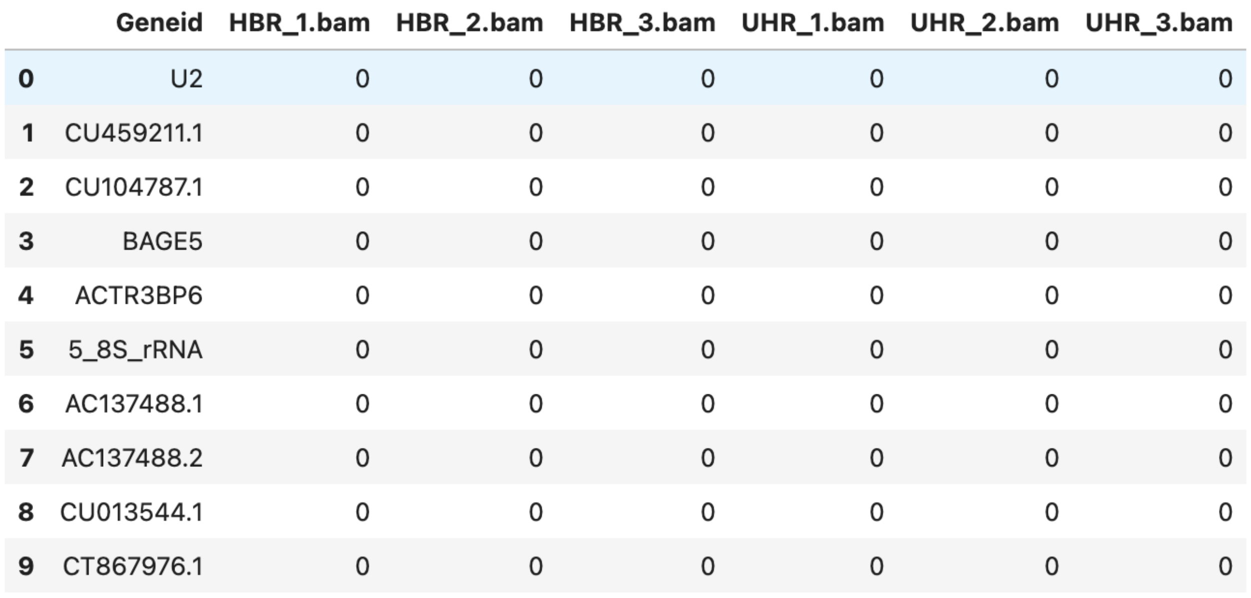


	Geneid	HBR_1.bam	HBR_2.bam	HBR_3.bam	UHR_1.bam	UHR_2.bam	UHR_3.bam
0	U2	0	0	0	0	0	0
1	CU459211.1	0	0	0	0	0	0
2	CU104787.1	0	0	0	0	0	0
3	BAGE5	0	0	0	0	0	0
4	ACTR3BP6	0	0	0	0	0	0

Figure 1: The first five rows of hbr_uhr_chr22_counts. The first column contains genes and the subsequent columns contain gene expression counts for each of the samples. The left most column of this data frame contains the row indices or names.

Because hbr_uhr_chr22_counts is a Pandas data frame (`type(hbr_uhr_chr22_counts)`, see lesson 2), it is possible to append one of the many Pandas commands to it. For instance, the `head` function was appended to display the first five rows of hbr_uhr_chr22_counts. The data frame name and function is separated by a period. This is perhaps one of the most appealing aspects of Python syntax. Note that the `head` function was followed by `()`. If the parentheses are blank, then the default first five lines will be shown. To view the first 10 rows of hbr_uhr_chr22_counts do the following.

```
hbr_uhr_chr22_counts.head(10)
```



	Geneid	HBR_1.bam	HBR_2.bam	HBR_3.bam	UHR_1.bam	UHR_2.bam	UHR_3.bam
0	U2	0	0	0	0	0	0
1	CU459211.1	0	0	0	0	0	0
2	CU104787.1	0	0	0	0	0	0
3	BAGE5	0	0	0	0	0	0
4	ACTR3BP6	0	0	0	0	0	0
5	5_8S_rRNA	0	0	0	0	0	0
6	AC137488.1	0	0	0	0	0	0
7	AC137488.2	0	0	0	0	0	0
8	CU013544.1	0	0	0	0	0	0
9	CT867976.1	0	0	0	0	0	0

Figure 2: Include an integer inside the parentheses of `pandas.dataframe.head()` function to view the specified number of lines in a tabular dataset.

The function `tail` can be used to view by default the bottom five lines of a tabular dataset. Similar to `head`, the number of lines shown can be customized by specifying an integer inside the parentheses.

```
hbr_uhr_chr22_counts.tail()
```

Get dimensions of a data frame

Pandas data frames have a function `shape` that informs of the number of rows and number of columns in a data frame (in other words the dimensions). To get the dimensions for hbr_uhr_chr22_counts, do the following

```
hbr_uhr_chr22_counts.shape
```

The hbr_uhr_chr22_counts data frame has 1335 rows and 7 columns.

```
(1335, 7)
```

Note

The elements in tabular data can be referred to by their row and column positions.

The `size` function returns the number elements in a data frame. For instance, hbr_uhr_chr22_counts has 1335 rows and 7 columns, which means that it has 1335 times 7 elements (or 9345).

Row indices/names

Figure 2 shows the first 10 rows of hbr_uhr_chr22_counts. The left most column, which contains labels starting with "0" is referred to as the row indices or row names. Users can specify a column in the dataset as the row indices or row names using the `index_col` options in `read_csv`. For instance, the hbr_uhr_chr22_rna_seq_counts.csv dataset could be imported with gene names as the row indices. To do this, add the `index_col=0` option to `read_csv`. Gene names in hbr_uhr_chr22_rna_seq_counts.csv is the first column and is denoted as column "0" in Python. Thus, setting `index_col=0` ensures that the gene names will be set as the row indices or row names (see Figure 3).

```
hbr_uhr_chr22_counts_1=pandas.read_csv("./hbr_uhr_chr22_rna_seq_coun
```

	HBR_1.bam	HBR_2.bam	HBR_3.bam	UHR_1.bam	UHR_2.bam	UHR_3.bam
Geneid						
U2	0	0	0	0	0	0
CU459211.1	0	0	0	0	0	0
CU104787.1	0	0	0	0	0	0
BAGE5	0	0	0	0	0	0
ACTR3BP6	0	0	0	0	0	0
...	...	...	...	...	...	...
ACR	0	0	0	0	2	0
AC002056.5	0	0	0	0	0	0
AC002056.3	0	0	0	0	0	0
RPL23AP82	41	59	54	32	23	34
RABL2B	74	62	54	68	50	47

Figure 3. The `index_col=0` option in `pandas.read_csv` sets the gene names as row names in the imported data frame.

Data wrangling

Subsetting

The command below will subset the expression counts for the RABL2B gene.

```
hbr_uhr_chr22_counts[hbr_uhr_chr22_counts["Geneid"]=="RABL2B"]
```

```
        Geneid   HBR_1.bam    HBR_2.bam    HBR_3.bam    UHR_1.bam    UHR_
1334    RABL2B       74           62           54           68
```

The "|" symbol can be used as the "or" operator so to also subset the counts for RPL23AP82

```
hbr_uhr_chr22_counts[(hbr_uhr_chr22_counts["Geneid"]=="RABL2B") | (hb
```

```
        Geneid       HBR_1.bam    HBR_2.bam    HBR_3.bam    UHR_1.bam
1333    RPL23AP82        41           59           54           32
1334    RABL2B           74           62           54           68
```

Alternatively, use the `isin` function and provide a list of genes to retrieve.

```
hbr_uhr_chr22_counts[hbr_uhr_chr22_counts["Geneid"].isin(["RABL2B", 
```

Use "." to reference a column.

```
hbr_uhr_chr22_counts[hbr_uhr_chr22_counts.Geneid=="RABL2B"]
```

Subsetting by integer positions

Given that the elements in a data frame are referenced by its row and column positions, what would be the approach for extracting the element in row 60 and column 5? The solution is the command below, which returns a result of 2. The row and column numbers are enclosed in "[]" and separated by a comma.

```
hbr_uhr_chr22_counts.iloc[60,5]
```

```
2
```

The above method for subsetting the element in row 60 and column 5 of hbr_uhr_chr22_counts is great if the goal is to extract the value and do numeric operation on it. But what if the user wants to return the element along with the corresponding gene in data frame format?

To do this, enclose the row and column indices to extract in their own inner set of square brackets as shown below. Column 0, which contains the gene name is also included in the brackets containing the column indices of interest.

```
hbr_uhr_chr22_counts.iloc[[60],[0,5]]
```

```
    Geneid  UHR_2.bam
60  CCT8L2      2
```

Pandas offers different approaches for subsetting rectangular data. One method is `iloc`.

> `iloc` is a "purely integer-location based indexing for selection by position" -- https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.iloc.html# *(https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.iloc.html#)*. The row and column positions are enclosed in "[]".

`iloc` allows for retrieval of elements in multiple rows and columns. For instance, the following can be used to retrieve the elements in rows 60 and 65 and columns 0, 4, 5, and 6 in hbr_uhr_chr22_counts. Note that the row and column positions are enclosed in an outer set of "[]". Within the outer set of "[]" the first set of "[]" enclose a comma separated list of row positions while the second set of "[]" enclose a comma separated list of column positions.

```
hbr_uhr_chr22_counts.iloc[[60,65],[0,4,5,6]]
```

```
    Geneid      UHR_1.bam   UHR_2.bam   UHR_3.bam
60  CCT8L2          1           2           0
65  SLC25A15P5      2           2           4
```

To get the first three rows of hbr_uhr_chr22_counts do the following. Note that it retrieves the rows with indices 0, 1, and 2.

```
hbr_uhr_chr22_counts.iloc[:3]
```

```
    Geneid   HBR_1.bam    HBR_2.bam    HBR_3.bam    UHR_1.bam    UHR_2.bar
0   U2           0            0            0            0            0
1   CU459211.1   0            0            0            0            0
2   CU104787.1   0            0            0            0            0
```

What will be the output for `hbr_uhr_chr22_counts.iloc[[3],:]`?

