Report Submission Information (must be completed before submitting report!)

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Workshop 2 - Machine Learning (ML) [2 weeks]

Topics Covered

- ML basics and definitions, supervised and unsupervised learning
- Linear regression, model selection, and regularisation
- · Clustering, k-means, and Gaussian Mixture Models
- Principal Component Analysis (PCA)
- Support Vector Machines (SVMs)
- · Logistic regression
- · Performance metrics and hyperparameter selection

Topic mindmap

Topic Notes

Optimisation is widely used in engineering (practice and research) today. That was not always so. I expect that in the future machine learning will be as prevalently used in engineering as optimisation is used today. The arguments in favour of it are (a) increasingly more powerful computing (b) lots of data (c) decreasing storage and computing costs. Machine learning benefits substantially from these trends. We will hopefully see together how engineering world will evolve in this century.

In this workshop, you will learn how to solve machine learning problems in practice and apply common algorithms to various data sets. Doing this yourself will give you a chance to connect theoretical knowledge and practical usage. We will start with simple, easy-to-visualise (2D) data sets so that concepts become clear. More interesting problems and data will be posed as open-ended (and optional) problems.

You will also familiarise yourself with machine learning libraries of Python, which is the de-facto language for ML these days. Still, the tools and data are chosen completely for educational reasons (simplicity, accessibility, cost). There are and will be better ML frameworks and more complex data sets but it is not realistic to cover all. Due to time limitations, we unfortunately do not focus on a big topic in this workshop and subject: data science (https://study.unimelb.edu.au/find/courses/graduate/master-of-data-science/what-will-i-study/). You should not get the wrong impression from the nice, cleaned-up data sets you are given in this workshop. In real life, data is messy and more than half of data science is about preparing data itself.

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Workflow and Assessment

This subject follows a problem- and project-oriented approach. In this learning workflow, the focus is on solving practical (engineering) problems, which motivate acquiring theoretical (background) knowledge at the same time.

Objectives

- Use these problems as a motivation to learn the fundamentals of machine learning covered in lectures.
- Gain hands-on experience with basic machine learning paradigms.
- Familiarise yourself with some of the practical software tools used for machine learning.
- Solve basic machine learning problems using Python Scipy and Scikit-learn.
- Connect theoretical knowledge and practical usage by doing it yourself.

Common objectives of all workshops

Gain hands-on experience and learn by doing! Understand how theoretical knowledge discussed in lectures relates to practice. Develop motivation for gaining further theoretical and practical knowledge beyond the subject material.

Self-learning is one of the most important skills that you should acquire as a student. Today, self-learning is much easier than it used to be thanks to a plethora of online resources.

Assessment Process

- Follow the procedures described below, perform the given tasks, and answer the workshop questions in this Python notebook itself! The resulting notebook will be your Workshop Report!
- 2. Submit the workshop report at the announced deadline
- Demonstrators will conduct a brief (5min) oral quiz on your submitted report in the subsequent weeks.

4. Your workshop marks will be a combination of the report you submitted and oral quiz results.

The goal is to learn, NOT blindly follow the procedures in the fastest possible way! Do not simply copy-paste answers (from Internet, friends, etc.). You can and should use all available resources but only to develop your own understanding. If you copy-paste, you will pay the price in the oral quiz!

Section 1: Linear Regression, Overfitting, and Regularisation

Example 1.1: Using curve fitting to model Diode characteristics

Diode characteristic

The diagram above shows the I-V curve of a <u>diode (https://en.wikipedia.org/wiki/Diode)</u> widely used in electronic circuits, see <u>1N4001-D spec sheet (right click to download) (1N4001-D.pdf)</u>.

We can use regression to model the I-V curve of this diode at 25° C.

