High Performance Data Analytics in Python

Scientists, engineers and professionals from many sectors are seeing an enormous growth in the size and number of datasets relevant to their domains. Professional titles have emerged to describe specialists working with data, such as data scientists and data engineers, but also other experts are finding it necessary to learn tools and techniques to work with big data. Typical tasks include preprocessing, analysing, modeling and visualising data.

Python is an industry-standard programming language for working with data on all levels of the data analytics pipeline. This is in large part because of the rich ecosystem of libraries ranging from generic numerical libraries to special-purpose and/or domain-specific packages, often supported by large developer communities and stable funding sources.

This lesson will give an overview of working with research data in Python using general libraries for storing, processing, analysing and sharing data. The focus is on high performance. After covering tools for performant processing on single workstations the focus shifts to profiling and optimising, parallel and distributed computing.

⚙ Prerequisites

- Basic experience with Python
- Basic experience in working in a Linux-like terminal
- Some prior experience in working with large or small datasets

Reading materials

- Python for Scientific Computing
- Using Python in an HPC Environment
- Python Performance Workshop
- ...

Setting Up Programming Environment

In order to run hands-on exercises in this course, you need the Python package and several depenencies.

- If you use your own computer to run exercises, you should follow the instructions described below to install relevant packages and setup specific programming environment before running hands-on exercises.

- You can use an HPC cluster if you have access to one to run hands-on exercises. Below we provide a short description to login to the **LUMI** cluster, load the modules, and run interactive/batch jobs.

Local Installation

Install miniforge

If you already have a preferred way to manage Python versions and libraries, you can stick to that. If not, we recommend that you install Python3 and all libraries using Miniforge, a free minimal installer for the package, dependency and environment manager conda.

Please follow the installation instructions to install Miniforge.

Make sure that conda is correctly installed:

```
$ conda --version
# conda 24.11.2
```

Install python programming environment on personal computer

For Mac users

With conda installed, install the required dependencies by running:

```
$ conda env create --yes -f https://raw.githubusercontent.com/ENCCS/hpda-
python/main/content/env/environment.yml
```

This will create a new environment pyhpda which you need to activate by:

```
$ conda activate pyhpda
```

Ensure that the Python version is fairly recent:

```
$ python --version
# Python 3.12.8
```

Finally, open Jupyter-Lab in your browser:

```
$ jupyter-lab
```

If you use VS code, you can come to the installed `pyhpda` programming environment via choosing `Select Kernel` ar the upper right corner, `Python Environents` and you will find the pre-installed `pyhpda` programming environment.

For Linux users

Please provide detailes instructures for linux users to install packages.

For Windows users

Please provide detailes instructures for windows users to install packages.

Using HPC Cluster

LUMI

Login to LUMI cluster

Follow practical instructions **HERE** to get your access to LUMI cluster.

- On Step 5, you can login to LUMI cluster through terminal.
- On Step 6, you can login to LUMI cluster from the web-interface.

Running jobs on LUMI cluster

If you want to run an interactive job asking for 1 node, 1 GPU, and 1 hour:

```
$ salloc -A project_XXXXX -N 1 -t 1:00:00 -p standard-g --gpus-per-node=1

$ srun <some-command>
```

Exit interactive allocation with `exit`.

You can also submit your job with a batch script submit.sh:

```
#!/bin/bash -l
#SBATCH --account=project_XXXXX
#SBATCH --job-name=example-job
#SBATCH --output=examplejob.o%j
#SBATCH --error=examplejob.e%j
#SBATCH --partition=standard-g
#SBATCH --nodes=1
#SBATCH --gpus-per-node=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=1:00:00

srun <some_command>
```

Some useful commands are listed below:

- Submit the job: `sbatch submit.sh`
- Monitor your job: `squeue --me`
- Kill job: `scancel <JOB_ID>`

Using `pyhpda` programming environment on LUMI cluster

We have installed the `pyhpda` programming environment on LUMI. You can follow instructions below to activate it and login to LUMI cluster, either via terminal or through the web-interface.

Login to LUMI cluster via terminal and then the commands below to check and activate the pyhpda environment.

```
$ /projappl/projecXXXXX10/miniconda3/bin/conda init

$ source ~/.bashrc

$ which
# you should get output as shown below
/project/project_XXXXX/miniconda3/condabin/cond

$ conda activate pyhpda

$ which python
# you should get output as shown below
/project/project_XXXXX/miniconda3/envs/pyhpda/bin/python
 conda
```

Login to LUMI cluster via web-interface and then select `Jupyter` (not `Jupyter for courses`) icon for an interactive session, and provide the following values in the form to launch the jupyter lab app.

- Project: `project_XXXXX`
- Partition: `interactive`

- Number of CPU cores: `2`
- Time: `4:00:00`
- Working directory: `/projappl/project_XXXXX`
- Python: `Custom`
- Path to python: `/project/project_XXXXX/miniconda3/envs/pyhpda/bin/python`
- `check` for *Enable system installed packages on venv creation*
- `check` for Enable packages under *~/.local/lib on venv start*
- Click the `Launch` button, wait for minutes until your requested session was created.
- Click the `Connect to Jupyter` button, and then select the Python kernel `Python 3 (venv)` for the created Jupyter notebooks.

