Python for biologists

Tutorial 2 - Read, process, and plot biological data

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In this tutorial you learn how to read data frames with python and how to select, transform, analyze, and plot the data. You can find a data file named `petal_sepal_length.txt` in the tutorial folder. This file contains the measured lengths of petals and sepals of 50 individuals of the plant species `Iris pythonica` (fake data). All individuals are classified as the same species and we want to test if we can find any clustering of these characters or if they are continuously distributed. Some of the following steps are not necessary for this purpose but are meant to provide some useful commands which can be used in many different situations.

1. Installation

For this tutorial we will need several addiitonal packages which you can install from your bash command line like this:

```
pip install pandas
pip install matplotlib
pip install sklearn
```

2. Use pandas to read a dataframe

Use the `read_csv()` function to read the csv file. You have to specify how the cells in the file are delimited (`,` is the default), which in this case is tab-delimited (`\t`).

Note: the pandas library also has a very hand `read_excel()` function which can be used to read excel files directly (no exporting of data in csv format necessary). Try it out if you have some excel file on your computer that you want to read into python.

In [4]:

```
import pandas as pd
data = pd.read_csv('../data/petal_sepal_length.txt',sep='\t')
```

View the first 10 lines of the dataframe using `head()` .

In [5]:

```
data.head(10)
```

Out[5]:

	sample_name	petal_length	sepal_length
0	sample1	2.037214	5.172704
1	sample2	4.915837	6.149615
2	sample3	1.614314	5.939969
3	sample4	1.525709	6.603432
4	sample5	3.729975	6.065105
5	sample6	0.778760	5.173370
6	sample7	5.291489	7.381162
7	sample8	5.486099	6.529424
8	sample9	1.588885	5.447183
9	sample10	3.506057	5.821899

Use the .iloc() function to extract a specific cell form the dataframe, e.g. the 2nd cell in the 2nd column (remember that python indexing starts with 0, so the element we want to print has the index 1,1):

```
In [6]: data.iloc[1,1]
```

```
Out[6]: 4.915837058559057
```

Check the column names of the dataframe:

```
In [7]: data.columns
```

```
Out[7]: Index(['sample_name', 'petal_length', 'sepal_length'], dtype='object')
```

Extract one of the columns by name. You can either do it this way:

```
In [8]: data.petal_length
```

```
Out[8]: 0     2.037214
        1     4.915837
        2     1.614314
        3     1.525709
        4     3.729975
        5     0.778760
        6     5.291489
        7     5.486099
        8     1.588885
        9     3.506057
        10    1.034731
        11    3.918415
        12    4.704223
        13    1.274312
        14    4.027879
        15    1.052670
        16    5.124328
        17    0.727854
        18    1.889160
        19    5.857770
        20    0.982377
        21    1.642252
        22    1.813812
        23    1.675574
        24    1.402000
        25    5.010073
        26    1.547179
        27    5.583385
        28    5.602358
        29    0.999512
        30    6.357546
        31    1.598450
        32    6.383405
        33    3.502309
        34    1.489134
        35    1.414486
        36    4.695659
        37    4.314651
        38    4.332901
        39    5.355377
        40    4.215726
        41    5.547972
        42    4.877986
        43    1.992262
        44    1.514988
        45    1.624965
        46    1.600432
        47    1.437563
        48    1.549250
        49    5.113597
        Name: petal_length, dtype: float64
```

Or this way:

```
In [9]: data['petal_length']
```

```
Out[9]: 0     2.037214
        1     4.915837
        2     1.614314
        3     1.525709
        4     3.729975
        5     0.778760
        6     5.291489
        7     5.486099
        8     1.588885
        9     3.506057
        10    1.034731
        11    3.918415
        12    4.704223
        13    1.274312
        14    4.027879
        15    1.052670
        16    5.124328
        17    0.727854
        18    1.889160
        19    5.857770
        20    0.982377
        21    1.642252
        22    1.813812
        23    1.675574
        24    1.402000
        25    5.010073
        26    1.547179
        27    5.583385
        28    5.602358
        29    0.999512
        30    6.357546
        31    1.598450
        32    6.383405
        33    3.502309
        34    1.489134
        35    1.414486
        36    4.695659
        37    4.314651
        38    4.332901
        39    5.355377
        40    4.215726
        41    5.547972
        42    4.877986
        43    1.992262
        44    1.514988
        45    1.624965
        46    1.600432
        47    1.437563
        48    1.549250
        49    5.113597
        Name: petal_length, dtype: float64
```

