

Introduction to Data Analysis and Machine Learning in Physics:

1. Introduction to python

Day 1: 6. April 2021

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Outline of the 1st day

- ▶ Technical instructions for your interactions with the CIP pool, like
 - ▶ using the jupyter hub
 - ▶ using python locally in your own linux environment (anaconda)
 - ▶ access the CIP pool from your own windows or linux system
 - ▶ transfer data from and to the CIP pool

Can be found in [CIPpoolAccess.PDF](#)

- ▶ Summary of NumPy
- ▶ Plotting with matplotlib
- ▶ Input / output of data
- ▶ Summary of pandas
- ▶ Fitting with iminuit and pyROOT

A glimpse into python classes

The following python classes are important to data analysis and machine learning will be used during the course

- ▶ **NumPy** - python library adding support for large, multi-dimensional arrays and matrices, along with high-level mathematical functions to operate on these arrays
- ▶ **matplotlib** - a python plotting library
- ▶ **SciPy** - extension of NumPy by a collection of mathematical algorithms for minimization, regression, fourier transformation, linear algebra and image processing
- ▶ **iminuit** - python wrapper to the data fitting toolkit **Minuit2** developed at CERN by F. James in the 1970ies
- ▶ **pyROOT** - python wrapper to the C++ data analysis toolkit ROOT used at the LHC
- ▶ **scikit-learn** - machine learning library written in python, which makes use extensively of NumPy for high-performance linear algebra algorithms

NumPy

NumPy (Numerical Python) is an open source Python library, which contains multidimensional array and matrix data structures and methods to efficiently operate on these. The core object is a homogeneous n-dimensional array object, `ndarray`, which allows for a wide variety of **fast operations and mathematical calculations with arrays and matrices** due to the extensive usage of compiled code.

- ▶ It is heavily used in numerous scientific python packages
- ▶ `ndarray` 's have a fixed size at creation → changing size leads to recreation
- ▶ Array elements are all required to be of the same data type
- ▶ Facilitates advanced mathematical operations on large datasets
- ▶ See for a summary, e.g.

<https://cs231n.github.io/python-numpy-tutorial/#numpy>

```
c = []  
for i in range(len(a)):  
    c.append(a[i]*b[i])
```

with NumPy
`c = a * b`

NumPy - array basics

- ▶ numpy arrays build a grid of **same type** values, which are indexed. The *rank* is the dimension of the array. There are methods to create and preset arrays.

```
myA = np.array([2, 5 , 11])           # create rank 1 array (vector like)
type(myA)                             # <class 'numpy.ndarray'>
myA.shape                              # (3,)
print(myA[2])                          # 11    access 3. element
myA[0] = 12                            # set 1. element to 12
myB = np.array([[1,5],[7,9]])         # create rank 2 array
myB.shape                              # (2,2)
print(myB[0,0],myB[0,1],myB[1,1])     # 1 5 9
myC = np.arange(6)                    # create rank 1 set to 0 - 5
myC.reshape(2,3)                      # change rank to (2,3)

zero = np.zeros((2,5))                # 2 rows, 5 columns, set to 0
one = np.ones((2,2))                  # 2 rows, 2 columns, set to 1
five = np.full((2,2), 5)              # 2 rows, 2 columns, set to 5
e = np.eye(2)                         # create 2x2 identity matrix
```

NumPy - array indexing (1)

- ▶ select slices of a numpy array

```
a = np.array([[1,2,3,4],
              [5,6,7,8],
              [9,10,11,12]])      # 3 rows 4 columns array
b = a[:2, 1:3]                  # subarray of 2 rows and
    array([[2, 3],              # column 1 and 2
           [6, 7]])
```

- ▶ a slice of an array points into the same data, *modifying* changes the original array!

```
b[0, 0] = 77                    # b[0,0] and a[0,1] are 77

r1_row = a[1, :]                # get 2nd row -> rank 1
r1_row.shape                    # (4,)
r2_row = a[1:2, :]              # get 2nd row -> rank 2
r2_row.shape                    # (1,4)
a=np.array([[1,2],[3,4],[5,6]]) # set a , 3 rows 2 cols
d=a[[0, 1, 2], [0, 1, 1]]       # d contains [1 4 6]
e=a[[1, 2], [1, 1]]            # e contains [4 6]
np.array([a[0,0],a[1,1],a[2,0]]) # address elements explicitly
```

