```python
In [1]: import numpy as np # Numpy is a fundamental package for scientific computation in python. Check it out if you don't kn
        import pandas as pd
        import matplotlib.pyplot as plt
```

Data visualisation with Pandas and Matplotlib

Pandas

import data as dataframe using pandas read_csv

Quick introduction can be found here : https://pandas.pydata.org/docs/user_guide/10min.html

```python
In [2]: data =  pd.read_csv('synth_data.txt',sep=';',names=['angle','intensity'],skiprows=1)
```

```python
In [3]: data
```

Out[3]:

	angle	intensity
0	-5.00000	3.035860
1	-4.98999	2.902397
2	-4.97998	2.890226
3	-4.96997	2.953325
4	-4.95996	2.847500
...	...	...
995	4.95996	2.919206
996	4.96997	2.864416
997	4.97998	2.920909
998	4.98999	2.922681
999	5.00000	2.934428

1000 rows × 2 columns

You can extract the values of this dataframe easily in several ways:

```python
In [4]: data['intensity'], data.intensity #Both give the same result
```

```
Out[4]: (0      3.035860
         1      2.902397
         2      2.890226
         3      2.953325
         4      2.847500
                  ...
         995    2.919206
         996    2.864416
         997    2.920909
         998    2.922681
         999    2.934428
         Name: intensity, Length: 1000, dtype: float64,
         0      3.035860
         1      2.902397
         2      2.890226
         3      2.953325
         4      2.847500
                  ...
         995    2.919206
         996    2.864416
         997    2.920909
         998    2.922681
         999    2.934428
         Name: intensity, Length: 1000, dtype: float64)
```

```python
In [5]: data.intensity.values; #Remove the ';' to see the full glory
```

Pandas has some neat built in functions for some quick maths e.g. to calculate the mean of a column

```python
In [6]: data.intensity.mean(), data.intensity.std(), data.intensity.min(), data.intensity.max()
```

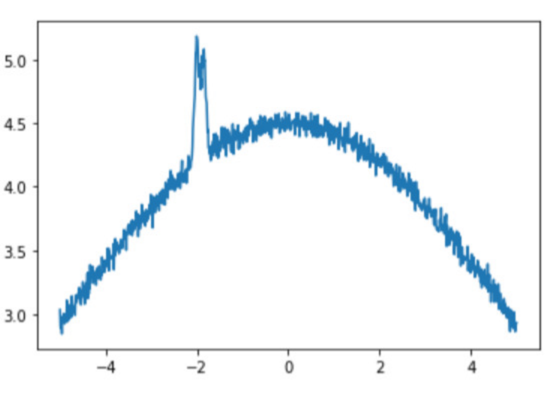
```
Out[6]: (3.9435234416869105, 0.5162251051659121, 2.847500417321436, 5.184228915730239)
```

Matplotlib pyplot

You can plot (and save) data easily using matplotlib pyplot https://matplotlib.org/stable/tutorials/introductory/pyplot.html

```python
In [7]: plt.plot(data['angle'],data['intensity'])
```

```
Out[7]: [<matplotlib.lines.Line2D at 0x21f03196df0>]
```

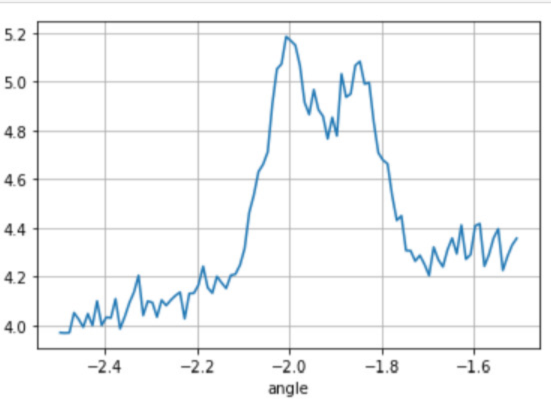


Select data of first peak using pandas.query

```python
In [8]: data_1st_peak = data.query('-2.5<angle<-1.5')
```