Check length of dataframe:

```
In [10]: len(data)
```

```
Out[10]: 50
```

3. Transform and filter data frame:

Sort the dataframe by one of the column values, e.g. by the column `petal_length` .

In the example command I'm not storing the sorted dataframe, but am simply printing it to the screen. If you want to store the sorted dataframe, you can define the sorted dataframe as a new variable or use the `inplace=True` flag inside the command.

In [15]:

```
data.sort_values(by=['petal_length'],ascending=False).head(15)
```

Out[15]:

	sample_name	petal_length	sepal_length
32	sample33	6.383405	5.473322
30	sample31	6.357546	6.109699
19	sample20	5.857770	4.775423
28	sample29	5.602358	5.734823
27	sample28	5.583385	6.768361
41	sample42	5.547972	6.519929
7	sample8	5.486099	6.529424
39	sample40	5.355377	6.257550
6	sample7	5.291489	7.381162
16	sample17	5.124328	5.799524
49	sample50	5.113597	5.029044
25	sample26	5.010073	6.460642
1	sample2	4.915837	6.149615
42	sample43	4.877986	5.499600
12	sample13	4.704223	6.241321

Let's say we want to find those samples, which have a petal length of more than 5. We can do that rather easily with pandas, using some simple indexing. If we use the square brackets `[]` it basically translates into "extract those elements where condition is fulfilled":

In [16]:

```
data[data.petal_length>5]
```

Out[16]:

	sample_name	petal_length	sepal_length
6	sample7	5.291489	7.381162
7	sample8	5.486099	6.529424
16	sample17	5.124328	5.799524
19	sample20	5.857770	4.775423
25	sample26	5.010073	6.460642
27	sample28	5.583385	6.768361
28	sample29	5.602358	5.734823
30	sample31	6.357546	6.109699
32	sample33	6.383405	5.473322
39	sample40	5.355377	6.257550
41	sample42	5.547972	6.519929
49	sample50	5.113597	5.029044

Now let's store the data from the dataframe into lists:

In [17]:
```
petal_list = list(data.petal_length)
sepal_list = list(data.sepal_length)
```

4. Plot the data

In order to plot in python you need to import the library `matplotlib.pyplot` .

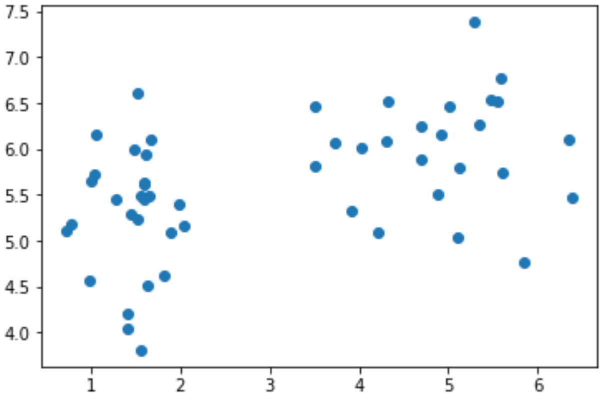
Import the matplotlib.pyplot library and activate the plotting option in the jupyter notebook (activation not required if you are working in spyder).

