Berkeley
MSSE
MOLECULAR SCIENCE &
SOFTWARE ENGINEERING

Lecture 06:

Data Visualization and File I/O

Markus Hohle

University California, Berkeley

Python for Molecular Sciences

MSSE 272, 3 Units

NOPE... IT CAN'T BE DONE ONLINE...
YOU ACTUALLY HAVE TO TAKE THE RAKE OUTSIDE
BISH TRIBUNE-REVIEW

Outline

Reading/Writing Files

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

Visualization

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

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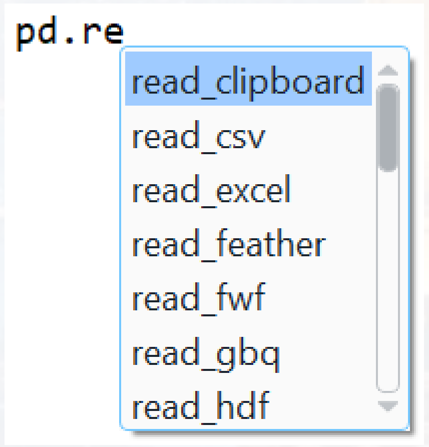
- `plt, ax, fig`

most common file formats

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

```
import pandas as pd
```



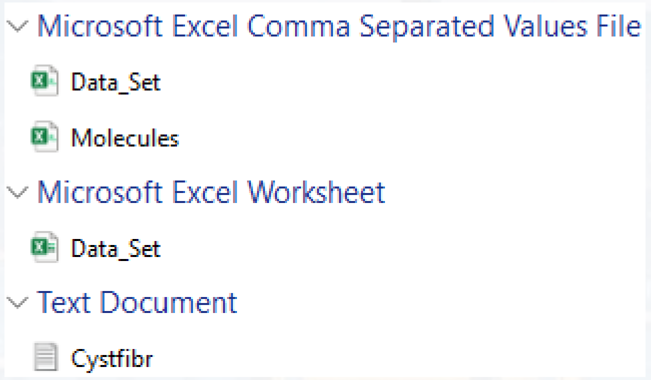
```
pd.re
```

Data Visualization and File I/O

most common file formats

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

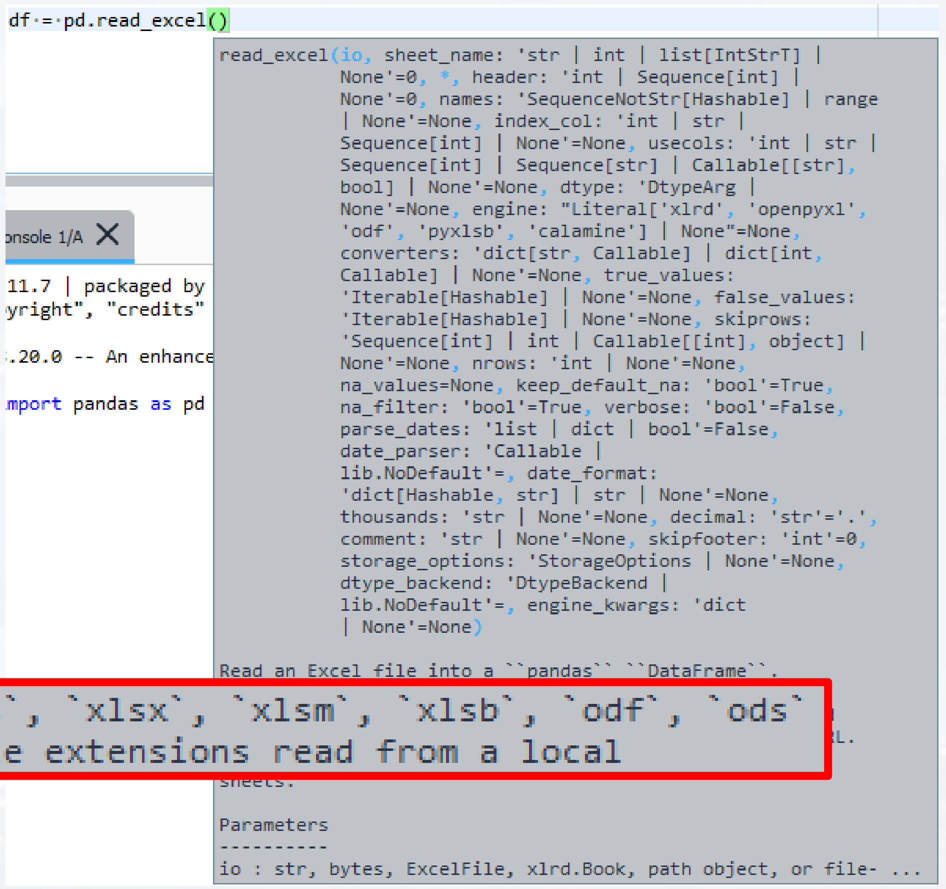
```
import pandas as pd
```



Microsoft Excel Comma Separated Values File
- Data_Set
- Molecules

Microsoft Excel Worksheet
- Data_Set

Text Document
- Cystfibr



```
df = pd.read_excel()
```

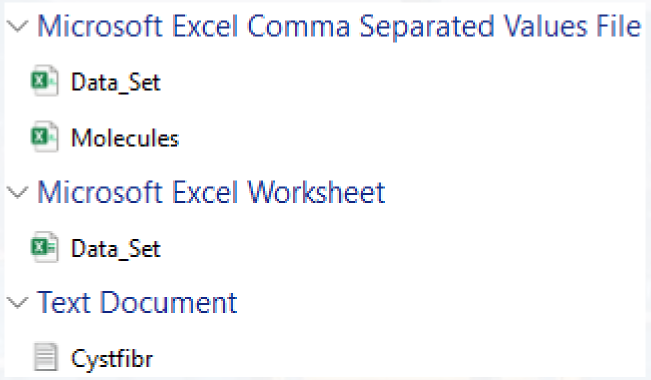
```
11.7 | packaged by
yright", "credits"
.20.0 -- An enhance
mport pandas as pd
```

```
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- ...
```

most common file formats

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

```
import pandas as pd
```

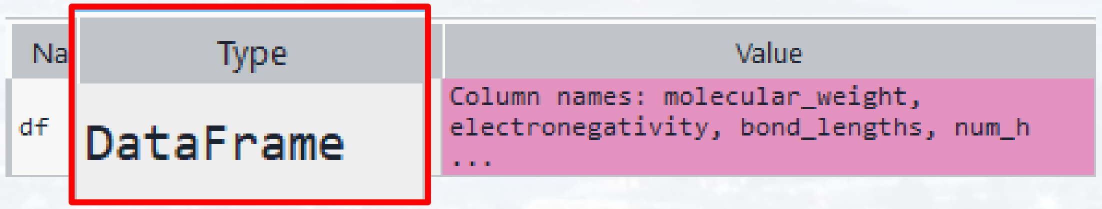


Microsoft Excel Comma Separated Values File
- Data_Set
- Molecules

Microsoft Excel Worksheet
- Data_Set

Text Document
- Cystfibr

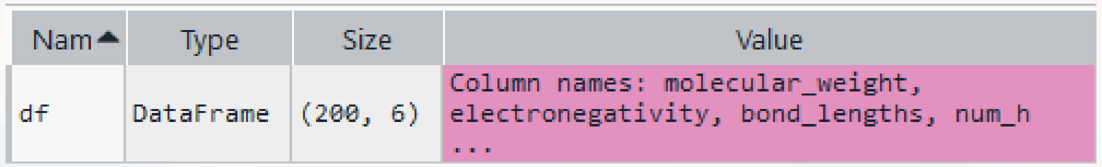
```
df = pd.read_csv('Molecules.csv')
```



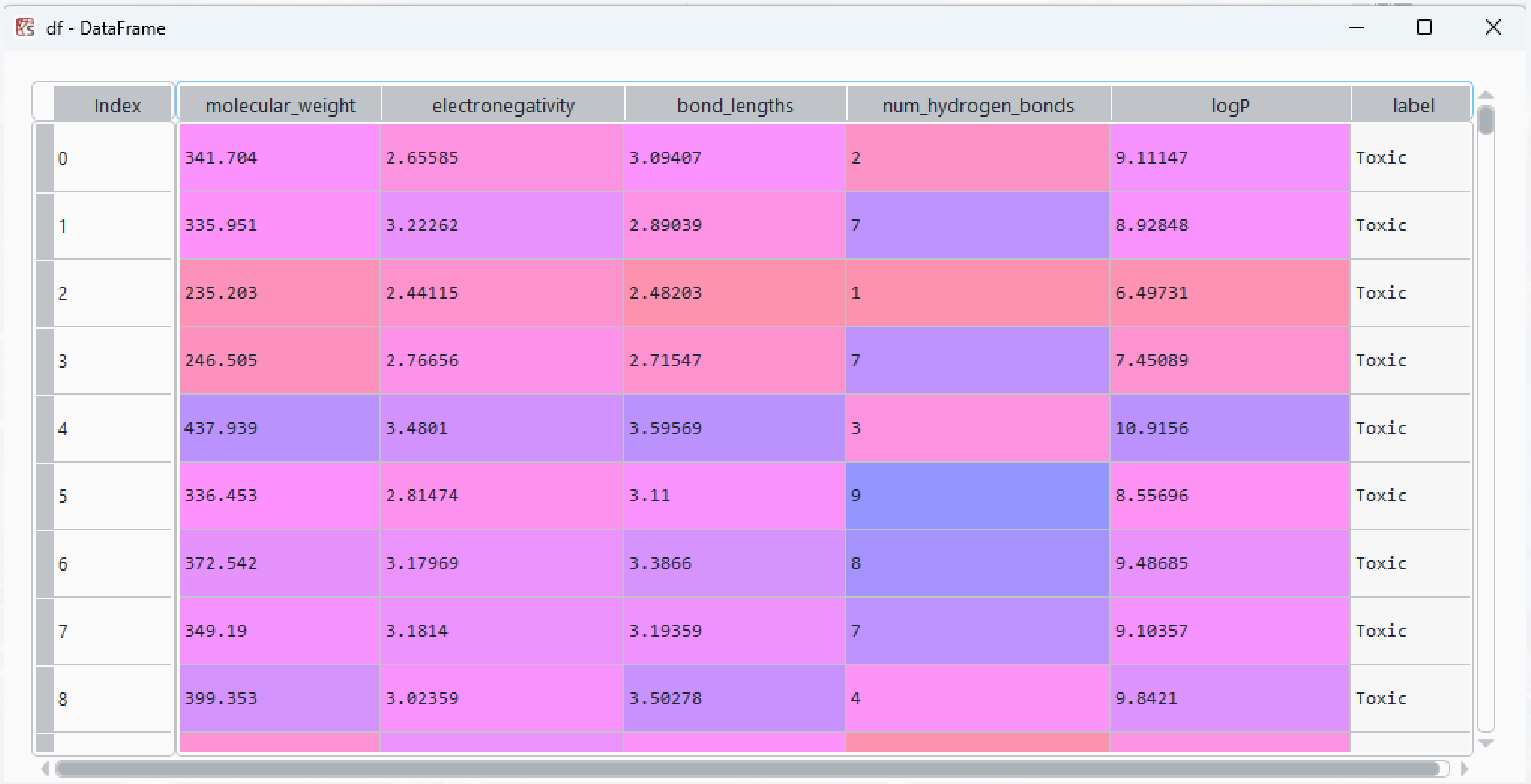
Na	Type	Value
df	DataFrame	Column names: molecular_weight, electronegativity, bond_lengths, num_h ...