Leonardo Booster

Login to Leonardo Booster cluster

Follow instructions at HERE to get your access to Leonardo Booster cluster.

Running jobs on Leonardo Booster cluster

Here are instructions to run jobs on Leonardo Booster cluster

- xxx
- xxx

Using `pyhpda` programming environment on Leonardo Booster cluster

Here are instructions to install the `pyhpda` programming environment on Leonardo Booster cluster

- xxx
- xxx

1. Motivation

This episode provides a broad overview of this course and the main motivation to attend this course.

Objectives

- What is big data
- What is the Python programming environment and the ecosystem
- What you will learn during this course

Instructor note

- 20 min teaching/type-along

- 0 min exercising

1.1 Big Data

- How large is the data you are working with?
- Are you experiencing performance bottlenecks when you try to analyse it?

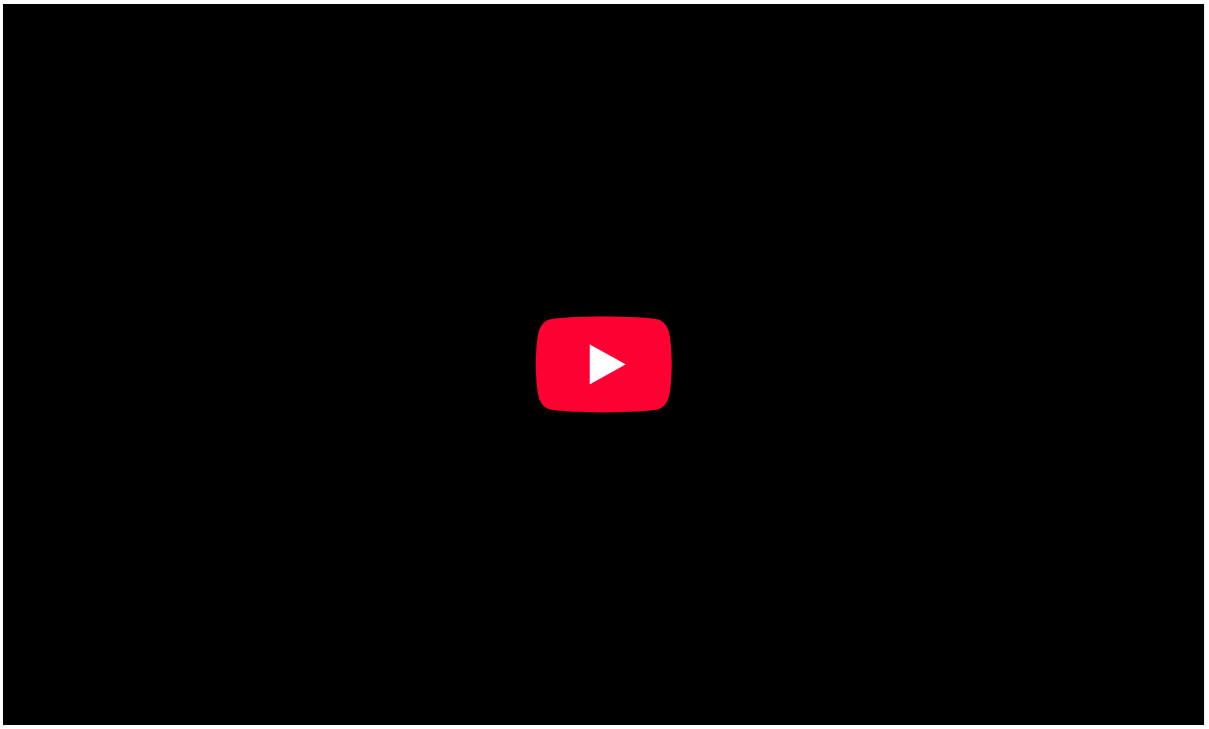
“Big data refers to data sets that are too large or complex to be dealt with by traditional data-processing application software. [...] Big data analysis challenges include capturing data, data storage, data analysis, search, sharing, transfer, visualization, querying, updating, information privacy, and data source.” (from Wikipedia)

“Big data” is a current buzzword used heavily in the tech industry, but many scientific research communities are increasingly adopting high-throughput data production methods which lead to very large datasets. One driving force behind this development is the advent of powerful machine learning methods which enable researchers to derive novel scientific insights from large datasets. Another is the strong development of high performance computing (HPC) hardware and the accompanying development of software libraries and packages which can efficiently take advantage of the hardware.

This course focuses on high-performace data analytics (HPDA), a subset of high-performance computing which focuses on working with large data. The data can come from either computer models and simulations or from experiments and observations, and the goal is to preprocess, analyse and visualise it to generate scientific results.

