

Lecture 02a:

Data Sampling and Pandas

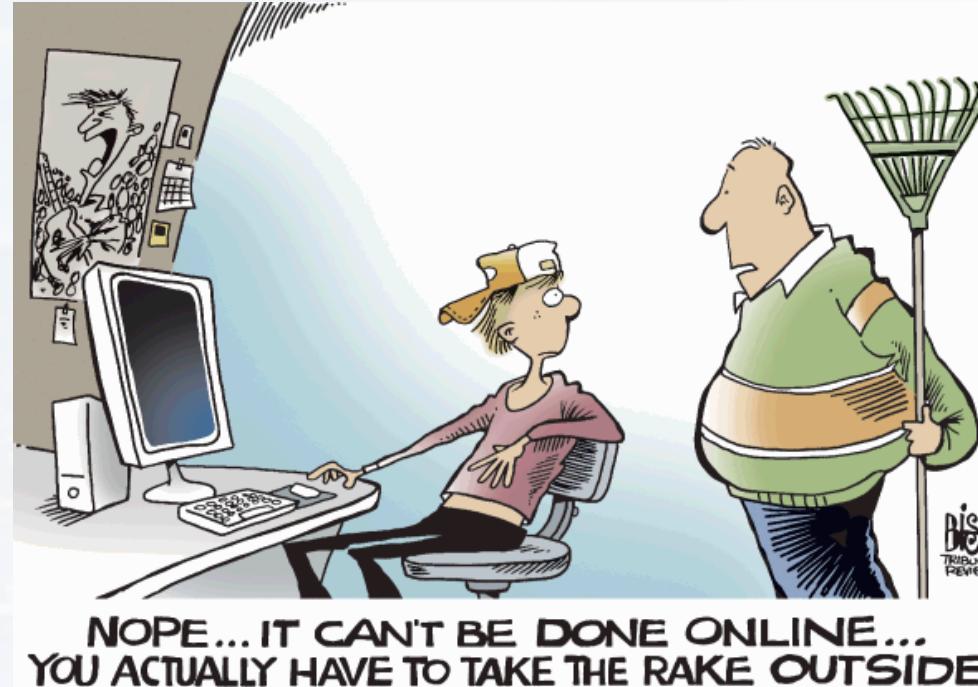


Markus Hohle

University California, Berkeley

Data Science for Scientific
Computing

MSSE 277A, 3 Units



Outline

Part I



Part I



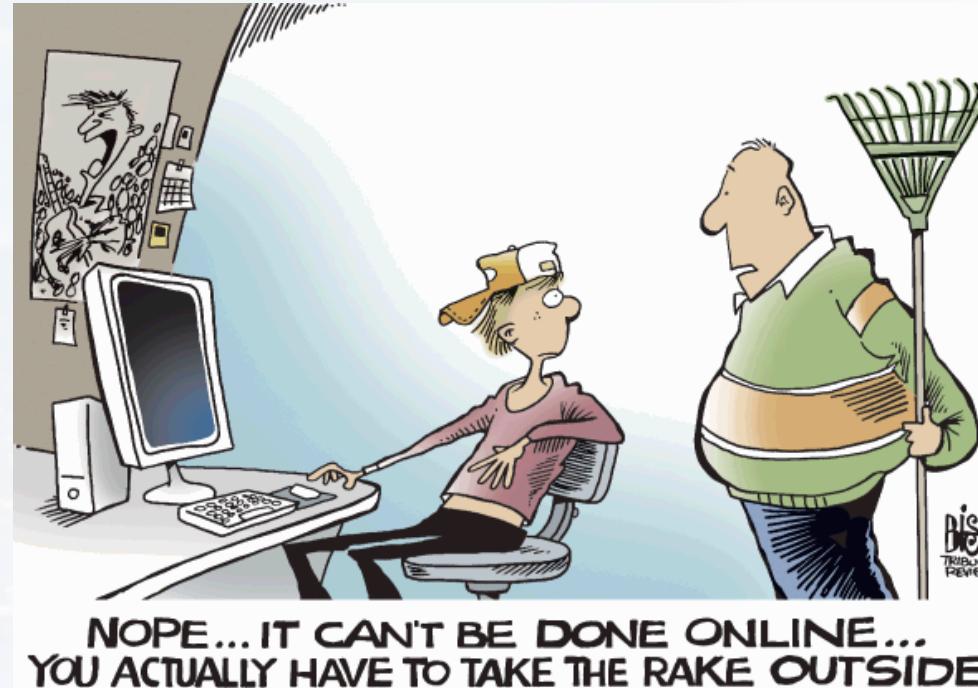
Outline

Reading/Writing Files

- Pandas and Data Frames
- Faster Alternatives
- More about .txt

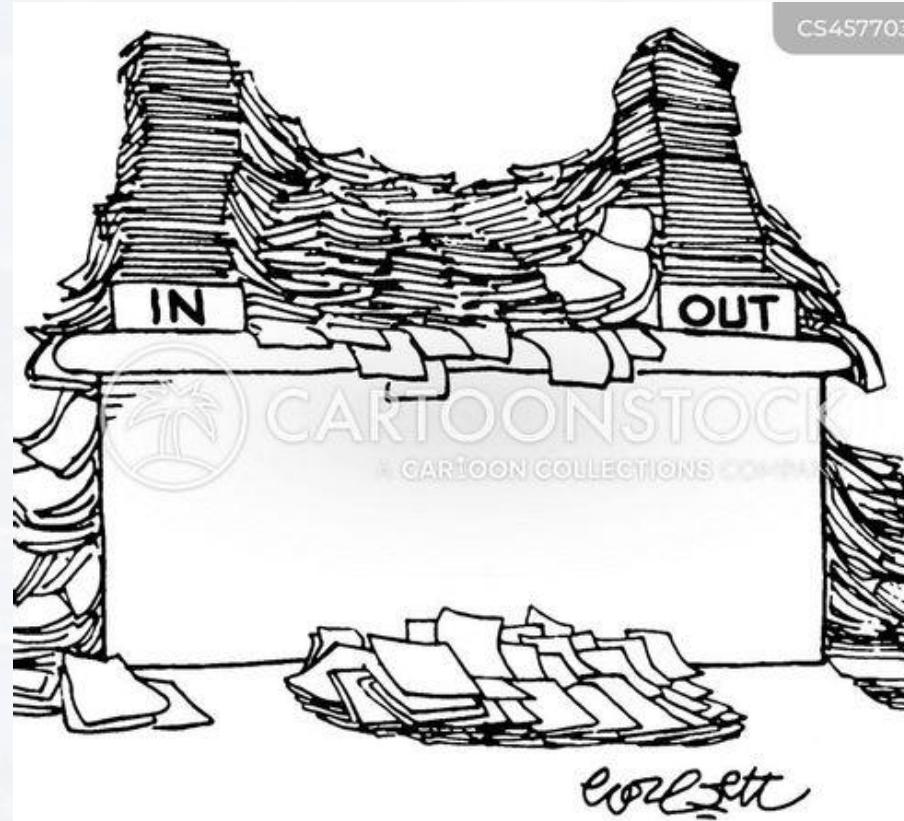
Visualization

- Matplotlib
- Seaborn
- plt, ax, fig



Outline

Part II



Outline

Standard Pandas

Line By Line

Chunks With Dask

PySpark



Outline

Reading/Writing Files

- Pandas and Data Frames
- Faster Alternatives
- More about .txt

Visualization

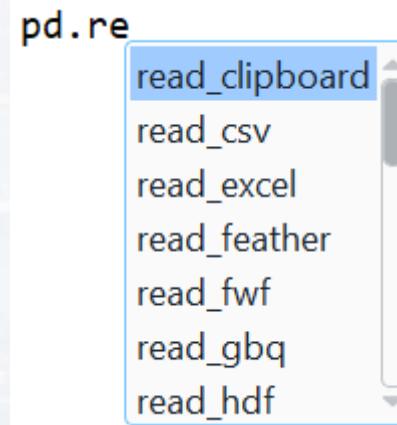
- Matplotlib
- Seaborn
- plt, ax, fig



most common file formats

plain text:	.dat .txt .fa
tables:	.csv .xls .xlsx
python:	.py .npy .pk1

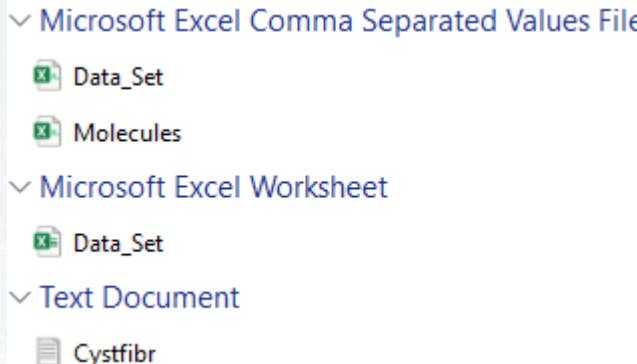
```
import pandas as pd
```





most common file formats

```
import pandas as pd
```



plain text:	.dat .txt .fa
tables:	.csv .xls .xlsx
python:	.py .npy .pkl

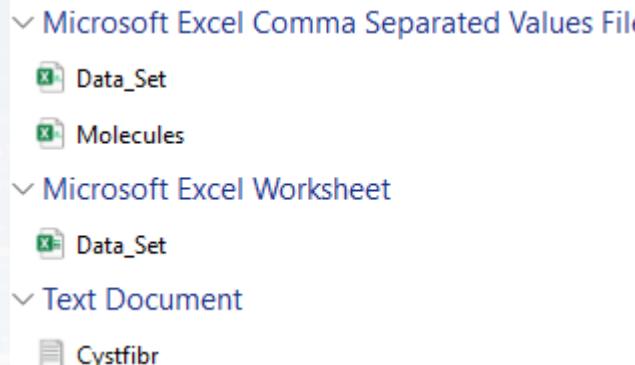
```
df = pd.read_excel()  
  
read_excel(io, sheet_name: 'str | int | list[IntStrT] |  
None'=0, *, header: 'int | Sequence[int]' |  
None'=0, names: 'SequenceNotStr[Hashable] | range'  
| None'=None, index_col: 'int | str |  
Sequence[int] | None'=None, usecols: 'int | str |  
Sequence[int] | Sequence[str] | Callable[[str],  
bool] | None'=None, dtype: 'DtypeArg' |  
None'=None, engine: 'Literal['xlrd', 'openpyxl',  
'odf', 'pyxlsb', 'calamine'] | None'=None,  
converters: 'dict[str, Callable] | dict[int,  
Callable] | None'=None, true_values:  
'Iterable[Hashable] | None'=None, false_values:  
'Iterable[Hashable] | None'=None, skiprows:  
'Sequence[int] | int | Callable[[int], object]' |  
None'=None, nrows: 'int | None'=None,  
na_values=None, keep_default_na: 'bool'=True,  
na_filter: 'bool'=True, verbose: 'bool'=False,  
parse_dates: 'list | dict | bool'=False,  
date_parser: 'Callable' |  
lib.NoDefault'=, date_format:  
'dict[Hashable, str] | str | None'=None,  
thousands: 'str | None'=None, decimal: 'str'='.',  
comment: 'str | None'=None, skipfooter: 'int'=0,  
storage_options: 'StorageOptions | None'=None,  
dtype_backend: 'DtypeBackend' |  
lib.NoDefault'=, engine_kwargs: 'dict  
| None'=None)  
  
Read an Excel file into a ``pandas`` ``DataFrame``.  
  
Supports ``xls``, ``xlsx``, ``xlsm``, ``xlsb``, ``odf``, ``ods``  
and ``odt`` file extensions read from a local  
sheets.  
Parameters  
-----  
io : str, bytes, ExcelFile, xlrd.Book, path object, or file- ...
```

Pandas &
Data Frames

most common file formats

plain text:	.dat .txt .fa
tables:	.csv .xls .xlsx
python:	.py .npy .pkl

```
import pandas as pd
```



```
df = pd.read_csv('Molecules.csv')
```

Name	Type	Value
df	DataFrame	Column names: molecular_weight, electronegativity, bond_lengths, num_h ...



```
import pandas as pd  
  
df = pd.read_csv('Molecules.csv')
```

Name	Type	Size	Value
df	DataFrame	(200, 6)	Column names: molecular_weight, electronegativity, bond_lengths, num_h ...

df - DataFrame

Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	341.704	2.65585	3.09407	2	9.11147	Toxic
1	335.951	3.22262	2.89039	7	8.92848	Toxic
2	235.203	2.44115	2.48203	1	6.49731	Toxic
3	246.505	2.76656	2.71547	7	7.45089	Toxic
4	437.939	3.4801	3.59569	3	10.9156	Toxic
5	336.453	2.81474	3.11	9	8.55696	Toxic
6	372.542	3.17969	3.3866	8	9.48685	Toxic
7	349.19	3.1814	3.19359	7	9.10357	Toxic
8	399.353	3.02359	3.50278	4	9.8421	Toxic



```
import pandas as pd

df = pd.read_csv('Molecules.csv')

df.head()
```