Pandas & Data Frames

```python
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 ...

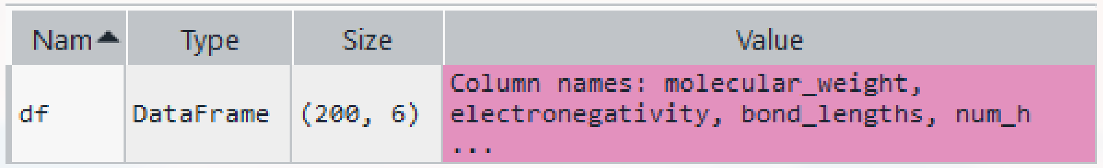


df - DataFrame

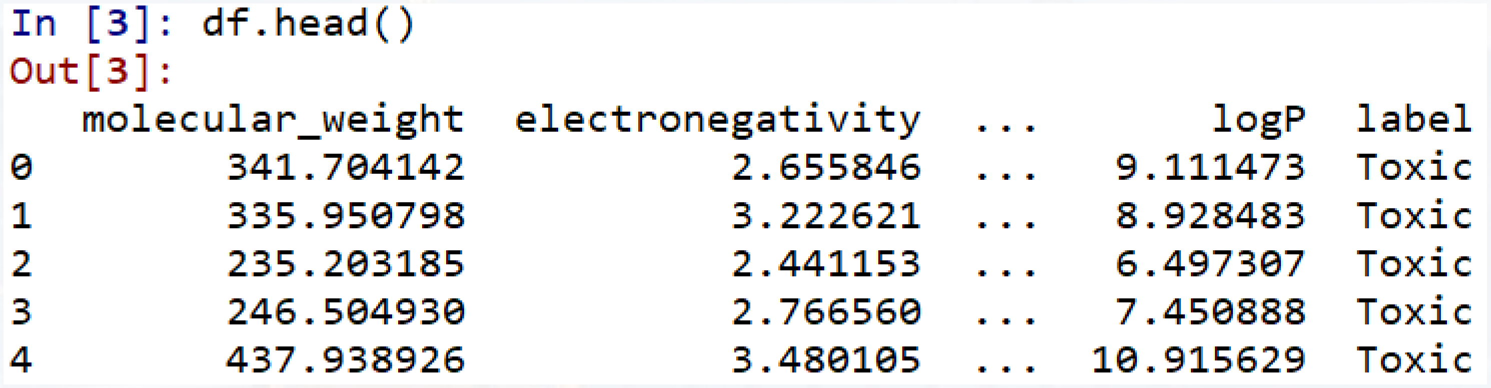
Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	341.704	2.65585	3.09407	2	9.11147	Toxic
1	335.951	3.22262	2.89039	7	8.92848	Toxic
2	235.203	2.44115	2.48203	1	6.49731	Toxic
3	246.505	2.76656	2.71547	7	7.45089	Toxic
4	437.939	3.4801	3.59569	3	10.9156	Toxic
5	336.453	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

Data Visualization and File I/O

```
import pandas as pd

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

df.head()
```



Nam	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('My_File.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

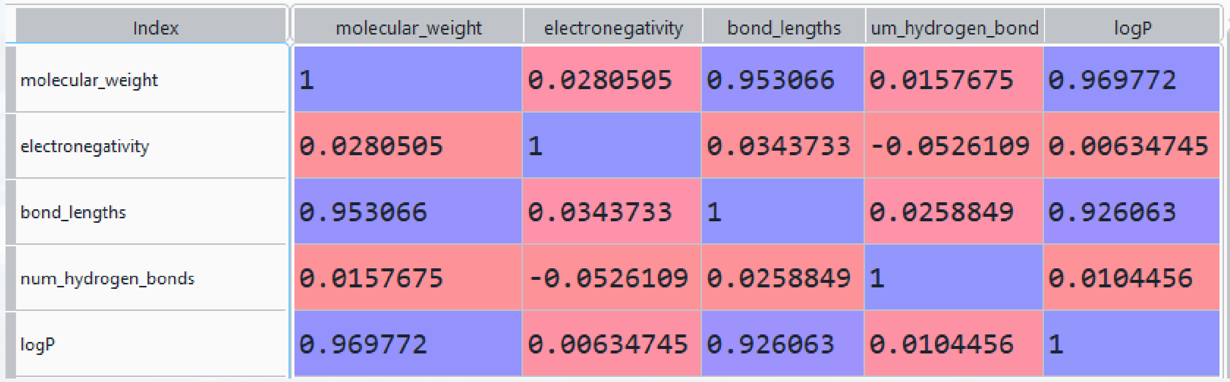
`df.columns` returns columns

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

`df.corr()` returns Pearsons' correlation coefficient

columns `0` to `4` contain `float`/`int`

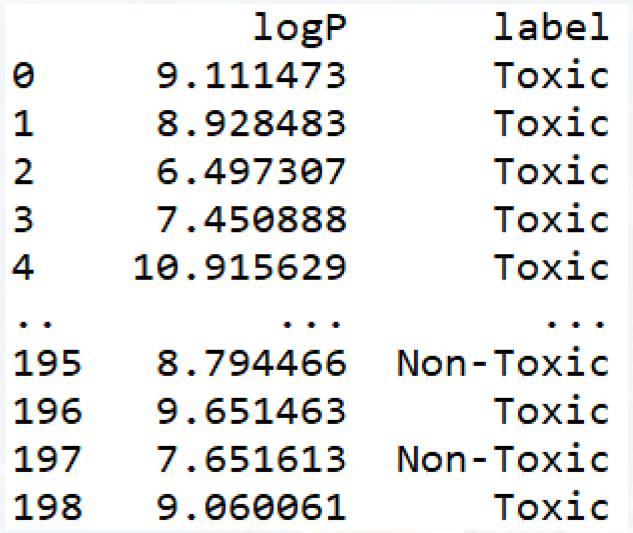
```
Corr = df[df.columns[:-1]].corr()
```



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

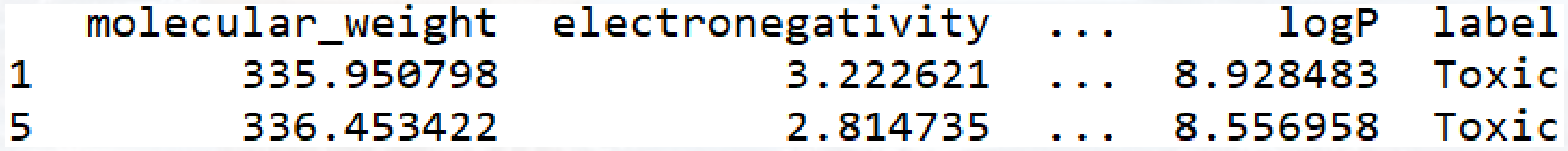
a data frame has numerous functions

`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

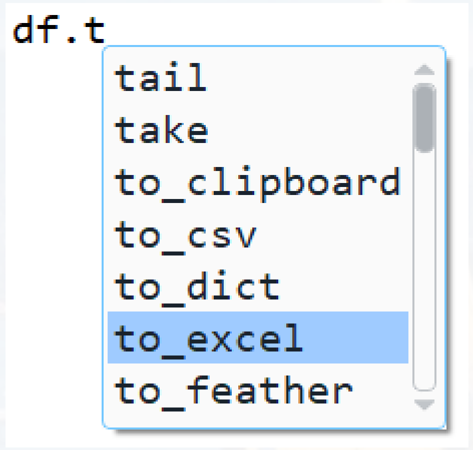
Try out the following commands!

`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

Pandas & Data Frames

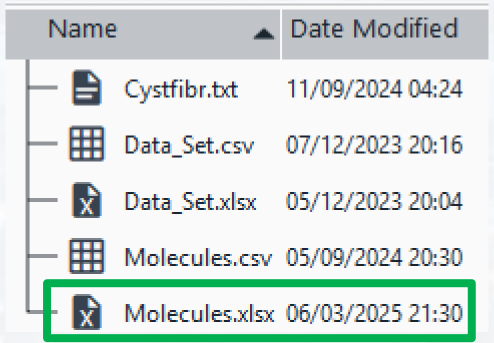
```python
import pandas as pd

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

finally, saving the data frame to an excel file

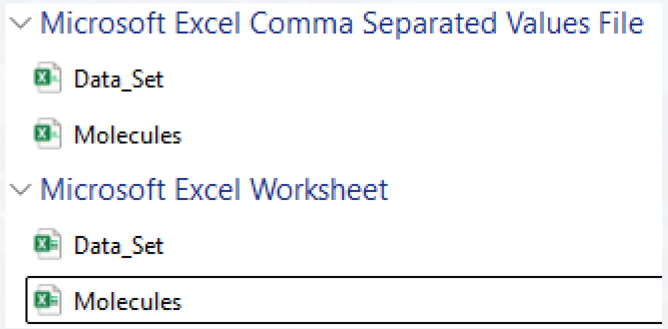


```
df.t
    tail
    take
    to_clipboard
    to_csv
    to_dict
    to_excel
    to_feather
```

```python
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



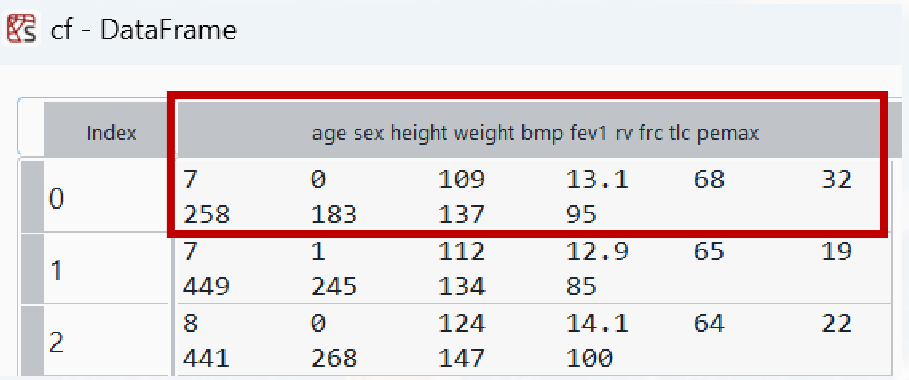
Microsoft Excel Comma Separated Values File
- Data_Set
- Molecules

Microsoft Excel Worksheet
- Data_Set
- Molecules

Data Visualization and File I/O

pandas can also read **text files**:

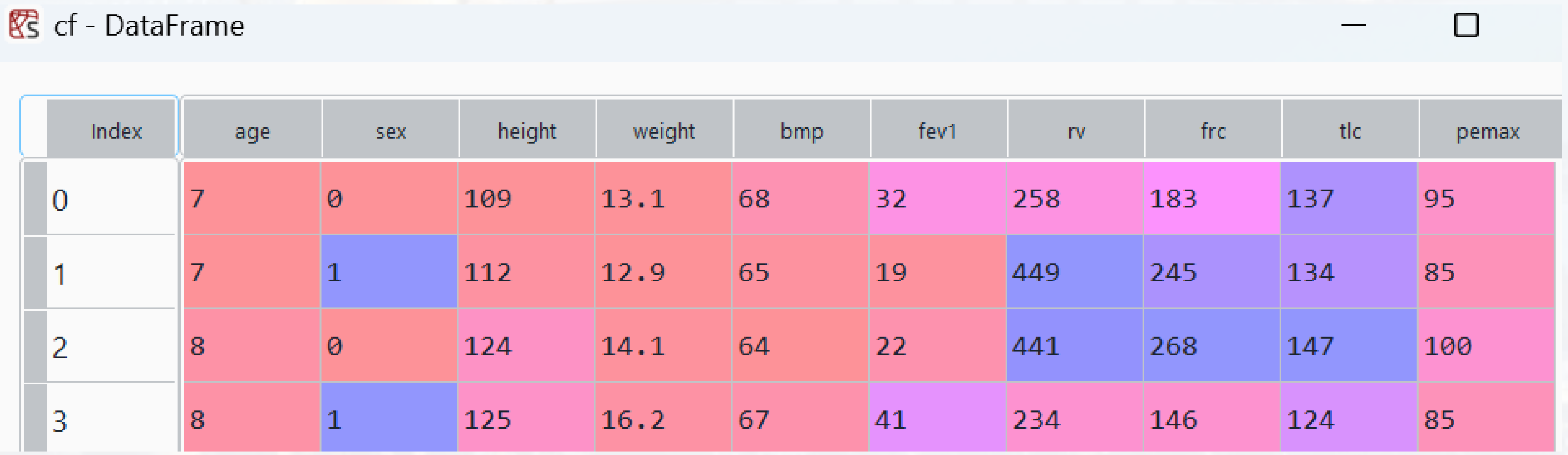
```
cf = pd.read_csv('cystfibr.txt')
```



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

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Data Visualization and File I/O

pandas is the standard library, but it is slow

reading a 130MB **excel file**:

```
import pandas as pd
import time


t1 = time.monotonic()

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

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


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

83 seconds

Data Visualization and File I/O

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

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
```

dask

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

Faster Alternatives

dask

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

```
import dask.dataframe as dd


t1 = time.monotonic()

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

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


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

0.016 seconds!

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

However, we might need to transform the output

Faster Alternatives

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

dask

```
import dask.dataframe as dd


t1 = time.monotonic()

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

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


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

1.7 seconds!

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

Faster Alternatives

polars

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

```
import polars as pl


t1 = time.monotonic()

df = pl.read_excel('Data_Set.xlsx')

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


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


df = pd.DataFrame(df)
```

8.2 seconds!

However, we might need to transform the output

Faster Alternatives

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

```
import polars as pl


t1 = time.monotonic()

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

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


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

10.2 seconds!