{{Sdet}}{{Ssum}}Solution{{Esum}}

The row with an index of 3 will be retrieved.

```
    Geneid   HBR_1.bam    HBR_2.bam    HBR_3.bam    UHR_1.bam    UHR_2.bar
3   BAGE5        0            0            0            0            0
```

{{Edet}}

Subsetting using column names

Panda's `loc` function allows for subsetting by row or column names. For instance, to retrieve the gene id column, do the following. The ":" denotes get every row.

```
hbr_uhr_chr22_counts.loc[:,['Geneid']]
```

```
        Geneid
0       U2
1       CU459211.1
2       CU104787.1
3       BAGE5
4       ACTR3BP6
...     ...
1330    ACR
1331    AC002056.5
1332    AC002056.3
1333    RPL23AP82
1334    RABL2B
```

To retrieve the counts for the gene SLC25A15P5, use the following where SLC25A15P5 is the subsetting criteria, where

- `hbr_uhr_chr22_counts.loc[:,'Geneid']` extracts the Geneid column.
- `=="SLC25A15P5"` will filter out the row with the SLC25A15P5 gene.

```
hbr_uhr_chr22_counts[hbr_uhr_chr22_counts.loc[:,'Geneid']=="SLC25A15I
```

```
    Geneid      HBR_1.bam    HBR_2.bam  HBR_3.bam   UHR_1.bam   UHR_
65  SLC25A15P5      0            0          0           2           
```

To retrieve counts for more than one gene, enclose the genes of interest in a list and use the `isin` function to filter out the rows containing the genes in the list.

```
hbr_uhr_chr22_counts[hbr_uhr_chr22_counts.loc[:,'Geneid'].isin(["SLC
```

```
    Geneid      HBR_1.bam   HBR_2.bam   HBR_3.bam   UHR_1.bam   UHR_
60  CCT8L2          0           0           0           1           
65  SLC25A15P5      0           0           0           2           
```

To find all of the SLC genes in hbr_uhr_chr22_counts, the following could be used where `str.startswith` searches for text that starts a pattern (ie. "SLC"). Other options for pattern matching include `str.endwith` and `str.contains`.

```
hbr_uhr_chr22_counts.loc[hbr_uhr_chr22_counts.loc[:,'Geneid'].str.st
```

```
        Geneid      HBR_1.bam   HBR_2.bam   HBR_3.bam   UHR_1.bam   
54      SLC9B1P4        0           0           0           0
65      SLC25A15P5      0           0           0           2
109     SLC25A18        100         111         74          6
181     SLC25A1         32          50          41          226
249     SLC9A3P2        0           0           0           0
268     SLC7A4          19          25          14          9
494     SLC2A11         54          63          46          28
726     SLC35E4         18          32          26          21
783     SLC5A1          0           0           0           0
795     SLC5A4          7           12          5           13
955     SLC16A8         9           13          11          11
1046    SLC25A17        39          39          40          119
1099    SLC25A5P1       0           0           1           0
```

Summary statistics of data frames

```
hbr_uhr_chr22_counts.describe()
```

```
        HBR_1.bam   HBR_2.bam   HBR_3.bam   UHR_1.bam   UHR_2.bam
count   1335.000000 1335.000000 1335.000000 1335.000000 1335.000000
mean    29.530337   36.264419   32.084644   50.694382   33.419476
std     99.177874   120.617793  108.237694  197.575081  122.598310
min     0.000000    0.000000    0.000000    0.000000    0.000000
25%     0.000000    0.000000    0.000000    0.000000    0.000000
50%     0.000000    0.000000    0.000000    1.000000    1.000000
75%     8.000000    10.000000   9.000000    13.000000   12.000000
max     1532.000000 1797.000000 1637.000000 4027.000000 2406.000000
```

Replacing column names

To view the column headings of a data frame use the `column` function. For instance,

```
hbr_uhr_chr22_counts.columns
```

```
HBR_1.bam
HBR_2.bam
HBR_3.bam
UHR_1.bam
UHR_2.bam
UHR_3.bam
```

The `str.replace` function can be used to replace a string with something else. Here, it used to remove ".bam" from the sample names in the column heading.

```
hbr_uhr_chr22_counts.columns=hbr_uhr_chr22_counts.columns.str.replac
```

Mathematical operations on data frames and filtering

Pandas enables mathematical operations on data frames. For instance, one might want to sum the total counts across all samples for each gene. The `sum` function can be used to this. Setting `axis=1` will sum up the counts for each row or gene. Because the Geneid column is a string, it is necessary to first subset only the sample columns.

```
hbr_uhr_chr22_counts.loc[:, ['HBR_1', 'HBR_2', 'HBR_3', 'UHR_1', 'UH
```

Below, genes with zero counts across all samples are removed from hbr_uhr_chr22_counts and stored as hbr_uhr_chr22_counts_filtered. To accomplish this set `hbr_uhr_chr22_counts.loc[:, ['HBR_1', 'HBR_2', 'HBR_3', 'UHR_1', 'UHR_2', 'UHR_3']].sum(axis=1) !=0` and use as a filter criteria.

```
hbr_uhr_chr22_counts_filtered=hbr_uhr_chr22_counts.loc[hbr_uhr_chr22_
```

Removing and adding columns to a data frame

For this exercise, stay in the /data/username/pies_2023 folder, which should be the present working directory (use `pwd` to check). If not in the /data/username/pies_2023 folder, change into it. Copy the hbr_uhr_deg_chr22.csv and hcc1395_deg_chr22.csv files from /data/classes/BTEP/pies_2023_data to the /data/username/pies_2023 directory.

```
cp /data/classes/BTEP/pies_2023_data/hbr_uhr_deg_chr22.csv .
```

```
cp /data/classes/BTEP/pies_2023_data/hcc1395_deg_chr22.csv .
```

The file hcc1395_deg_chr22.csv will be needed for the practice questions.

This exercise will use the differential gene expression analysis table from the hbr and uhr study.

```
hbr_uhr_deg_chr22=pandas.read_csv("./hbr_uhr_deg_chr22.csv")
```

The `info()` function will retrieve information regarding the hbr_uhr_deg_chr22 data frame, which includes the column names.

```
hbr_uhr_deg_chr22.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1335 entries, 0 to 1334
Data columns (total 18 columns):
 #   Column          Non-Null Count  Dtype
---  ------          --------------  -----
 0   name            1335 non-null   object
 1   baseMean        1335 non-null   float64
 2   baseMeanA       1335 non-null   float64
 3   baseMeanB       1335 non-null   float64
 4   foldChange      971 non-null    float64
 5   log2FoldChange  971 non-null    float64
 6   lfcSE           971 non-null    float64
 7   stat            971 non-null    float64
```

```
  8   PValue          971 non-null    float64
  9   PAdj            971 non-null    float64
  10  FDR             639 non-null    float64
  11  falsePos        639 non-null    float64
  12  HBR_1.bam       1335 non-null   float64
  13  HBR_2.bam       1335 non-null   float64
  14  HBR_3.bam       1335 non-null   float64
  15  UHR_1.bam       1335 non-null   float64
  16  UHR_2.bam       1335 non-null   float64
  17  UHR_3.bam       1335 non-null   float64
dtypes: float64(17), object(1)
memory usage: 187.9+ KB
```

The hbr_uhr_deg_chr22 table contains differential gene expression analysis results. Relevant columns include

- name: gene names
- log2FoldChange: the gene expression change between the two treatment groups
- PAdj: the adjusted p-value associated with statistical confidence of the expression change
- The columns labeled with the sample names (ie. columns 12 through 17) are the normalized gene expression counts

Use `str.replace` to remove ".bam" from the sample names in columns 12 through 17.

```
hbr_uhr_deg_chr22.columns=hbr_uhr_deg_chr22.columns.str.replace(".ba
```

To drop columns in a Pandas data frame, use the `.drop` function and specify the name(s) of the column(s) to remove. The example below removes columns baseMean, baseMeanA,and baseMeanB

```
hbr_uhr_deg_chr22.drop(columns=["baseMean","baseMeanA", "baseMeanB"]
```

Subset the name, log2FoldChange, and PAdj columns in hbr_uhr_deg_chr22 and save to a new data frame hbr_uhr_deg_chr22_1.

```
hbr_uhr_deg_chr22_1=hbr_uhr_deg_chr22.loc[:,["name", "log2FoldChange
```

```
hbr_uhr_deg_chr22_1.head()
```

```
    name    log2FoldChange      PAdj
0   SYNGR1       -4.6        5.200000e-217
1   SEPT3        -4.6        4.500000e-204
2   YWHAH        -2.5        4.700000e-191
3   RPL3         1.7         5.400000e-134
4   PI4KA        -2.0        2.900000e-118
```

Next, add a column called "-log10PAdj" to hbr_uhr_deg_chr22_1, which will contain the negative of log10 of the values in the PAdj column. "-log10PAdj" is used in volcano plots that depict gene expression change versus statistical confidence. To calculate -log10PAdj, the package numpy will be used. Numpy *(https://numpy.org)* enables scientific calculations.

```
import numpy
```

```
hbr_uhr_deg_chr22_1["-log10PAdj"]=numpy.negative(numpy.log10(hbr_uhr_
```

Take a look at the first several lines of hbr_uhr_deg_chr22_1

```
hbr_uhr_deg_chr22_1.head()
```

```
    name    log2FoldChange      PAdj            -log10PAdj
0   SYNGR1  -4.6                5.200000e-217   216.283997
1   SEPT3   -4.6                4.500000e-204   203.346787
2   YWHAH   -2.5                4.700000e-191   190.327902
3   RPL3    1.7                 5.400000e-134   133.267606
4   PI4KA   -2.0                2.900000e-118   117.537602
```

Other methods for adding new column to a Pandas data frame include `insert` and `assign`.

The final task for this lesson is to add a column that indicates whether a gene is up regulated, down regulated, or has no change based on the log2FoldChange and PAdj values. The criteria are as follows.

- PAdj >= 0.01: no change (marked as ns in the column)
- Absolute value of log2FoldChange <2: no change (marked as ns in the column)
- log2FoldChange >= 2 and PAdj < 0.01: (up regulated)
- log2FoldChange <=2 and PAdj < 0.01: (down regulated)

To code this in Python, the first step is to drop the NA values from the hbr_uhr_deg_chr22_1 using `dropna`.

```
hbr_uhr_deg_chr22_1=hbr_uhr_deg_chr22_1.dropna()
```

Next, create a list called significance_criteria that contains the criteria shown above. In the criteria list below, "&" is the Boolean for "and". To calculate the absolute value of log2FoldChange, `numpy.absolute` is used.

```
significance_criteria=[(hbr_uhr_deg_chr22_1["PAdj"]>=0.01),
                       (numpy.absolute(hbr_uhr_deg_chr22_1["log2Fold(
                      (hbr_uhr_deg_chr22_1["log2FoldChange"]>=2) & (I
                      (hbr_uhr_deg_chr22_1["log2FoldChange"]<=-2) &
```

Then, create a list called significance_status that indicates whether the criteria are ns (not significant), up, or down. These statuses have to correspond to the order in which the criteria were listed in significance_criteria.

```
significance_status=["ns","ns","up","down"]
```

Finally, `numpy.select` will be used to assign values to the significance column.

```
hbr_uhr_deg_chr22_1["significance"]=numpy.select(significance_criter
```

```
hbr_uhr_deg_chr22_1.head(4)
```

```
    name    log2FoldChange         PAdj        -log10PAdj  signific
0   SYNGR1      -4.6          5.200000e-217   216.283997  down
1   SEPT3       -4.6          4.500000e-204   203.346787  down
2   YWHAH       -2.5          4.700000e-191   190.327902  down
3   RPL3         1.7          5.400000e-134   133.267606  ns
```

Write this data frame to a csv file in the /data/username/pies_2023 folder, which should be the present working directory. Replace username with the user's Biowulf account ID. The `to_csv` command in Pandas is used to write data frames to csv files. Setting `index=False` ensures that the csv file will not have row names.

```
hbr_uhr_deg_chr22_1.to_csv("./hbr_uhr_deg_chr22_with_significance_le
```

This lesson has shown the participants various data wrangling approaches using the Python package Pandas. The capabability of Pandas expand to more than what is covered here, participants are encouraged to check out the Pandas documentations *(https://pandas.pydata.org/docs/)* to learn more.