In [18]:
```
import matplotlib.pyplot as plt
%matplotlib inline
```

Now plot the data as a scatter plot

In [19]:
```
plt.scatter(petal_list,sepal_list)
```

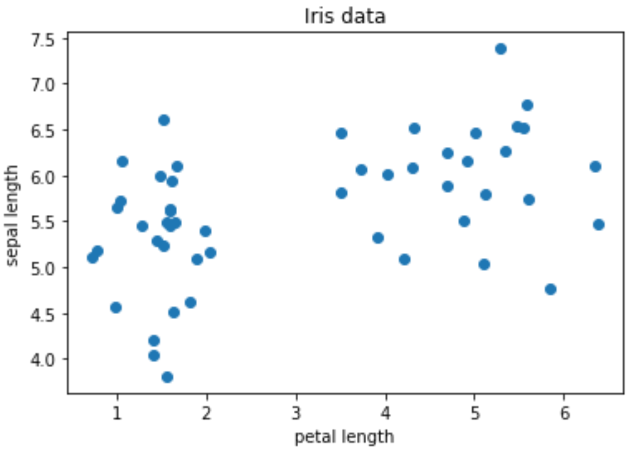
Out[19]:
```
<matplotlib.collections.PathCollection at 0x1221cf990>
```



You can modify the plot by adding labels to the axis. In python the plot is being modified in "layers", which means, every modification/addition is stated in a new line:

In [20]:
```
plt.scatter(petal_list,sepal_list)
plt.xlabel('petal length')
plt.ylabel('sepal length')
plt.title('Iris data')
```

Out[20]:
```
Text(0.5, 1.0, 'Iris data')
```



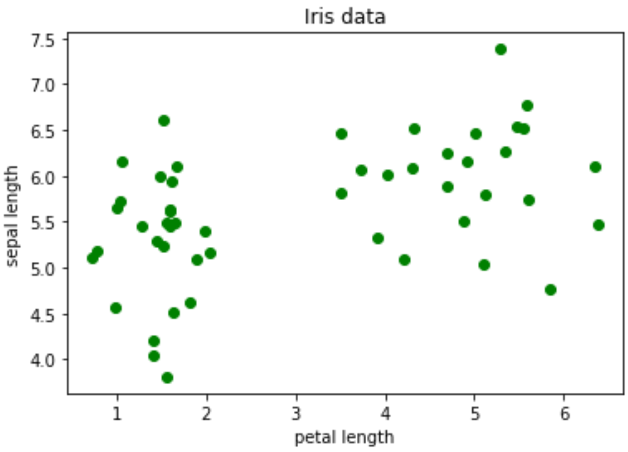
You can change the color of the plot like this:

In [21]:

```
plt.scatter(petal_list,sepal_list,color='green')
plt.xlabel('petal length')
plt.ylabel('sepal length')
plt.title('Iris data')
```

Out[21]:

```
Text(0.5, 1.0, 'Iris data')
```



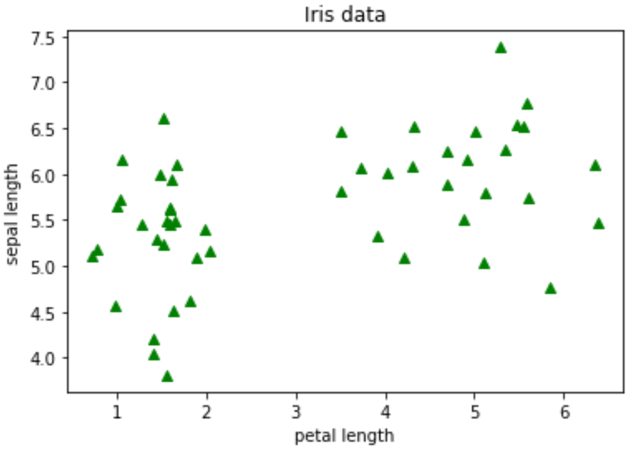
Or change the shape of the plotted points:

In [22]:

```
plt.scatter(petal_list,sepal_list,color='green',marker='^')
plt.xlabel('petal length')
plt.ylabel('sepal length')
plt.title('Iris data')
```

Out[22]:

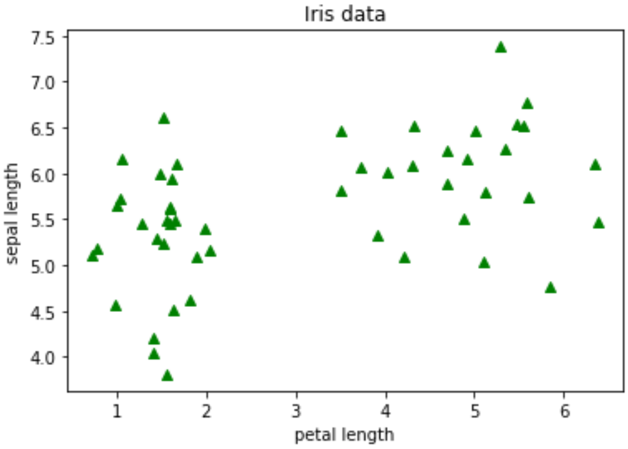
```
Text(0.5, 1.0, 'Iris data')
```



If you want to save a plot as a figure, you first need to define a figure object and after all your plotting commands you can use the function `savefig()`

In [23]:

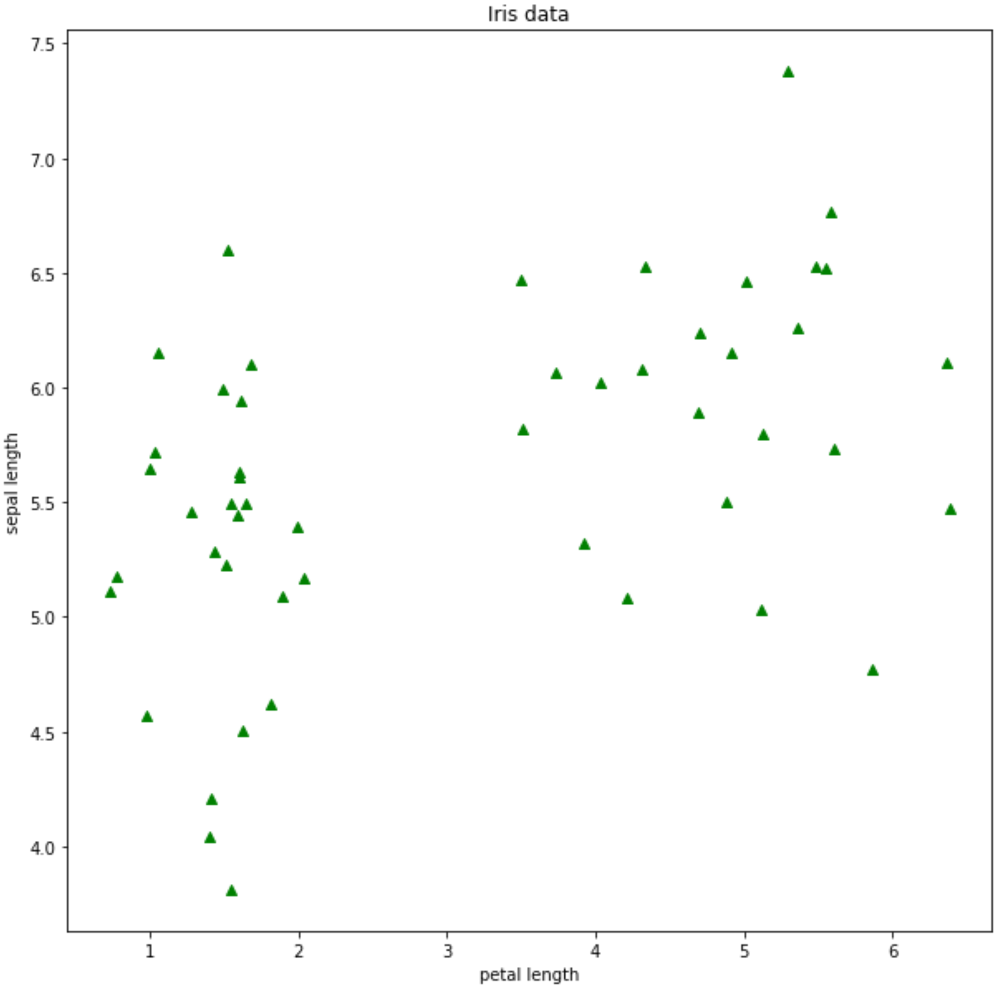
```
fig = plt.figure()
plt.scatter(petal_list,sepal_list,color='green',marker='^')
plt.xlabel('petal length')
plt.ylabel('sepal length')
plt.title('Iris data')
fig.savefig('./scatter_plot.pdf',bbox_inches='tight', dpi = 500)
```



