Python Homework

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This pdf is generated from jupyter notebook because we have to submit the homework this way.
For convinence, you can find original jupyter notebook on my github here.

Numpy

[ ]:
```
import numpy as np
```

1. How to get common elements between two arrays?

[ ]:
```
a = np.array([1,2,3,2,3,4,3,4,5,6])
b = np.array([4,7,15,3,5,6,9,1,12,14])
```

[ ]:
```
np.intersect1d(a,b)
```

[ ]:
```
array([1, 3, 4, 5, 6])
```

2. How to remove from array a items that exist in array b?

[ ]:
```
# Definition of two arrays
a = np.array([1,3,5,7,9])
b = np.array([2,4,6,8,10])
```

[ ]:
```
# Solution
a[~np.isin(a,b)]
```

[ ]:
```
array([1, 3, 5, 7, 9])
```

3. Replace all even numbers in array 'a' with the new value '-2':

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

[ ]:
```
# Solution
a[a%2 == 0] = -2
a # Show the result
```

[ ]:
```
array([-2,  1, -2,  3, -2,  5, -2,  7, -2,  9])
```

4. Swap the last two rows of the following array:

[ ]:
```
a = np.arange(25).reshape(5,5)
```

[ ]:
```
#Solution
a[[-1,-2]] = a[[-2,-1]]
a # Show the result
```

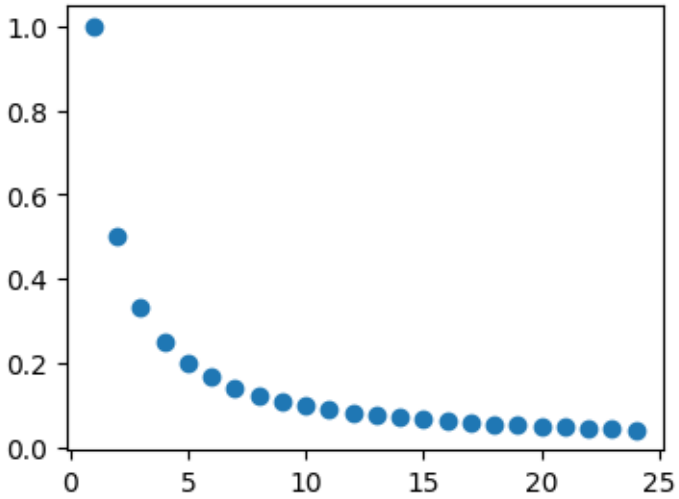
[ ]:
```
array([[ 0,  1,  2,  3,  4],
       [ 5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14],
       [20, 21, 22, 23, 24],
       [15, 16, 17, 18, 19]])
```

Matplotlib

5. Draw a scatter plot with the following data: s_x and s_y

[ ]:
```
s_x = range(1, 25)
s_y = [1 / x for x in s_x]
s_z = [1 / (25 - x) for x in s_x]
```

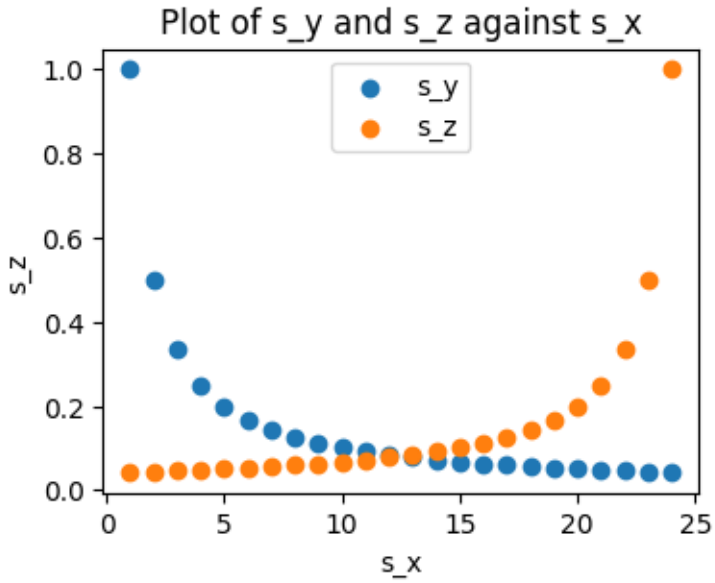
[ ]:
```
import matplotlib.pyplot as plt
fig, ax = plt.subplots()
ax.scatter(s_x,s_y, label="s_y");
```