The video shown below provide more descriptions of the big data.

```
from IPython.display import YouTubeVideo

YouTubeVideo('qydP7cOH4qc', width=600, height=360)
```



1.2 Python

💬 Discussion

Performance bottlenecks in Python

- Have you ever written Python scripts that look something like the one below?
- Compared to C/C++/Fortran, this for-loop will probably be orders of magnitude slower

```
f = open("mydata.dat", "r")
for line in f.readlines():
    fields = line.split(",")
    x, y, z = fields[1], fields[2], fields[3]
    # some analysis with x, y and z
f.close()
```

Despite early design choices of the Python language which made it significantly slower than conventional HPC languages, a rich and growing ecosystem of open source libraries have established Python as an industry-standard programming language for working with data on all levels of the data analytics pipeline. These range from generic numerical libraries to special-purpose and/or domain-specific packages. This lesson is focused on introducing modern packages from the Python ecosystem to work with large data. Specifically, we will learn to use:

- Numpy
- Scipy
- Pandas
- Xarray

- Numba
- Cython
- multithreading
- multiprocessing
- Dask

1.3 What You Will Learn

This lesson provides a broad overview of methods to work with large datasets using tools and libraries from the Python ecosystem. Since this field is fairly extensive we will not have time to go into much depth. Instead, the objective is to expose just enough details on each topic for you to get a good idea of the big picture and an understanding of what combination of tools and libraries will work well for your particular use case.

Specifically, **this course covers**:

- Tools for efficiently storing data and writing/reading data to/from disk
- How to share datasets and mint digital object identifiers (DOI)
- Main methods of efficiently working with tabular data and multidimensional arrays
- How to measure performance and boost performance of time consuming Python functions
- Various methods to parallelise Python code

The course does not cover the following episodes but the lesson materials for these episodes are provided at other modules. Please refer to the links provided below to the other course materials.

- Visualisation techniques
- Machine learning
- GPU programming

1.4 Keypoints

- Datasets are getting larger across nearly all scientific and engineering domains
- The Python ecosystem has many libraries and packages for working with big data efficiently

2. Efficient Array Computing

This episode introduces how to write high-performance numerical code in Python packages (Numpy, Pandas, and Scipy) by leveraging tools and libraries designed to optimize computation speed and memory usage. It explores strategies such as vectorization with NumPy, just-in-time compilation using Numba, and parallelization techniques that can significantly reduce execution time. These methods help Python developers overcome the traditional performance limitations of the language, making it suitable for intensive scientific and engineering applications.

Objectives

- Understand limitations of Python's standard library for large data processing
- Understand limitations of Python's standard library for large data processing
- Understand the logic behind NumPy ndarrays and learn to use some NumPy numerical computing tools
- Learn to use data structures and analysis tools from Panda

Instructor note

- 25 min teaching/type-along
- 25 min exercising

2.1 Why can Python be slow?

Computer programs are nowadays practically always written in a high-level human readable programming language and then translated to the actual machine instructions that a processor understands. There are two main approaches for this translation:

- For **compiled** programming languages, the translation is done by a compiler before the execution of the program
- For **interpreted** languages, the translation is done by an interpreter during the execution of the program

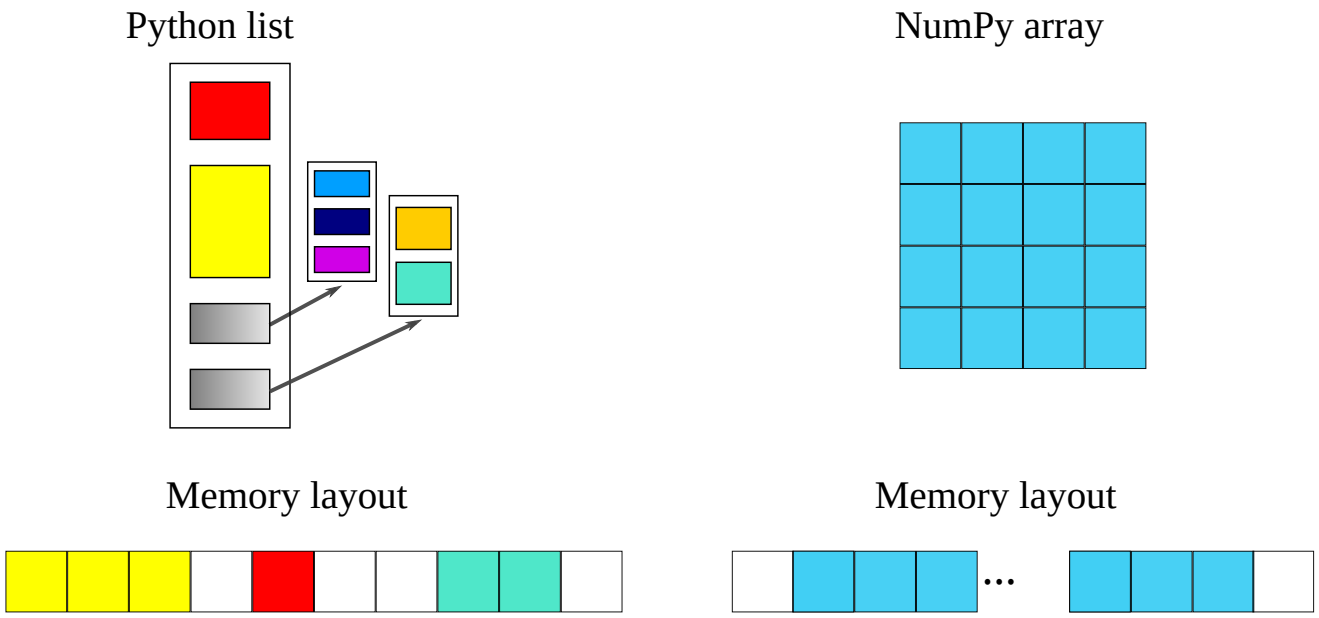
2.2 NumPy

NumPy is based on well-optimized C code, which gives much better performace than regular Python. In particular, by using homogeneous data structures, NumPy *vectorizes* mathematical operations where fast pre-compiled code can be applied to a sequence of data instead of using traditional `for` loops.