Name	Type	Size	Value
df	DataFrame	(200, 6)	Column names: molecular_weight, electronegativity, bond_lengths, num_h ...

```
In [3]: df.head()
Out[3]:
   molecular_weight  electronegativity  ...      logP  label
0        341.704142          2.655846  ...    9.111473  Toxic
1        335.950798          3.222621  ...    8.928483  Toxic
2        235.203185          2.441153  ...    6.497307  Toxic
3        246.504930          2.766560  ...    7.450888  Toxic
4        437.938926          3.480105  ...   10.915629  Toxic
```

fully equivalent for excel files:

```
df = pd.read_excel('Molecules.xlsx')
```



a data frame has numerous functions

df.head () shows header

```
molecular_weight  electronegativity ...      logP  label
0            341.704142          2.655846 ...    9.111473  Toxic
1            335.950798          3.222621 ...    8.928483  Toxic
2            235.203185          2.441153 ...    6.497307  Toxic
```

df.index returns rows

```
df.index
RangeIndex(start=0, stop=200, step=1)
```

df.columns returns columns

```
Index(['molecular_weight', 'electronegativity', 'bond_lengths',
       'num_hydrogen_bonds', 'logP', 'label'],
      dtype='object')
```



a data frame has numerous functions

df.columns returns columns

```
Index(['molecular_weight', 'electronegativity', 'bond_lengths',
       'num_hydrogen_bonds', 'logP', 'label'],
      dtype='object')
```

df.corr() returns Pearson's correlation coefficient

columns 0 to 4 contain float/int

Corr = df[df.columns[:-1]].corr()

Index	molecular_weight	electronegativity	bond_lengths	um_hydrogen_bond	logP
molecular_weight	1	0.0280505	0.953066	0.0157675	0.969772
electronegativity	0.0280505	1	0.0343733	-0.0526109	0.00634745
bond_lengths	0.953066	0.0343733	1	0.0258849	0.926063
num_hydrogen_bonds	0.0157675	-0.0526109	0.0258849	1	0.0104456
logP	0.969772	0.00634745	0.926063	0.0104456	1



a data frame has numerous functions

```
df[['logP', 'label']]
```

returns **data frame of selected columns**

```
      logP    label
0    9.111473  Toxic
1    8.928483  Toxic
2    6.497307  Toxic
3    7.450888  Toxic
4   10.915629  Toxic
...
195  8.794466 Non-Toxic
196  9.651463  Toxic
197  7.651613 Non-Toxic
198  9.060061  Toxic
```

```
df.loc[[1, 5]]
```

returns **data frame of selected rows**

```
      molecular_weight  electronegativity ...      logP    label
1            335.950798           3.222621 ...  8.928483  Toxic
5            336.453422           2.814735 ...  8.556958  Toxic
```



a data frame has numerous functions

Try out the following commands!

```
df.iloc[4:6, 5:9]
```

slicing **data frame** using **iloc**

```
df.iloc[4,5] = 999
```

manipulating individual entries

```
df.insert(2, 'New', df.iloc[:,1])
```

inserting another column called *New*

```
df.rename(index = {1: 'bbb'})
```

changing name of row **1**

```
df.rename(columns = {'Label': 'Toxic or Not'})
```

changing column name



```
import pandas as pd  
  
df = pd.read_csv('Molecules.csv')
```

finally, saving the data frame to an excel file

```
df.t  
tail  
take  
to_clipboard  
to_csv  
to_dict  
to_excel  
to_feather
```

```
df.to_excel('Molecules.xlsx')
```

Name	Date Modified
Cystfibr.txt	11/09/2024 04:24
Data_Set.csv	07/12/2023 20:16
Data_Set.xlsx	05/12/2023 20:04
Molecules.csv	05/09/2024 20:30
Molecules.xlsx	06/03/2025 21:30

▼ Microsoft Excel Comma Separated Values File
Data_Set
Molecules
▼ Microsoft Excel Worksheet
Data_Set
Molecules



pandas can also read **text files**:

```
cf = pd.read_csv('cystfibr.txt')
```



cf - DataFrame

Index	age	sex	height	weight	bmp	fev1	rv	frc	tlc	pemax
0	7	0	109	13.1	68	32	258	183	137	95
1	7	1	112	12.9	65	19	449	245	134	85
2	8	0	124	14.1	64	22	441	268	147	100

```
cf = pd.read_csv('cystfibr.txt', sep = '\s+')
```

cf - DataFrame

Index	age	sex	height	weight	bmp	fev1	rv	frc	tlc	pemax
0	7	0	109	13.1	68	32	258	183	137	95
1	7	1	112	12.9	65	19	449	245	134	85
2	8	0	124	14.1	64	22	441	268	147	100
3	8	1	125	16.2	67	41	234	146	124	85



note: data frames are

- very **user friendly** and
- have many **useful functions**

but:

- they are **slow** when working with bigger data sets
- and for any computational operation

therefore:

- **don't use data frames** for the **data analysis** part!
- use **numpy** arrays instead!
- pandas data frames are more like a **nice summary for the user**





Outline

Reading/Writing Files

- Pandas and Data Frames
- Faster Alternatives
- More about .txt

Visualization

- Matplotlib
- Seaborn
- plt, ax, fig



Faster
Alternatives

pandas is the standard library, but it is slow

reading a 130MB **excel file**:

```
import pandas as pd
import time
```

```
t1 = time.monotonic()
```

83 seconds

```
df = pd.read_excel('Data_Set.xlsx')
```

```
t2 = time.monotonic()
```

```
dt = t2 - t1
```

```
print("Total runtime: " + str(dt) + ' seconds')
```



Faster
Alternatives

pandas is the standard library, but it is slow

reading a 180MB **csv file** with the **same content**:

```
import pandas as pd
import time

t1 = time.monotonic()

df = pd.read_csv('Data_Set.csv')

t2 = time.monotonic()
dt = t2 - t1

print("Total runtime: " + str(dt) + ' seconds')
```

1.2 seconds!



Faster Alternatives

pandas:

excel file:	83.0 sec
csv file:	1.2 sec

reading a 180MB **txt file** with the **same content**:

```
import pandas as pd
import time
```

```
t1 = time.monotonic()

df = pd.read_csv('Data_Set.txt')

t2 = time.monotonic()
dt = t2 - t1

print("Total runtime: " + str(dt) + ' seconds')
```

1.5 seconds!



Faster Alternatives

pandas:

excel file:	83.0 sec
csv file:	1.2 sec
txt file:	1.5 sec



faster than pandas,
but fewer functions

dask

polars

fireducks



FireDucks



Faster
Alternatives

pandas:

excel file:	83.0 sec
csv file:	1.2 sec
txt file:	1.5 sec

```
pip install dask  
pip install polars  
pip install xlsx2csv #for excel API  
pip install fastexcel
```



```
import dask.dataframe as dd
```



Faster
Alternatives



```
import dask.dataframe as dd
```

```
t1 = time.monotonic()
```

```
df = dd.read_csv('Data_Set.csv')
```

```
t2 = time.monotonic()
```

```
dt = t2 - t1
```

0.016 seconds!

```
print("Total runtime: " + str(dt) + ' seconds')
```

```
df = pd.DataFrame(df)
```

However, we might need to
transform the output

pandas:

excel file:	83.0 sec
csv file:	1.2 sec
txt file:	1.5 sec



Faster
Alternatives



dask

```
import dask.dataframe as dd\n\n    t1 = time.monotonic()\n\n    df = pd.DataFrame(dd.read_csv('Data_Set.csv'))\n\n    t2 = time.monotonic()\n    dt = t2 - t1\n\n    print("Total runtime: " + str(dt) + ' seconds')
```

pandas:

excel file:	83.0 sec
csv file:	1.2 sec
txt file:	1.5 sec

1.7 seconds!

As of Dec 2025, dask **doesn't have an excel API**



Faster
Alternatives



```
import polars as pl
```

```
t1 = time.monotonic()  
  
df = pl.read_excel('Data_Set.xlsx')
```

```
t2 = time.monotonic()  
dt = t2 - t1
```

8.2 seconds!

```
print("Total runtime: " + str(dt) + ' seconds')
```

```
df = pd.DataFrame(df)
```

However, we might need to
transform the output

pandas:

excel file:	83.0	sec
csv file:	1.2	sec
txt file:	1.5	sec

dask

csv file:	0.016 sec
to df	1.7 sec



Faster
Alternatives



```
import polars as pl
```

```
t1 = time.monotonic()
```

```
df = pd.DataFrame(pl.read_excel('Data_Set.xlsx'))
```

```
t2 = time.monotonic()
```

```
dt = t2 - t1
```

10.2 seconds!

```
print("Total runtime: " + str(dt) + ' seconds')
```

pandas:

excel file:	83.0	sec
csv file:	1.2	sec
txt file:	1.5	sec

dask

csv file:	0.016 sec
to df	1.7 sec



Faster
Alternatives



```
import polars as pl

t1 = time.monotonic()

df = pl.read_csv('Data_Set.csv')

t2 = time.monotonic()
dt = t2 - t1

print("Total runtime: " + str(dt) + ' seconds')
```

pandas:

	excel file:	83.0	sec
	csv file:	1.2	sec
	txt file:	1.5	sec

dask

	csv file:	0.016	sec
	to df	1.7	sec

polars

	excel file	8.2	sec
	to df	10.2	sec

0.27 seconds!



Faster
Alternatives



```
import polars as pl

t1 = time.monotonic()

df = pd.DataFrame(pl.read_csv('Data_Set.csv'))
```

```
t2 = time.monotonic()
dt = t2 - t1
```

```
print("Total runtime: " + str(dt) + ' seconds')
```

pandas:

	excel file:	83.0	sec
	csv file:	1.2	sec
	txt file:	1.5	sec

dask

	csv file:	0.016	sec
	to df	1.7	sec

polars

	excel file	8.2	sec
	to df	10.2	sec

0.20 seconds!



Faster
Alternatives

pandas



dask

polars

.xlsx

83 sec

na

8.2 sec

10.2 sec

.csv

1.2 sec

0.016 sec

1.6 sec

0.27 sec

0.20 sec

.txt

1.5 sec

0.016 sec

0.92 sec

0.25 sec

0.23 sec



Faster
Alternatives



.xlsx

83 sec

na

8.2 sec
10.2 sec

.csv

1.2 sec

0.016 sec
1.6 sec

0.27 sec
0.20 sec

.txt

1.5 sec

0.016 sec
0.92 sec

0.25 sec
0.23 sec

check out Benchmark_Pandas_Dask_Polars.py



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- Pandas and Data Frames
- Faster Alternatives
- More about .txt

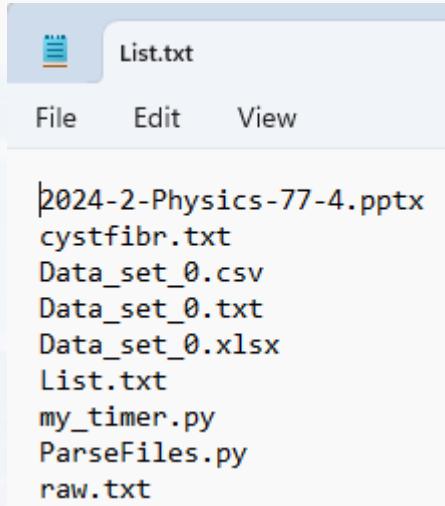
Visualization

- Matplotlib
- Seaborn
- plt, ax, fig



More about
.txt

sometimes txt files don't come in a nice format



→ using `open`

```
with open('List.txt', errors = "ignore") as f:  
    text = f.read()
```

Text editor - text

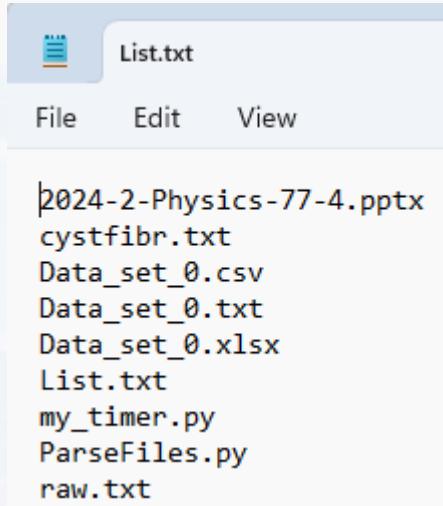
```
2024-2-Physics-77-4.pptx  
cystfibr.txt  
Data_set_0.csv  
Data_set_0.txt  
Data_set_0.xlsx  
List.txt  
my_timer.py  
ParseFiles.py  
raw.txt
```

reads file line by line and stops automatically when has reached the end

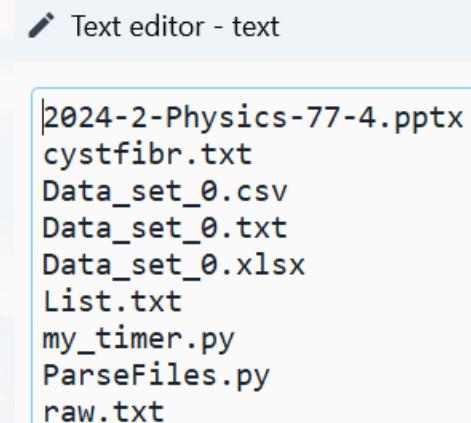


More about
.txt

sometimes txt files don't come in a nice format



```
with open('List.txt', errors = "ignore") as f:  
    text = f.read()
```



```
T = list(text.split())
```