Lesson 4: Data visualization using Python

Learning objectives

This lesson will provide participants with enough knowledge to start using Python for data visualization. Specifically, participants should

- Be able to use the package Seaborn to
    - Construct plots that range from very basic to elegant as well as biologically relevant
    - Customize plots including altering font size and adding custom annotations

Python data visualization tools

Seaborn *(https://seaborn.pydata.org)* is a popular Python plotting package, which is the tool that will be introduced in this lesson. Seaborn is an extension of and builds on Matplotlib *(https://matplotlib.org)* and is oriented towards statistical data visualization. However, there are other packages, including those that are domain specific, implement grammar of graphics, and are used for creating web-based visualization dashboards. A non-exhaustive list of Python plotting packages is shown below.

- Matplotlib *(https://matplotlib.org)*
- Plotnine: implements grammar of graphics for those familiar with R's ggplot2 *(https://plotnine.readthedocs.io/en/stable/)*
- bioinfokit: genomic data visualization *(https://github.com/reneshbedre/bioinfokit)*
- pygenomeviz: visuazlize comparative genomics data *(https://moshi4.github.io/pyGenomeViz/)*
- Dash bio: create interactive data visualizations and web dashboards *(https://dash.plotly.com/dash-bio)*

Visualization using Seaborn

Load packages

```
import pandas
import numpy
import matplotlib.pyplot as plt
import seaborn
```

Modify the basic plot elements with Seaborn.

To plot using Seaborn, start the command with `seaborn` followed by the plot type, separated by a period.

```
seaborn.plot_type
```

This section will use Seaborn's `scatterplot` to explore how to work with and modify basic elements of plotting. The foundations learned in this section form the basis for creating advanced and elegant plots.

The data that will be plotted is a point located at 5 on the x axis and 5 on the y axis. To generate x and y, `numpy.array` was used. Here, x and y are single element arrays that store the number 5.

```
x=numpy.array([5])
y=numpy.array([5])
```

Plot x and y using Seaborn's `scatterplot` function (see Figure 1 for results), which takes data frames or Numpy arrays as input. Here, x will be plotted on the x axis, and y will be plotted on the y axis. The plot can be stored as a variable, which in this example is plot0.

```
plot0=seaborn.scatterplot(x=x, y=y)
plt.show()
```

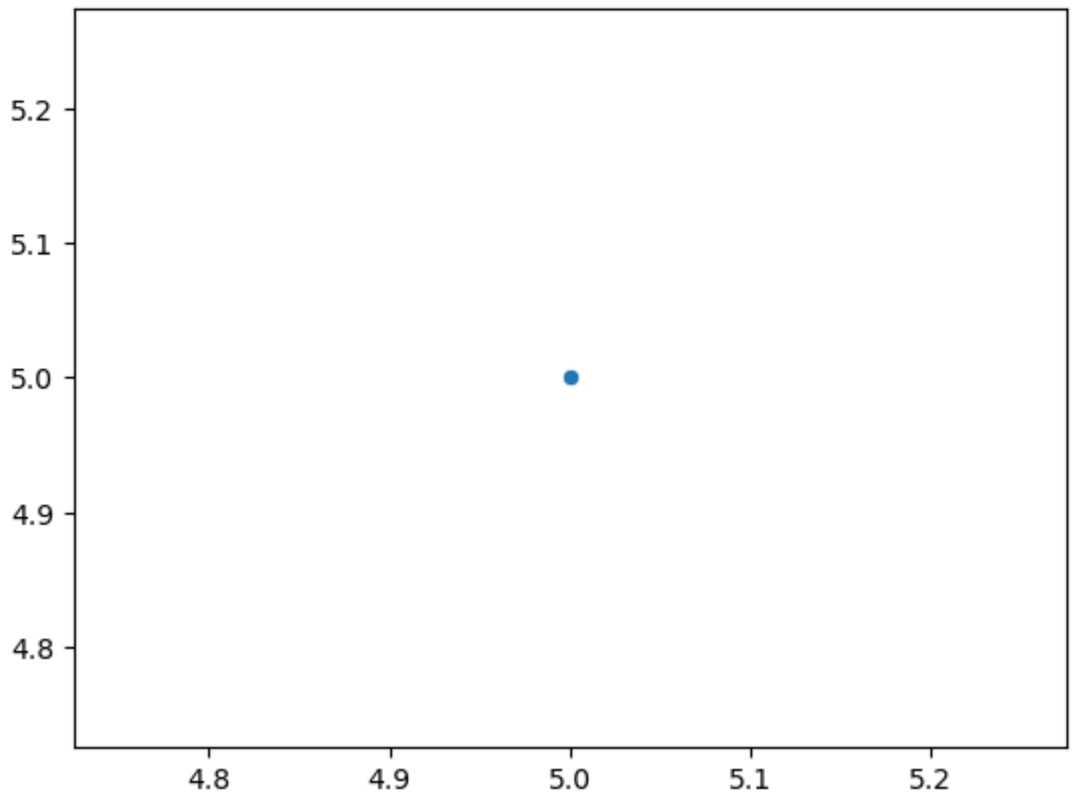


Figure 1

The plot in Figure 1 has no axes labels. Axes labels are an integral part of an informative data visualization. It might also be useful to include meaningful x and y limits. To do this, append the various `.set*` attributes to the plot. See Figure 2a for result.

- `set_xlabel`: specify x axis label (`size` is used to set the label font size)
- `set_ylabel`: specify y axis
- `set_xlim`: sets the x axis limits
- `set_ylim`: sets the y axis limits
- `set_xticks`: sets the location of x axis tick marks
- `set_xticklabels`: sets the x axis tick mark labels, `size` is used to set the tick mark label font size
- `set_yticks`: sets the location of y axis tick marks
- `set_yticklabels`: sets the y axis tick mark labels, `size` is used to set the tick mark label font size

```
plot0=seaborn.scatterplot(x=x, y=y)
plot0.set_xlabel("x axis", size=14)
plot0.set_ylabel("y axis", size=14)
plot0.set_xlim(0,10)
plot0.set_ylim(0,10)
plot0.set_xticks([0,2,4,6,8,10])
plot0.set_xticklabels(labels=["0","2","4","6","8","10"], size=15)
```

```
plot0.set_yticks([0,2,4,6,8,10])
plot0.set_yticklabels(labels=["0","2","4","6","8","10"], size=15)
plt.show()
```

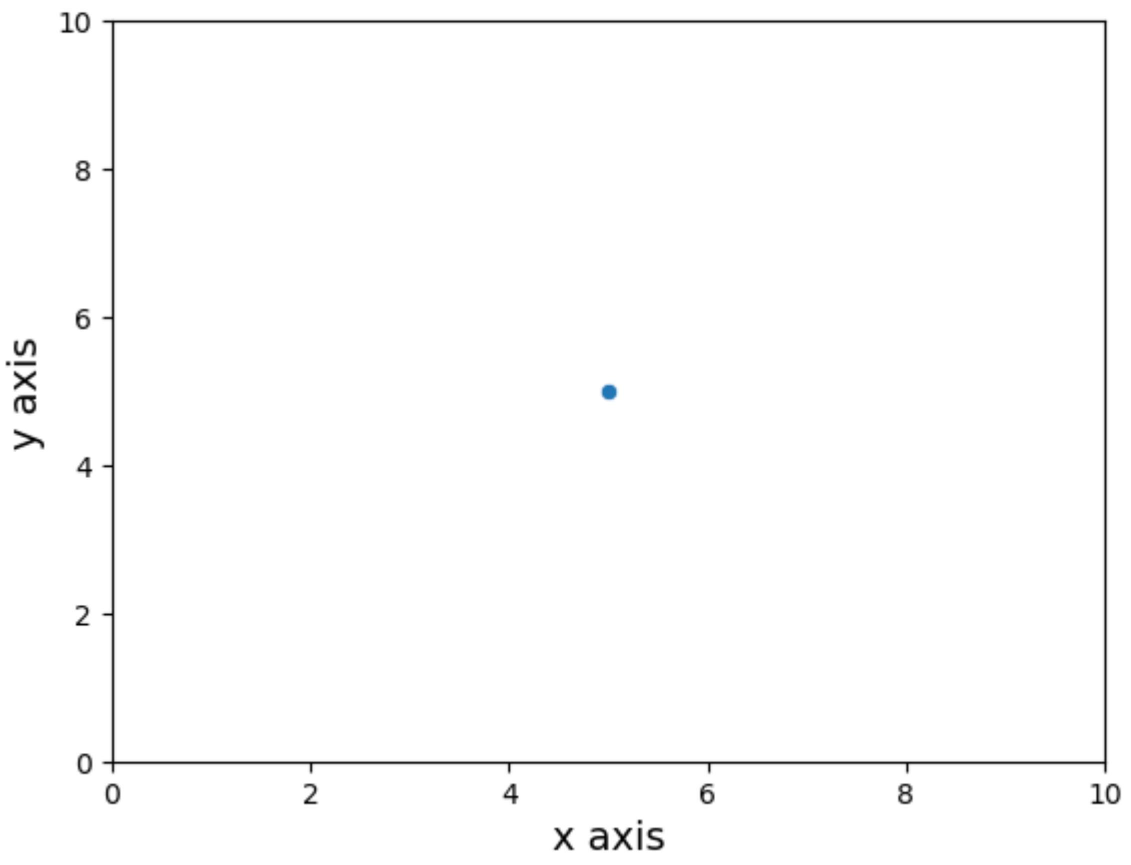


Figure 2

The `plotting_context` of a Seaborn plot contains parameters that determine scaling of plot elements (see https://seaborn.pydata.org/generated/seaborn.plotting_context.html *(https://seaborn.pydata.org/generated/seaborn.plotting_context.html)*). To view these parameters, do the following, which will return the plot scaling parameters as a dictionary.

```
print(seaborn.plotting_context())
```

```
{'font.size': 12.0, 'axes.labelsize': 12.0, 'axes.titlesize': 12.0,
```

These parameters can be changed using the `set_context` function by providing a customized dictionary and assigning it to the `rc` argument.

```
help(seaborn.set_context)
```

```
Help on function set_context in module seaborn.rcmod:

set_context(context=None, font_scale=1, rc=None)
    Set the parameters that control the scaling of plot elements.

    This affects things like the size of the labels, lines, and othe
    of the plot, but not the overall style. This is accomplished usi
    matplotlib rcParams system.

    The base context is "notebook", and the other contexts are "pape
    and "poster", which are version of the notebook parameters scale
    values. Font elements can also be scaled independently of (but r
    the other values.

    See :func:`plotting_context` to get the parameter values.

    Parameters
    ----------
    context : dict, or one of {paper, notebook, talk, poster}
        A dictionary of parameters or the name of a preconfigured se
    font_scale : float, optional
        Separate scaling factor to independently scale the size of t
        font elements.
    rc : dict, optional
        Parameter mappings to override the values in the preset seab
        context dictionaries. This only updates parameters that are
        considered part of the context definition.
```

To change the x and y axes tick label font size to 20, use `seaborn.set_context(rc={'xtick.labelsize': 20, 'ytick.labelsize': 20})` prior to constructing a Seaborn plot.