Faster Alternatives

polars

```
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

polars

```
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

	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

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Outline

Reading/Writing Files

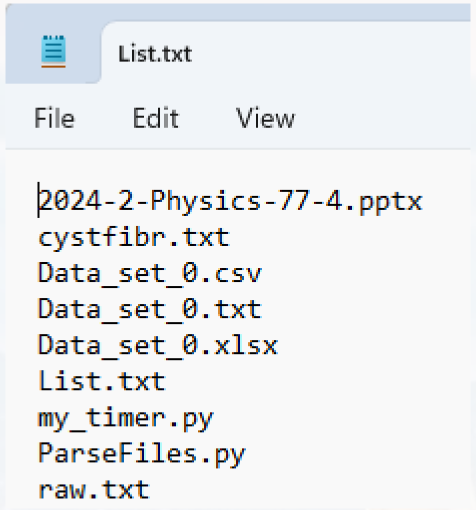
- Pandas and Data Frames
- Faster Alternatives
- **More about `.txt`**

Visualization

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

More about .txt

sometimes txt files don't come in a nice format

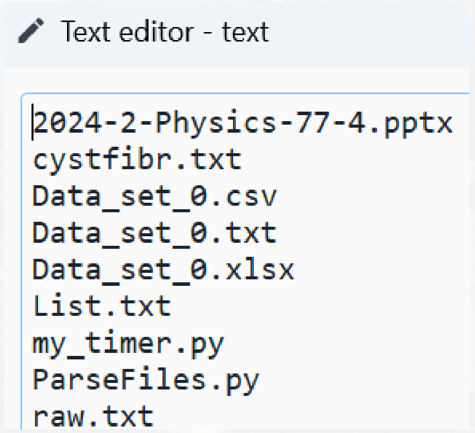


```
2024-2-Physics-77-4.pptx
cystfibr.txt
Data_set_0.csv
Data_set_0.txt
Data_set_0.xlsx
List.txt
my_timer.py
ParseFiles.py
raw.txt
```

→ using open

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

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

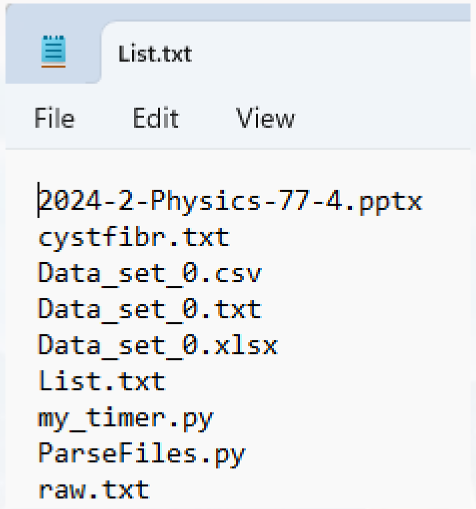


```
2024-2-Physics-77-4.pptx
cystfibr.txt
Data_set_0.csv
Data_set_0.txt
Data_set_0.xlsx
List.txt
my_timer.py
ParseFiles.py
raw.txt
```

Data Visualization and File I/O

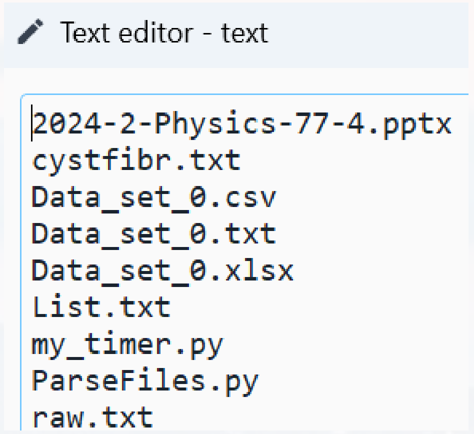
More about .txt

sometimes txt files don't come in a nice format



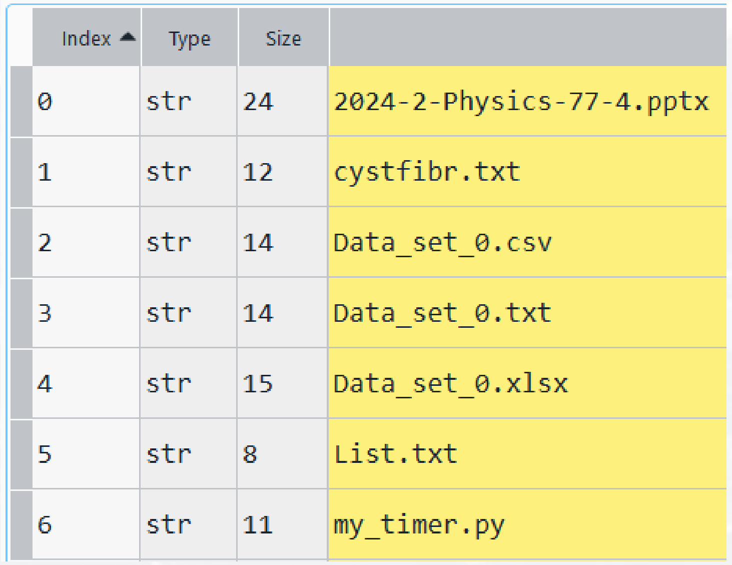
```
2024-2-Physics-77-4.pptx
cystfibr.txt
Data_set_0.csv
Data_set_0.txt
Data_set_0.xlsx
List.txt
my_timer.py
ParseFiles.py
raw.txt
```

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



```
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
```

```python
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

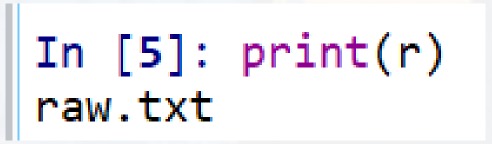
syntax of open

```python
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)
```

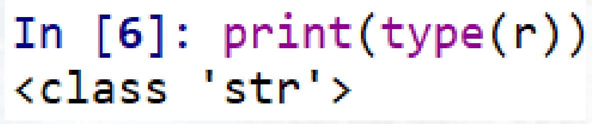
opens file line by line

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'>
```

NOPE... IT CAN'T BE DONE ONLINE...
YOU ACTUALLY HAVE TO TAKE THE RAKE OUTSIDE
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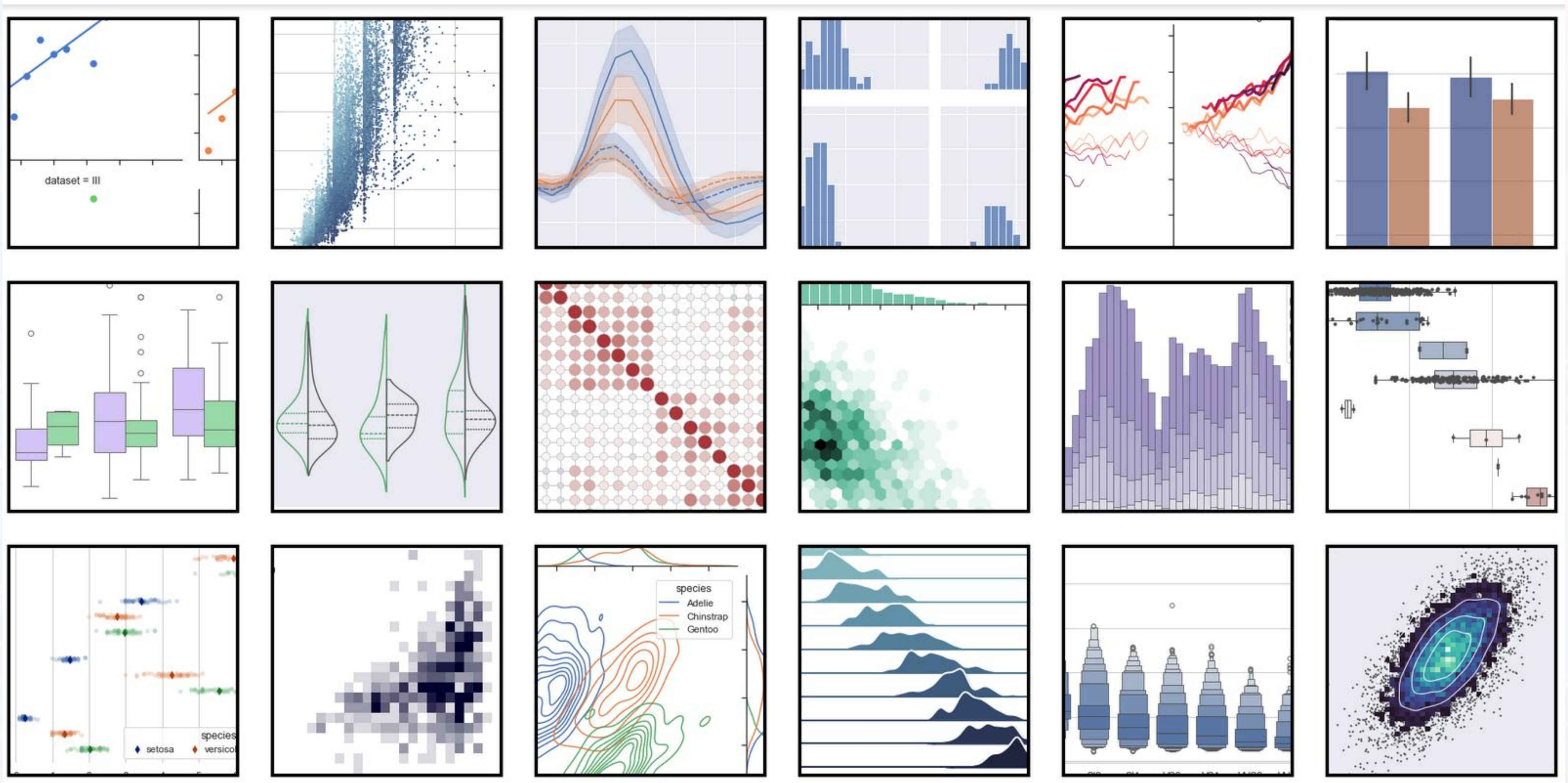
TRIBUNE-REVIEW

Data Visualization and File I/O

Python Graph Gallery

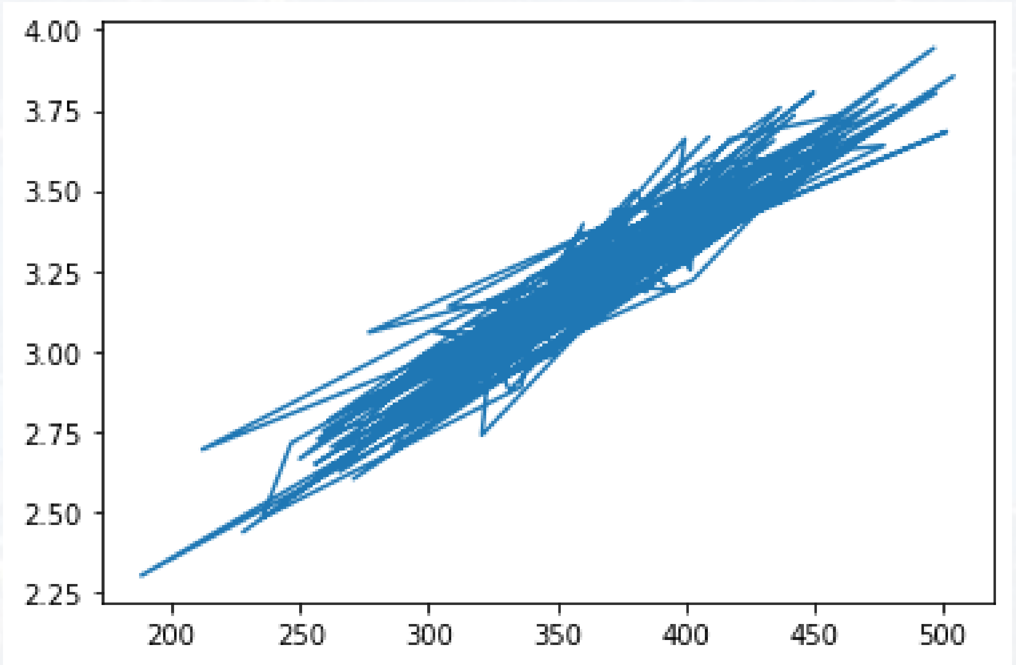
https://seaborn.pydata.org/examples/index.html



Data Visualization and File I/O

basic plots
arguments
settings

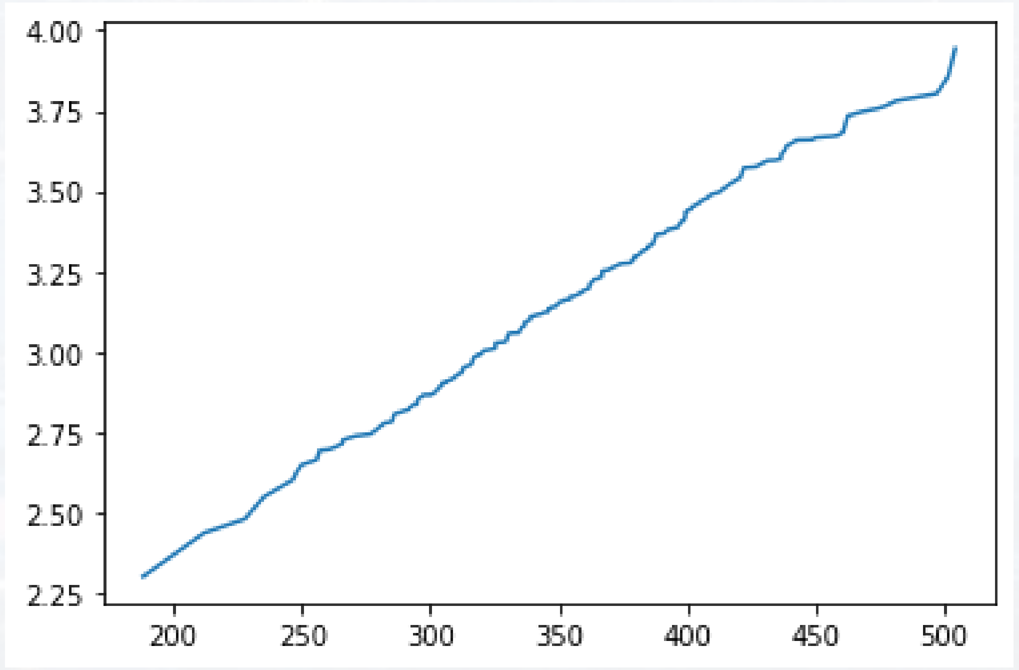
```
import pandas as pd
import matplotlib.pyplot as plt

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

x    = Data.molecular_weight
y    = Data.bond_lengths


plt.plot(x,y)
```