Index ▲	Type	Size	
0	str	24	2024-2-Physics-77-4.pptx
1	str	12	cystfibr.txt
2	str	14	Data_set_0.csv
3	str	14	Data_set_0.txt
4	str	15	Data_set_0.xlsx
5	str	8	List.txt
6	str	11	my_timer.py



More about

.txt

syntax of `open`

```
with open('my_file.txt', flags, errors = "ignore") as f:
```

```
    text = f.read()
```

finishes once it has reached the end
and closes *f*

flags/modes:

- '*r*' opens file for reading only.
- '*w*' opens file for writing. If the file exists, it overwrites it, otherwise, it creates a new file.
- '*a*' opens file for appending only. If the file doesn't exist, it creates the file.
- '*x*' creates new file. If the file exists, it fails.
- '*+*' opens file for updating
- '*t*' opens file in text mode (default)
- '*b*' opens file in binary mode

flags can be combined like, eg '*wb*'

`with` opens a loop for reading the file line by line



More about
.txt

syntax of `open`

```
with open('List.txt', 'r') as read_f:  
    with open('List_copy.txt', 'w') as write_f:  
        for r in read_f:  
            write_f.write(r)
```

opens file line by line

opens new file line by line
for writing

writes each line to new file

In [5]: `print(r)`
`raw.txt`

In [6]: `print(type(r))`
`<class 'str'>`



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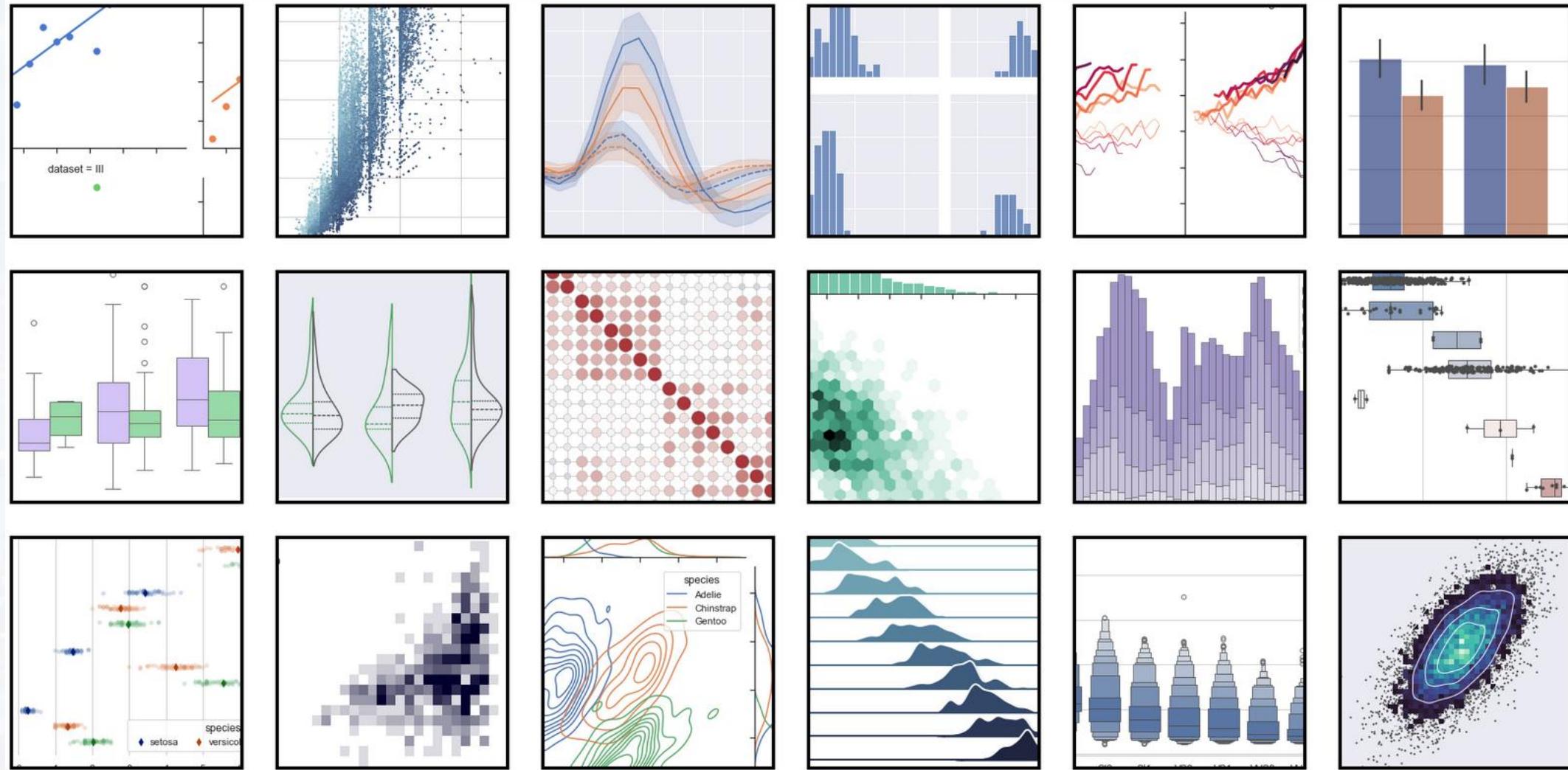
Data Sampling and Pandas:

Data Sampling and Pandas

matplotlib

Python Graph Gallery

<https://seaborn.pydata.org/examples/index.html>





matplotlib

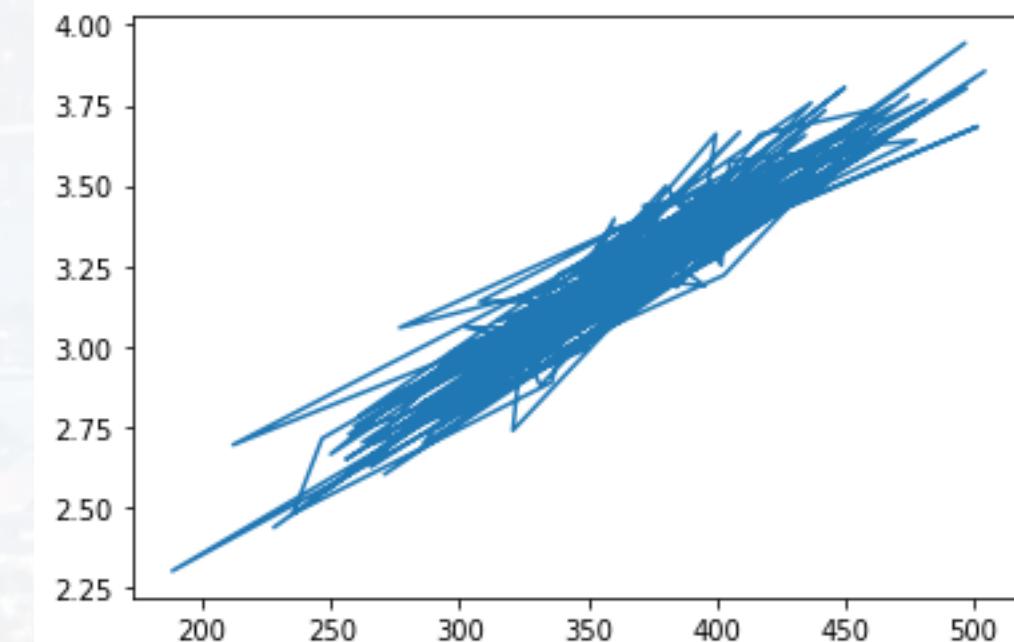
```
import pandas as pd
import matplotlib.pyplot as plt

Data = pd.read_csv('Molecules.csv')

x      = Data.molecular_weight
y      = Data.bond_lengths

plt.plot(x,y)
```

basic plots
arguments
settings





matplotlib

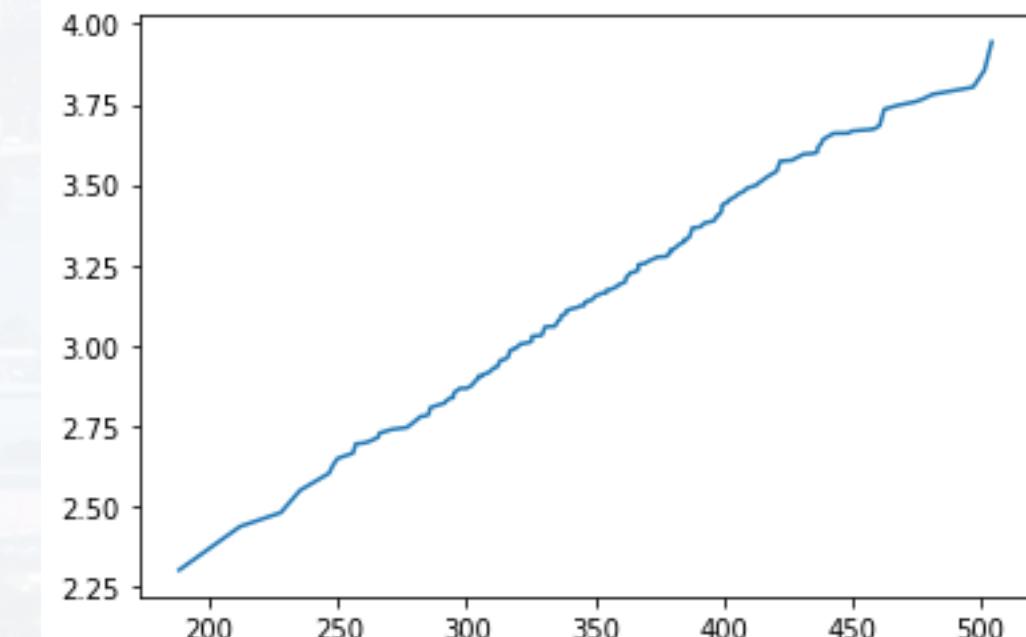
```
import pandas as pd  
import matplotlib.pyplot as plt
```

```
Data = pd.read_csv('Molecules.csv')
```

```
x      = Data.molecular_weight  
y      = Data.bond_lengths
```

```
plt.plot(sorted(x), sorted(y))
```

basic plots
arguments
settings





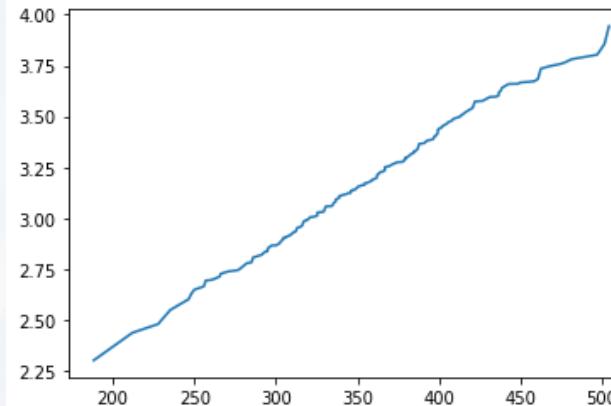
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Data Sampling and Pandas:

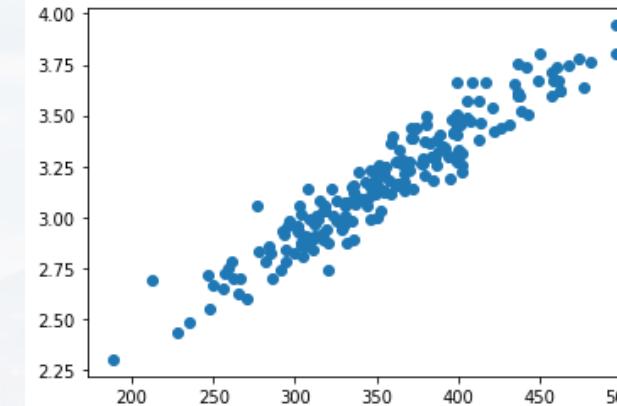
Data Sampling and Pandas

matplotlib

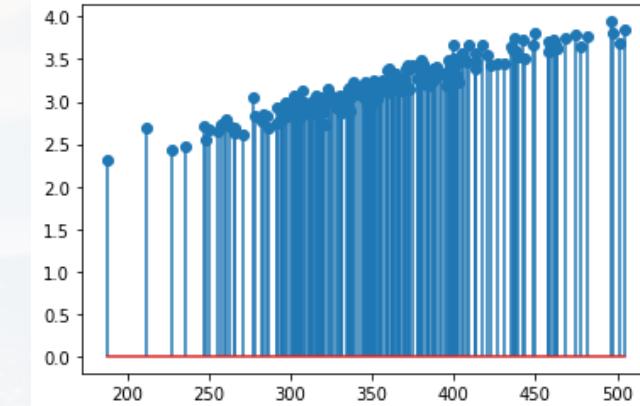
```
plt.plot(sorted(x),  
         sorted(y))
```