The code above can be modified to generate a more complex scatter plot that has more points. For instance, the inputs for x and y can be changed to numeric arrays of five 6 elements each.

```
x=numpy.array([0,1,2,3,4,5])
y=numpy.multiply(2,x)
print("x is a numeric array composed of: ", x)
print("y is a numeric array composed of: ", y)
```

```
x is a numeric array composed of:  [0 1 2 3 4 5]
y is a numeric array composed of:  [ 0  2  4  6  8 10]
```

The code used to generate Figure 2 can then be run again with modifications to the x and y axes limits to generate the plot shown in Figure 3. To produce a line plot representation of Figure 3, simply change the plot type to lineplot (`seaborn.lineplot`).

```
plot0=seaborn.scatterplot(x=x, y=y)
plot0.set_xlabel("x axis", size=14)
plot0.set_ylabel("y axis", size=14)
plot0.set_xlim(0,6)
plot0.set_ylim(0,12)
plot0.set_xticks([0,2,4,6])
plot0.set_xticklabels(labels=["0","2","4","6"], size=15)
plot0.set_yticks([0,2,4,6,8,10,12])
plot0.set_yticklabels(labels=["0","2","4","6","8","10","12"], size=1!
plt.show()
```

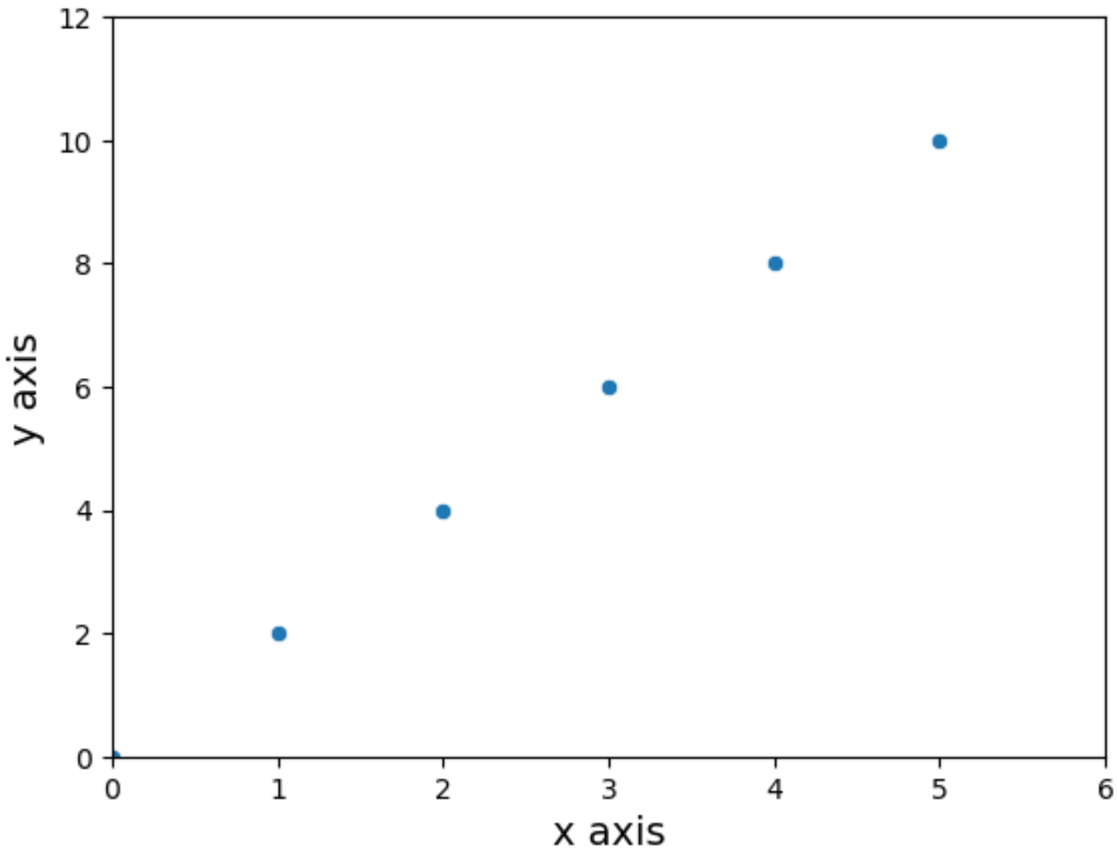


Figure 3

Constructing biologically relevant plots

The next exercise is to practice creating a scatter plot on a biologically relevant dataset. Namely, the differential expression results from the hbr and uhr RNA sequencing study will be used to create a scatter plot depicting log2 fold change of gene expression on the x axis and negative log10 of the adjusted p-values on the y axis. This special case of scatter plot is called a volcano plot.

Step one is to import the data using Panda's `read.csv` command.

```
hbr_uhr_deg_chr22=pandas.read_csv("./hbr_uhr_deg_chr22_with_signific
```

Now, review the contents of this data table by doing the following.

```
hbr_uhr_deg_chr22.head(4)
```

```
    name    log2FoldChange      PAdj         -log10PAdj  significance
0   SYNGR1        -4.6        5.200000e-217  216.283997  down
1   SEPT3         -4.6        4.500000e-204  203.346787  down
2   YWHAH         -2.5        4.700000e-191  190.327902  down
3   RPL3          1.7         5.400000e-134  133.267606  down
```

To create the volcano plot, provide the following arguments. See Figure 4 for result.

- The data frame (ie. hbr_uhr_deg_chr22)
- What to plot on the x axis (ie. log2FoldChange)
- What to plot on the y axis (ie. "-log10PAdj")

```
plot1=seaborn.scatterplot(hbr_uhr_deg_chr22,x="log2FoldChange", y="-
```

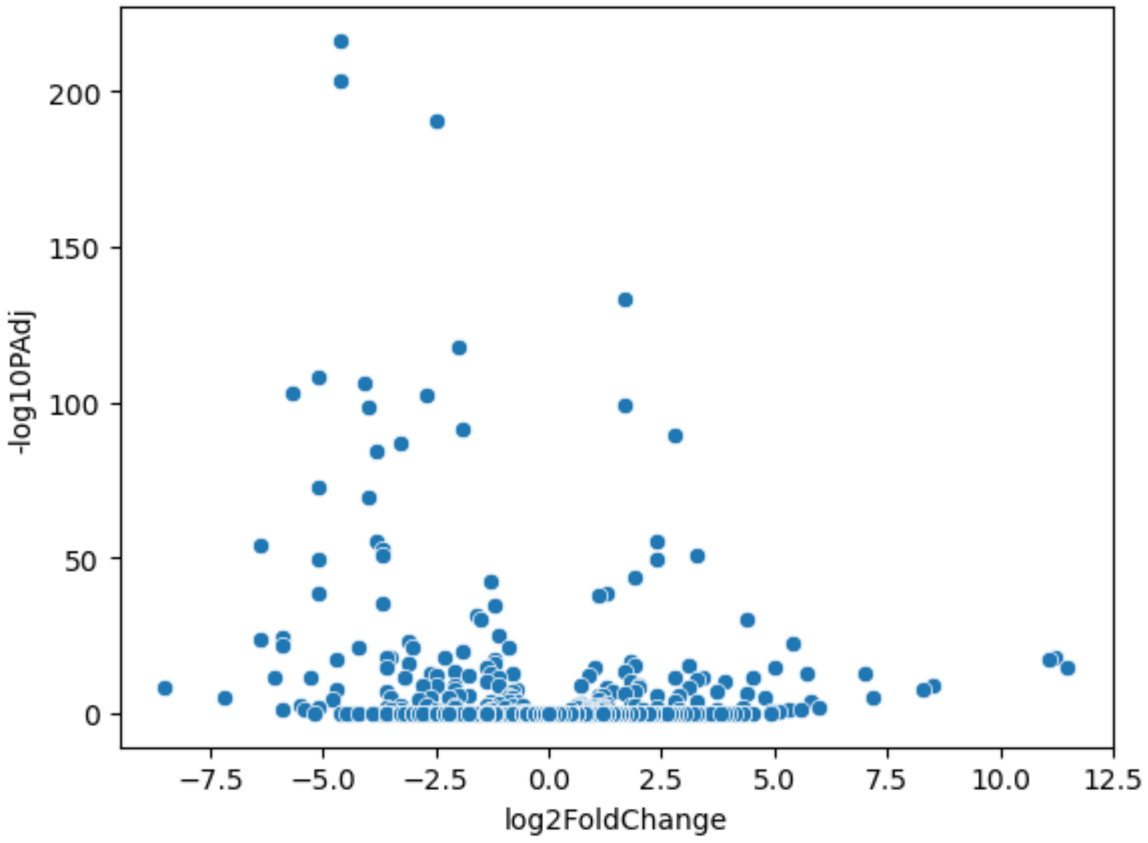


Figure 4

The volcano plot in Figure 4 does not help with visualizing the up, down, an non-significant genes. Fortunately, the `hue` option can be used to distinguish these. See Figure 5.

```
plot1=seaborn.scatterplot(hbr_uhr_deg_chr22,x="log2FoldChange", y="-
```