Data Visualization and File I/O

basic plots
arguments
settings

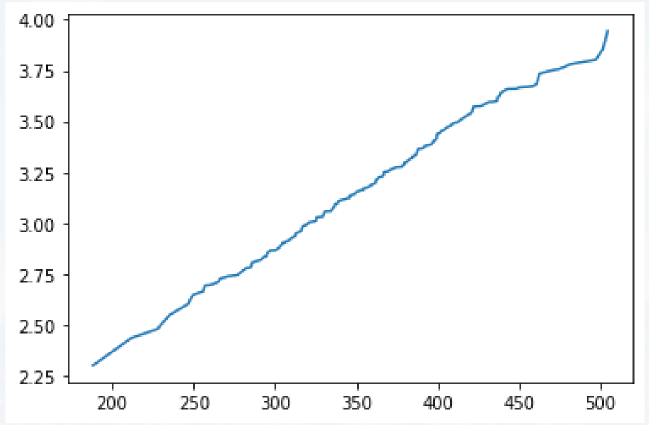
```
import pandas as pd
import matplotlib.pyplot as plt

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

x     = Data.molecular_weight
y     = Data.bond_lengths


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



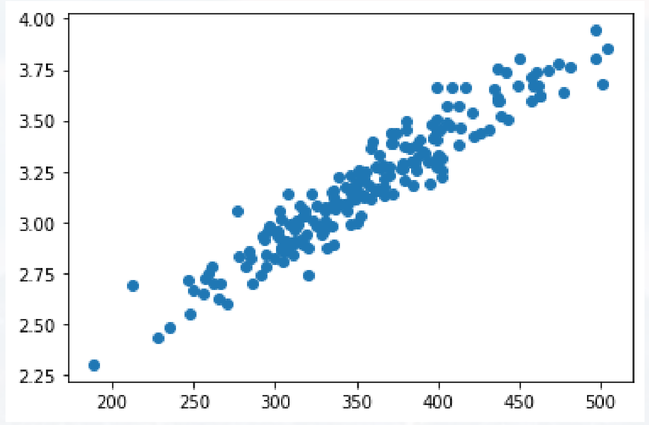
Data Visualization and File I/O

basic plots
arguments
settings

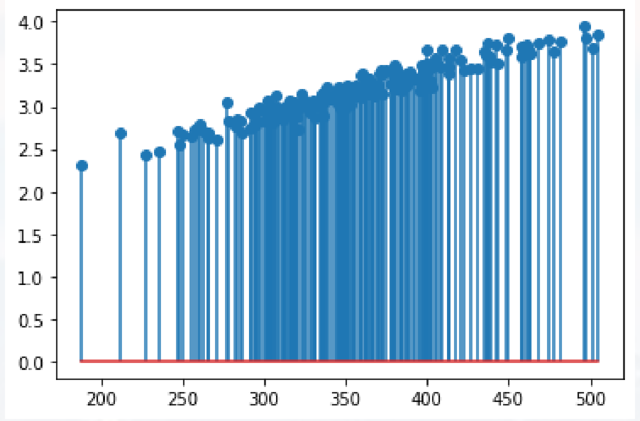
```
plt.plot(sorted(x),
         sorted(y))
```



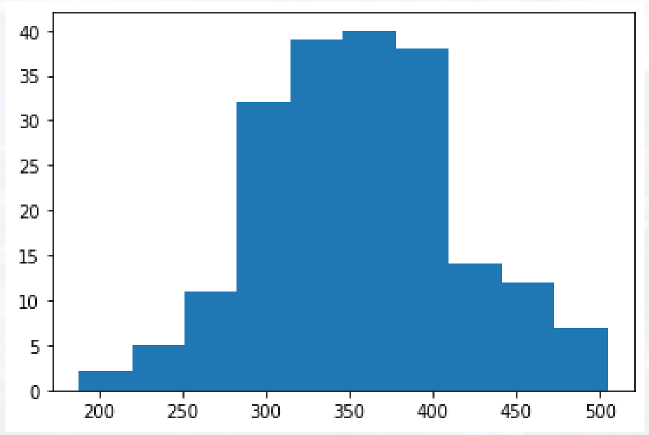
```
plt.scatter(x, y)
```



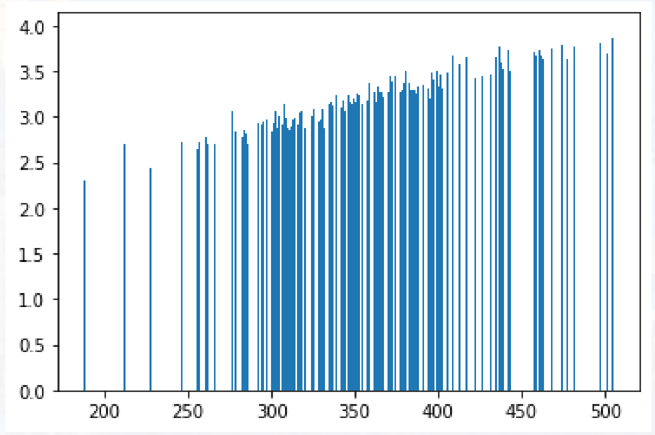
```
plt.stem(x, y)
```



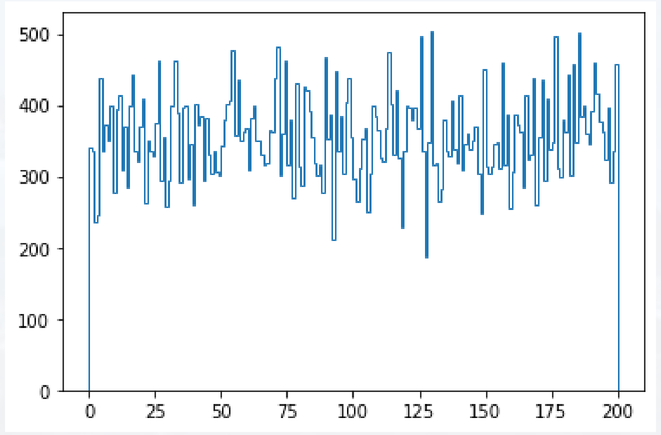
```
plt.hist(x)
```



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

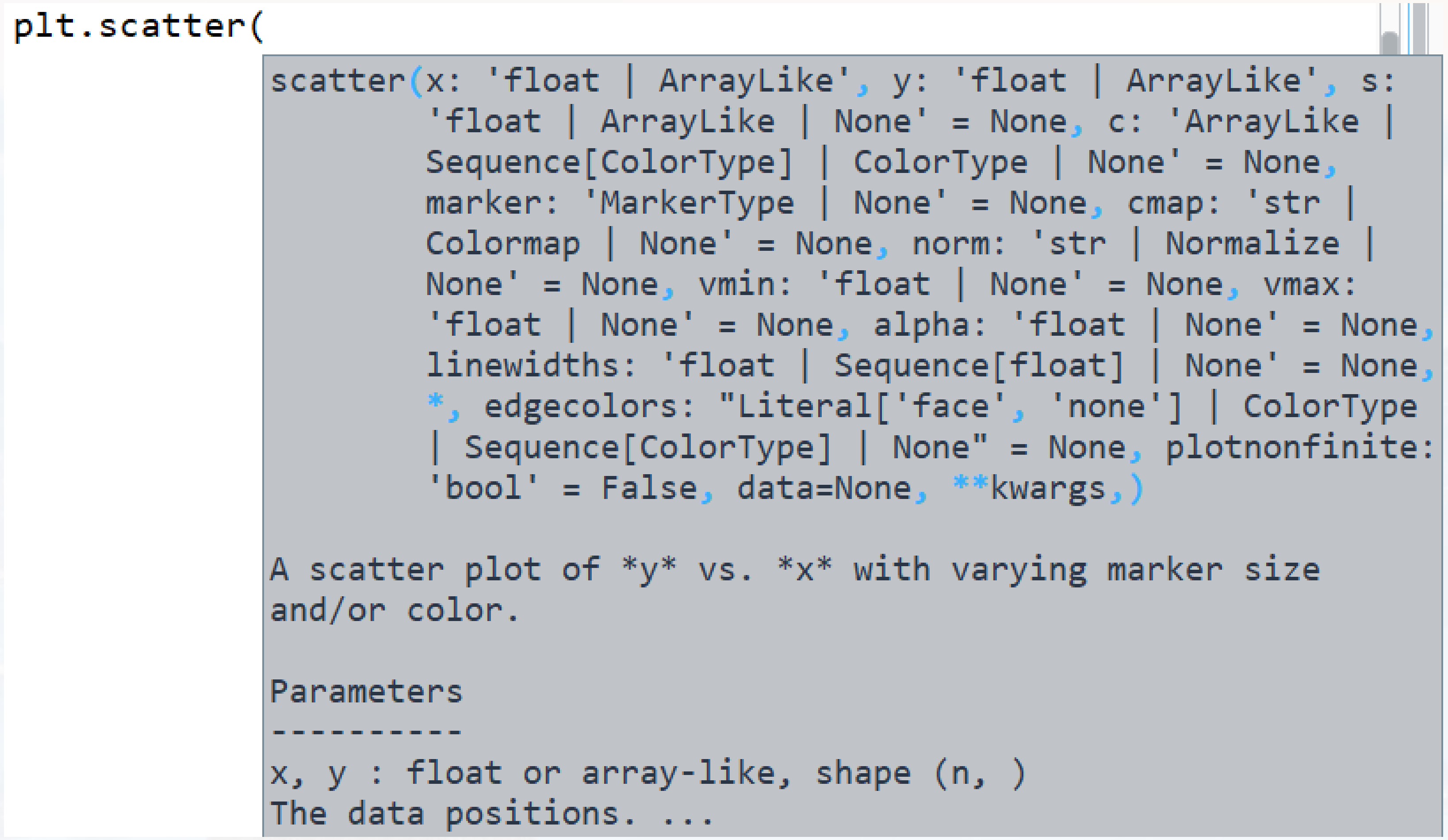


```
plt.stairs(x)
```



Data Visualization and File I/O

basic plots
arguments
settings



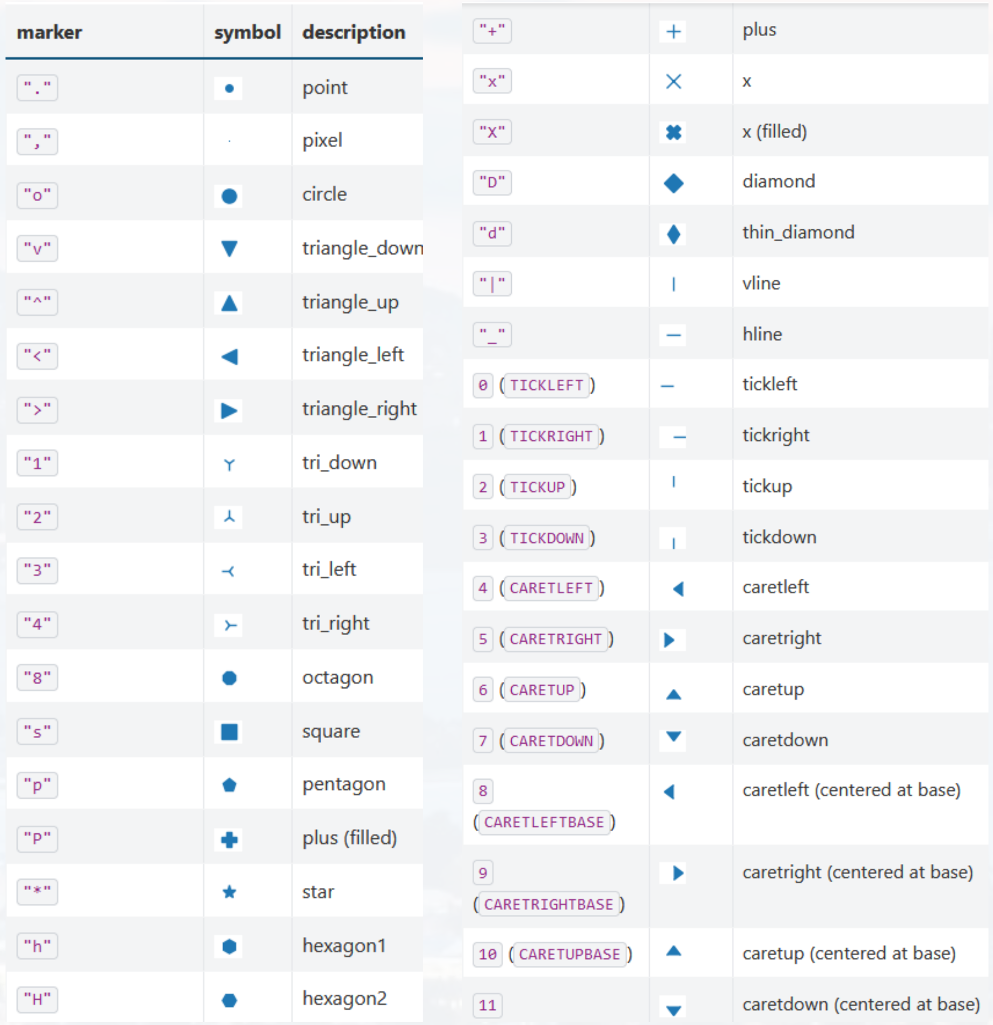
```
plt.scatter(
```