NumPy - array indexing (2)

- ▶ integer array indexing by setting an array of indices → selecting/changing elements

```
a = np.array([[1,2,3,4],
              [5,6,7,8],
              [9,10,11,12]])
# 3 rows 4 columns array

p_a = np.array([0,2,0])
# Create an array of indices
s = a[np.arange(3), p_a]
# number the rows, p_a points to cols
# s contains [1 7 9]
print (s)
a[np.arange(3),p_a] += 10
# add 10 to corresponding elements
x=np.array([[8,2],[7,4]])
# create 2x2 array
bool = (x > 5)
# bool : array of boolians
# [[True False]
#  [True False]]
print(x[x>5])
# select elements, prints [8 7]
```

- ▶ data type in numpy - create according to input numbers or set explicitly

```
x = np.array([1.1, 2.1])
# create float array
print(x.dtype)
# print float64
y=np.array([1.1,2.9],dtype=np.int64)
# create float array [1 2]
```

NumPy - functions

- ▶ math functions operate elementwise either as operator overload or as methods

```
x=np.array([[1,2],[3,4]],dtype=np.float64) # define 2x2 float array
y=np.array([[3,1],[5,1]],dtype=np.float64) # define 2x2 float array
s = x + y # elementwise sum
s = np.add(x,y)
s = np.subtract(x,y)
s = np.multiply(x,y) # no matrix multiplication!
s = np.divide(x,y)
s = np.sqrt(x), np.exp(x), ...
x @ y , or np.dot(x, y) # matrix product
np.sum(x, axis=0) # sum of each column
np.sum(x, axis=1) # sum of each row
xT = x.T # transpose of x
x = np.linspace(0,2*pi,100) # get equal spaced points in x

r = np.random.default_rng(seed=42) # constructor random number class
b = r.random((2,3)) # random 2x3 matrix
```


► broadcasting in numpy

The term broadcasting describes how numpy treats arrays with different shapes during arithmetic operations

- add a scalar b to a 1D array $a = [a_1, a_2, a_3]$ → expand b to $[b, b, b]$
- add a scalar b to a 2D [2,3] array $a = [[a_{11}, a_{12}, a_{13}], [a_{21}, a_{22}, a_{23}]]$ → expand b to $b = [[b, b, b], [b, b, b]]$ and add element wise
- add 1D array $b = [b_1, b_2, b_3]$ to a 2D [2,3] array $a = [[a_{11}, a_{12}, a_{13}], [a_{21}, a_{22}, a_{23}]]$ → 1D array is broadcast across each row of the 2D array $b = [[b_1, b_2, b_3], [b_1, b_2, b_3]]$ and added element wise

Arithmetic operations can only be performed when the shape of each dimension in the arrays are equal or one has the dimension size of 1. Look [here](#) for more details

```
# Add a vector to each row of a matrix
x = np.array([[1,2,3], [4,5,6]]) # x has shape (2, 3)
v = np.array([1,2,3])           # v has shape (3,)
x + v      # [[2 4 6]
           #  [5 7 9]]
```

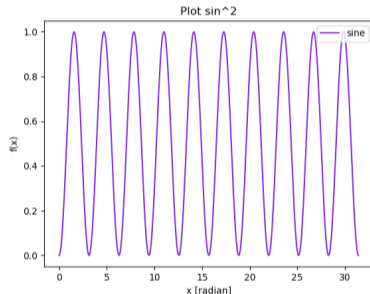
Plot data

A popular library to present data is the `pyplot` module of `matplotlib`.

- ▶ Drawing a function in one plot

```
import numpy as np
import matplotlib.pyplot as plt
# generate 100 points from 0 to 2 pi
x = np.linspace( 0, 10*np.pi, 100 )
f = np.sin(x)**2
# plot function
plt.plot(x,f, 'blueviolet', label='sine')
plt.xlabel('x [radian]')
plt.ylabel('f(x)')
plt.title('Plot sin^2')
plt.legend(loc='upper right')
plt.axis([0,30,-0.1,1.2]) # limit the plot range

# show the plot
plt.show()
```