2.2.1 Arrays

The core of NumPy is the NumPy `ndarray` (n-dimensional array). Compared to a Python list, an ndarray is similar in terms of serving as a data container. Some differences between the two are:

- ndarrays can have multiple dimensions, *e.g.* a 1-D array is a vector, a 2-D array is a matrix
- ndarrays are fast only when all data elements are of the same type



2.2.2 Creating NumPy arrays

One way to create a NumPy array is to convert from a Python list, but make sure that the list is homogeneous (contains same data type) otherwise performace will be downgraded. Since appending elements to an existing array is slow, it is a common practice to preallocate the necessary space with `np.zeros` or `np.empty` when converting from a Python list is not possible.

```
import numpy as np

a = np.array((1, 2, 3, 4), float)
print(f"a = {a}\n")
# array([ 1., 2., 3., 4.])

list1 = [[1, 2, 3], [4, 5, 6]]
mat = np.array(list1, complex)
# create complex array, with imaginary part equal to zero
print(f"mat = \n {mat} \n")
# array([[ 1.+0.j, 2.+0.j, 3.+0.j],
#        [ 4.+0.j, 5.+0.j, 6.+0.j]])

print(f"mat.shape={mat.shape}, mat.size={mat.size}")
# mat.shape=(2, 3), mat.size=6
```

Caution

You should copy the code above to a separate code block, or change its cell type from from `Markdown` to `Code`.

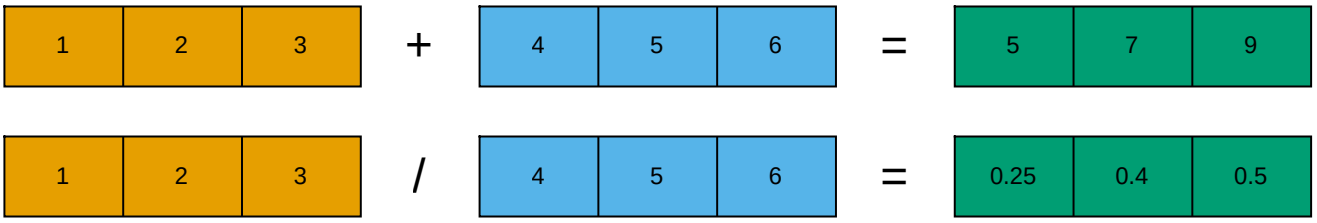
`arange` and `linspace` can generate ranges of numbers:

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

b = np.arange(0.1, 0.2, 0.02)
print(b)
# array([0.1 , 0.12, 0.14, 0.16, 0.18])

c = np.linspace(-4.5, 4.5, 5)
print(c)
# array([-4.5 , -2.25, 0. , 2.25, 4.5 ])
```

2.2.3 Array operations and manipulations

All the familiar arithmetic operators in NumPy are applied elementwise:

```
# 1D example

import numpy as np
a = np.array([1, 2, 3])
b = np.array([4, 5, 6])

print(f" a+b = {a+b}\n a/b = {a/b}")
```



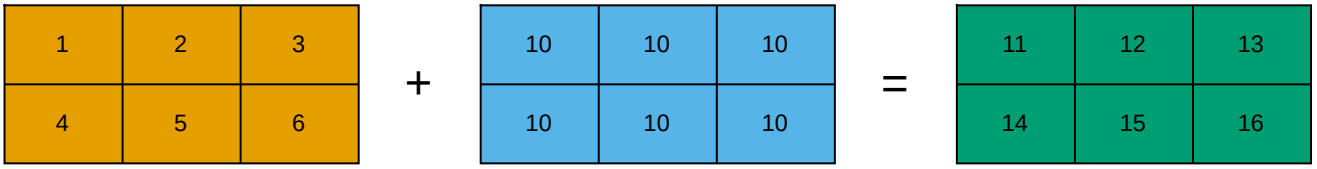
✍ Exercise

Run the code below to get familiar with indexing in a 2D example.

```
# 2D example

import numpy as np
a = np.array([[1, 2, 3], [4, 5, 6]])
b = np.array([[10, 10, 10], [10, 10, 10]])

print(a+b)
# [[11, 12, 13],
#  [14, 15, 16]]
```

Caution

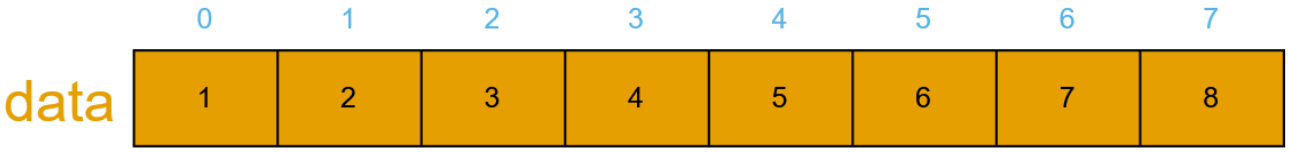
You can download the code example from HERE.



2.2.4 Array indexing

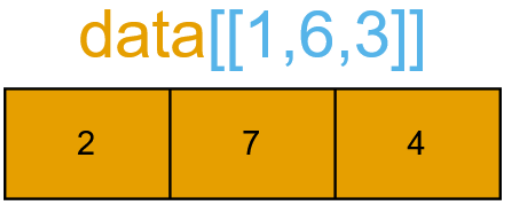
Basic indexing is similar to Python lists. Note that advanced indexing creates copies of arrays.