You can adjust the figure size using the `figsize=()` argument inside the `plt.figure()` function:

In [25]:

```
fig = plt.figure(figsize=(10,10))
plt.scatter(petal_list,sepal_list,color='green',marker='^')
plt.xlabel('petal length')
plt.ylabel('sepal length')
plt.title('Iris data')
fig.savefig('../output_files/scatter_plot.pdf',bbox_inches='tight', dpi = 500)
```



5. Identify clusters

We can see in the plots above that the data points seem to cluster into two separate clusters (maybe representing separate populations or cryptic species. We can use the kmeans algorithm to identify clusters and automatically assign the data points belonging to each cluster. For this we use the `sklearn` python library, which contains many useful machine learning algorithms.

Before we can use the `KMeans()` function of this library we need to slightly transform our data. This function want the data in tuple format, which means every datapoint should be contained in a seaprate tuple, which looks like this `(x_value1, y_value1), (x_value2, y_value2), ...` .

Currently our data is in list format, looking like this `[x_value1,x_value2,...]` and `[y_value1,y_value2,...]` . To transform these lists into the desired format we can use the `zip()` function. The zip function returns an object which we have to transform into a list again to make it visible, which we can do with the `list()` function:

In [26]:
```
tuple_data = list(zip(petal_list, sepal_list))
print(tuple_data)
```

```
[(2.037213545574565, 5.172704440755738), (4.915837058559057, 6.149615365303662),
(1.6143144404422318, 5.939969222731516), (1.5257094629553694, 6.60343155818193
8), (3.7299754141452683, 6.065105089620714), (0.7787600224579809, 5.173369526730
656), (5.291488606290831, 7.381162369515891), (5.486099357579179, 6.529423906221
606), (1.5888847511006476, 5.447182516437644), (3.506056546470821, 5.82189871198
8933), (1.0347308723897142, 5.719114159495453 5), (3.9184146064300767, 5.32433750
535842), (4.704222691916959, 6.241320619454233), (1.2743118663460602, 5.46019514
5790823), (4.027879380970228, 6.018648753254772), (1.0526702377383088, 6.1491582
372113704), (5.124327526301326, 5.799524450012601), (0.7278537859299755, 5.11105
45058489665), (1.889159752975209, 5.09323743199745), (5.8577698329937276, 4.7754
23113784206), (0.9823765564976252, 4.5701405527312895), (1.642251547933402, 5.49
6335497225293), (1.8138118759285808, 4.62066074530137), (1.6755744474602847, 6.0
98174133374835), (1.4019996878544254, 4.044936687505984), (5.010073235092442, 6.
460642131711677), (1.5471793166899546, 3.81078255673585), (5.583384761827779, 6.
768361361219995), (5.602358230386057, 5.734823297994679), (0.999512446749096, 5.
644809160886201), (6.357546048970175, 6.1096992728792765), (1.5984496681847908,
5.633241635573474), (6.383405004182108, 5.473321810175103), (3.502308512726084,
6.4668535112453975), (1.4891339583350467, 5.992310194737472), (1.414486358056965
8, 4.2119740358904725), (4.695659246296348, 5.8898347763694945), (4.314650886027
9305, 6.078577681601839), (4.332901307434329, 6.525604264626423), (5.35537688921
0996, 6.257550125001438), (4.215725527898536, 5.083585059284203), (5.54797209958
0166, 6.519929044689162), (4.877986170333111, 5.499600054451635), (1.99226235756
93024, 5.392825131125007), (1.514988105180589, 5.229604218306541), (1.6249645875
023282, 4.50732836329002), (1.6004321884727593, 5.609623442827154), (1.437563393
8613075, 5.288216939487398), (1.5492498365689618, 5.496505964948804), (5.1135973
948012285, 5.029043605683267)]
```