► Drawing subplots in one canvas

```
...
g = np.exp(-0.2*x)
# create figure
plt.figure(num=2,figsize=(10.0,7.5),dpi=150,facecolor='lightgrey')
plt.suptitle('1 x 2 Plot')
# create subplot and plot first one
plt.subplot(1,2,1)
# plot first one
plt.title('exp(x)')
plt.xlabel('x')
plt.ylabel('g(x)')
plt.plot(x,g,'blueviolet')
# create subplot and plot second one
plt.subplot(1,2,2)
plt.plot(x,f,'orange')
plt.plot(x,f*g,'red')
plt.legend(['sine^2','exp*sine'])
# show the plot
plt.show()
```

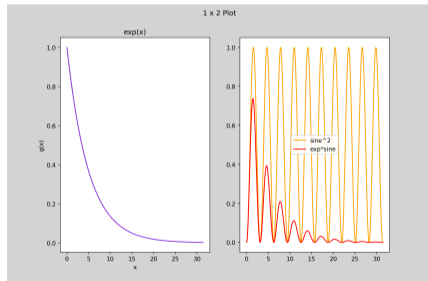


Image data

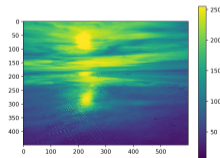
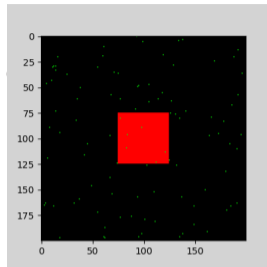
The `image` class of the `matplotlib` library can be used to load the image to numpy arrays and to render the image.

- ▶ There are 3 common formats for the numpy array
 - ▶ (M, N) scalar data used for greyscale images
 - ▶ (M, N, 3) for RGB images (each pixel has an array with RGB color attached)
 - ▶ (M, N, 4) for RGBA images (each pixel has an array with RGB color and transparency attached)

The method `imread` loads the image into an `ndarray`, which can be manipulated. The method `imshow` renders the image data

▶ Drawing pixel data and images

```
....  
# create data array with pixel position and RGB color  
width, height = 400, 400  
data = np.zeros((height, width, 3), dtype=np.uint8)  
# red patch in the center  
data[175:225, 175:225] = [255, 0, 0]  
x = np.random.randint(0,width-1,100)  
y = np.random.randint(0,height-1,100)  
data[x,y]= [0,255,0] # random green pixel  
plt.imshow(data)  
plt.show()  
....  
import matplotlib.image as mpimg  
#read image into numpy array  
pic = mpimg.imread('picture.jpg')  
mod_pic = pic[:, :, 0] # grab slice 0 of the colors  
plt.imshow(mod_pic) # use default color code also  
plt.colorbar() # try cmap='hot'  
plt.show()
```



Input / output

For the analysis of measured data efficient input / output plays an important role. In numpy, ndarrays can be saved and read in from files. `load()` and `save()` functions handle numpy binary files (`.npy` extension) which contain data, shape, dtype and other information required to reconstruct the ndarray of the disk file.

```
r = np.random.default_rng()           # instantiate random number generator
a = r.random((4,3))                   # random 4x3 array
np.save('myBinary.npy', a)           # write array a to binary file myBinary.npy
b = np.arange(12)
np.savez('myComp.npz', a=a, b=b)     # write a and b in compressed binary file
.....
b = np.load('myBinary.npy')          # read content of myBinary.npy into b
```

The storage and retrieval of array data in text file format is done with `savetxt()` and `loadtxt()` methods. Parameter controlling delimiter, line separators, file header and footer can be specified.

```
x = np.array([1,2,3,4,5,6,7])        # create ndarray
np.savetxt('myText.txt',x,fmt='%d')  # write array x to text file myText.txt
.....
```

Exercise 1

- i) Display a numpy array as figure of a blue cross. The size should be 200 by 200 pixel. Use as array format (M, N, 3), where the first 2 specify the pixel positions and the last 3 the rgb color from 0:255.
- ▶ Draw in addition a red square of arbitrary position into the figure.
 - ▶ Draw a circle in the center of the figure. Try to create a mask which selects the inner part of the circle using the indexing.

Solution: 01_intro_ex_1a_sol.py

- ii) Read data which contains pixels from the binary file horse.py into a numpy array. Display the data and the following transformations in 4 subplots: scaling and translation, compression in x and y, rotation and mirroring.

Solution: 01_intro_ex_1b_sol.py

Pandas

`pandas` is a software library written in Python for [data manipulation and analysis](#).