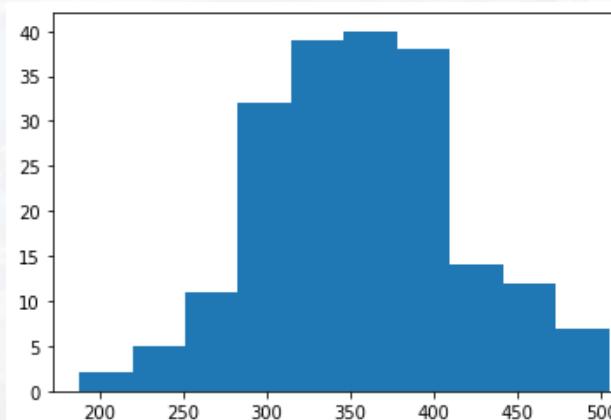
```
plt.scatter(x, y)
```



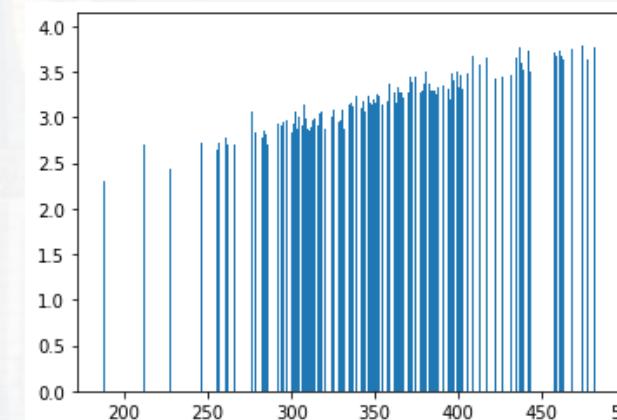
```
plt.stem(x, y)
```



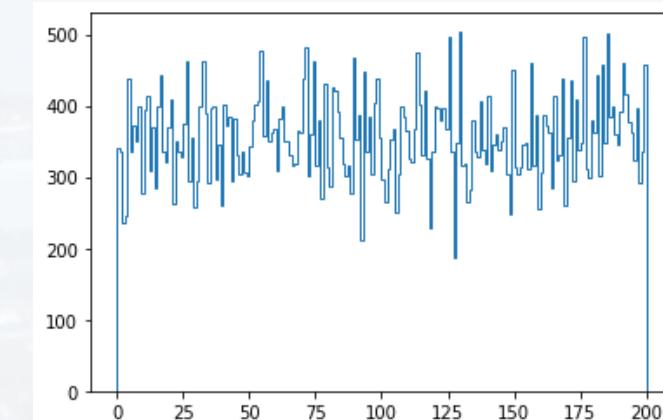
```
plt.hist(x)
```



```
plt.bar(x, y)
```



```
plt.stairs(x)
```



basic plots
arguments
settings



matplotlib

```
plt.scatter(
```

```
    scatter(x: 'float | ArrayLike', y: 'float | ArrayLike', s:
            'float | ArrayLike | None' = None, c: 'ArrayLike |
            Sequence[ColorType] | ColorType | None' = None,
            marker: 'MarkerType | None' = None, cmap: 'str |
            Colormap | None' = None, norm: 'str | Normalize |
            None' = None, vmin: 'float | None' = None, vmax:
            'float | None' = None, alpha: 'float | None' = None,
            linewidths: 'float | Sequence[float] | None' = None,
            *, edgecolors: "Literal['face', 'none'] | ColorType |
            Sequence[ColorType] | None" = None, plotnonfinite:
            'bool' = False, data=None, **kwargs,)
```

A scatter plot of *y* vs. *x* with varying marker size and/or color.

Parameters

x, y : float or array-like, shape (n,)

The data positions. ...

basic plots

arguments

settings



matplotlib

```
plt.scatter(x, y,  
            marker = 'p',  
            s = 135,  
            color = [0.5, 0.1, 0.1],  
            edgecolor = 'black',  
            alpha = 0.3)
```

marker style: str

basic plots
arguments
settings

marker	symbol	description			
"."	●	point	"+"	+	plus
"_"	.	pixel	"x"	×	x
"o"	●	circle	"D"	◆	diamond
"v"	▼	triangle_down	"d"	◆	thin_diamond
"^"	▲	triangle_up	" "		vline
"<"	◀	triangle_left	"_"	—	hline
">"	▶	triangle_right	0 (TICKLEFT)	—	tickleft
"1"	▼	tri_down	1 (TICKRIGHT)	—	tickright
"2"	▲	tri_up	2 (TICKUP)		pickup
"3"	◀	tri_left	3 (TICKDOWN)		tickdown
"4"	▶	tri_right	4 (CARETLEFT)	◀	caretleft
"8"	●	octagon	5 (CARETRIGHT)	▶	caretright
"s"	■	square	6 (CARETUP)	▲	caretup
"p"	◆	pentagon	7 (CARETDOWN)	▼	caretdown
"P"	◆	plus (filled)	8 (CARETLEFTBASE)	◀	caretleft (centered at base)
"*"	★	star	9 (CARETRIGHTBASE)	▶	caretright (centered at base)
"h"	⬢	hexagon1	10 (CARETUPBASE)	▲	caretup (centered at base)
"H"	⬢	hexagon2	11	▼	caretdown (centered at base)



matplotlib

```
plt.scatter(x, y,  
            marker = 'p',  
            s = 135,  
            color = [0.5, 0.1, 0.1],  
            edgecolor = 'black',  
            alpha = 0.3)
```

basic plots
arguments
settings

marker size in
pixel: int



matplotlib

```
plt.scatter(x, y,  
            marker = 'p',  
            s = 135,  
            color = [0.5, 0.1, 0.1],  
            edgecolor = 'black',  
            alpha = 0.3)
```

basic plots
arguments
settings

color:

array RGB code if **three** values, RGB code plus alpha, if **four** values

str	full string:	'green' 'yellow'
	abbreviation:	'g' 'y'
	HEX code:	'#4b8333' '#fff8de'



matplotlib

```
plt.scatter(x, y,  
            marker = 'p',  
            s = 135,  
            color = [0.5, 0.1, 0.1],  
            edgecolor = 'black',  
            alpha = 0.3)
```

basic plots
arguments
settings

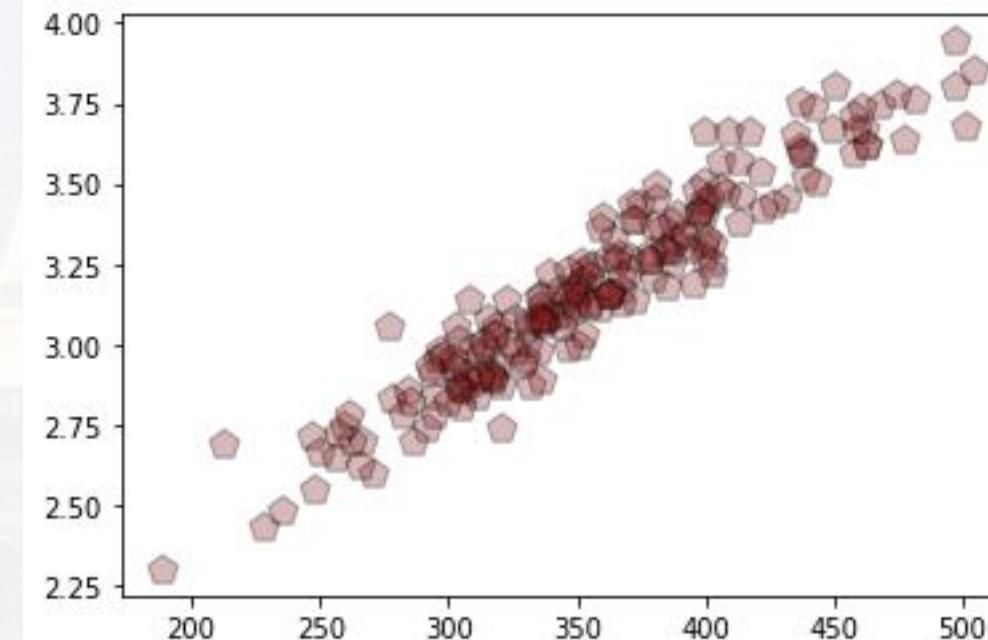
alpha (opaqueness-opacity): float



matplotlib

```
plt.scatter(x, y,  
            marker = 'p',  
            s = 135,  
            color = [0.5, 0.1, 0.1],  
            edgecolor = 'black',  
            alpha = 0.3)
```

basic plots
arguments
settings





matplotlib

```
plt.scatter(x, y, marker = 'p', s = 135, color = [0.5, 0.1, 0.1],  
            edgecolor = 'black', alpha = 0.3)
```

```
plt.xlabel(r'x values $\tau^{ij}_{def}$')  
plt.ylabel('y values')  
plt.title('first plot')  
plt.legend(['data'])  
plt.xscale('log')  
plt.savefig('new_plot.pdf')  
plt.show()
```

basic plots
arguments
settings

Python speaks LaTeX, but needs
raw string



matplotlib

```
plt.scatter(x, y, marker = 'p', s = 135, color = [0.5, 0.1, 0.1],  
            edgecolor = 'black', alpha = 0.3)
```

basic plots
arguments
settings

```
plt.xlabel(r'x values $\tau^{ij}_{\text{def}}$')  
plt.ylabel('y values')  
plt.title('first plot')  
plt.legend(['data'])  
plt.xscale('log')  
plt.savefig('new_plot.pdf')  
plt.show()
```

legend needs to be
a list



matplotlib

```
plt.scatter(x, y, marker = 'p', s = 135, color = [0.5, 0.1, 0.1],  
            edgecolor = 'black', alpha = 0.3)
```

basic plots
arguments
settings

```
plt.xlabel(r'x values $\tau^{ij}_{\text{def}}$')  
plt.ylabel('y values')  
plt.title('first plot')  
plt.legend(['data'])  
plt.xscale('log')  
plt.savefig('new_plot.pdf')  
plt.show()
```

plots can be saved
to any common
format



matplotlib

```
plt.scatter(x, y, marker = 'p', s = 135, color = [0.5, 0.1, 0.1],  
            edgecolor = 'black', alpha = 0.3)
```

basic plots
arguments
settings

```
plt.xlabel(r'x values $\tau^{ij}_{\text{def}}$')  
plt.ylabel('y values')  
plt.title('first plot')  
plt.legend(['data'])  
plt.xscale('log')  
plt.savefig('new_plot.pdf')  
plt.show()
```

sometimes plots don't show up
(depending on settings)
type plt.show()
at the **very end**



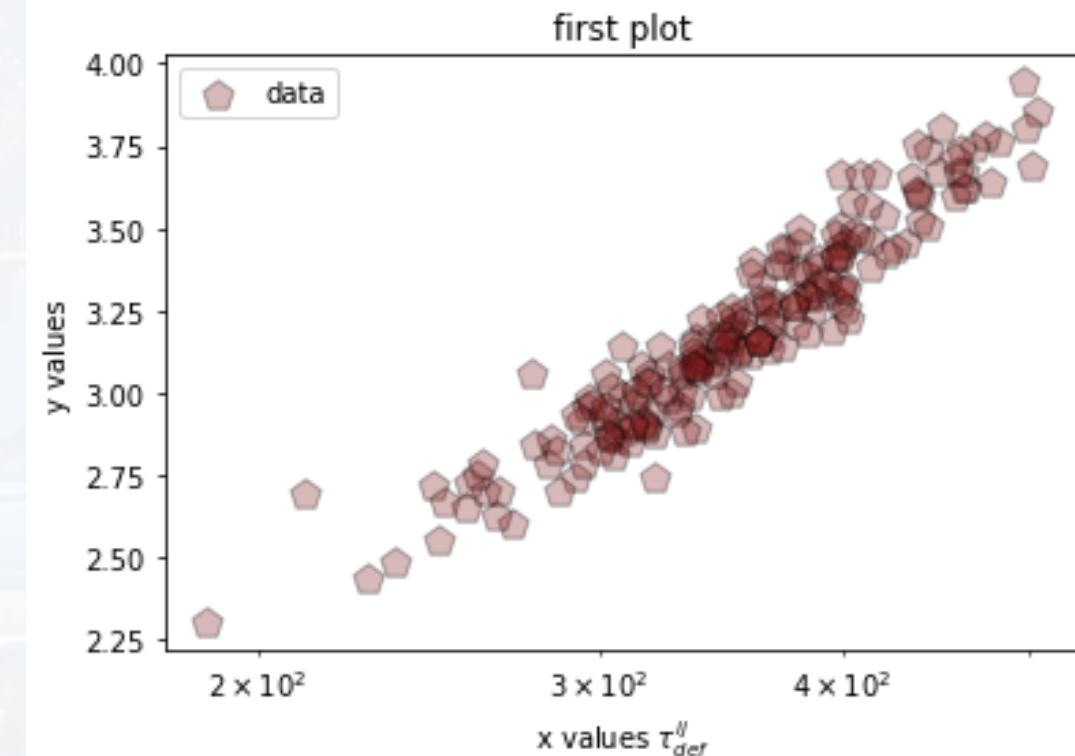
matplotlib

```
plt.scatter(x, y, marker = 'p', s = 135, color = [0.5, 0.1, 0.1],  
            edgecolor = 'black', alpha = 0.3)
```

basic plots
arguments
settings

```
plt.xlabel(r'x values $\tau^{ij}_{def}$')  
plt.ylabel('y values')  
plt.title('first plot')  
plt.legend(['data'])  
plt.xscale('log')  
plt.savefig('new_plot.pdf')  
plt.show()
```