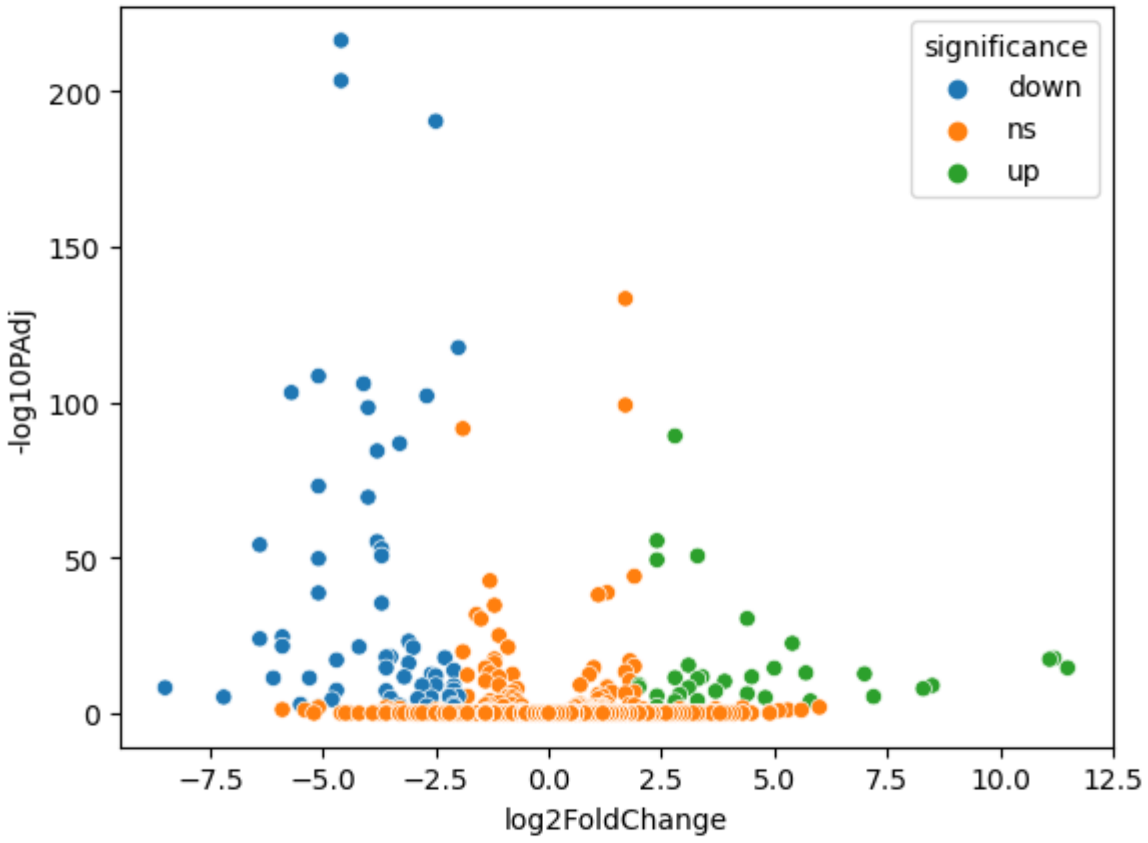


Figure 5

It would be informative to label some of the top significant differentially expressed genes in the volcano plot. To do this, import the file hbr_uhr_deg_chr22_top_genes.csv and assign it to the data frame hbr_uhr_deg_chr22_top_genes.

```
hbr_uhr_deg_chr22_top_genes=pandas.read_csv("./hbr_uhr_deg_chr22_top_
```

```
hbr_uhr_deg_chr22_top_genes
```

The table contains the top two differentially expressed genes according to the adjusted p-value (PAdj). The task to do is to label the points corresponding to these two genes on the volcano plot. The values for log2FoldChange and -log10PAdj will serve as the x and y coordinates for plotting the gene name.

```
     name     log2FoldChange       PAdj         -log10PAdj   significance
0    XBP1          2.8         7.300000e-90     89.136677    up
1    SYNGR1       -4.6         5.200000e-217    216.283997   down
```

To label the two top differentially expressed genes, start by constructing the volcano plot from Figure 5. Then, use a `for` loop to iterate through the name column in the data frame hbr_uhr_deg_chr22_top_genes. In the `for` loop

- `i`: the number that keeps track of the row number in the data frame hbr_uhr_deg_chr22_top_genes and is used to
  - reference the x coordinate or log2FoldChange value in that row
  - reference the y coordinate or -log10PAdj value in that row
- `enumerate`: iterate through the name column in hbr_uhr_deg_chr22_top_genes and stores the name to variable gene_name. `i` is incremented as it iterates through the name column within the `for` loop

```
plot1=seaborn.scatterplot(hbr_uhr_deg_chr22,x="log2FoldChange", y="-
for i, gene_name in enumerate(hbr_uhr_deg_chr22_top_genes["name"]):
    plot1.text(hbr_uhr_deg_chr22_top_genes["log2FoldChange"][i],
                 hbr_uhr_deg_chr22_top_genes["-log10PAdj"][i],gene_name
```

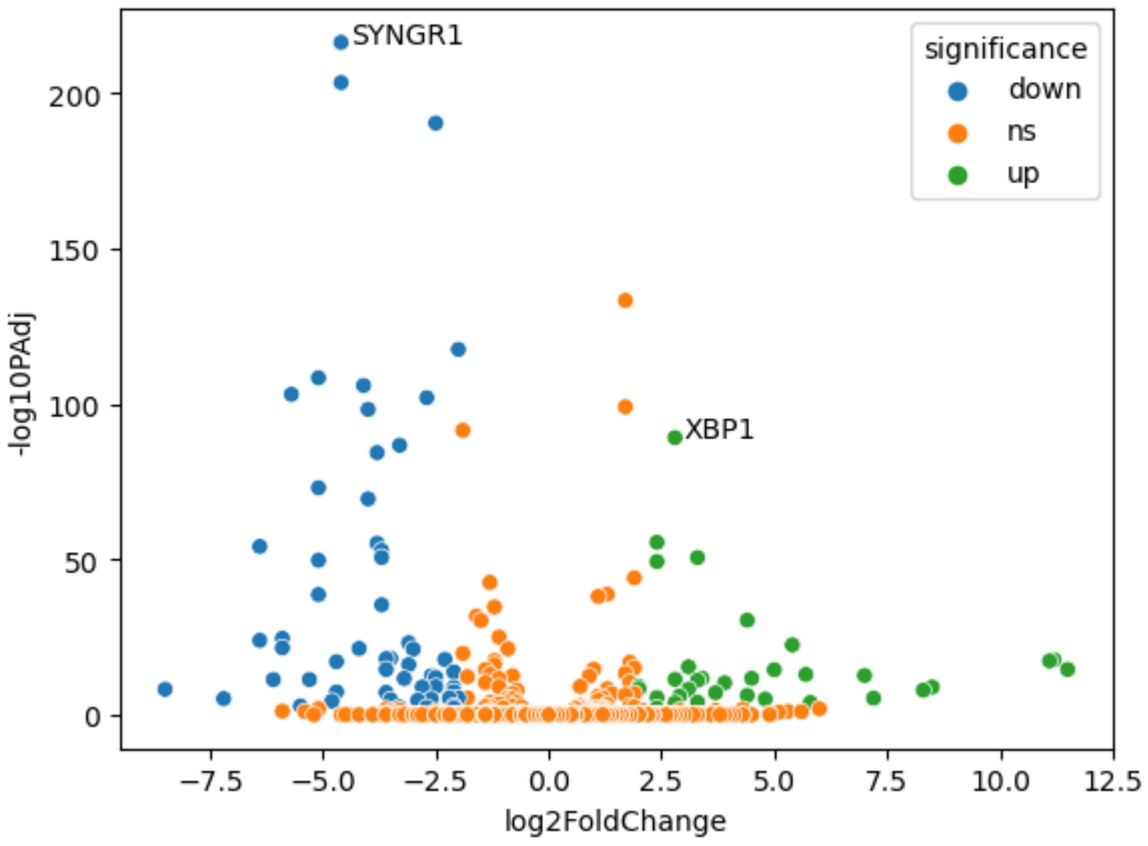


Figure 6

The next visualization is the heatmap and dendrogram combination, which helps with visualizing clusters and patterns. Heatmap and dendrogram can be used in RNA sequencing studies to inspect whether there are cluster of genes with similar expression patterns among treatment groups. The normalized counts for the top differential expressed genes in the hbr and uhr study will be used to construct a heatmap/dendrogram using Seaborn's `clustermap`.

Import the data.

```
hbr_uhr_top_deg_normalized_counts=pandas.read_csv("./hbr_uhr_top_deg_
```

The `seaborn.clustermap` command below generates a clustermap of the top differential expressed genes in the hbr and uhr study. The arguments and options are as follows.

- Argument: The dataset (ie. hbr_uhr_top_deg_normalized_counts)
- Options:
    - `z_score=0`: scale the rows by z-score
    - `cmap`: specify color palette (ie. viridis)
    - `figsize`: specify figure size
    - `vmin`: minimum value on the color scale bar
    - `vmax`: maximum value on the color scale bar
    - `cbar_kws`: dictionary containing key value pair that specifies the title to the color scale bar
    - `cbar_pos`: coordinates for placement of the color scale bar

```
plot4=seaborn.clustermap(hbr_uhr_top_deg_normalized_counts,z_score=0
                        figsize=(8,8),vmin=-1.5, vmax=1.5,cbar_kws=(
                        cbar_pos=(0.855,0.8,0.025,0.15))
```