You can easily adjust your plot and give it labels for example. For details have a look at the documentation and remember: Google is your friend

```python
In [9]: plt.plot(data_1st_peak['angle'],data_1st_peak['intensity'])
        plt.xlabel('angle')
        plt.grid()
```



Fitting data using lmfit

Define the function that we want to model. Note that the most common functions are usually included in lmfit already.

```python
In [10]: def Gaussian(x, a, x0, sigma, offset=0):
             """
             1-dimensional Gaussian distribution

             Parameters
             ----------
             x : np.array
                 Coordinates
             a : float
                 Amplitude
             x0 : float
                 Center
             sigma : float
                 Standard deviation
             offset : float, optional
                 Absolute offset value, defaults to 0

             Returns
             -------
             np.array
             """
             gauss = a * (1 / (sigma * np.sqrt(2 * np.pi))) * np.exp(-0.5 * np.square((x-x0)/sigma))
             return offset + gauss
```

```python
In [11]: def Double_Gaussian_lin_off(x,a1,x01,sigma1,a2,x02,sigma2,ax,bx):
             '''Sum of two Gaussians and a linear offset
             '''
             return Gaussian(x,a1,x01,sigma1)+Gaussian(x,a2,x02,sigma2)+ax*x+bx
```

Use lmfit to model data

```python
In [12]: import lmfit
```

Quick introduction to lmfit: https://lmfit.github.io/lmfit-py/model.html

```python
In [13]: gmodel = lmfit.Model(Double_Gaussian_lin_off)
```

```python
In [14]: print(f'parameter names: {gmodel.param_names}')
         print(f'independent variables: {gmodel.independent_vars}')
```

```
parameter names: ['a1', 'x01', 'sigma1', 'a2', 'x02', 'sigma2', 'ax', 'bx']
independent variables: ['x']
```

Set the initial parameters for our model

```python
In [15]: init_params = dict(a1=0.11, x01=-2, sigma1=0.04,
                            a2=0.11, x02=-1.85, sigma2=0.04,
                            ax=0, bx=4)
```

```python
In [16]: params = gmodel.make_params(**init_params)
```

```python
In [17]: params
```

Out[17]:

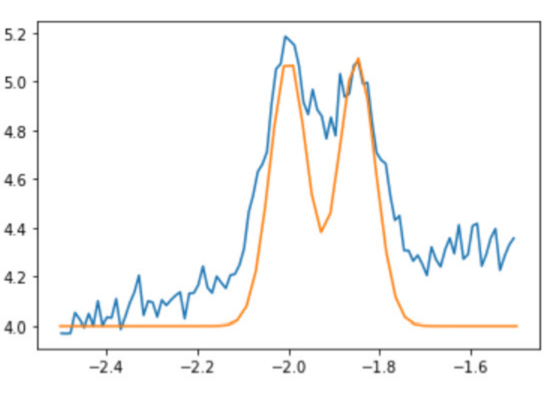
name	value	initial value	min	max	vary
a1	0.11000000	None	-inf	inf	True
x01	-2.00000000	None	-inf	inf	True
sigma1	0.04000000	None	-inf	inf	True
a2	0.11000000	None	-inf	inf	True
x02	-1.85000000	None	-inf	inf	True
sigma2	0.04000000	None	-inf	inf	True
ax	0.00000000	None	-inf	inf	True
bx	4.00000000	None	-inf	inf	True

Test our model guess to see if it roughly fits the data

```python
In [18]: x_eval = np.linspace(-2.5,-1.5)
         y_eval = gmodel.eval(x=x_eval,params = params)
```

```python
In [19]: plt.plot(data_1st_peak['angle'],data_1st_peak['intensity'])
         plt.plot(x_eval,y_eval)
```

```
Out[19]: [<matplotlib.lines.Line2D at 0x21f0d6f9940>]
```



Now perform the actual fit with our parameter guess

```python
In [20]: result = gmodel.fit(data=data_1st_peak['intensity'], params=params, x=data_1st_peak['angle'])
```

retrieve the parameters and their uncertainties from the fit

```python
In [21]: result.params
```