```
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. ...
```

Data Visualization and File I/O

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

marker style: `str`



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

Data Visualization and File I/O

basic plots
arguments
settings

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

marker size in pixel: `int`

Data Visualization and File I/O

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

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'`

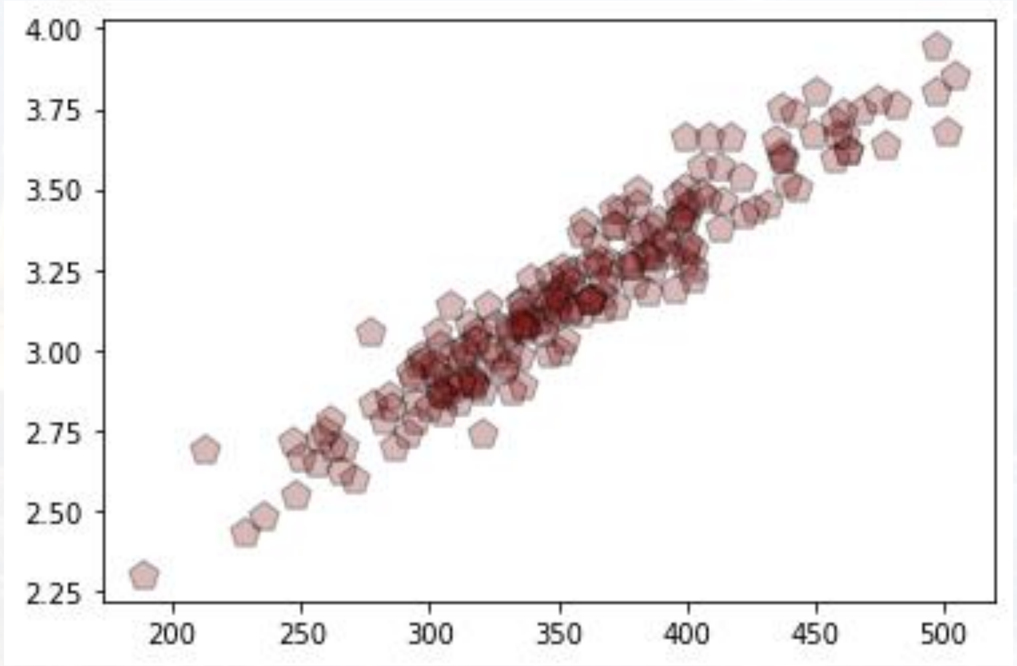
Data Visualization and File I/O

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

alpha (opaqueness/opacity): `float`

Data Visualization and File I/O

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



Data Visualization and File I/O

```
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()
```

Python speaks LaTeX, but needs raw string

```
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()
```

legend needs to be a `list`

basic plots
arguments
settings

```
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()
```

plots can be saved to any common format

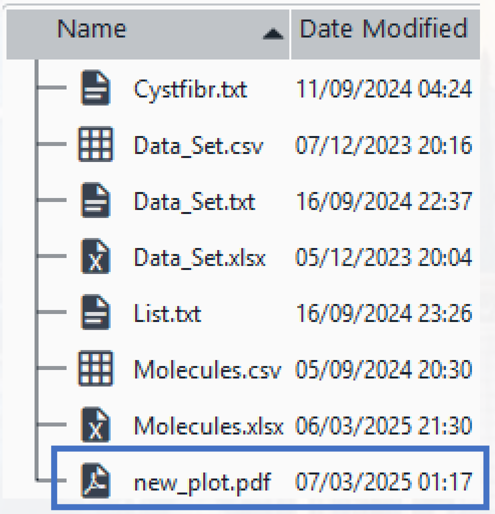
Data Visualization and File I/O

```
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()
```

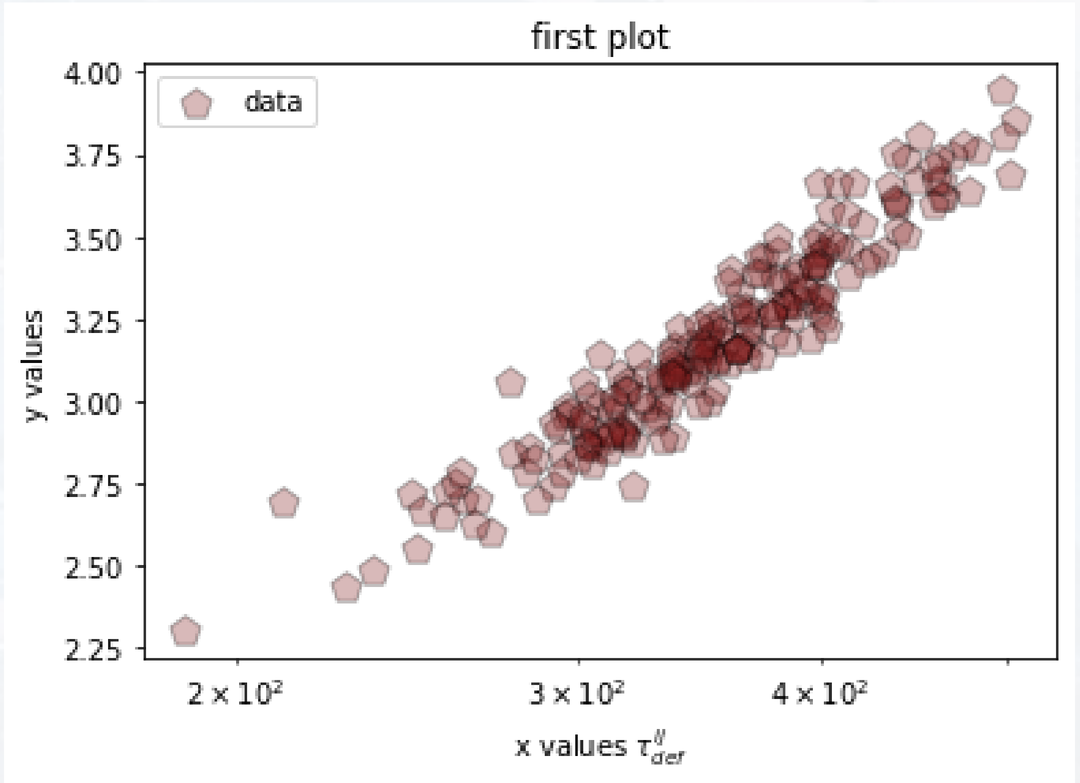
sometims plots don‘t show up (depending on settings)
type `plt.show()`
at the **very end**

Data Visualization and File I/O

```
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()
```



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



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

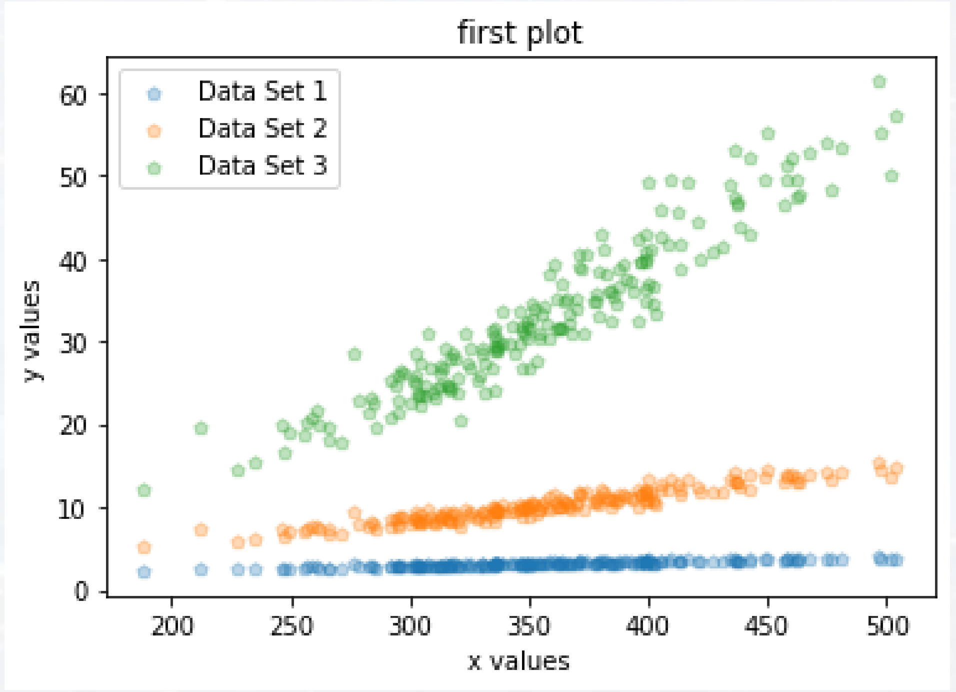
assigns a label to each data set → stored for legend

calling the legend (no input argument)

Data Visualization and File I/O

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



NOPE... IT CAN'T BE DONE ONLINE...
YOU ACTUALLY HAVE TO TAKE THE RAKE OUTSIDE
BISH
TRIBUNE-REVIEW

Outline

Reading/Writing Files

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

Visualization

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

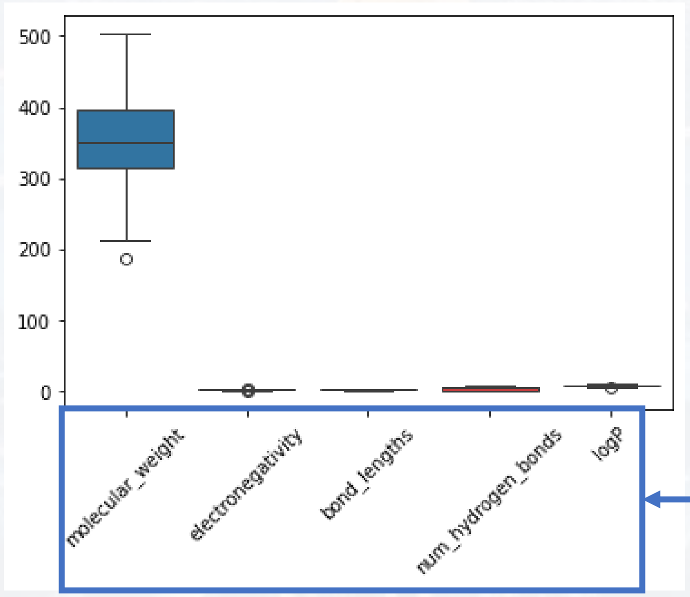
Data Visualization and File I/O

sophisticated plots:

```
import seaborn as sns
```

starting from **data frames** right away

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

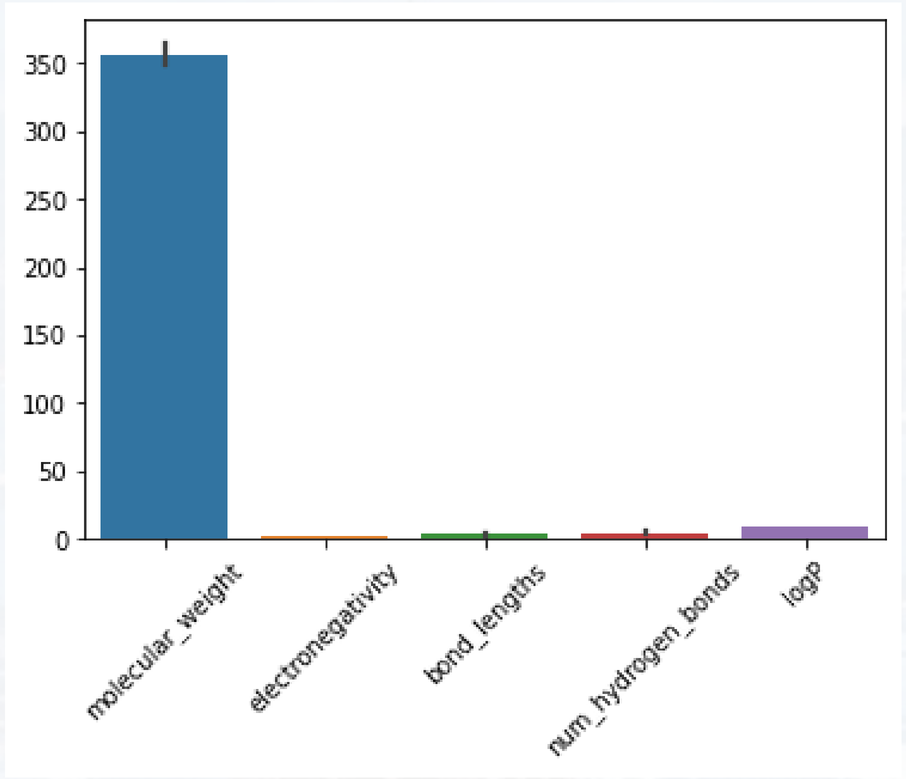


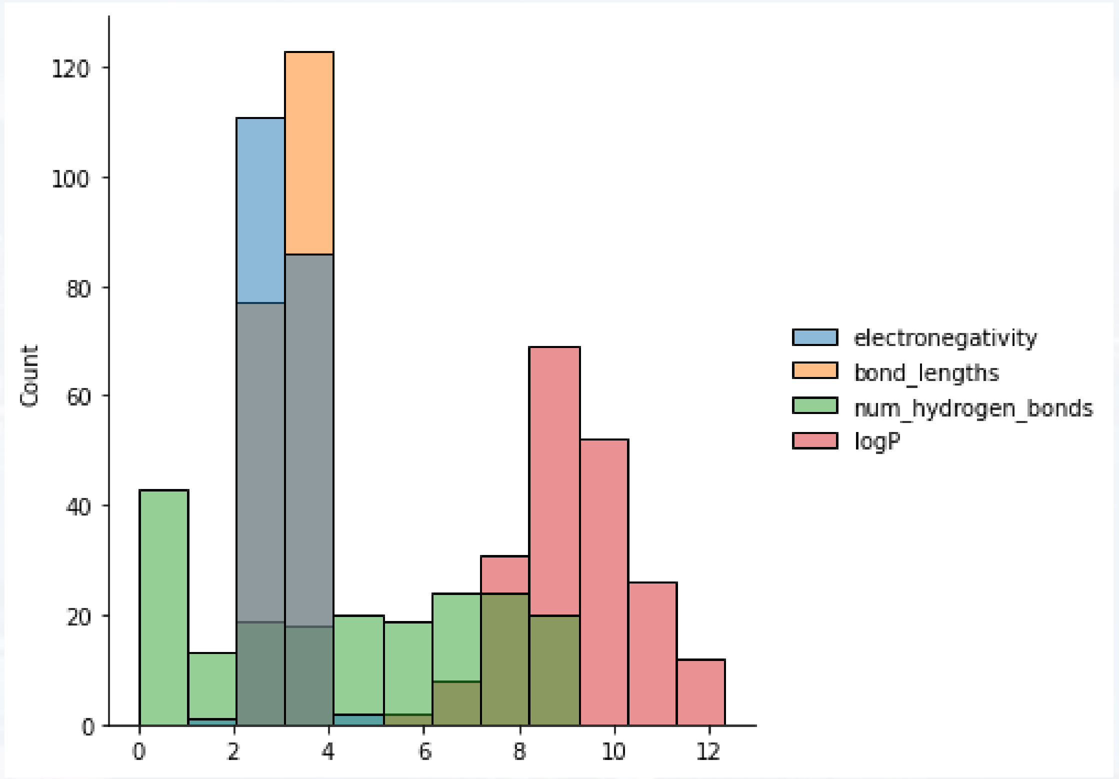
reads labels from data frame

Data Visualization and File I/O

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

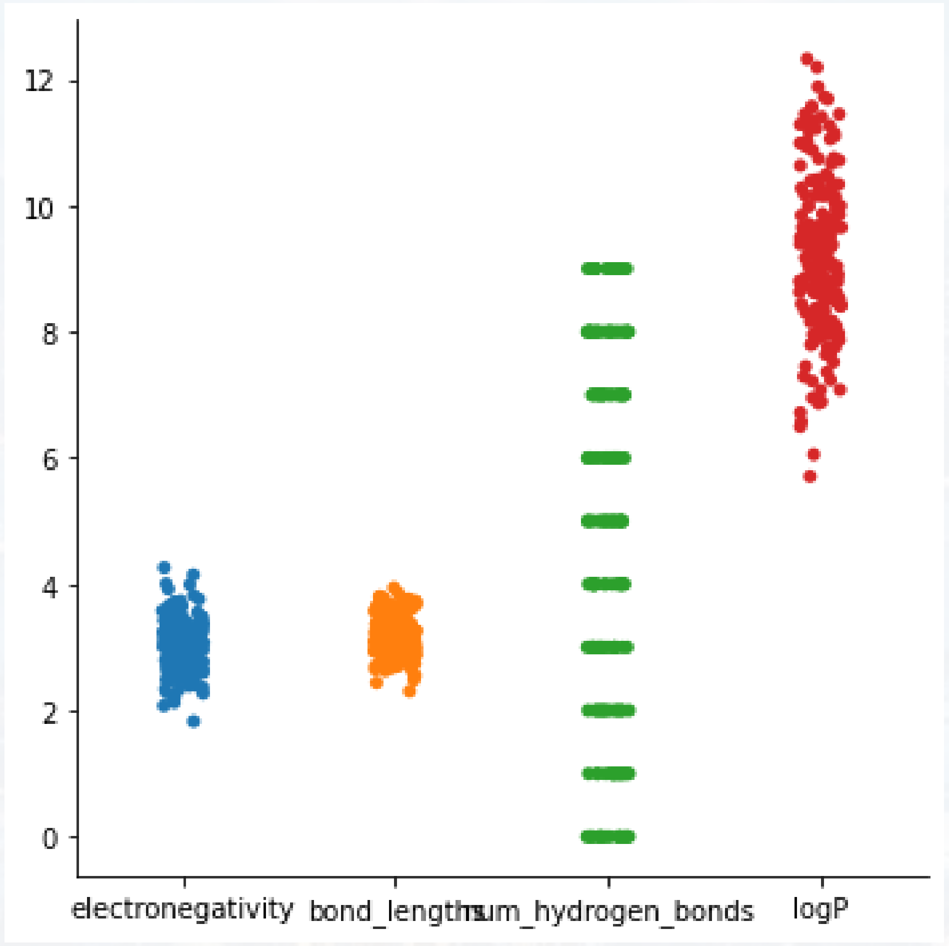
```
sns.displot(Data[Data.columns[1:-1]])
plt.show()
```





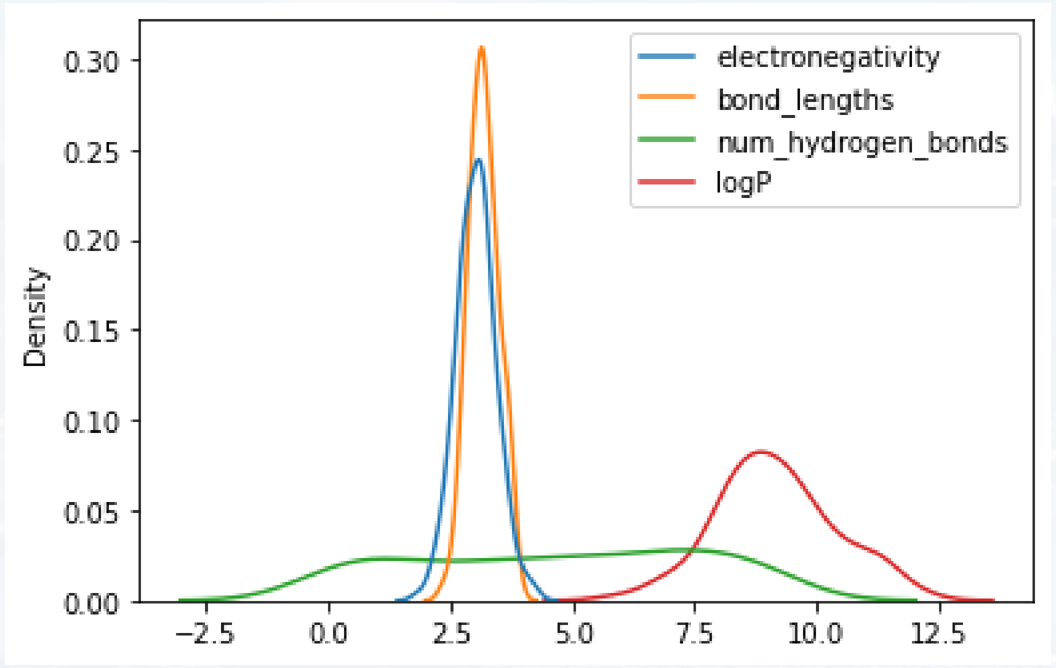
Data Visualization and File I/O

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



Data Visualization and File I/O

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

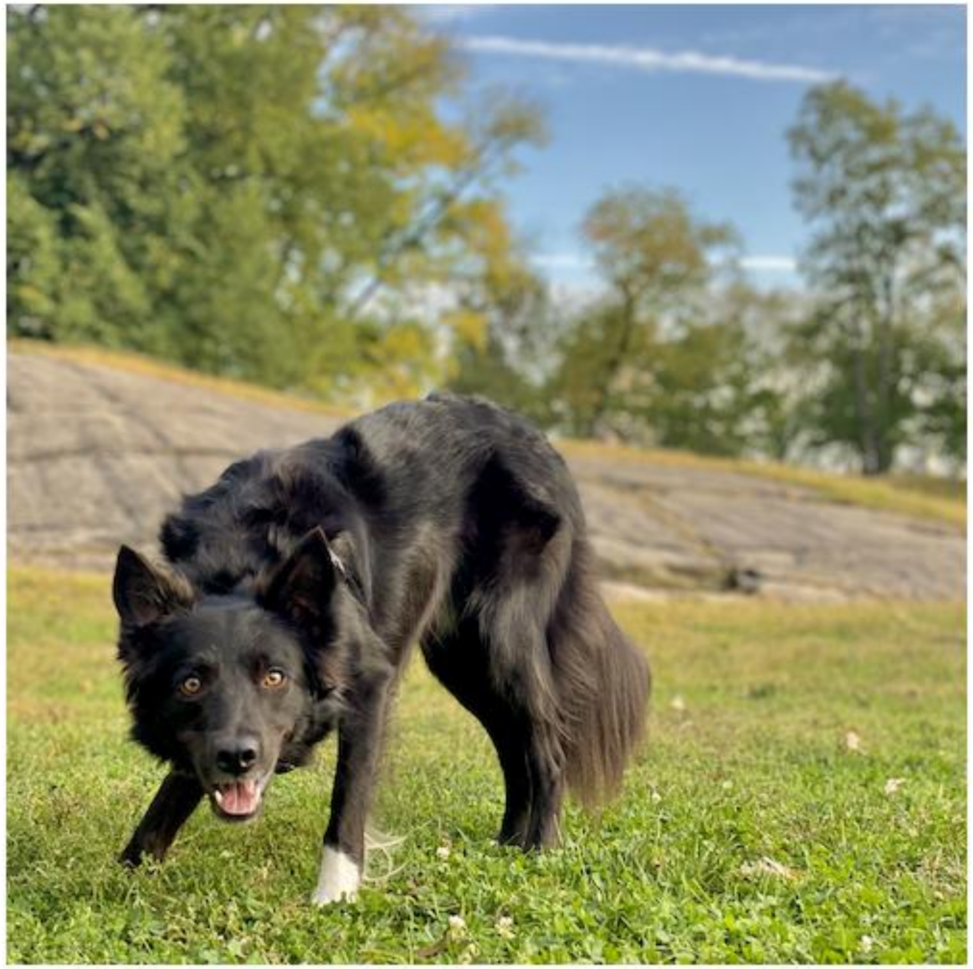


Graph Gallery with examples

Data Visualization and File I/O

```
sns.dogplot()
```

```
sns.dogplot(1)
```



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NOPE... IT CAN'T BE DONE ONLINE... YOU ACTUALLY HAVE TO TAKE THE RAKE OUTSIDE

Outline

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- Faster Alternatives
- More about `.txt`

Visualization

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

Data Visualization and File I/O

`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

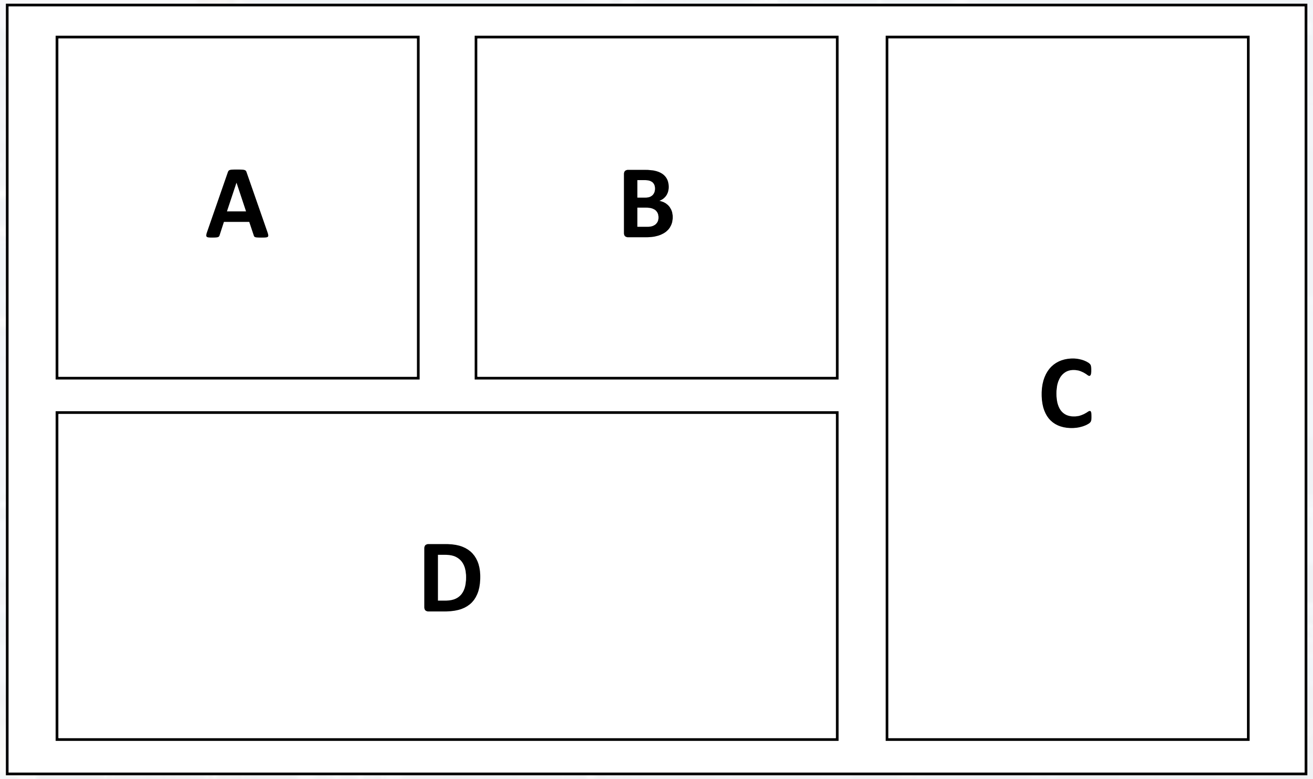
Data Visualization and File I/O

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'],\
                                  ['D', 'D', 'C']], layout = "constrained")
```