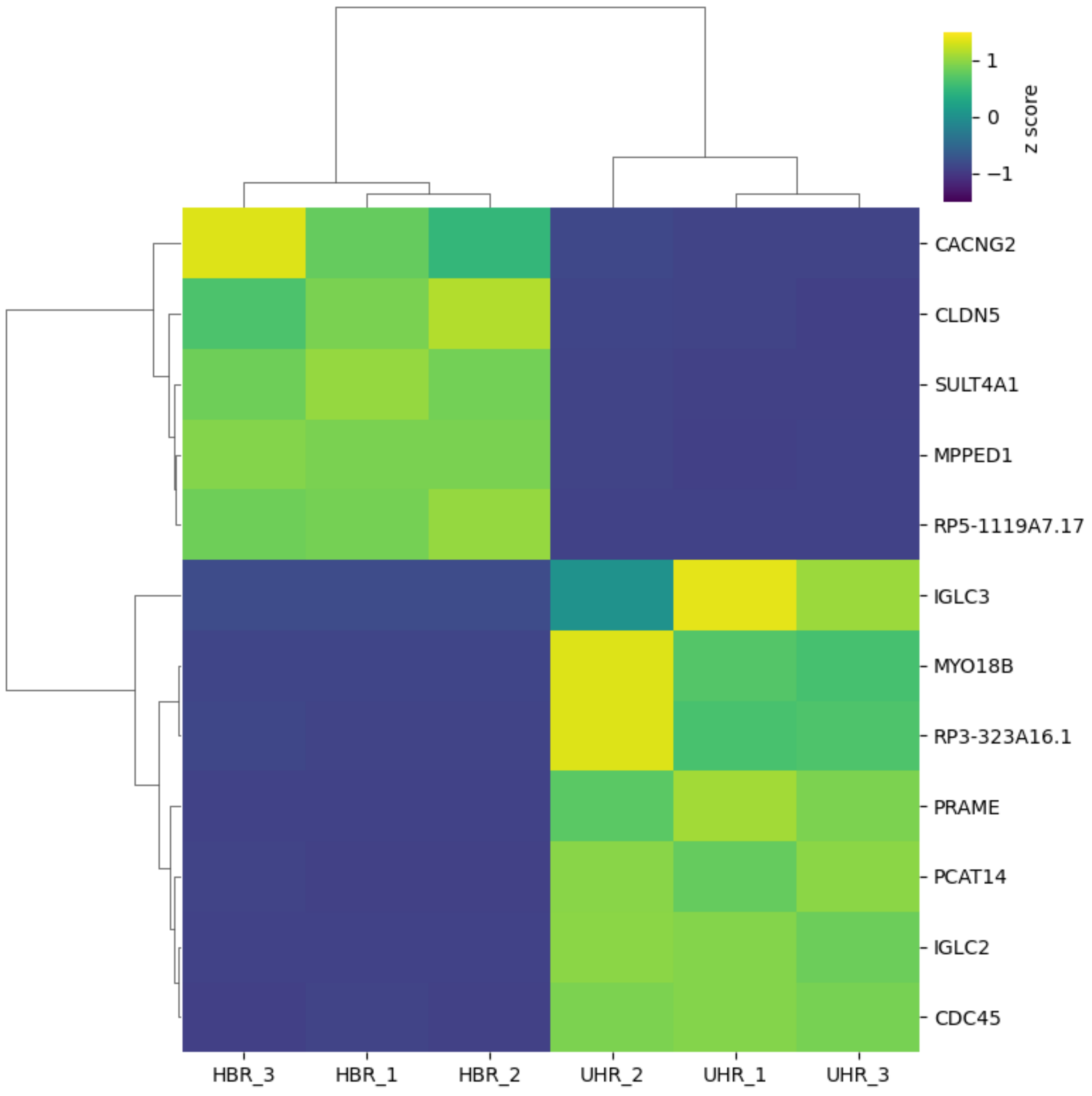


Figure 9: Expression heatmap of the top 12 differentially expressed genes in the HBR and UHR study

Below, a Pandas Series, called samples that contains a mapping of colors to study samples is created.

```
samples=pandas.Series({"HBR_1":"orangered", "HBR_2":"orangered", "HB
```

Then a variable, column_colors is created that contains a mapping of the hbr_uhr_top_deg_normalized_counts column headings to the colors specified in samples. This is accomplished using the `map` command.

```
column_colors=hbr_uhr_top_deg_normalized_counts.columns.map(samples)
```

The option `col_colors`, which is set to column_colors is added to display a color bar on the top of the heatmap that helps to distinguish treatment groups (ie. hbr or uhr).

Other options added include

- `ax_heatmap.set_xticklabels`: allows for customizing the x axis labels' fontsize and rotation. This requires using `ax_heatmap.get_xmajorticklabels()` to get the x axis tick labels
- `ax_cbar.tick_params`: sets the size for the color scale bar labels
- `ax_col_colors.set_title`: sets the title and location bar displaying the treatment group to color mapping

```
plot4=seaborn.clustermap(hbr_uhr_top_deg_normalized_counts,z_score=0
                        figsize=(8,8),vmin=-1.5, vmax=1.5,cbar_kws=(
                        col_colors=column_colors, cbar_pos=(0.855,0.
plot4.ax_heatmap.set_xticklabels(plot4.ax_heatmap.get_xmajorticklabe
plot4.ax_cbar.tick_params(labelsize=12)
plot4.ax_col_colors.set_title("treatment",x=-0.1,y=0.01)
plt.show()
```

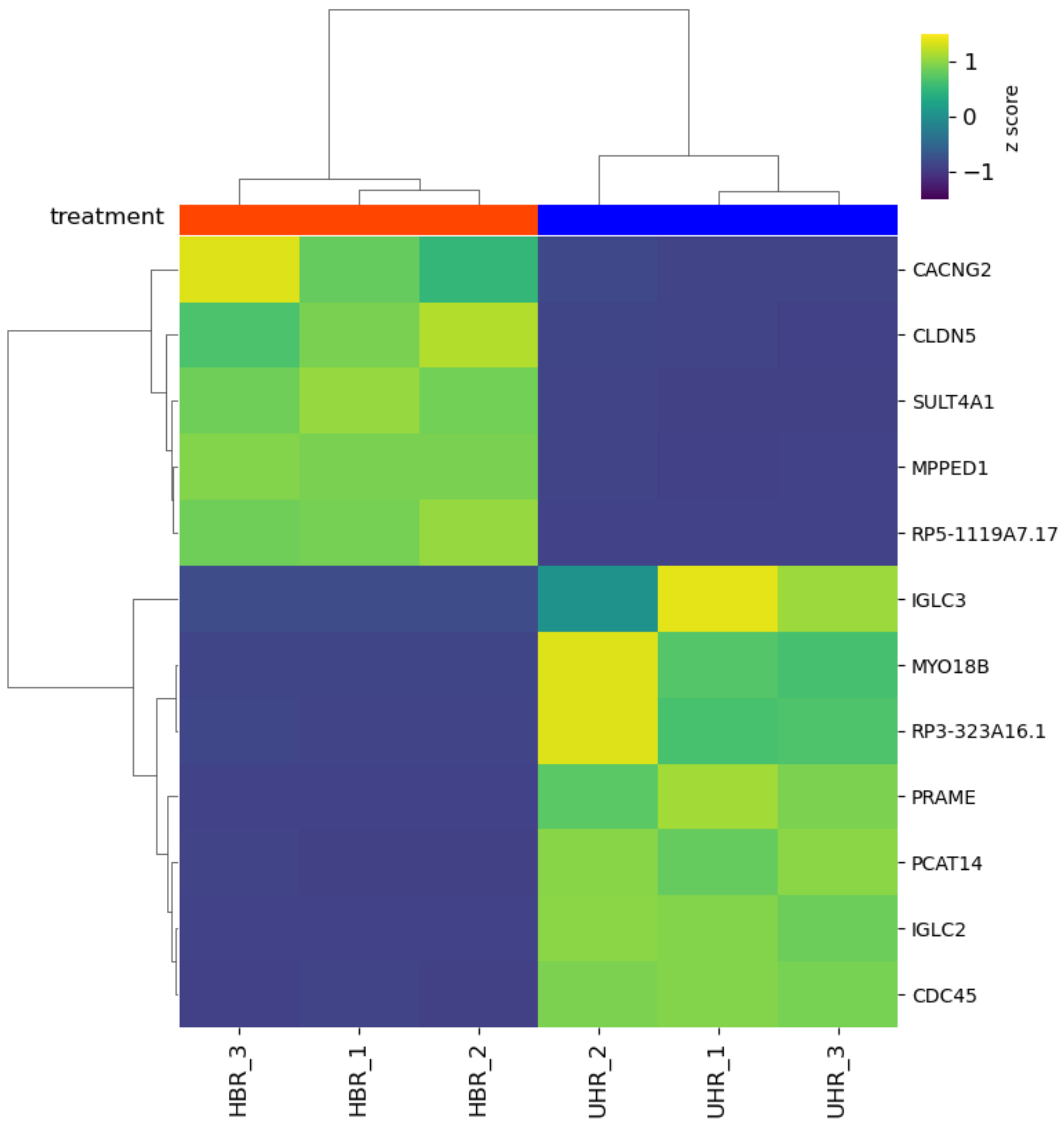


Figure 10: Expression heatmap of the top 12 differentially expressed genes in the HBR and UHR study with treatment group annotations.

Practice questions

Lesson 2 practice questions

Question 1

Create a variable that stores the value for pi.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
pi=3.14
```

{{Edet}}

Question 2

What data type is stored in the variable pi? And why?

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
type(pi)
```

```
float
```

The variable pi has decimals, thus it is a float.

{{Edet}}

Question 3

Create a variable that stores Avogadro's number.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
avogadro=6.02e23
```

{{Edet}}

Question 4

How do we check if Avogadro's number is greater than pi?

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
avogadro > pi
```

```
True
```

{{Edet}}

Question 5

Use the `if` statement to print out something if Avogadro's number is greater than pi.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
if avogadro > pi:
    print("Avogadro's number is greater than pi")
else:
    print("No conclusion can be made")
```

```
Avogadro's number is greater than pi
```

{{Edet}}

Question 6

Create a list of five random things that you can think of and then use a `for` loop to print each item in the list.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
town=["Curry","Thompson","Green","Igoudala","Durant"]
```

```
for player in range(0,5):
    print(town[player])
```

Alternative solution

```
for player in town:
    print(player)
```

{{Edet}}

Lesson 3 practice questions

Question 1

Import hcc1395_chr22_rna_seq_counts.csv and store it as hcc1395_chr22_counts.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
import pandas
```

```
hcc1395_chr22_counts=pandas.read_csv("./hcc1395_chr22_rna_seq_counts
```

{{Edet}}

Question 2

How many rows and columns are in hcc1395_chr22_counts?

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_chr22_counts.shape
```

```
(1335, 7)
```

{{Edet}}

Question 3

What are the column names in hcc1395_chr22_counts and how to view the first 10 rows of this data set?

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_chr22_counts.head(10)
```

Alternatively, use `hcc1395_chr22_counts.columns` to get the column headings for this data frame.

{{Edet}}

Question 4

How many genes start with the letter "C" in hcc1395_chr22_counts?

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_chr22_counts.loc[hcc1395_chr22_counts.loc[:,'Geneid'].str.sta
```

{{Edet}}

Question 5

Import hcc1395_deg_chr22.csv and store it as hcc1395_deg_chr22.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_deg_chr22=pandas.read_csv("./hcc1395_deg_chr22.csv")
```

{{Edet}}

Question 6

Remove ".bam" from the column headers of hcc1395_deg_chr22.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_deg_chr22.columns=hcc1395_deg_chr22.columns.str.replace(".bar
```

{{Edet}}

Question 7

Subset out the following columns from hcc1395_deg_chr22 and store it as hcc1395_deg_chr22_1.

- name
- log2FoldChange
- PAdj

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_deg_chr22_1=hcc1395_deg_chr22.loc[:,["name", "log2FoldChange'
```

Use the `.head` function to check of the subsetting was done correctly.