```
# 1D example

import numpy as np

data = np.array([1,2,3,4,5,6,7,8])

# integer indexing
print("Integer indexing")
print(f"data = {data}")
print(f"data[3] = {data[3]}")
print(f"data[0:2] = {data[0:2]}")
print(f"data[-2] = {data[-2]}")
print(f"data[::-4] = {data[::-4]}")

# fancy indexing
print("\nFancy indexing")
print(f"data[[1,6,3]] = {data[[1,6,3]]}")

# boolean indexing
print("\nBoolean indexing")
print(f"data[data>5] = {data[data>5]}")
```

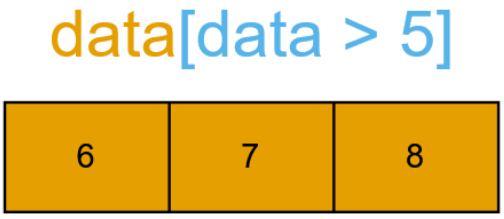


Integer indexing:

Fancy indexing:



Boolean indexing:



✍ Exercise

Run the code below to get familiar with indexing in a 2D example.

```
# 2D example

data = np.array([[1, 2, 3, 4],[5, 6, 7, 8],[9, 10, 11, 12]])

# integer indexing
print("Integer indexing")
print(f"data[1] = {data[1]}")
print(f"data[:, 1] = {data[:, 1]}")
print(f"data[1:3, 2:4] = {data[1:3, 2:4]}")

# fancy indexing
print("\nFancy indexing")
print(f"data[[0,2,1], [2,3,0]] = {data[[0,2,1], [2,3,0]]}")

# boolean indexing
print("\nBoolean indexing")
print(f"data[data>10] = {data[data>10]}")
```

Caution

Again, you should move the code above to a separate code block, or change its cell type from from `Markdown` to `Code`.

2.2.5 I/O with NumPy

Numpy provides functions for reading from/writing to files. Both ASCII and binary formats are supported with the CSV and npy/npz formats.

CSV

The `numpy.loadtxt()` and `numpy.savetxt()` functions can be used. They save in a regular column layout and can deal with different delimiters, column titles and numerical representations.

```
a = np.array([1, 2, 3, 4])
np.savetxt("my_array.csv", a)
b = np.loadtxt("my_array.csv")

print(a == b) # [ True  True  True  True]
```

Attention

If you get an eror like xxx, you should import numpy before the first line `import numpy as np`.

Binary

The npy format is a binary format used to dump arrays of any shape. Several arrays can be saved into a single npz file, which is simply a zipped collection of different npy files. All the arrays to be saved into a npz file can be passed as kwargs to the `numpy.savez()` function. The data can then be recovered using the `numpy.load()` method, which returns a dictionary-like object in which each key points to one of the arrays.

```
a = np.array([1, 2, 3, 4])
b = np.array([5, 6, 7, 8])

np.savez("my_arrays.npz", array_1=a, array_2=b)
data = np.load("my_arrays.npz")

print(data['array_1'] == a) # [ True  True  True  True]
print(data['array_2'] == b) # [ True  True  True  True]
```

2.2.6 Random numbers

The module `numpy.random` provides several functions for constructing random arrays

- `random()`: uniform random numbers
- `normal()`: normal distribution
- `choice()`: random sample from given array
- ...

```
import numpy as np

print(np.random.random((2,2)),'\n')