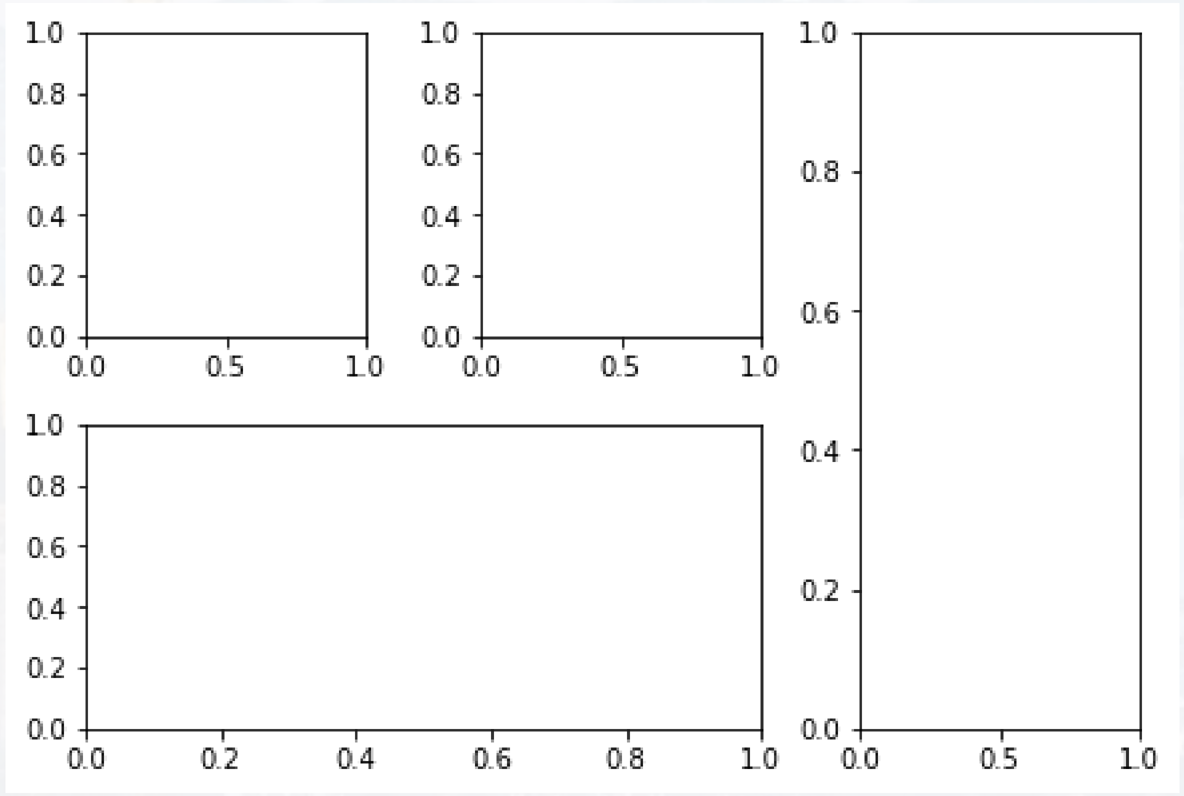
Data Visualization and File I/O

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'],\
                                   ['D', 'D', 'C']], layout = "constrained")
```



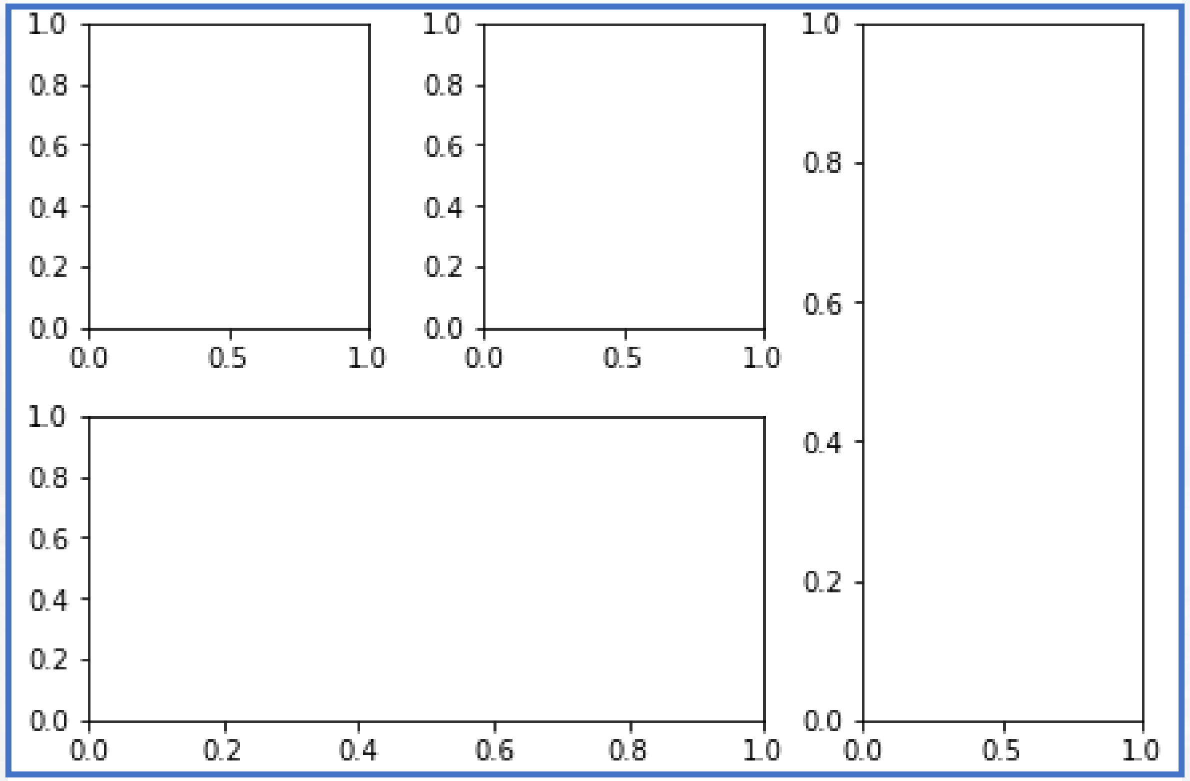
Data Visualization and File I/O

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'],\
                                  ['D', 'D', 'C']], layout = "constrained")
```



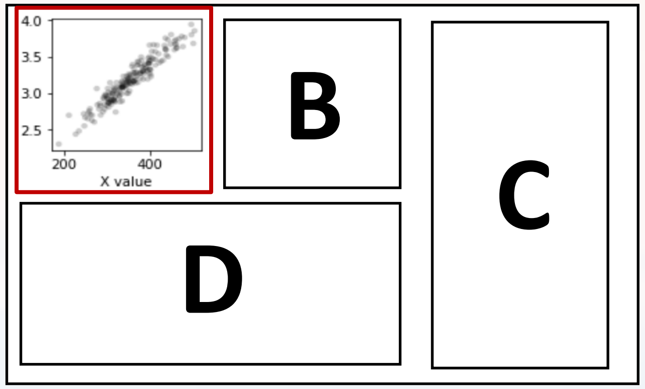
points to the current figure

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



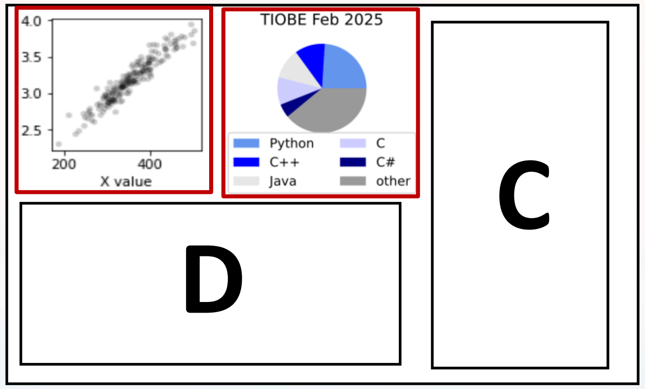
```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\
                                  ['D', 'D', 'C']], layout = "constrained")

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**

Data Visualization and File I/O

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'],\
                                  ['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',\
              '#000080', '#999999'])
axes['B'].set(title = 'TIOBE Feb 2025')
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\
                bbox_to_anchor = (0.5,-0.5), loc = 'lower center',\
                ncol = 2)
```

populating the second axis object with a **pie chart**

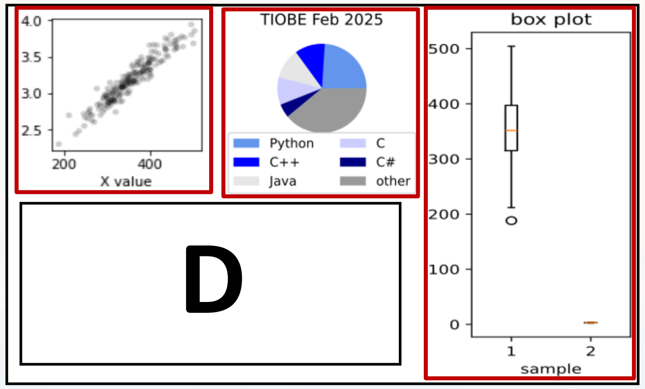
Data Visualization and File I/O

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



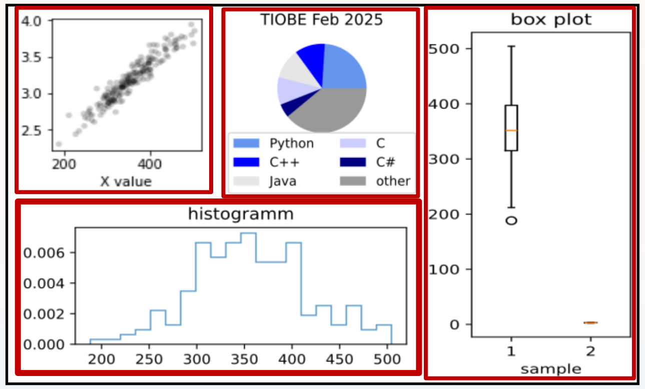
```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\
                                  ['D', 'D', 'C']], layout = "constrained")

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',\
                                                 '#000080', '#999999'])
axes['B'].set(title = 'TIOBE Feb 2025')
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\
                 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')
```

and so on...

Data Visualization and File I/O

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'],\
                                  ['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',\
                                                 '#000080', '#999999'])
axes['B'].set(title = 'TIOBE Feb 2025')
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\
                 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',\
               alpha = 0.75)
axes['D'].set(title = 'histogram')
```

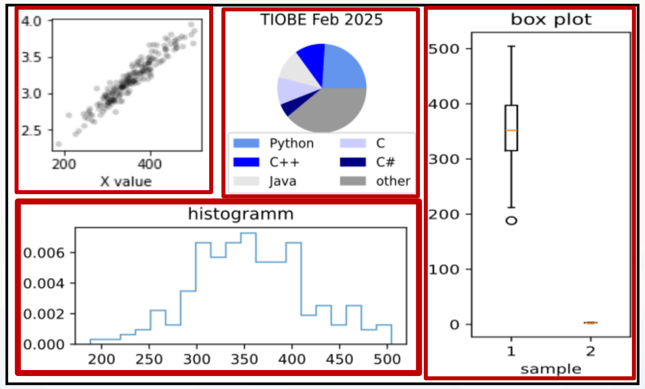
and so on...

Data Visualization and File I/O

Three levels in Python:		
	plt	the plot itself
	ax	referring to axis of specific plot
	fig	referring to a figure

mosaic subplots

classical subplots

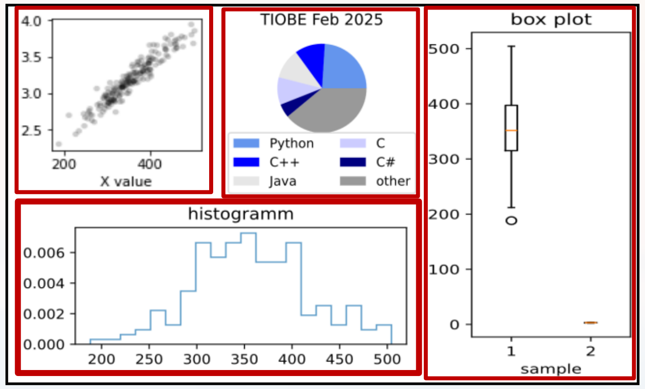


reference to the individual axes

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\
                                  ['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',\
                                                 '#000080', '#999999'])
axes['B'].set(title = 'TIOBE Feb 2025')
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\
                 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',\
          alpha = 0.75)
axes['D'].set(title = 'histogram')
```