```
hcc1395_deg_chr22_1.head()
```

{{Edet}}

Question 8

Add a column to hcc1395_deg_chr22_1 that contains the negative log10 of the PAdj value.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
import numpy
```

```
hcc1395_deg_chr22_1["-log10PAdj"]=numpy.negative(numpy.log10(hcc1395_
```

{{Edet}}

Lesson 4 practice questions

Question 1

Create a volcano plot for the differential expression analysis results for the hcc1395 data (hint: import hcc1395_deg_chr22_with_significance.csv)

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
import pandas
import matplotlib.pyplot as plt
import seaborn
```

```
hcc1395_deg_chr22=pandas.read_csv("./hcc1395_deg_chr22_with_signific
```

```
plot1=seaborn.scatterplot(hcc1395_deg_chr22,x="log2FoldChange", y="-
plt.show()
```

{{Edet}}

Question 2

Label the two most differential expressed genes in the volcano plot. As a hint, first import hcc1395_deg_chr22_top_genes.csv.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_deg_chr22_top_genes=pandas.read_csv("./hcc1395_deg_chr22_top_
```

```
plot1=seaborn.scatterplot(hcc1395_deg_chr22,x="log2FoldChange", y="-
for i, gene_name in enumerate(hcc1395_deg_chr22_top_genes["name"]):
    plot1.text(hcc1395_deg_chr22_top_genes["log2FoldChange"][i],
               hcc1395_deg_chr22_top_genes["-log10PAdj"][i],gene_name
plt.show()
```

{{Edet}}

Question 3

Import hcc1395_top_deg_normalized_counts.csv and create an expression heatmap. Use the Viridis color palette.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
hcc1395_top_deg_normalized_counts=pandas.read_csv("./hcc1395_top_deg_
```

```
plot2=seaborn.clustermap(hcc1395_top_deg_normalized_counts,z_score=0
                        figsize=(8,8),vmin=-1.5, vmax=1.5,cbar_kws=(
plt.show()
```

{{Edet}}

Question 4

Add a bar on the top of the heatmap that shows which treatment group the samples belong to.

{{Sdet}}{{Ssum}}Solution{{Esum}}