- Offers data structures and operations for manipulating numerical tables with integrated indexing
- Imports data from various file formats, e.g. comma-separated values, JSON, SQL or Excel
- Tools for reading and writing data structures, allows analyzing, filtering, splitting, merging and joining
- Built on top of NumPy
- Visualize the data with `matplotlib`
- Most machine learning tools support `pandas` → it is widely used to preprocess data sets for machine learning

Pandas micro introduction

Goal: Exploring, cleaning, transforming, and visualization of data. The basic indexable objects are

- Series -> vector (list) of data elements of arbitrary type
- DataFrame -> tabular arrangement of data elements of column wise arbitrary type

Both allow cleaning data by removing of empty or nan data entries

```
import numpy as np
import pandas as pd # use together with numpy
s = pd.Series([1, 3, 5, np.nan, 6, 8]) # create a Series of float64
r = pd.Series(np.random.randn(4)) # Series of random numbers float64
dates = pd.date_range("20130101", periods=3) # index according to dates
df = pd.DataFrame(np.random.randn(3,4), index=dates, columns=list("ABCD"))
print (df) # print the DataFrame
```

	A	B	C	D
2013-01-01	1.618395	1.210263	-1.276586	-0.775545
2013-01-02	0.676783	-0.754161	-1.148029	-0.244821
2013-01-03	-0.359081	0.296019	1.541571	0.235337

```
new_s = s.dropna() # return a new Data Frame with no empty cells
```

- pandas data can be saved in different file formats (CSV, JASON, html, XML, Excel, OpenDocument, HDF5 format,). NaN entries are kept in the output file.

- ▶ csv file

```
df.to_csv("myFile.csv") # Write the DataFrame df to a csv file
```

- ▶ HDF5 output

```
df.to_hdf("myFile.h5",key='df',mode='w') # Write the DataFrame df to HDF5  
s.to_hdf("myFile.h5", key='s',mode='a')
```

- ▶ Writing to an excel file

```
df.to_excel("myFile.xlsx", sheet_name="Sheet1")
```

- Deleting file with data in python

```
import os  
os.remove('myFile.h5')
```

■ read in data from various formats

▶ csv file

```
.....  
df = pd.read_csv('heart.csv') # read csv data table  
print(df.info())  
    <class 'pandas.core.frame.DataFrame'>  
    RangeIndex: 303 entries, 0 to 302  
    Data columns (total 14 columns):  
    #   Column      Non-Null Count  Dtype  
    ---  ---  
    0   age          303 non-null    int64  
    1   sex          303 non-null    int64  
    2   cp           303 non-null    int64  
    print(df.head(5))          # prints the first 5 rows of the data table  
    print(df.describe())      # shows a quick statistic summary of your data
```

▶ Reading an excel file

```
df = pd.read_excel("myFile.xlsx", "Sheet1", na_values=["NA"])
```

There are many options specifying details for IO.

■ Various functions exist to select and view data from pandas objects

- ▶ Display column and index

```
df.index                # show datetime index of df
DatetimeIndex(['2013-01-01', '2013-01-02', '2013-01-03'],
              dtype='datetime64[ns]', freq='D')

df.columns              # show columns info
Index(['A', 'B', 'C', 'D'], dtype='object')
```

- ▶ `DataFrame.to_numpy()` gives a NumPy representation of the underlying data

```
df.to_numpy()          # one dtype for the entire array, not per column!
[[-0.62660101 -0.67330526  0.23269168 -0.67403546]
 [-0.53033339  0.32872063 -0.09893568  0.44814084]
 [-0.60289996 -0.22352548 -0.43393248  0.47531456]]
```

Does not include the index or column labels in the output

- ▶ more on viewing

```
df.T                    # transpose the DataFrame df
df.sort_values(by="B")  # Sorting by values of a column of df
df.sort_index(axis=0, ascending=False) # Sorting by index descending values
df.sort_index(axis=0, ascending=False) # Display columns in inverse order
```

■ Selecting data of pandas objects → keep or reduce dimensions

- ▶ get a named column as a Series

```
df["A"]           # selects a column A from df, similar to df.A
df.iloc[:, 1:2]   # slices column A explicitly from df, df.loc[:, ["A"]]
```

- ▶ select rows of a DataFrame

```
df[0:2]           # selects row 0 and 1 from df,
df["20130102":"20130103"] # use indices endpoint are included!
df.iloc[3]        # Select with the position of the passed integers
df.iloc[1:3, :]   # selects row 1 and 2 from df
```