Now we are ready to run the KMeans() function on our transformed tuple data. We have to provide how many clusters we believe there are in the data. Let's go with `2` for now (`n_clusters=2`):

In [27]:
```
from sklearn.cluster import KMeans

kmeans = KMeans(n_clusters=2).fit(tuple_data)
```

The output of the `KMeans()` command is stored as a variable which we named `kmeans` . From this variable we can extract the labels, which is the assignment of our data points to cluster 0 or cluster 1:

In [28]:
```
kmeans.labels_
```

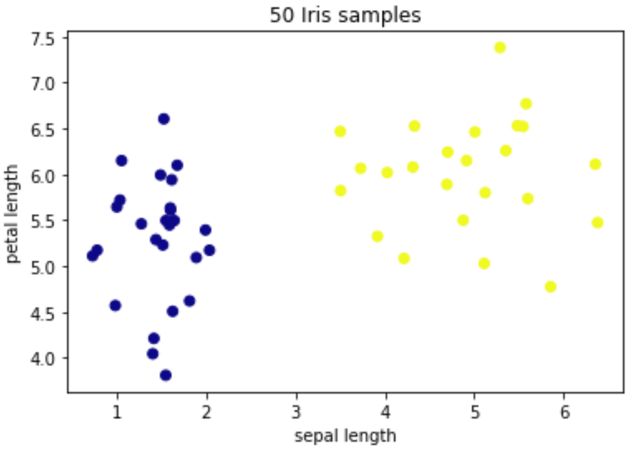
Out[28]:
```
array([0, 1, 0, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 0, 0, 1, 0, 0,
       0, 0, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1, 0,
       0, 0, 0, 0, 0, 1], dtype=int32)
```

We can use that label array to color the points accordingly, using the `c=` flag in the `scatter()` function. Let's save the label array as a new variable `labels` which we then parse into the `scatter()` function:

In [29]:
```
labels = kmeans.labels_

plt.scatter(petal_list,sepal_list,c=labels,cmap='plasma')
plt.xlabel('sepal length')
plt.ylabel('petal length')
plt.title('50 Iris samples')
```

Out[29]:
```
Text(0.5, 1.0, '50 Iris samples')
```



From the kmeans output you can also export the center points of each cluster. These are stored as the values `cluster_centers_` in the kmeans output:

In [30]:
```
center0,center1 = kmeans.cluster_centers_
print(center0)
print(center1)
```

```
[1.45414789 5.289111  ]
[4.89395901 6.00016191]
```

You can plot a point (or a list of points) using the `plot()` function. The `plot()` function needs the input data as x and y coordinates (`plot(x_coord,y_coord)`). Since our variables contain the x and y coordinates for each modpoint, we can plot each of these points by typing `plt.plot(center0[0],center0[1])` and `plt.plot(center1[0],center1[1]` respectively:

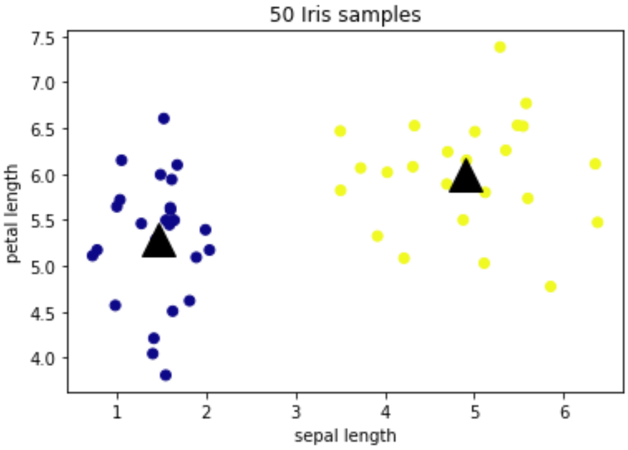
In [31]:

```
plt.scatter(petal_list,sepal_list,c=labels,cmap='plasma')
plt.plot(center0[0],center0[1],marker='^',color='black',markersize=20)
plt.plot(center1[0],center1[1],marker='^',color='black',markersize=20)

plt.xlabel('sepal length')
plt.ylabel('petal length')
plt.title('50 Iris samples')
```