```
samples=pandas.Series({"hcc1395_normal_rep1":"orangered", "hcc1395_n
column_colors = hcc1395_top_deg_normalized_counts.columns.map(sample
plot2=seaborn.clustermap(hcc1395_top_deg_normalized_counts,z_score=0
                        figsize=(8,8),vmin=-1.5, vmax=1.5,cbar_kws=(
                        col_colors=column_colors, cbar_pos=(0.05,0.8
plot2.ax_heatmap.set_xticklabels(plot2.ax_heatmap.get_xmajorticklabe
plot2.ax_cbar.tick_params(labelsize=12)
plot2.ax_col_colors.set_title("treatment",x=1.09,y=-0.3)
plt.show()
```

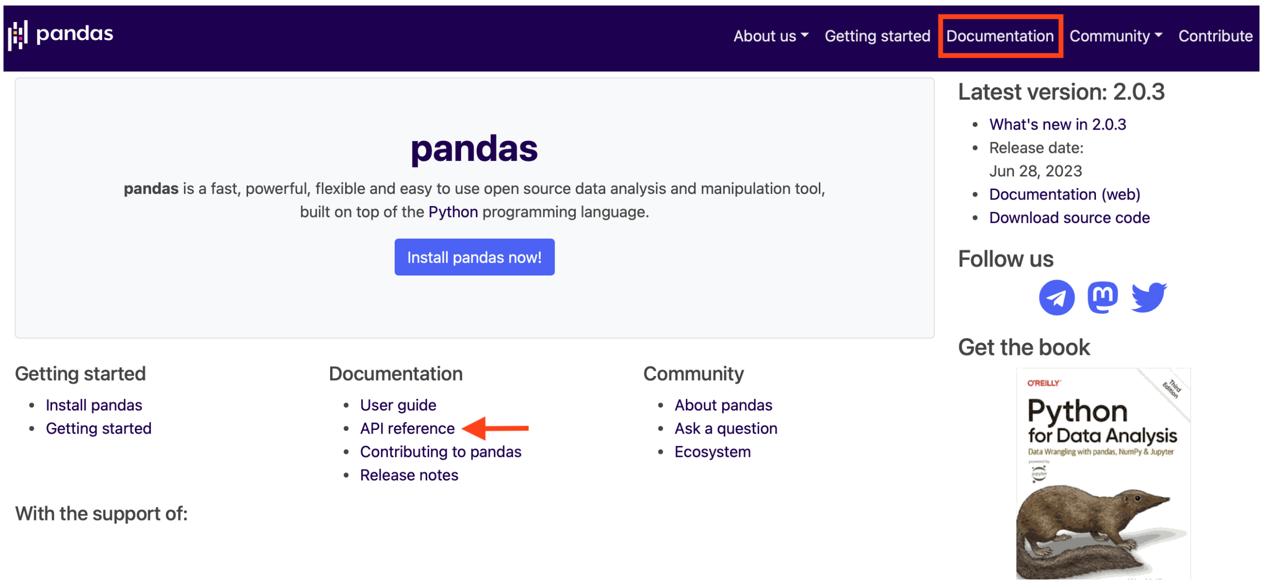
{{Edet}}

Finding help

The document provides useful links where participants can find help for the Python packages that were addressed during the course series.

Pandas - package for working with tabular data *(https://pandas.pydata.org)*

- Pandas API reference gives instructions for each command *(https://pandas.pydata.org/docs/reference/index.html)*. To get to the API reference, either
    - Navigate to the the Documentation section at the Pandas homepage and click on API reference (Figure 1).
    - OR, click on the the Documentation tab at the top of the Pandas homepage and click on the tile labeled API reference in the subsequent page (Figure 2).



pandas

pandas is a fast, powerful, flexible and easy to use open source data analysis and manipulation tool, built on top of the Python programming language.

Latest version: 2.0.3

- What's new in 2.0.3
- Release date: Jun 28, 2023
- Documentation (web)
- Download source code

Getting started

- Install pandas
- Getting started

Documentation

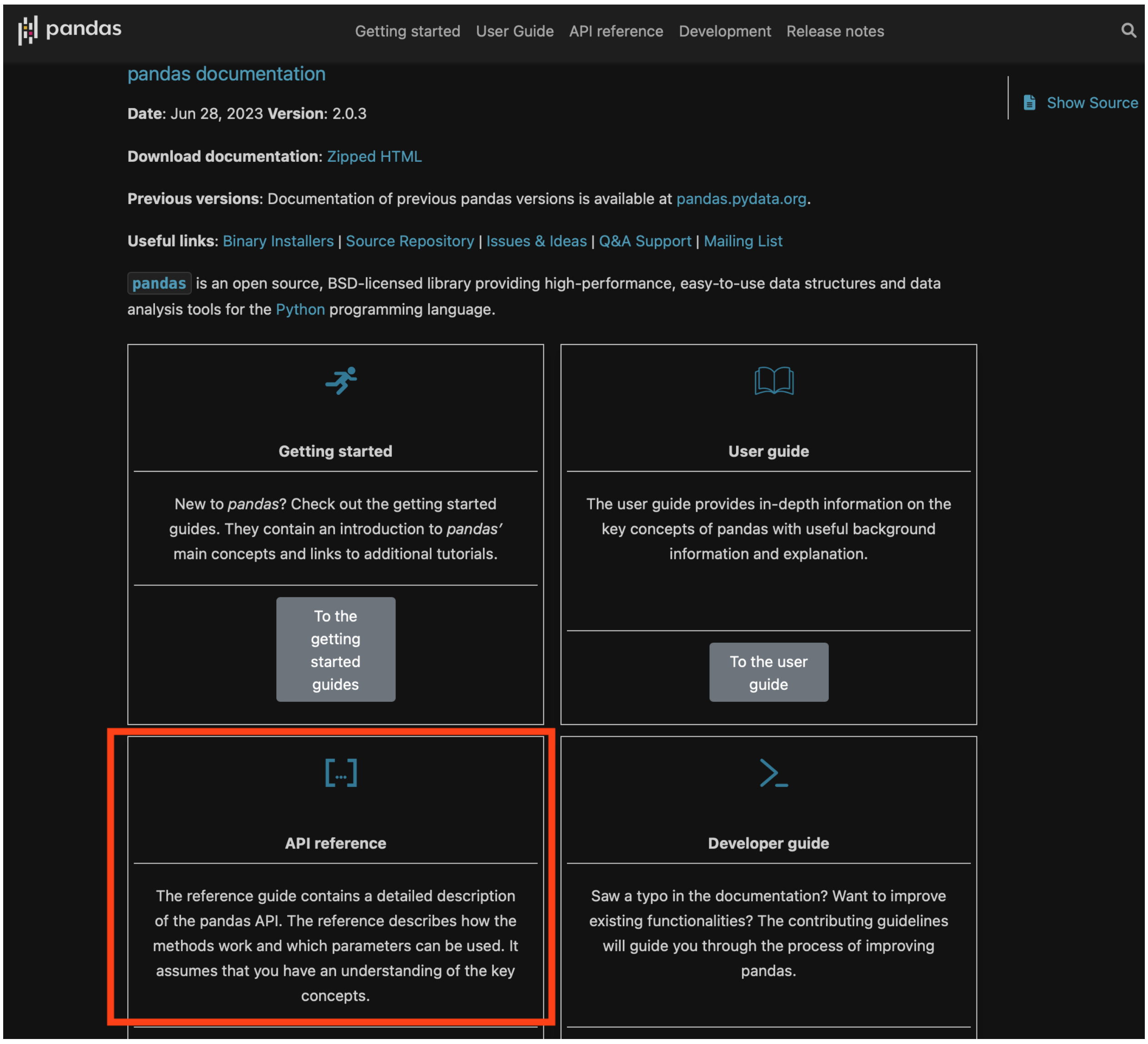
- User guide
- API reference
- Contributing to pandas
- Release notes

Community

- About pandas
- Ask a question
- Ecosystem

With the support of:

Figure 1



pandas documentation

Date: Jun 28, 2023 **Version**: 2.0.3

Download documentation: Zipped HTML

Previous versions: Documentation of previous pandas versions is available at pandas.pydata.org.

Useful links: Binary Installers | Source Repository | Issues & Ideas | Q&A Support | Mailing List

`pandas` is an open source, BSD-licensed library providing high-performance, easy-to-use data structures and data analysis tools for the Python programming language.

Getting started

New to *pandas*? Check out the getting started guides. They contain an introduction to *pandas'* main concepts and links to additional tutorials.

To the getting started guides

User guide

The user guide provides in-depth information on the key concepts of pandas with useful background information and explanation.

To the user guide

API reference

The reference guide contains a detailed description of the pandas API. The reference describes how the methods work and which parameters can be used. It assumes that you have an understanding of the key concepts.

Developer guide

Saw a typo in the documentation? Want to improve existing functionalities? The contributing guidelines will guide you through the process of improving pandas.

Figure 2

Seaborn for data visualization *(https://seaborn.pydata.org/index.html)*

- Seaborn API reference gives instructions for each command *(https://seaborn.pydata.org/api.html)*. To get to the Seaborn API reference, click on API at the top of the Seaborn website.

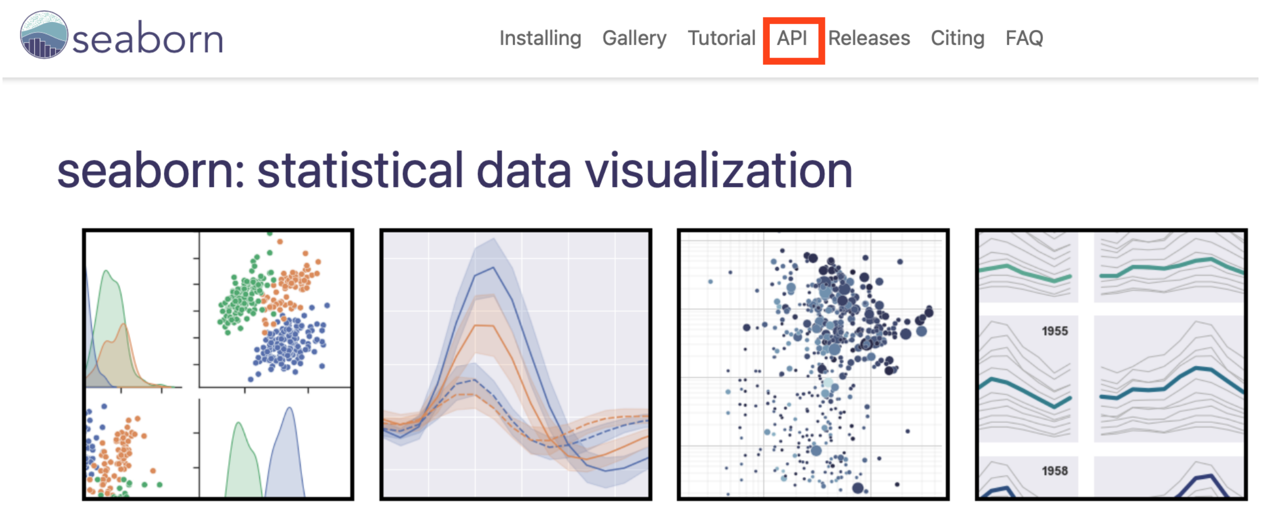


Figure 3

Numpy for scientific computing *(https://numpy.org/doc/stable/index.html)*

- Numpy API reference *(https://numpy.org/doc/stable/reference/index.html)*. To get to this, select Documentation at the top of the Numpy homepage (Figure 4) and then click on either of the links to the API reference (Figure 5).

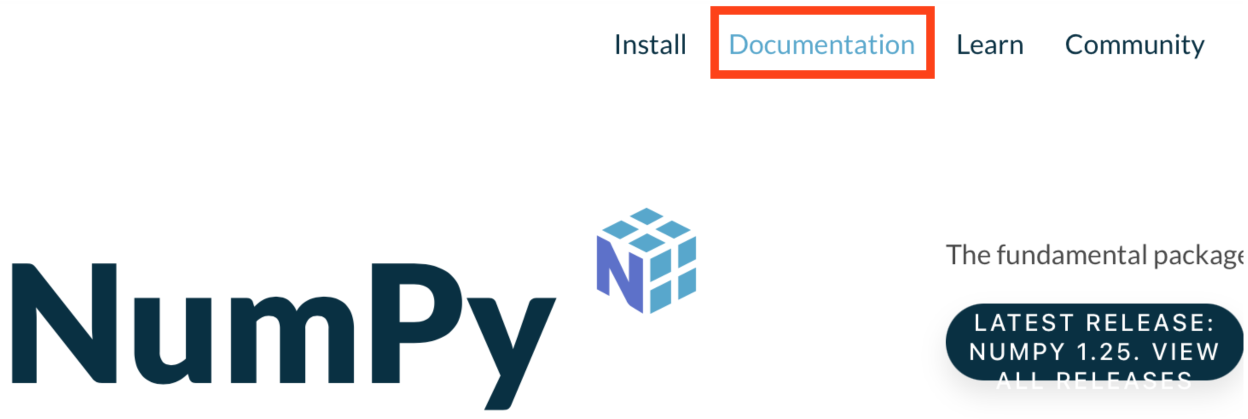
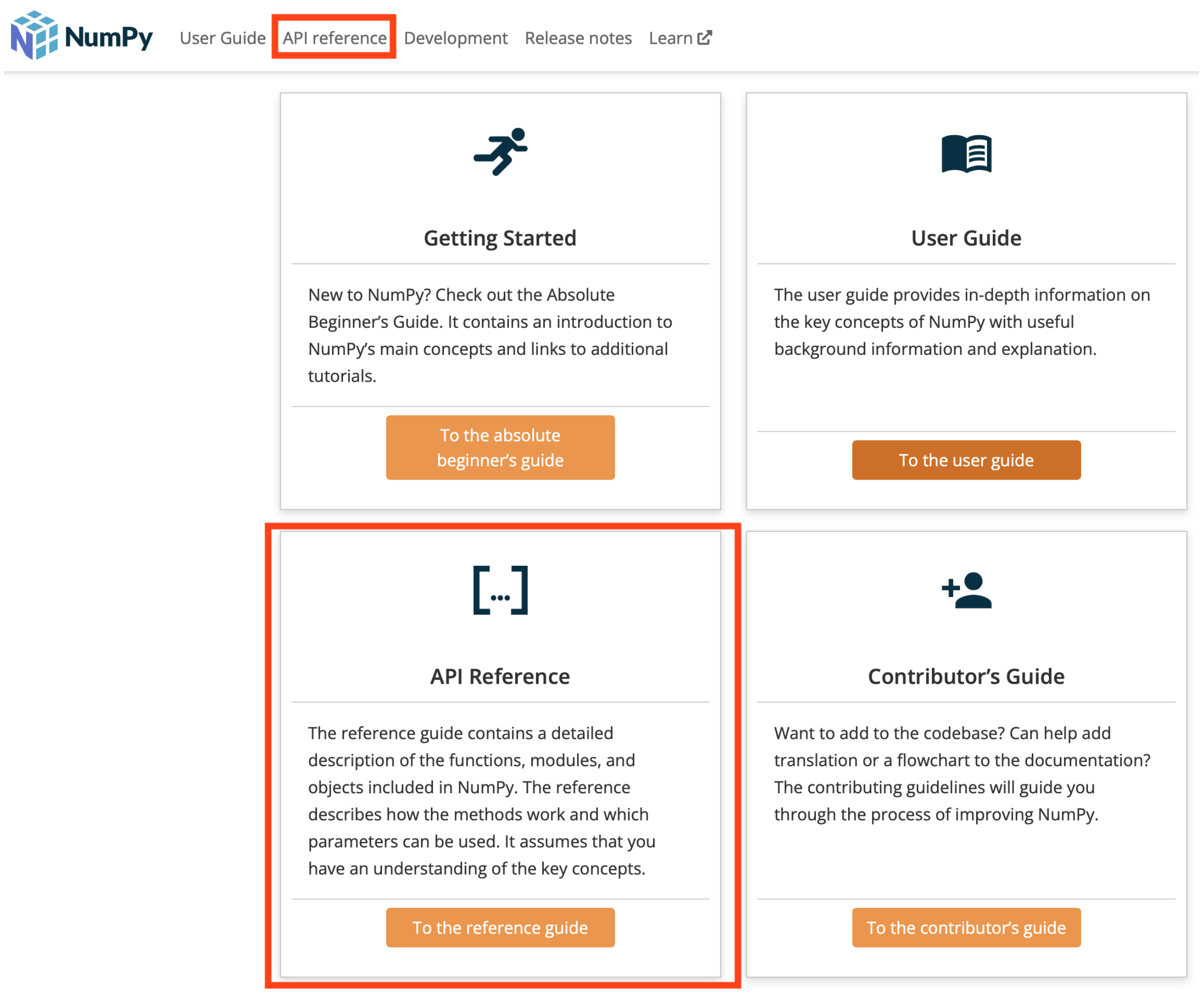


Figure 4



Getting Started

New to NumPy? Check out the Absolute Beginner's Guide. It contains an introduction to NumPy's main concepts and links to additional tutorials.

To the absolute beginner's guide

User Guide

The user guide provides in-depth information on the key concepts of NumPy with useful background information and explanation.

To the user guide

API Reference

The reference guide contains a detailed description of the functions, modules, and objects included in NumPy. The reference describes how the methods work and which parameters can be used. It assumes that you have an understanding of the key concepts.

To the reference guide

Contributor's Guide

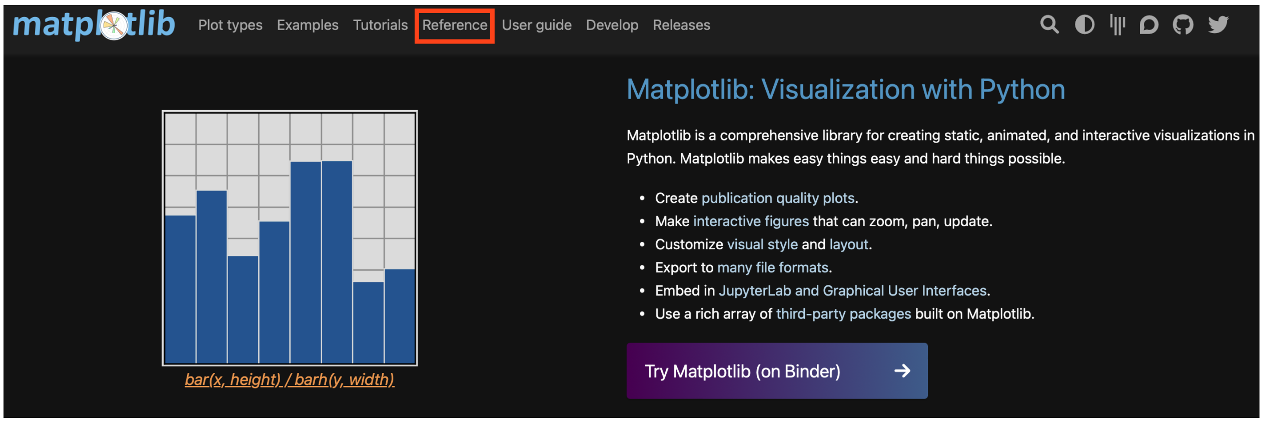
Want to add to the codebase? Can help add translation or a flowchart to the documentation? The contributing guidelines will guide you through the process of improving NumPy.

To the contributor's guide

Figure 5

Matplotlib for data visualization *(https://matplotlib.org)*

- Matplotlib API reference *(https://matplotlib.org/stable/api/index)*. To get to this, click on reference at the top of the Matplotlib homepage (Figure 6).



Matplotlib: Visualization with Python

Matplotlib is a comprehensive library for creating static, animated, and interactive visualizations in Python. Matplotlib makes easy things easy and hard things possible.

- Create publication quality plots.
- Make interactive figures that can zoom, pan, update.
- Customize visual style and layout.
- Export to many file formats.
- Embed in JupyterLab and Graphical User Interfaces.
- Use a rich array of third-party packages built on Matplotlib.

Try Matplotlib (on Binder)

Figure 6