- ▶ select by label

```
df.loc["20130102":"20130103", ["C", "D"]] # selects row 1 and 2 and only C and D
df.loc[dates[0], "A"]                       # selects a single value (scalar)
```

- ▶ select by lists of integer position (as in NumPy)

```
df.iloc[[0, 2], [1, 3]] # select row 1 and 3 and col B and D
df.iloc[1, 1]           # get a value explicitly
```

- ▶ select according to expressions

```
df.query('B<C')           # select rows where B < C
df1=df[(df["B"]==0)&(df["D"]==0)] # conditions on rows
```

■ Selecting data of pandas objects continued

▶ Boolean indexing

```
df[df["A"] > 0]           # select df where all values of column A are >0
df[df > 0]                # select values from the entire DataFrame
```

more complex example

```
df2 = df.copy()          # copy df
df2["E"] = ["eight", "one", "four"] # add column E
df2[df2["E"].isin(["two", "four"])] # test if elements "two" and "four" are
                                     # contained in Series column E
```

▶ Operations (in general exclude missing data)

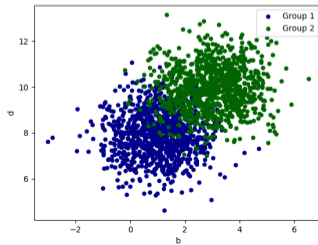
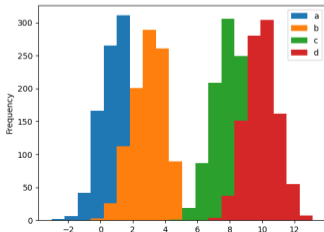
```
df2[df2 > 0] = -df2      # All elements > 0 change sign
df.mean(0)              # get column wise mean (numbers=axis)
df.mean(1)              # get row wise mean
df.std(0)               # standard deviation according to axis
df.cumsum()             # cumulative sum of each column
df.apply(np.sin)        # apply function to each element of df
df.apply(lambda x: x.max() - x.min()) # apply lambda function column wise
df + 10                 # add scalar 10
df - [1, 2, 10, 100]    # subtract values of each column
df.corr()               # Compute pairwise correlation of columns
```

Pandas - plotting data

Visualization is integrated in pandas using matplotlib. Here are only 2 examples

- ▶ Plot random data in histogram and scatter plot

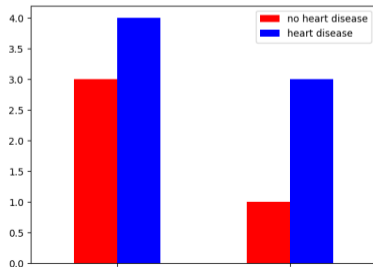
```
# create DataFrame with random normal distributed data
df = pd.DataFrame(np.random.randn(1000,4),columns=["a","b","c","d"])
df = df + [1, 3, 8, 10] # shift mean to 1, 3, 8, 10
plt.figure()
df.plot.hist(bins=20) # histogram all 4 columns
g1 = df.plot.scatter(x="a",y="c",color="DarkBlue",label="Group 1")
df.plot.scatter(x="b",y="d",color="DarkGreen",label="Group 2",ax=g1)
```



Pandas - plotting data

The function `crosstab()` takes one or more array-like objects as indexes or columns and constructs a new DataFrame of variable counts on the inputs

```
df = pd.DataFrame(                                # create DataFrame of 2 categories
    {"sex":    np.array([0,0,0,0,1,1,1,1,0,0,0]),
     "heart":  np.array([1,1,1,0,1,1,1,0,0,0,1])
    } )                                           # closing bracket goes on next line
pd.crosstab(df2.sex,df2.heart)                  # create cross table of possibilities
pd.crosstab(df2.sex,df2.heart).plot(kind="bar",color=['red','blue']) # plot counts
```



Exercise 2

Read the file `heart.csv` into a DataFrame. [Information on the dataset](#)

- Which columns do we have
- Print the first 3 rows
- Print the statistics summary and the correlations
- Print mean values for each column with and without disease
- Select the data according to sex and target (heart disease 0=no 1=yes).
- Plot the age distribution of male and female in one histogram
- Plot the heart disease distribution according to chest pain type cp
- Plot `thalach` according to target in one histogramm
- Plot sex and target in a histogramm figure
- Correlate age and max heart rate according to target
- Correlate age and cholesterol according to target

Solution: `01_intro_ex_2_sol.py`