Name	Date Modified
Cystfibr.txt	11/09/2024 04:24
Data_Set.csv	07/12/2023 20:16
Data_Set.txt	16/09/2024 22:37
Data_Set.xlsx	05/12/2023 20:04
List.txt	16/09/2024 23:26
Molecules.csv	05/09/2024 20:30
Molecules.xlsx	06/03/2025 21:30
new_plot.pdf	07/03/2025 01:17





matplotlib

more than one data set:

```
for a in range(3):
    a += 1
    plt.scatter(x, y**a,
                marker = 'p',
                s      = 30,
                alpha  = 0.3,
                label  = 'Data Set ' + str(a))
```

```
plt.xlabel('x values')
plt.ylabel('y values')
plt.title('first plot')
plt.legend()
plt.show()
```

basic plots
arguments
settings

assigns a label to each data set → stored for legend

calling the legend (no input argument)



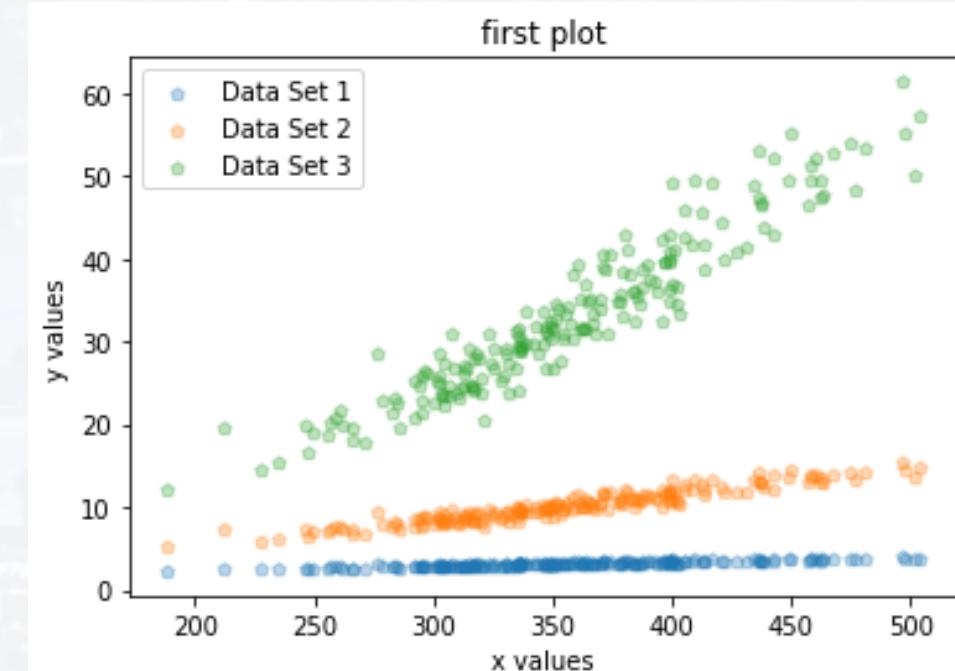
matplotlib

more than one data set:

```
for a in range(3):
    a += 1
    plt.scatter(x, y**a,
                marker = 'p',
                s      = 30,
                alpha  = 0.3,
                label  = 'Data Set ' + str(a))
```

```
plt.xlabel('x values')
plt.ylabel('y values')
plt.title('first plot')
plt.legend()
plt.show()
```

basic plots
arguments
settings





Outline

Reading/Writing Files

- Pandas and Data Frames
- Faster Alternatives
- More about .txt

Visualization

- Matplotlib
- Seaborn
- plt, ax, fig



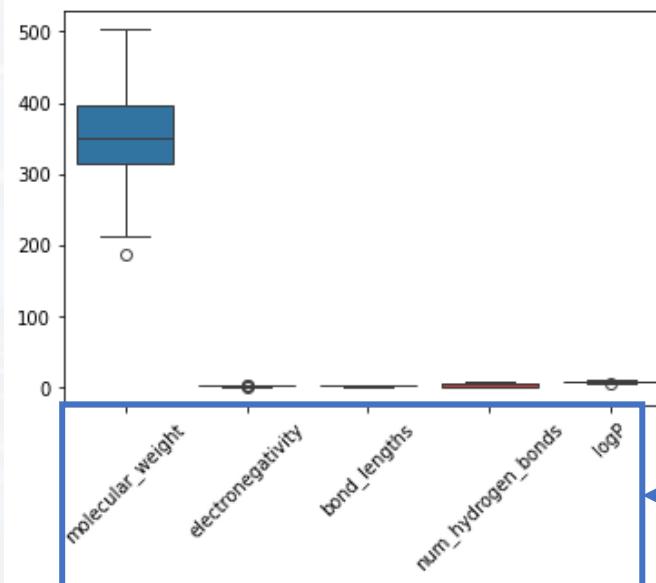
seaborn

sophisticated plots:

```
import seaborn as sns
```

starting from **data frames** right away

```
sns.boxplot(Data)
plt.xticks(rotation = 45)
plt.show()
```

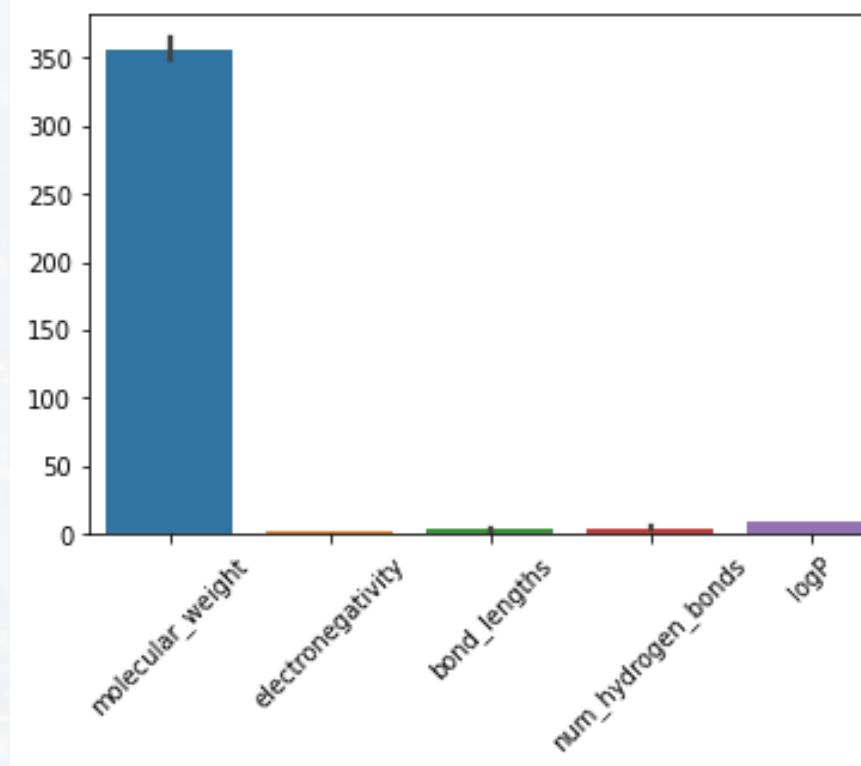


reads labels from data frame

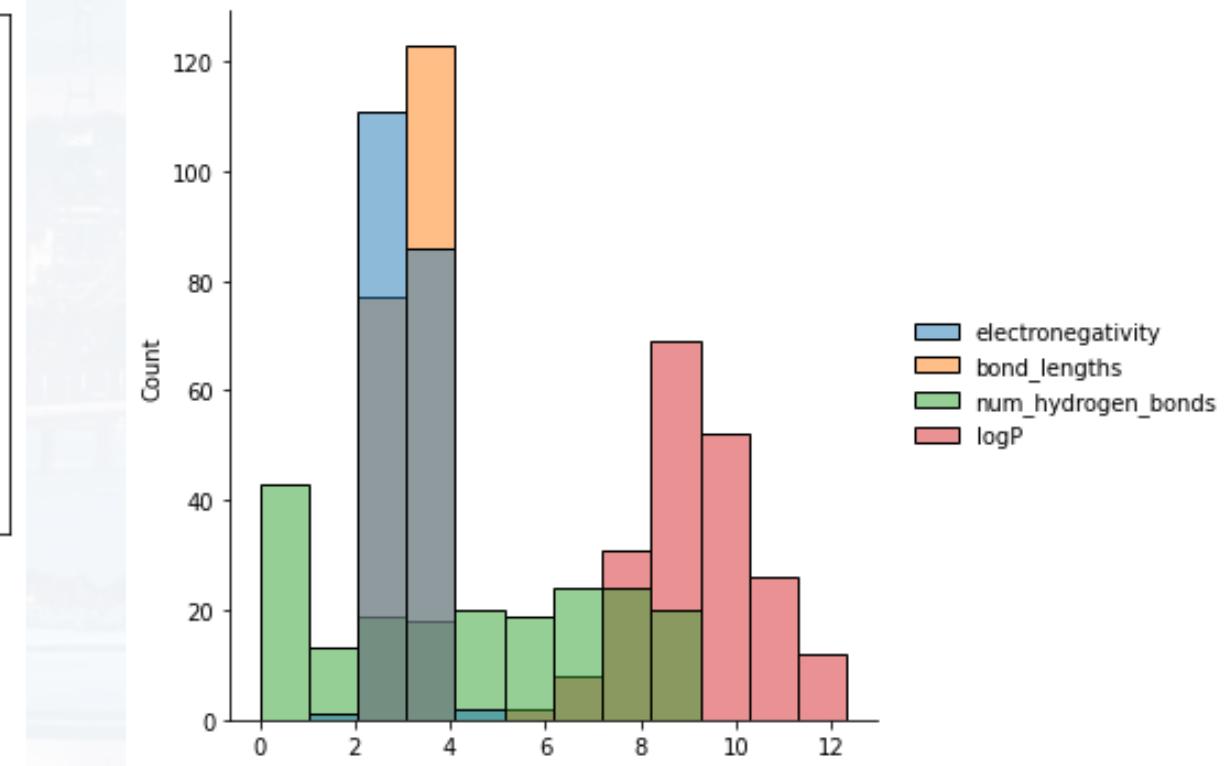


seaborn

```
sns.barplot(Data)
plt.xticks(rotation = 45)
plt.show()
```



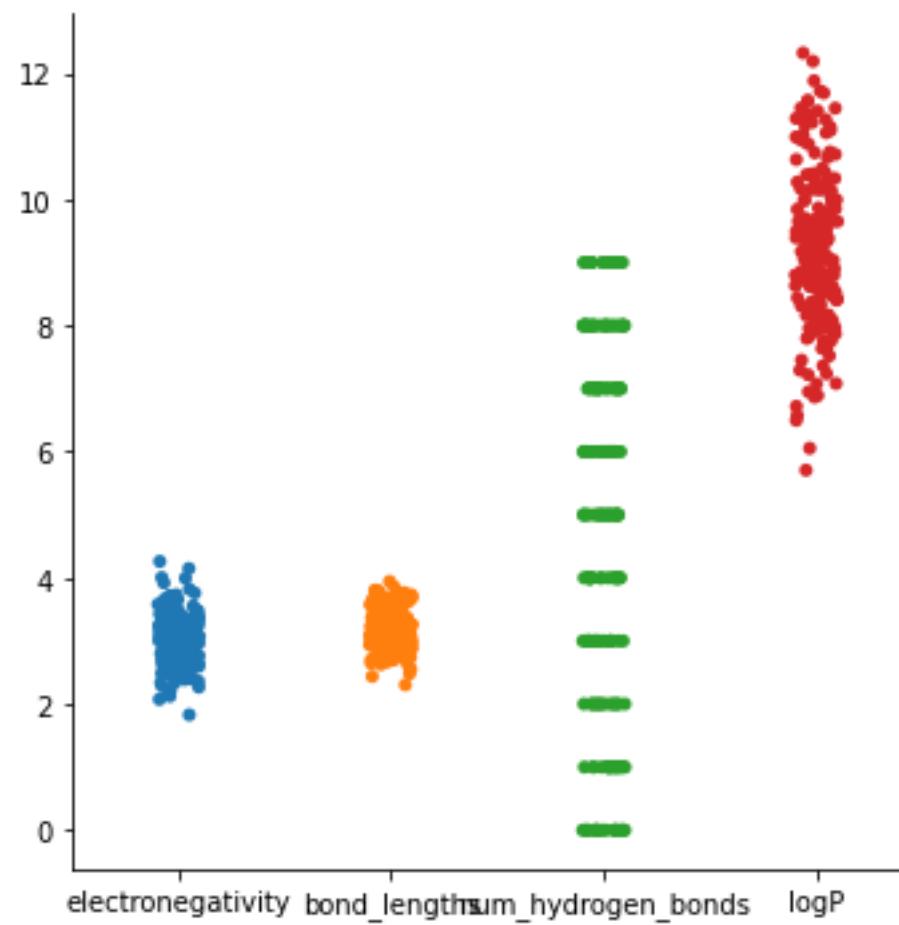
```
sns.displot(Data[Data.columns[1:-1]])
plt.show()
```





seaborn

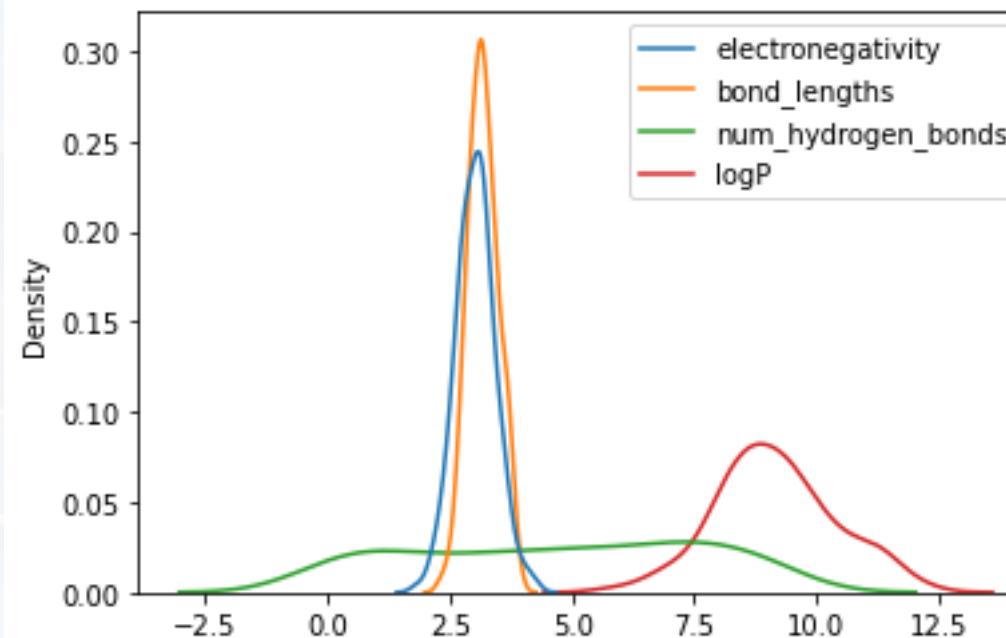
```
sns.catplot(Data[Data.columns[1:-1]])  
plt.show()
```





seaborn

```
sns.kdeplot(Data[Data.columns[1:-1]])  
plt.show()
```



[Graph Gallery with examples](#)