Out[31]:

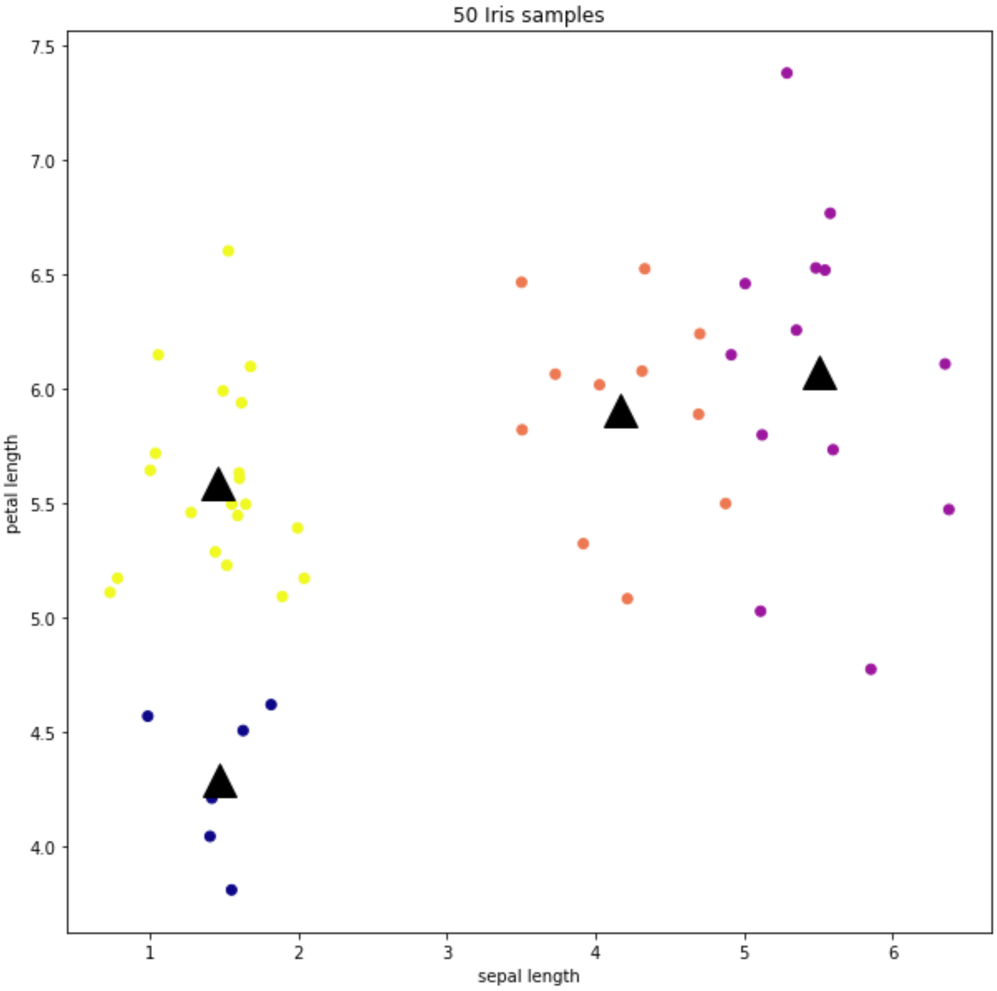
```
Text(0.5, 1.0, '50 Iris samples')
```



Task: Run the kmeans algorithm for 4 clusters (`n_clusters=4`), plot all four clusters including the center points, and save the plot as a pdf file.

The output should look like this:

In [99]:



Let's move on to [tutorial 3 (https://github.com/tobiashofmann88/python_for_biologists/blob/master/tutorials/tutorial_3.ipynb)](https://github.com/tobiashofmann88/python_for_biologists/blob/master/tutorials/tutorial_3.ipynb)