1. Overlap in this plot the additional dataset s_z, and add a proper legend to the plot, axes labels and a title

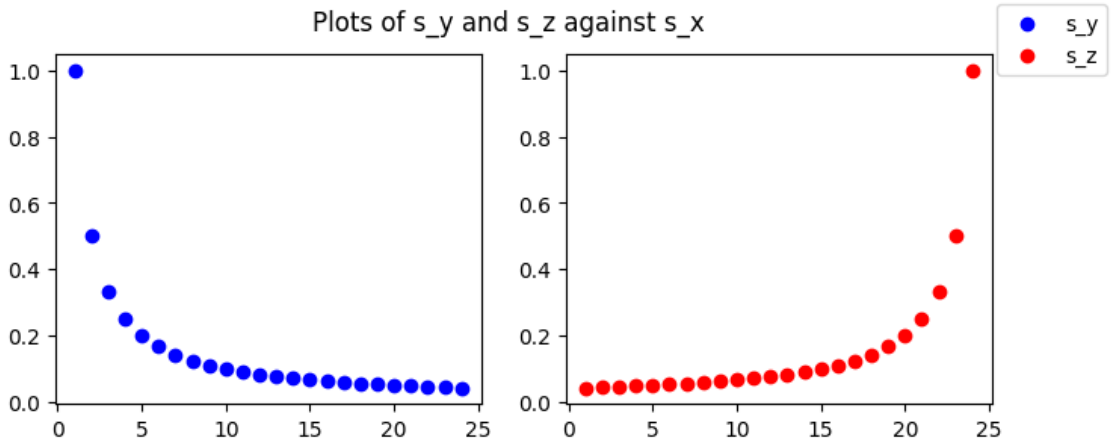
[ ]:
```
ax.scatter(s_x,s_z, label="s_z")
ax.set_title("Plot of s_y and s_z against s_x")
ax.set_xlabel("s_x")
ax.set_ylabel("s_z")
ax.legend()
fig # Show the figure again
```

[ ]:



2. Generate 2 subplots in a figure using datasets s_y and s_z, and add a proper legend to the plots and a title

[ ]:
```
fig, axes = plt.subplots(1,2,figsize=(8, 3))
axes[0].scatter(s_x,s_y,label="s_y", color='blue')
axes[1].scatter(s_x,s_z,label="s_z", color='red')
fig.suptitle("Plots of s_y and s_z against s_x")
fig.legend();
# If the labels for axes are necessary, it's possible to add like this:
#for ax, y_label in zip(axes,["s_y", "s_z"]):
#    ax.set_xlabel("s_x")
#    ax.set_ylabel(y_label)
```



Pandas

6. Prepare the plot "Root Mean Square Fluctuation vs Residue Number" (Potasium Ion Channel Kv1.2) by using the following input file 'rmsf.xvg'

- First we will load the data into dataframe object and print it

[ ]:
```
import pandas as pd
columns = ["Residue_Number", "RMSF"]
#Load data with numpy, as it supports multiple comment delimiters (unlike␣
 ↪pandas)
clean_data = np.loadtxt("rmsf.xvg",comments=["#","@"])
df = pd.DataFrame(clean_data,columns=columns).convert_dtypes()
df # Show the dataframe
```

[ ]:
```
      Residue_Number    RMSF
0                  1  0.3253
1                  2  0.2577
2                  3   0.233
3                  4  0.1791
4                  5  0.1793
…                  …       …
2843            2844  0.1707
2844            2845  0.1805
2845            2846  0.1921
2846            2847  0.1935
2847            2848  0.2433

[2848 rows x 2 columns]
```

- Let's see a random sample of 10 rows from the data

[ ]:
```
df.sample(10)
```

[ ]:

	Residue_Number	RMSF
1861	1862	0.29
1477	1478	0.1851
2682	2683	0.298
628	629	0.1212
2386	2387	0.3519
2306	2307	0.1064
138	139	0.1146
572	573	0.2476
837	838	0.1297
1756	1757	0.1528

- Now let's see the basic statistic of the data

[ ]:
```
df.describe()
```

[ ]:

	Residue_Number	RMSF
count	2848.0	2848.0
mean	1424.5	0.205974
std	822.291108	0.078368
min	1.0	0.0852
25%	712.75	0.147175
50%	1424.5	0.1878
75%	2136.25	0.246525
max	2848.0	0.6545

- Thanks to *convert_dtypes*( ) method, we can see that each column is represented by best possible datatype

[ ]:
```
df.dtypes
```

[ ]:
```
Residue_Number      Int64
RMSF              Float64
dtype: object
```

Let's create a new dataframe df2 and add a new column to that dataframe *RMSF_2*, where we store squares of *RMSF* column values

[ ]:
```
df2 = df.copy()
df2["RMSF_2"] = df2["RMSF"]**2
df2.to_parquet("RMSD_2")
df2 # Show the dataframe
```

[ ]:

	Residue_Number	RMSF	RMSF_2
0	1	0.3253	0.10582
1	2	0.2577	0.066409

```
2                    3   0.233  0.054289
3                    4  0.1791  0.032077
4                    5  0.1793  0.032148
…                  …      …        …
2843              2844  0.1707  0.029138
2844              2845  0.1805   0.03258
2845              2846  0.1921  0.036902
2846              2847  0.1935  0.037442
2847              2848  0.2433  0.059195

[2848 rows x 3 columns]
```

- Finally, let's plot the RMSF vs Residue_Number and save it as *jpeg* picture

[ ]:
```
ax = df.plot(x=columns[0],y=columns[1])
#Optinally we can set the y label
#ax.set_ylabel("nm")
ax.figure.savefig("RMSF_plot.jpeg")
```