Berkeley
UNIVERSITY OF CALIFORNIA

Data Sampling and Pandas:

Data Sampling and Pandas

seaborn

`sns.dogplot()`



`sns.dogplot(1)`





Outline

Reading/Writing Files

- Pandas and Data Frames
- Faster Alternatives
- More about .txt

Visualization

- Matplotlib
- Seaborn
- `plt, ax, fig`



.plt.
fig

Three levels in Python:

plt	the plot itself
ax	referring to axis of specific plot
fig	referring to a figure (which can include numerous subplots)

mosaic subplots
classical subplots



.plt.
fig

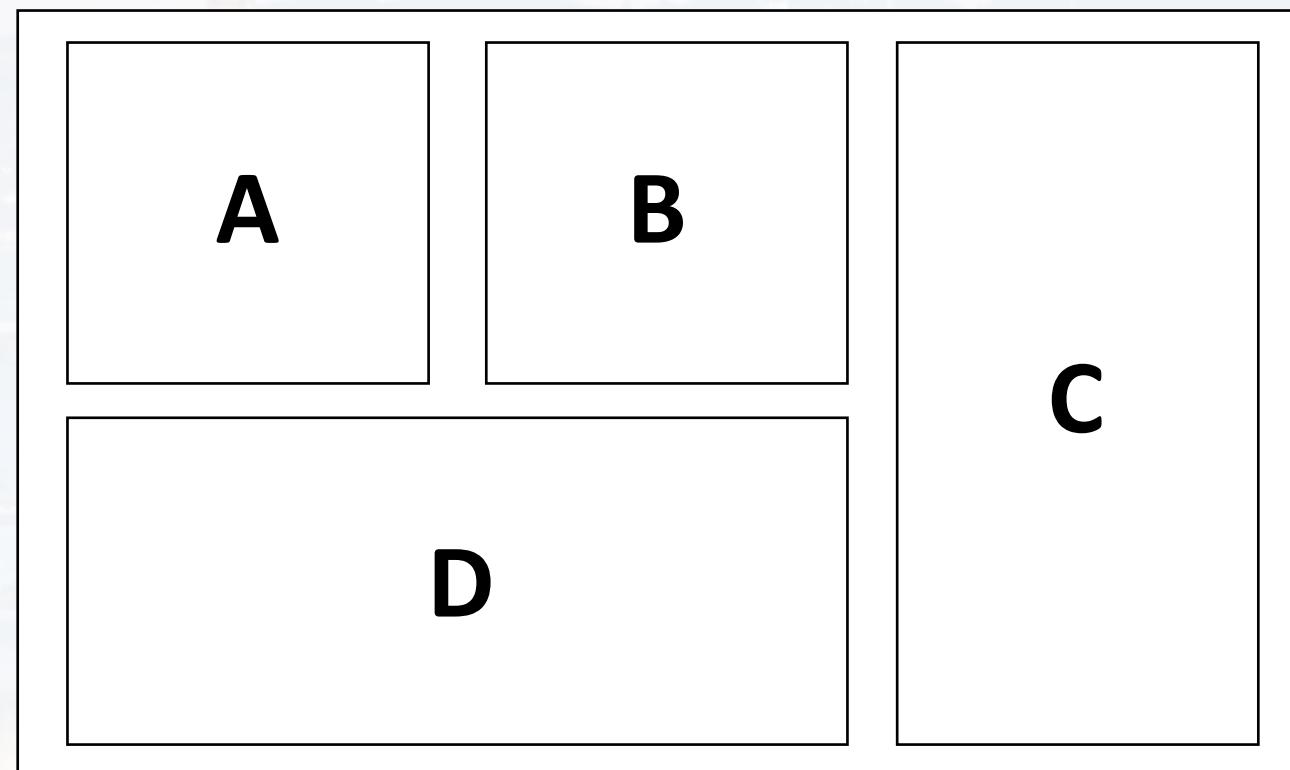
Three levels in Python:

plt	the plot itself
ax	referring to axis of specific plot
fig	referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```





.plt.
ax
fig

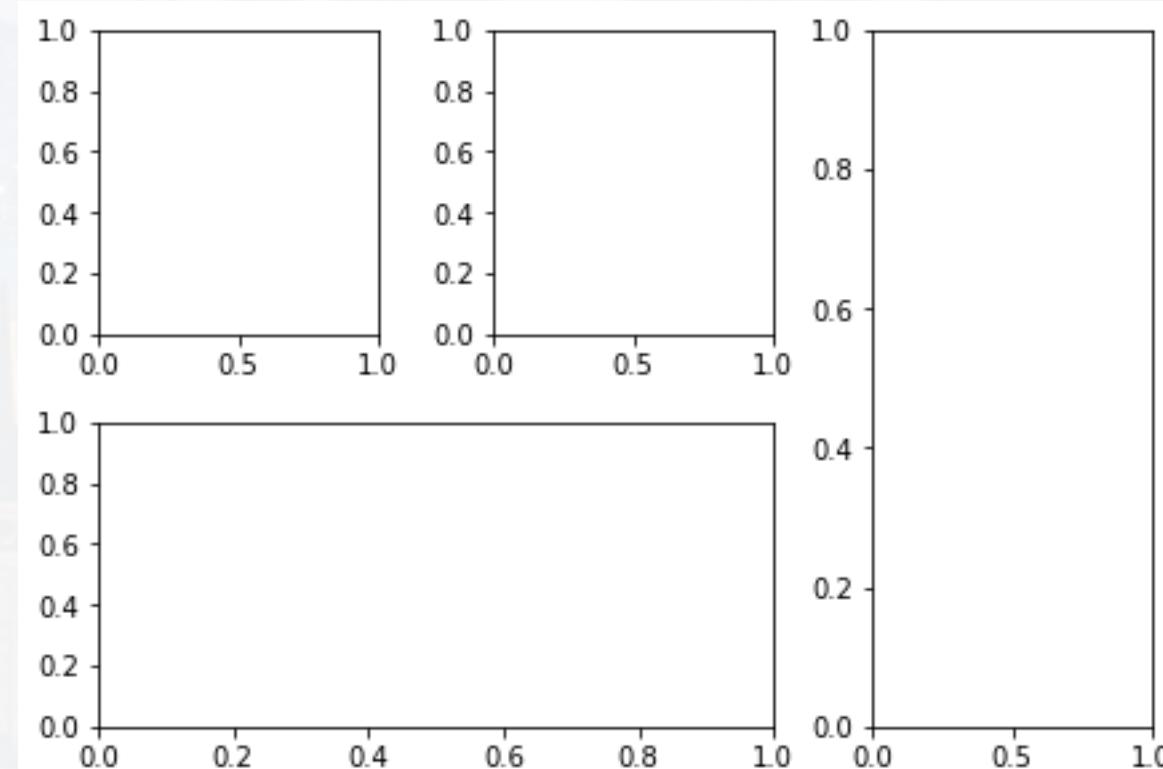
Three levels in Python:

plt	the plot itself
ax	referring to axis of specific plot
fig	referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([[ 'A', 'B', 'C'],\n                                  [ 'D', 'D', 'C']]), layout = "constrained")
```





.plt.
ax
fig

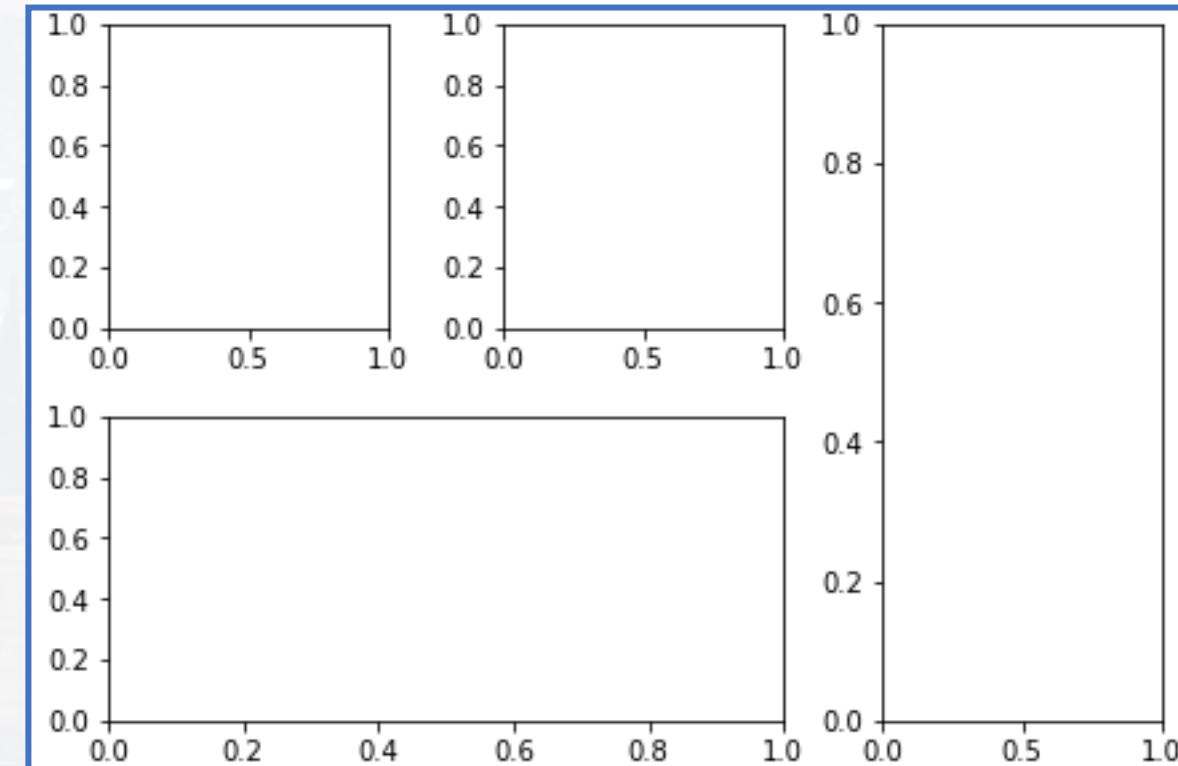
Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```



points to the current
figure



.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

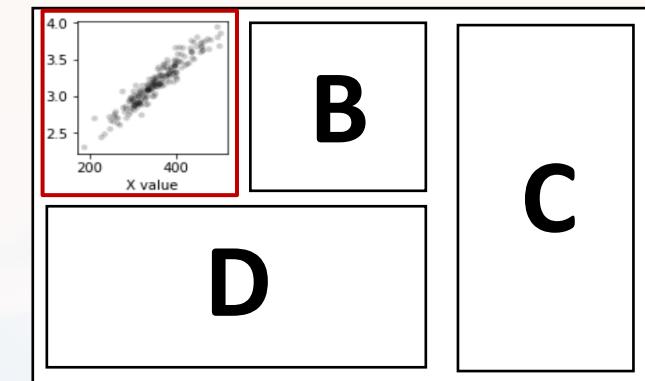
mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([[ 'A', 'B', 'C'],\n                                  [ 'D', 'D', 'C']]), layout = "constrained")
```

```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes['A'].set(xlabel = 'X value')
```

populating the
first axis object
with a **scatter plot**





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

mosaic subplots

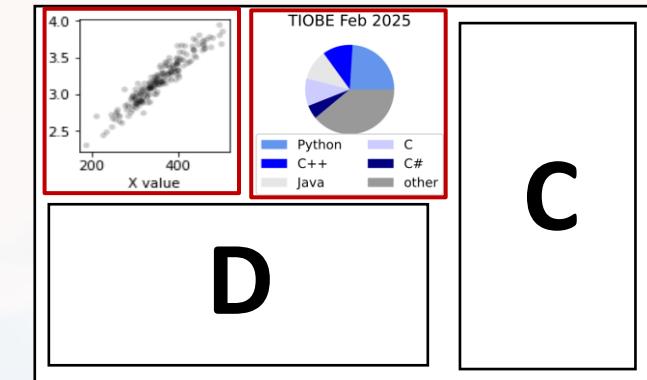
classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes['A'].set(xlabel = 'X value')
```