Data Visualization and File I/O

Three levels in Python:	plt	the plot itself
	ax	referring to axis of specific plot
	fig	referring to a figure



mosaic subplots

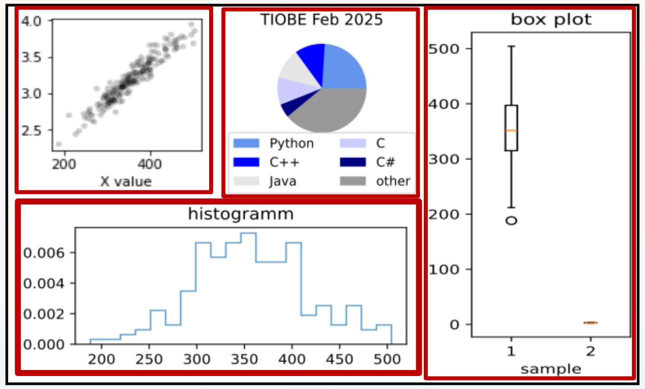
classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\
                                   ['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',\
                                                 '#000080', '#999999'])
axes['B'].set(title = 'TIOBE Feb 2025')
axes['B'].legend(['Python', 'C++', 'Java', 'C', 'C#', 'other'],\
                 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',\
          alpha = 0.75)
axes['D'].set(title = 'histogram')
```

notice the different color codes

Data Visualization and File I/O

Three levels in Python:	plt	the plot itself
	ax	referring to axis of specific plot
	fig	referring to a figure



mosaic subplots

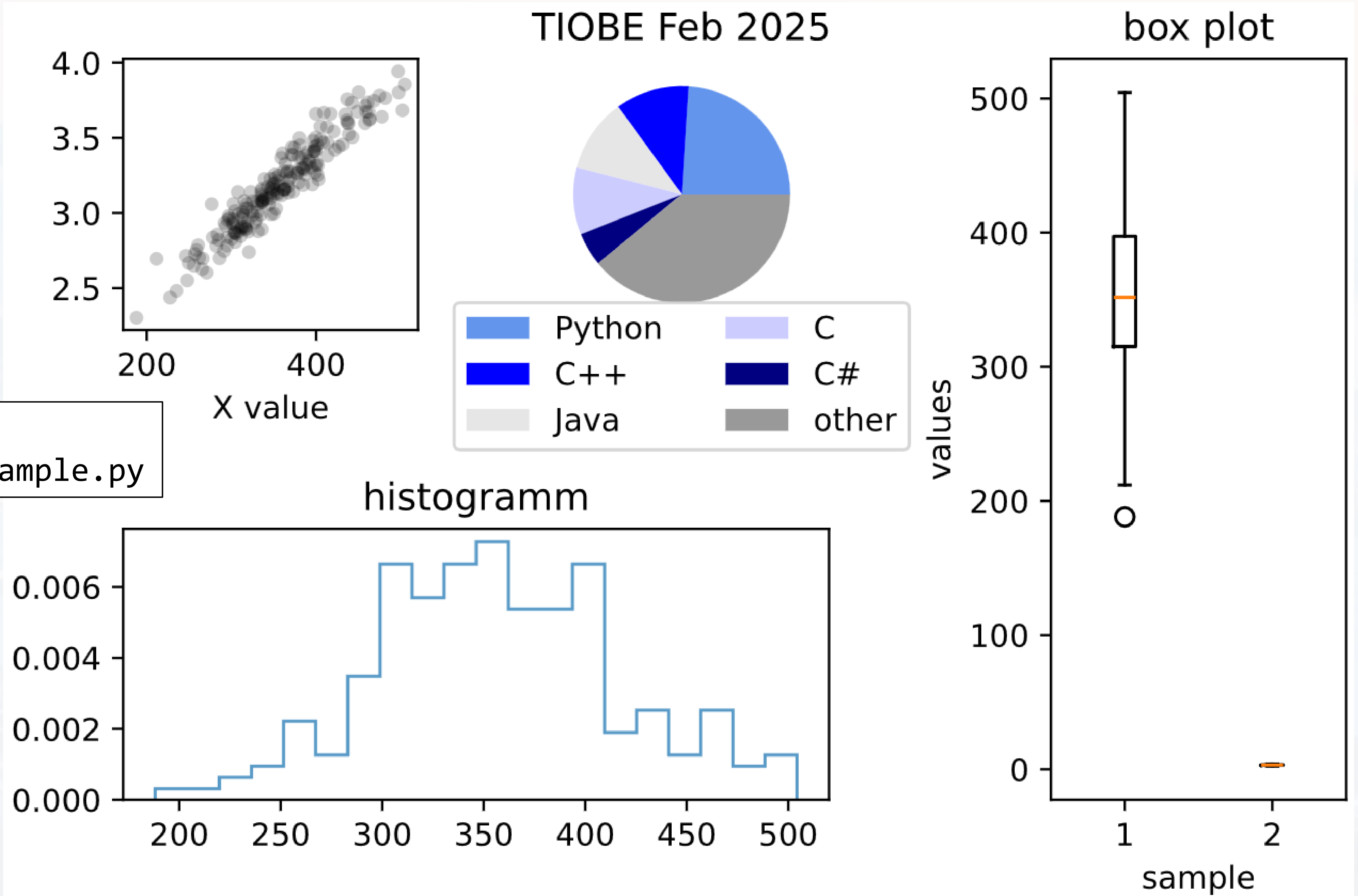
classical subplots

```
figMo, axes = plt.subplot_mosaic([['A', 'B', 'C'],\
                                  ['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',\
         alpha = 0.75)
axes['D'].set(title = 'histogram')


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

referring to the specific figure

Data Visualization and File I/O

`plt, ax, fig`



check out
`PlotMosaicExample.py`

Data Visualization and File I/O

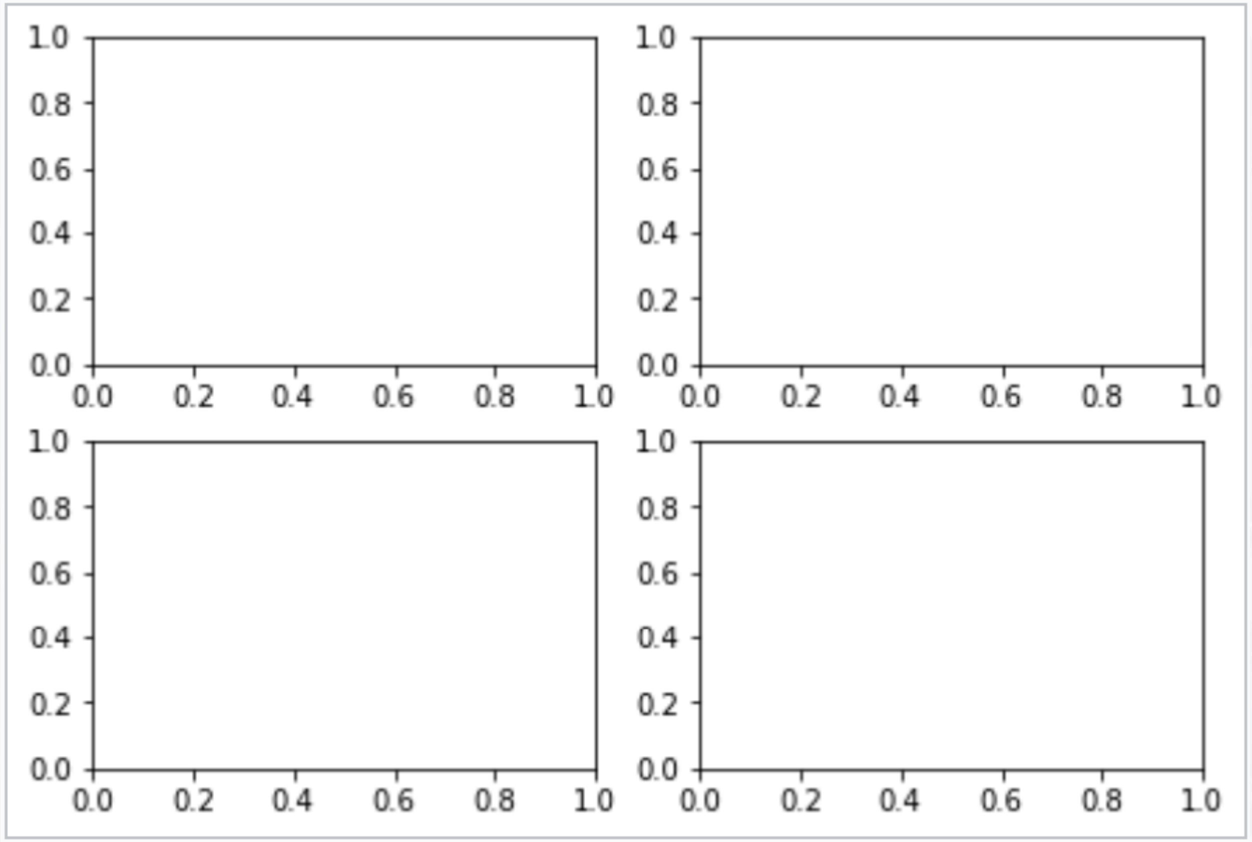
`plt, ax, fig`

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")
```



Data Visualization and File I/O

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!**

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

```
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')
```

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Data Visualization and File I/O

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)

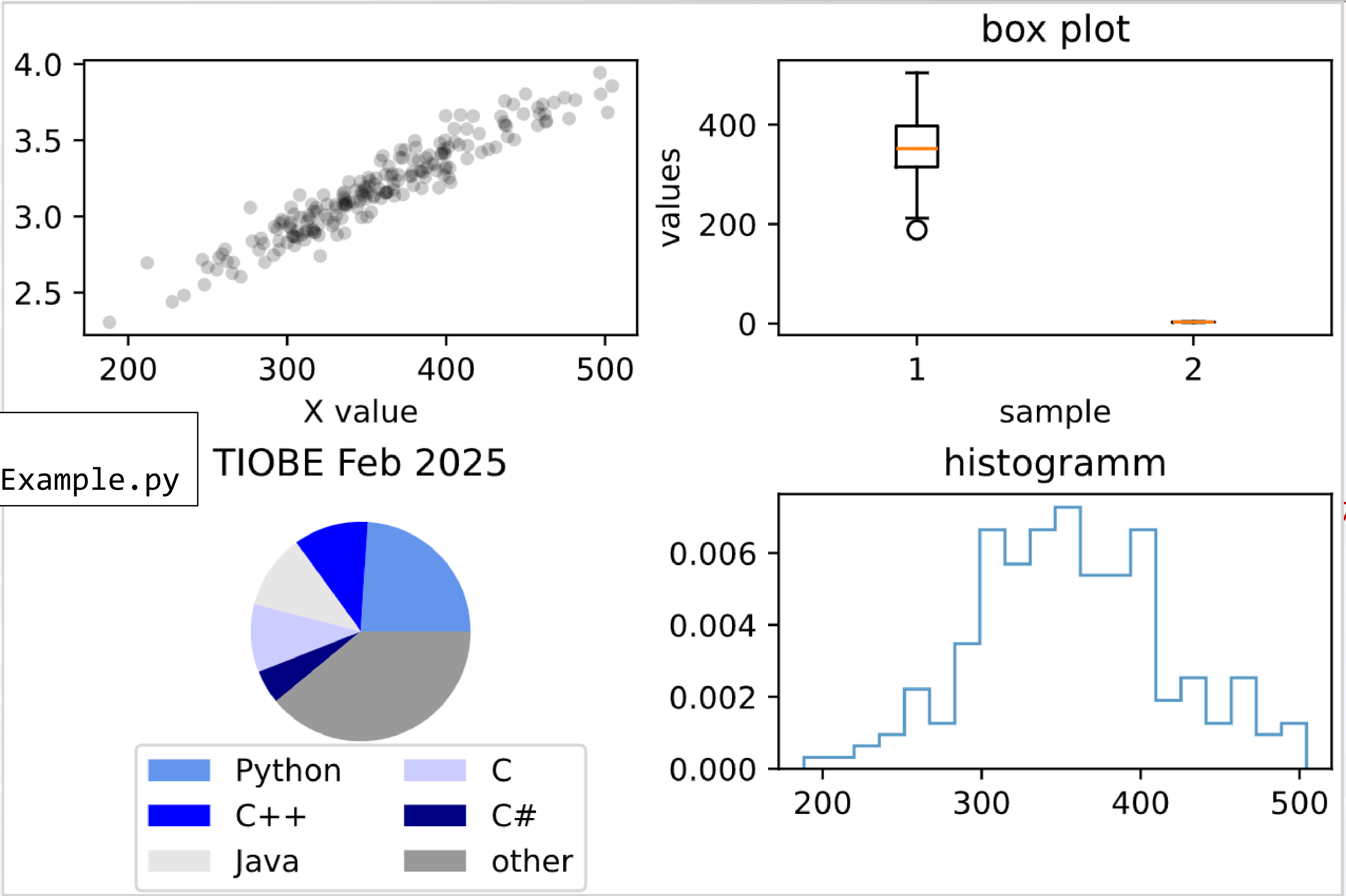
mosaic subplots

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, 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)
```

Data Visualization and File I/O

`plt, ax, fig`



check out
`PlotStandardExample.py`

75)

Thank you very much for your attention!