print(np.random.choice(np.arange(4), 10))
```

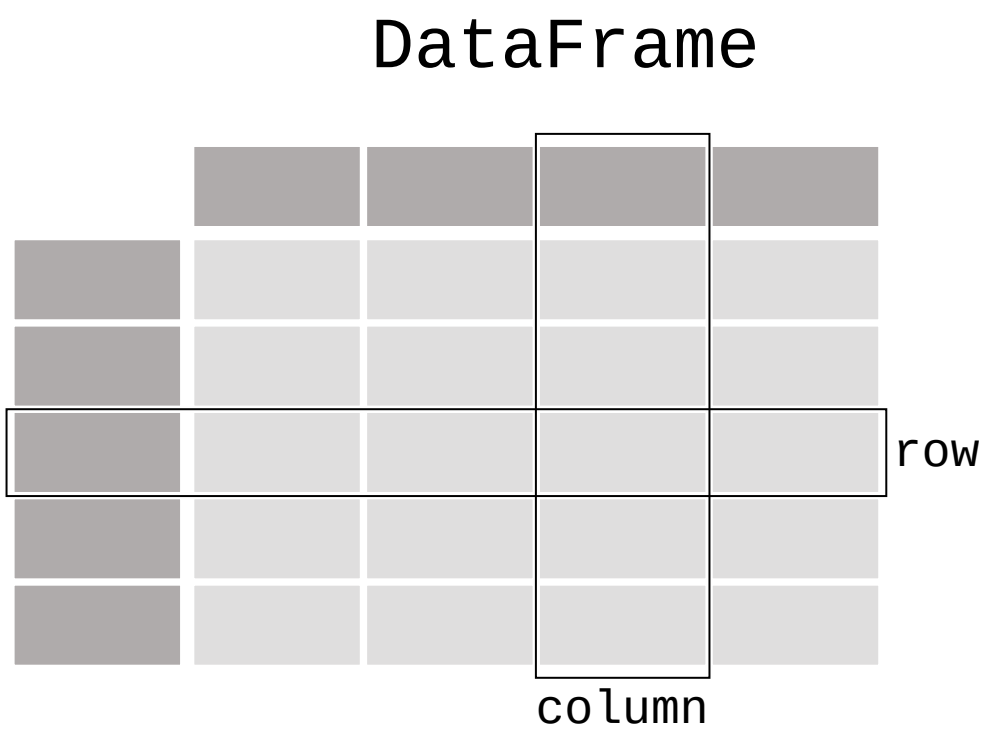
Warning

You might get different results from this code example.

2.3 Pandas

Pandas is a Python package that provides high-performance and easy to use data structures and data analysis tools. The core data structures of Pandas are Series and Dataframes.

- a Pandas `series` is a one-dimensional NumPy array with an index which we could use to access the data
- a `dataframe` consist of a table of values with labels for each row and column. A dataframe can combine multiple data types, such as numbers and text, but the data in each column is of the same type.
- each column of a dataframe is a series object - a dataframe is thus a colle tion of series.



2.3.1 Data analysis workflow

Pandas is a powerful tool for many steps of a data analysis pipeline:

To explore some of the capabilities, we start with an example dataset containing the passenger list from the Titanic, which is often used in Kaggle competitions and data science tutorials. First step is to load Pandas and download the dataset into a dataframe.

```
import pandas as pd

url = "https://raw.githubusercontent.com/pandas-dev/pandas/master/doc/data/titanic.csv"

# set the index to the "Name" column
titanic = pd.read_csv(url, index_col="Name")
```

Note

Pandas also understands multiple other formats, for example `read_excel()`, `read_hdf()`, `read_json()`, *etc.* (and corresponding methods to write to file: `to_csv()`, `to_excel()`, `to_hdf()`, `to_json()`, ...)...)

We can now view the dataframe to get an idea of what it contains and print some summary statistics of its numerical data:

```
# print the first 5 lines of the dataframe
print(titanic.head())

# print some information about the columns
print(titanic.info())

# print summary statistics for each column
print(titanic.describe())
```

2.3.2 Missing/invalid data

What if your dataset has missing data? Pandas uses the value np.nan to represent missing data, and by default does not include it in any computations. We can find missing values, drop them from our dataframe, replace them with any value we like or do forward or backward filling.

```
titanic.isna()                          # returns boolean mask of NaN values

print(titanic.dropna())                 # drop missing values
print(titanic.dropna(how="any"))        # or how="all"
print(titanic.dropna(subset=["Cabin"])) # only drop NaNs from one column
print(titanic.fillna(0))                # replace NaNs with zero
```

2.4 Scipy

Let us look more closely into one out of the countless useful functions available in SciPy. `curve_fit()` is a non-linear least squares fitting function. NumPy has least-squares fitting via the `np.linalg.lstsq()` function, but we need to go to SciPy to find non-linear curve fitting. This example fits a power-law to a vector.

```
import numpy as np
from scipy.optimize import curve_fit

def powerlaw(x, A, s):
    return A * np.power(x, s)

# data
Y = np.array([9115, 8368, 7711, 5480, 3492, 3376, 2884, 2792, 2703, 2701])
X = np.arange(Y.shape[0]) + 1.0

# initial guess for variables
p0 = [100, -1]
# fit data
params, cov = curve_fit(f=powerlaw, xdata=X, ydata=Y, p0=p0, bounds=(-np.inf, np.inf))

print("A =", params[0], "+/-", cov[0,0]**0.5)
print("s =", params[1], "+/-", cov[1,1]**0.5)

# optionally plot
import matplotlib.pyplot as plt
plt.plot(X,Y)
plt.plot(X, powerlaw(X, params[0], params[1]))
plt.show()
```

2.5 Exercises

✍ Working effectively with dataframes

Recall the `curve_fit()` method from SciPy discussed above, and imagine that we want to fit powerlaws to every row in a large dataframe. How can this be done effectively?

First define the `powerlaw()` function and another function for fitting a row of numbers:

```
import numpy as np
import pandas as pd
from scipy.optimize import curve_fit

def powerlaw(x, A, s):
    return A * np.power(x, s)

def fit_powerlaw(row):
    X = np.arange(row.shape[0]) + 1.0
    params, cov = curve_fit(f=powerlaw, xdata=X, ydata=row, p0=[100, -1], bounds=(-
np.inf, np.inf))
    return params[1]
```

Next load a dataset with multiple rows similar to the one used in the example above:

```
df = pd.read_csv("https://raw.githubusercontent.com/ENCCS/hpda-
python/main/content/data/results.csv")
# print first few rows
df.head()
```

Now consider these four different ways of fitting a powerlaw to each row of the dataframe:

```
# 1. Loop

powers = []
for row_indx in range(df.shape[0]):
    row = df.iloc[row_indx,1:]
    p = fit_powerlaw(row)
    powers.append(p)
```

```
# 2. `iterrows()

powers = []
for row_indx,row in df.iterrows():
    p = fit_powerlaw(row[1:])
    powers.append(p)
```

```
# 3. `apply()

powers = df.iloc[:,1:].apply(fit_powerlaw, axis=1)
```

```
# 4. `apply()` with `raw=True`

# raw=True passes numpy ndarrays instead of series to fit_powerlaw
powers = df.iloc[:,1:].apply(fit_powerlaw, axis=1, raw=True)
```

Which one do you think is most efficient? You can measure the execution time by adding `%%timeit` to the first line of a Jupyter code cell. More on timing and profiling in a later episode.

✔ Solution

The execution time for four different methods are described below. Note that you may get different numbers when you run these examples.

```
# 1 Loop

%%timeit
powers = []
for row_indx in range(df.shape[0]):
   row = df.iloc[row_indx,1:]
   p = fit_powerlaw(row)
   powers.append(p)

# 33.6 ms ± 682 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

```
# 2. `iterrows()`

%%timeit
powers = []
for row_indx,row in df.iterrows():
   p = fit_powerlaw(row[1:])
   powers.append(p)

# 28.7 ms ± 947 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

```
# 3. `apply()`

%%timeit
powers = df.iloc[:,1:].apply(fit_powerlaw, axis=1)

# 26.1 ms ± 1.19 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

```
# 4. `apply()` with `raw=True`

%%timeit
powers = df.iloc[:,1:].apply(fit_powerlaw, axis=1, raw=True)

# 24 ms ± 1.27 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

✍ Further analysis of Titanic passenger list dataset

Consider the titanic dataset.

> If you haven't done so already, load it into a dataframe before the exercises: `import pandas as pd; url = "https://raw.githubusercontent.com/pandas-dev/pandas/master/doc/data/titanic.csv"; titanic = pd.read_csv(url, index_col="Name")`

- Compute the mean age of the first 10 passengers by slicing and the `mean` method
- Using boolean indexing, compute the survival rate (mean of "Survived" values) among passengers over and under the average age. Now investigate the family size of the passengers (*i.e.* the "SibSp" column):
- What different family sizes exist in the passenger list?
  - Hint: try the `unique()` method
- What are the names of the people in the largest family group?
- (Advanced) Create histograms showing the distribution of family sizes for passengers split by the fare, i.e. one group of high-fare passengers (where the fare is above average) and one for low-fare passengers
  - **Hint**: instead of an existing column name, you can give a lambda function as a parameter to `hist` to compute a value on the fly. For example `lambda x: "Poor" if titanic["Fare"].loc[x] < titanic["Fare"].mean() else "Rich"`).

✔ Solution

1. Mean age of the first 10 passengers:
   - `titanic.iloc[:10,:]["Age"].mean()` or
   - `titanic.iloc[:10,4].mean()` or
   - `titanic.loc[:"Nasser, Mrs. Nicholas (Adele Achem)", "Age"].mean()`

2. Survival rate among passengers over and under average age:
   - `titanic[titanic["Age"] > titanic["Age"].mean()]["Survived"].mean()` and
   - `titanic[titanic["Age"] < titanic["Age"].mean()]["Survived"].mean()`
3. Existing family sizes: `titanic["SibSp"].unique()`
4. Names of members of largest family(ies): `titanic[titanic["SibSp"] == 8].index`
5. `titanic.hist("SibSp", lambda x: "Poor" if titanic["Fare"].loc[x] < titanic["Fare"].mean() else "Rich", rwidth=0.9)`

2.6 Keypoints

- NumPy provides a static array data structure, fast mathematical operations for arrays and tools for linear algebra and random numbers
- Pandas dataframes are a good data structure for tabular data
- Dataframes allow both simple and advanced analysis in very compact form

➡ See also

- Introduction to running R, Python, Julia, and Matlab in HPC
- Practical Intro to GPU Programming using Python
- Using Python in an HPC environment
- Python for Scientific Computing
- ...

✍ Homework

Choice questions

Why are Python lists inefficient for numerical computations?

- **A) They store elements as generic objects with dynamic typing**
- B) They are statically typed
- C) They don't support indexing
- D) They don't support loops

What is the main advantage of NumPy arrays (ndarray) over Python lists for numerical tasks?

- A) They can hold multiple data types
- B) They automatically parallelize loops
- **C) They store data in a compact, contiguous block of memory**
- D) They have larger memory overhead

What is "vectorization" in the context of NumPy?

- A) A way to convert lists to dictionaries
- B) A process of compiling Python code
- C) A plotting technique
- **D) Replacing explicit loops with whole-array operations**

How does a pandas DataFrame differ from a NumPy array?

- A) DataFrames are slower and less powerful
- **B) DataFrames support heterogeneous data types and labeled axes**
- C) Arrays use less memory
- D) DataFrames cannot be indexed

What does `scipy.optimize.curve_fit()` do?

- A) Performs numerical integration
- **B) Fits data to a model function**
- C) Solves a linear system
- D) Computes a histogram

Coding questions

Generate a 1D NumPy array of 1 million random floats. Compute the square root of each element using:

- a) a Python for loop
- b) NumPy's vectorized np.sqrt

Load a CSV file of weather data (*e.g.*, temperature, humidity, wind).

- a) filter rows where temperature > 30°C
- b) compute the average humidity for each month using `groupby`

Create a random 100×100 matrix A and a vector b.

- a) use `scipy.linalg.solve` to solve the system $Ax = b$
- b) verify the solution by checking the residual norm

Simulate a DataFrame with missing values in numerical columns.

- a) fill missing values with the column mean (using NumPy)
- b) compute basic statistics before and after imputation

Generate noisy data for a quadratic function $y = ax^2 + bx + c$

- a) use `scipy.optimize.curve_fit` to fit the data and recover the original parameters

- b) plot the original *vs* fitted curve

3. Sphinx Directives

Directives

There are directives in Sphinx to highlight code blocks

- `discussion` , `demo` , `exercises` , `solution` , `homework` , `seealso` ...
- `note` , `hint` , `important` , `attention` , `caution` , `warning` , `danger` , ...

In Jupyter NB, there is no such stryling settings. We can ask course developers to provide some keywords (as listed below) before the code block. and we can convert these Jupyter NB blocks to Sphinx blocks.

The format in the Jupyter NB should look like the content below:

```
<font color='purple'>**Discussion**</font>: How large is your data?

- How large is the data you are working with?
- Are you experiencing performance bottlenecks when you try to analyse it?
</div>
```

- Highlight the keyword (here it is `Discussion`) using the corresponding font color
- the Jupyter NB code block starts with `<font color=` and ends with `</div>`

💬 How large is your data?

- How large is the data you are working with?
- Are you experiencing performance bottlenecks when you try to analyse it?

Attention

Do not remove the following line.

Caution

Do not remove the following line.

Warning

Do not remove the following line.

Danger

Here is a danger!

Error

Here is an error!

Hint

In this exercise, you can use A instead of B.

Tip

In this exercise, you can use A instead of B.

Important

You should use the latest version of Python.

✍ Exercise

Description of exercise

- Do this
- then do this
- finally observe what happens when you do this...do this...

✍ With an option "Click to show"

Description of exercise

- Do this
- then do this
- finally observe what happens when you do this...do this...

✔ Solution

Here is the solution for above exercises.

📝 Homework

Here are the homework assignments for this episode.

Note

Here we chose to summarize the data by its mean, but many other common statistical functions are available as dataframe methods, like `std()`, `min()`, `max()`, `cumsum()`, `median()`, `skew()`, `var()`, *etc.*

👀 Demo

Code for demonstration

➡ See also

publications and webpages for references

Define addition keywords

- `suggestion`, `recommendation`, ...

Suggestion

It is recommended to use the CUDA version > 10.0.

Badges

Here is one badge after we publish this module at Zenodo.

We can design other badges with different colors.

Learning outcomes

This material is for all researchers and engineers who work with large or small datasets and who want to learn powerful tools and best practices for writing more performant, parallelised, robust and reproducible data analysis pipelines.

By the end of a workshop covering this lesson, learners should:

- Have a good overview of available tools and libraries for improving performance in Python (**link to leaves in skill tre**)
- Knowing libraries for efficiently storing, reading and writing large data (**link to leaves in skill tree**)
- Be comfortable working with NumPy arrays and Pandas dataframes for data analysis using Python (**link to leaves in skill tree**)
- …

Instructor's guide

Teaching hours and number of participants

This module is developed for one instructor and two teaching assistants during teaching for 40 students. The teaching can be delivered online, onsite, or in a hybrid format, providing flexibility to accommodate different learning preferences and circumstances. Whether students attend in person or remotely, the course materials and exercises are designed to ensure a consistent and engaging learning experience. Instructors can leverage virtual tools such as video conferencing and shared coding environments alongside traditional classroom setups to support all modes of delivery effectively.

Students are expected to dedicate 2-4 hours in total. This estimate combines contact hours, such as lectures or exercises (1~2 hours), with independent learning time (1-2 hours), which include self-study, assignments, and revision. Balancing these components ensures students have sufficient guided instruction while allowing ample time for personal engagement with the material.

Mode of teaching and exercising

Before teaching this module, the instructor is expected to set up the programming environment on the HPC cluster or assist students with installing the necessary packages on their personal computers. During exercises, instructors may use Jupyter notebooks for demonstrations or copy and paste code examples from the webpage into script files. These scripts can then be executed on students' personal computers or the HPC cluster, providing a flexible learning experience.

Hardware requirements on HPC clusters

The HPC cluster used for this course should be equipped with modern NVIDIA GPUs that support CUDA programming. It is recommended that the cluster allocates a minimum of 20 GPU hours per person throughout the course duration. This allocation ensures sufficient time for code development, testing, and running computationally intensive workloads. A minimum of 16 GB GPU memory is recommended to handle large datasets and complex computations efficiently.

Credit

Don't forget to check out additional **course materials** from XXX. Please **contact us** if you want to reuse these course materials in your teaching. You can also join the **XXX channel** to share your experience and get more help from the community.