Out[21]:

name	value	standard error	relative error	initial value	min	max	vary
a1	0.12589582	0.00557085	(4.42%)	0.11	-inf	inf	True
x01	-2.00066809	0.00247830	(0.12%)	-2	-inf	inf	True
sigma1	0.05319513	0.00238031	(4.47%)	0.04	-inf	inf	True
a2	0.09771845	0.00558466	(5.72%)	0.11	-inf	inf	True
x02	-1.85089183	0.00283757	(0.15%)	-1.85	-inf	inf	True
sigma2	0.04933394	0.00267577	(5.42%)	0.04	-inf	inf	True
ax	0.32966960	0.01989471	(6.03%)	0	-inf	inf	True
bx	4.84270815	0.04140036	(0.85%)	4	-inf	inf	True

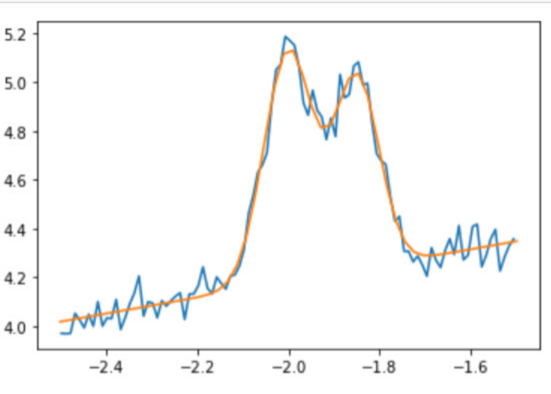
Extracting the actual value (and its uncertainty) of a fitted parameter is a bit tricky but works as follows:

```python
In [22]: result.params['x01'].value, result.params['x01'].stderr
```

```
Out[22]: (-2.0006680890686153, 0.0024782961672320646)
```

Compare fit to data and save the plot

```python
In [23]: plt.plot(data_1st_peak['angle'],data_1st_peak['intensity'])
         plt.plot(x_eval,result.eval(params=result.params,x=x_eval))
         plt.savefig('fitted_data.png')
```



recieve the fit report that includes a lot of interesting parameters like red. chi-square

```python
In [24]: result
```

Out[24]:

Model

Model(Double_Gaussian_lin_off)

Fit Statistics

fitting method	leastsq
# function evals	46
# data points	100
# variables	8
chi-square	0.26870287
reduced chi-square	0.00292068
Akaike info crit.	-575.931928
Bayesian info crit.	-555.090567

Variables

name	value	standard error	relative error	initial value	min	max	vary
a1	0.12589582	0.00557085	(4.42%)	0.11	-inf	inf	True
x01	-2.00066809	0.00247830	(0.12%)	-2	-inf	inf	True
sigma1	0.05319513	0.00238031	(4.47%)	0.04	-inf	inf	True
a2	0.09771845	0.00558466	(5.72%)	0.11	-inf	inf	True
x02	-1.85089183	0.00283757	(0.15%)	-1.85	-inf	inf	True
sigma2	0.04933394	0.00267577	(5.42%)	0.04	-inf	inf	True
ax	0.32966960	0.01989471	(6.03%)	0	-inf	inf	True
bx	4.84270815	0.04140036	(0.85%)	4	-inf	inf	True

Correlations (unreported correlations are < 0.100)

ax	bx	0.9855
a1	sigma1	0.8545
a2	sigma2	0.8535
a1	x02	0.7481
x01	a2	-0.7469
sigma1	x02	0.7272
x01	x02	0.7249
x01	sigma2	-0.7173
sigma1	a2	-0.6749
a1	a2	-0.6608
a1	sigma2	-0.6498
a1	x01	0.6434
a2	x02	-0.6307
x01	sigma1	0.6290
x02	sigma2	-0.6026
sigma1	sigma2	-0.5967
a2	bx	-0.2953
a2	ax	-0.2593
sigma2	bx	-0.2154
sigma2	ax	-0.1952

If you have questions or feedback regarding this notebook please feel free to write an email to nk7@uni-bonn.de . Cheers, Nick