```
axes['B'].pie([24, 11, 11, 10, 5, 39],\n              colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9], '#CCCCFF',\n              '#000080', '#999999'])  
axes['B'].set(title = 'TIOBE Feb 2025')  
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\n                bbox_to_anchor = (0.5,-0.5), loc = 'Lower center',\n                ncol = 2)
```

populating the
second axis object
with a pie chart





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

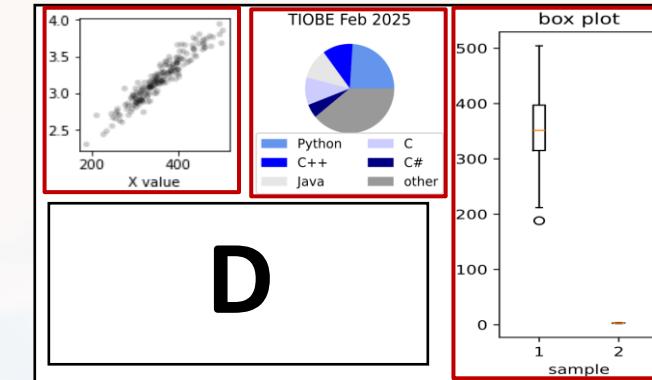
```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes['A'].set(xlabel = 'X value')
```

```
axes['B'].pie([24, 11, 11, 10, 5, 39], colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9], '#CCCCFF',\n                                         '#000080', '#999999'])
```

```
axes['B'].set(title = 'TIOBE Feb 2025')  
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\n                bbox_to_anchor = (0.5,-0.5), loc = 'lower center', ncol = 2)
```

and so on...

```
axes['C'].boxplot([x,y])  
axes['C'].set(xlabel = 'sample')  
axes['C'].set(ylabel = 'values')  
axes['C'].set(title = 'box plot')
```





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes['A'].set(xlabel = 'X value')
```

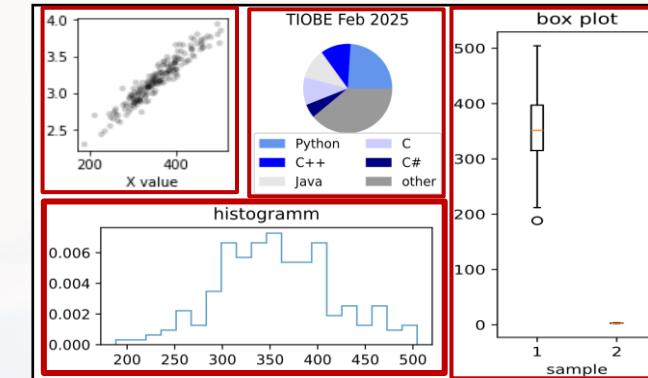
```
axes['B'].pie([24, 11, 11, 10, 5, 39], colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9], '#CCCCFF',\n                                         '#000080', '#999999'])
```

```
axes['B'].set(title = 'TIOBE Feb 2025')  
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\n                bbox_to_anchor = (0.5, -0.5), loc = 'lower center', ncol = 2)
```

```
axes['C'].boxplot([x,y])  
axes['C'].set(xlabel = 'sample')  
axes['C'].set(ylabel = 'values')  
axes['C'].set(title = 'box plot')
```

```
axes['D'].hist(x, 20, density = True, histtype = 'step', facecolor = 'g',\n               alpha = 0.75)  
axes['D'].set(title = 'histogram')
```

and so on...





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

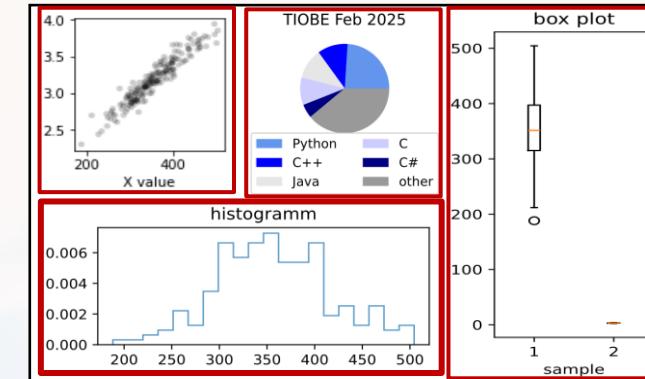
mosaic subplots

classical subplots

reference to the individual axes

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')\naxes['A'].set(xlabel = 'X value')\n\naxes['B'].pie([24, 11, 11, 10, 5, 39], colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9], '#CCCCFF',\n              '#000080', '#999999'])\naxes['B'].set(title = 'TIOBE Feb 2025')\naxes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\n                bbox_to_anchor = (0.5,-0.5), loc = 'lower center', ncol = 2)\naxes['C'].boxplot([x,y])\naxes['C'].set(xlabel = 'sample')\naxes['C'].set(ylabel = 'values')\naxes['C'].set(title = 'box plot')\n\naxes['D'].hist(x, 20, density = True, histtype = 'step', facecolor = 'g',\n               alpha = 0.75)\naxes['D'].set(title = 'histogram')
```





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

mosaic subplots

classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

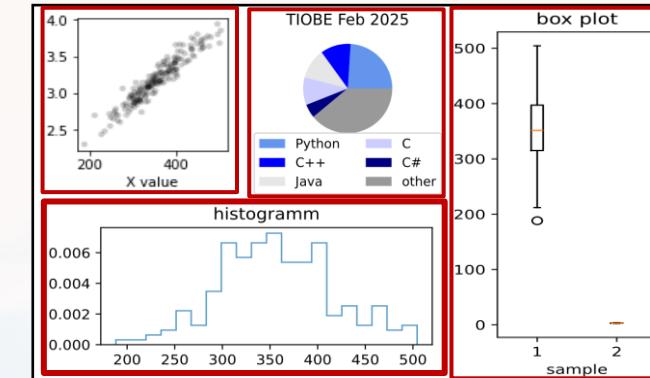
```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')\naxes['A'].set(xlabel = 'X value')
```

```
axes['B'].pie([24, 11, 11, 10, 5, 39], colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9], '#CCCCFF',\n                                         '#000080', '#999999'])
```

```
axes['B'].set(title = 'TIOBE Feb 2025')\naxes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\n                bbox_to_anchor = (0.5, -0.5), loc = 'lower center', ncol = 2)
```

```
axes['C'].boxplot([x,y])\naxes['C'].set(xlabel = 'sample')\naxes['C'].set(ylabel = 'values')\naxes['C'].set(title = 'box plot')
```

```
axes['D'].hist(x, 20, density = True, histtype = 'step', facecolor = 'g',\n               alpha = 0.75)\naxes['D'].set(title = 'histogram')
```



notice the
different color
codes



.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure

mosaic subplots

classical subplots

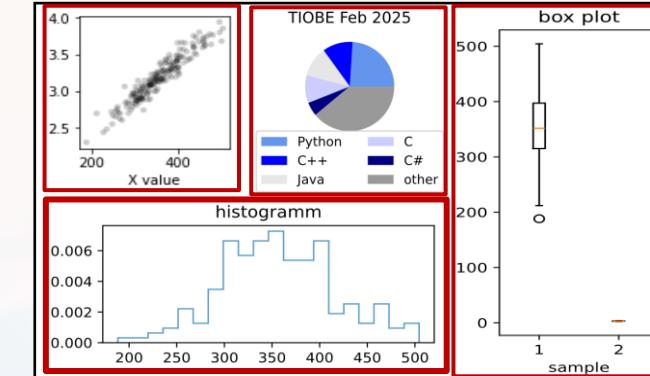
```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\n                                  ['D', 'D', 'C']], layout = "constrained")
```

```
axes['A'].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes['A'].set(xlabel = 'X value')
```

...

```
axes['D'].hist(x, 20, density = True, histtype = 'step', facecolor = 'g',\n                alpha = 0.75)  
axes['D'].set(title = 'histogram')
```

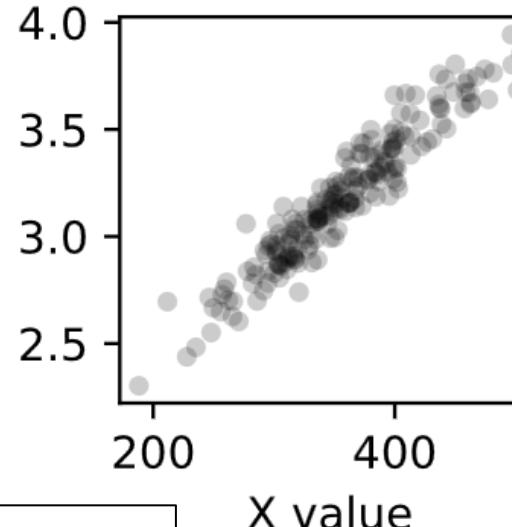
```
figMo.savefig('test.pdf', dpi = 1600)
```



referring to the
specific figure

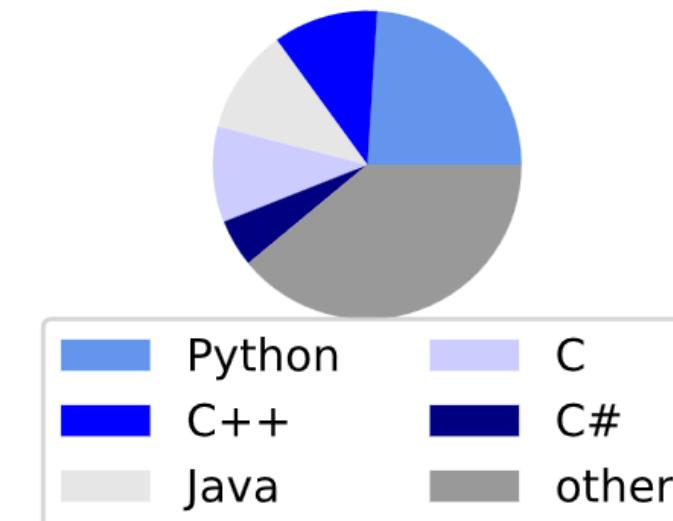


.plt. ax
fig

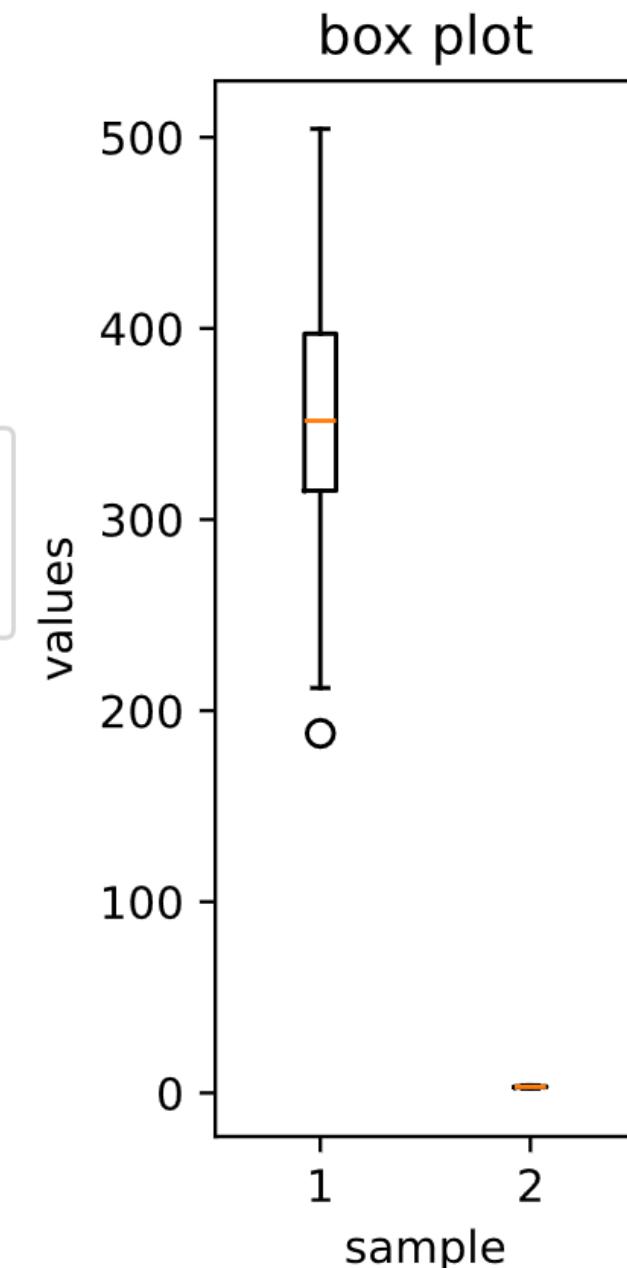
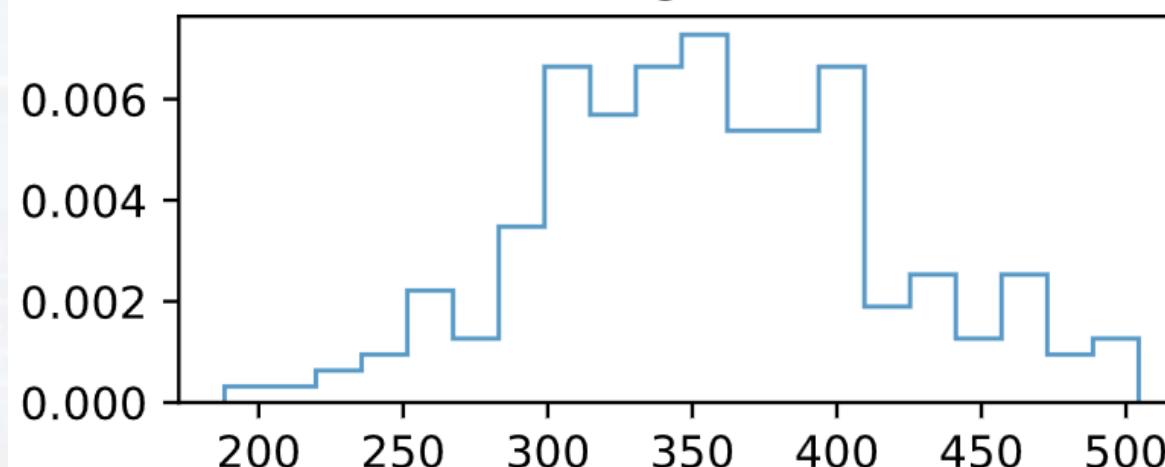


check out
PlotMosaicExample.py

TIOBE Feb 2025



histogramm





.plt.
ax
fig

Three levels in Python:

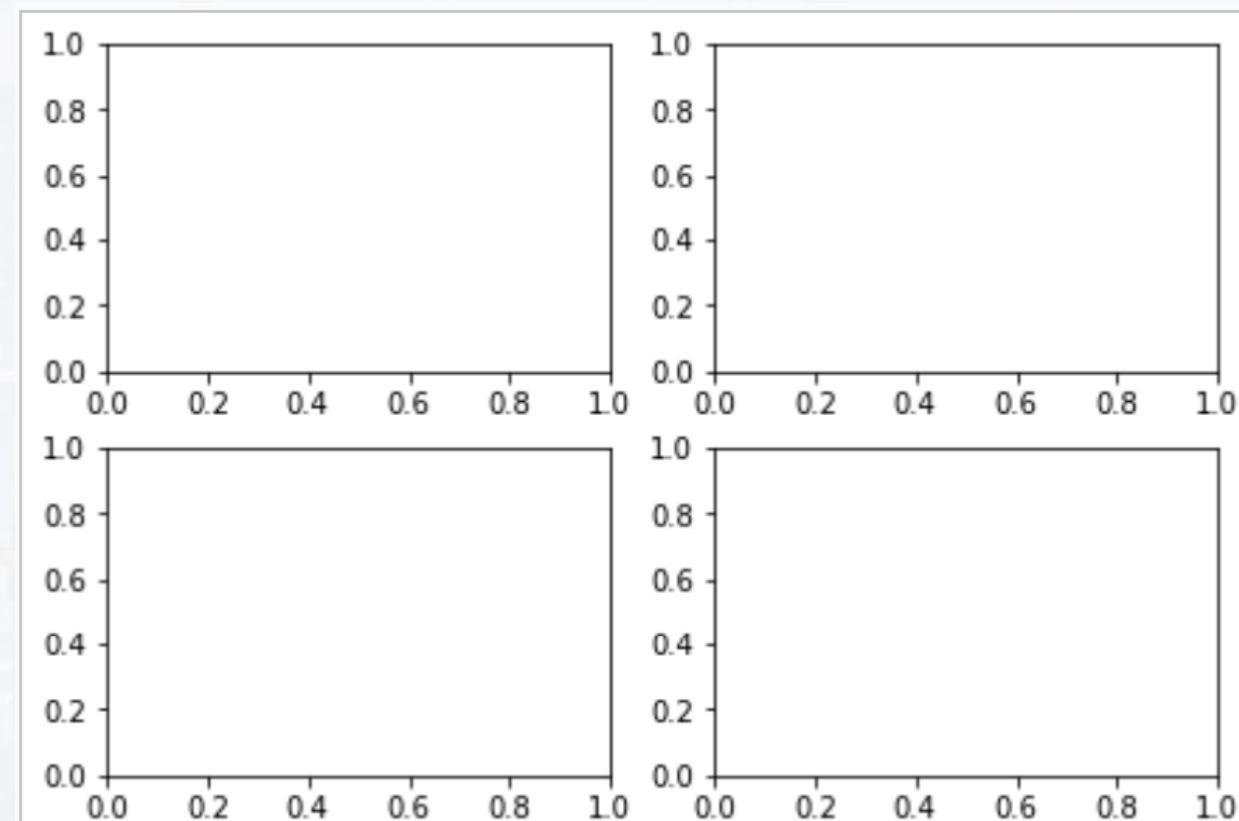
plt	the plot itself
ax	referring to axis of specific plot
fig	referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

Same idea!

```
figSt, axes = plt.subplots(nrows = 2, ncols = 2, layout = "constrained")
```





.plt.
ax
fig

Three levels in Python:

plt the plot itself
ax referring to axis of specific plot
fig referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

Same idea!

```
figSt, axes = plt.subplots(nrows = 2, ncols = 2, layout = "constrained")  
  
axes[0, 0].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')  
axes[0, 0].set(xlabel = 'X value')  
  
axes[1, 0].pie([24, 11, 11, 10, 5, 39], colors = ['#6495ED', 'blue', [0.9, 0.9, 0.9],  
                 '#CCCCFF', '#000080', '#999999'])  
axes[1, 0].set(title = 'TIOBE Feb 2025')  
axes[1, 0].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],  
                 bbox_to_anchor = (0.5, -0.5), loc = 'Lower center', ncol = 2)  
  
axes[0, 1].boxplot([x, y])  
axes[0, 1].set(xlabel = 'sample')  
axes[0, 1].set(ylabel = 'values')  
axes[0, 1].set(title = 'box plot')  
  
axes[1, 1].hist(x, 20, density = True, histtype = 'step', facecolor = 'g', alpha = 0.75)  
axes[1, 1].set(title = 'histogram')
```

in mosaic mode:
label can be
numeric or str.
here: has to be
int (referres to
locaton in
figure)



.plt.
fig

Three levels in Python:

plt	the plot itself
ax	referring to axis of specific plot
fig	referring to a figure (which can include numerous subplots)

mosaic subplots

classical subplots

Same idea!

```
figSt, axes = plt.subplots(nrows = 2, ncols = 2, layout = "constrained")
axes[0, 0].scatter(x, y, s = 20, c = 'k', alpha = 0.2, edgecolors = 'none')
axes[0, 0].set(xlabel = 'X value')

...
axes[1, 1].hist(x, 20, density=True, histtype = 'step', facecolor = 'g', alpha = 0.75)
axes[1, 1].set(title = 'histogramm')

figSt.savefig('test.pdf', dpi = 1600)
```

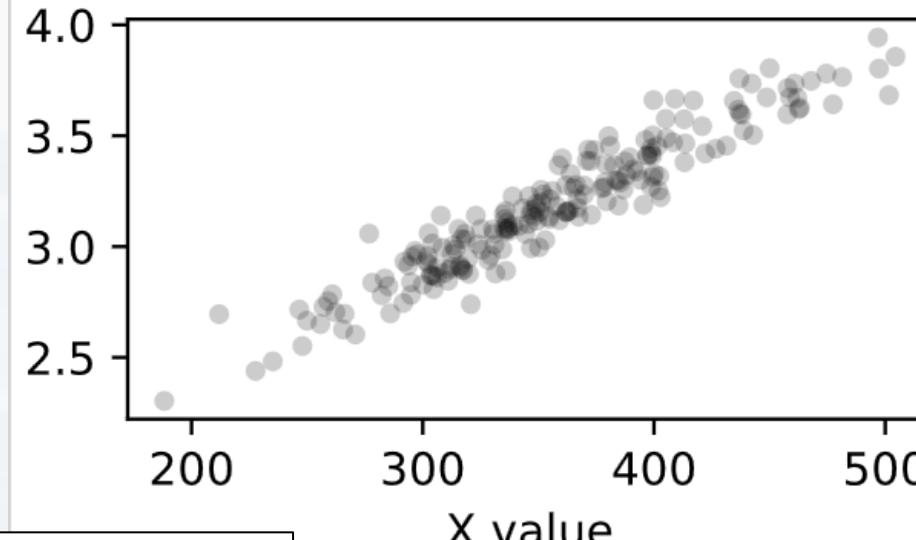


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Data Sampling and Pandas:

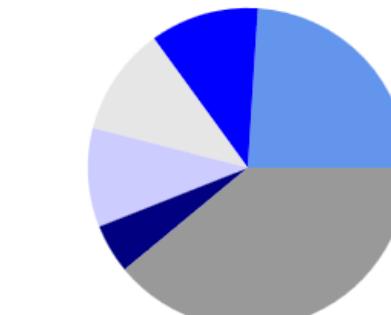
Data Sampling and Pandas

.plt. ax
fig

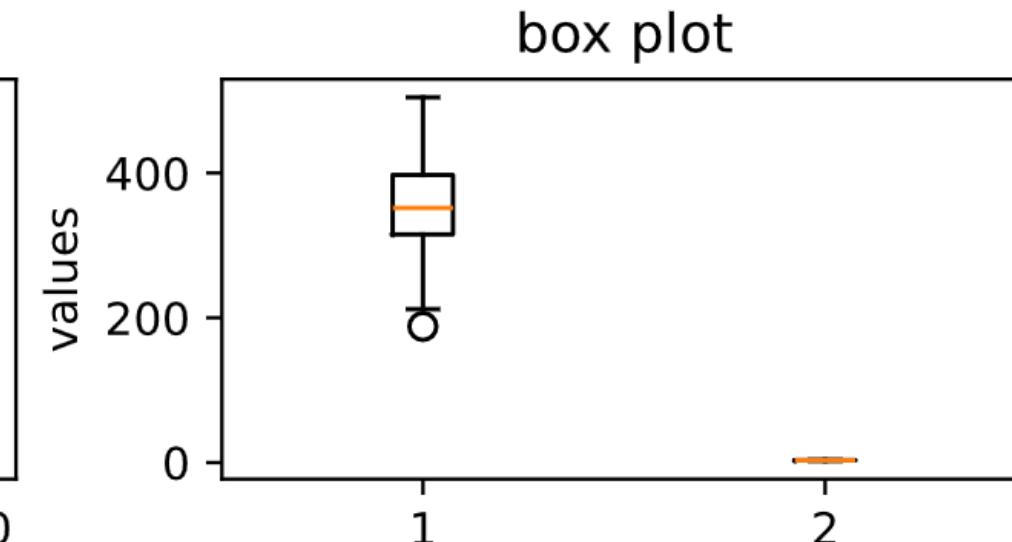


check out
PlotStandardExample.py

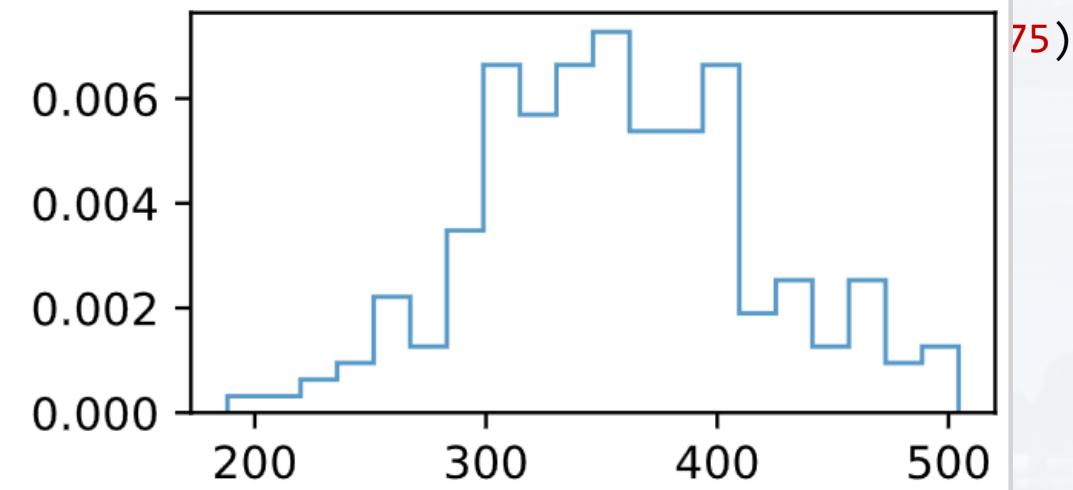
X value
TIOBE Feb 2025



Python	C
C++	C#
Java	other



sample
histogramm



75)



Thank you very much for your attention!