Using the nice tool, WebPlotDigitizer (https://automeris.io/WebPlotDigitizer/), a small and clean data set is generated and stored in <u>csv format (https://en.wikipedia.org/wiki/Comma-separated_values)</u>. We now use the famous <u>pandas library (https://pandas.pydata.org/)</u> to read the **csv** file.

```
In [1]: %matplotlib notebook
import pandas as pd
import numpy as np
from scipy import optimize
import matplotlib.pyplot as plt
import matplotlib

dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
# Note that if you don't put names to csv or into the function as above,
# pandas ignores the first row in calculations!
```

Out[1]:

```
        Vf
        If

        0
        0.794737
        0.100714

        1
        0.801316
        0.111255

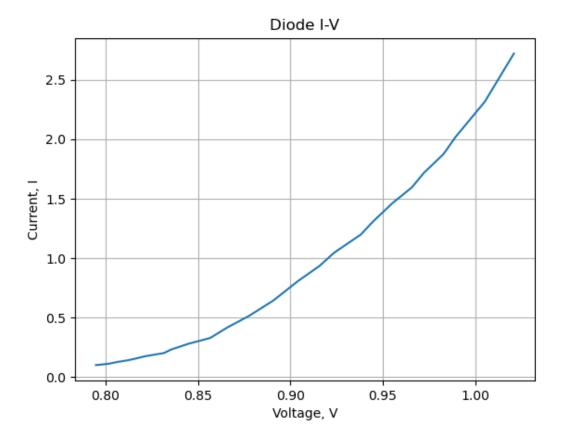
        2
        0.806579
        0.127593

        3
        0.811842
        0.140954

        4
        0.815789
        0.153793
```

```
In [2]: plt.figure()
    plt.plot(dataset.values[:,0], dataset.values[:,1])
    plt.xlabel('Voltage, V')
    plt.ylabel('Current, I')
    plt.title('Diode I-V')
    plt.grid()
```

<IPython.core.display.Javascript object>



Note that the figure above is convex but the one above was looking concave! Can you see why?

Question 1.1 [20%]

Now let's consider the linear model I=f(V)=a+bV, for $a,b\in\mathbb{R}$ for simplicity.

We can find the best (a, b) that minimises the error between the N data points (I_j, V_j) and this linear model by solving the optimisation problem

$$\min_{a,b} \sum_{j=1}^{N} (I_j - (a + bV_j))^2$$

This is equivalent *in spirit* to what the machine learning libraries such as *scikit-learn (sklearn)* do to solve this problem! As you will repeatedly see, there is a deep and close relationship between optimisation and many learning methods.

- 1. Find the optimal a, b pair by solving the unconstrained optimisation problem above using **pyomo**. Using the formula and the parameters, a, b, you derived, plot the linear I-V curve with the additional constraint $I \ge 0$ or $\max(I, 0)$.
- First, fit a <u>linear model (https://scikit-learn.org/stable/modules/linear_model.html)</u> using "linear_model.LinearRegression()". Plot the result, find the coefficients, and calculate the mean squared error (MSE).
- 3. Next, fit a polynomial model (https://scikit-learn.org/stable/modules/linear_model.html#polynomial-regression-extending-linear-models-with-basis-functions) of second degree, i.e. a quadratic model. Plot the model, find the coefficients, and calculate MSE. Interpret and discuss the results.
- 4. Add a regularisation term, i.e use <u>ridge regression (https://scikit-learn.org/stable/modules /linear_model.html#ridge-regression)</u>. Do you observe an improvement? Discuss.
- 5. Try a couple of higher order models (e.g. 4, 6) without regularisation, and provide the results as before. What do you observe when you compare the coefficients? Find validation and training errors for the models and discuss/interpret your results.

Hints

- you will need to use <u>pipelines (https://scikit-learn.org/stable/modules/compose.html#pipeline)</u>. To access coefficients use model.named_steps['linearregression'].coef_ or model.named_steps['ridge'].coef_
- 2. the train_test_split function provides a very convenient way of shuffling the data and dividing it into training and test sets (3:1 default ratio), see https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.train_test_split.html)
 /sklearn.model_selection.train_test_split.html

```
In [3]: from sklearn import linear_model
    from sklearn.metrics import mean_squared_error
    from sklearn.linear_model import Ridge
    from sklearn.preprocessing import PolynomialFeatures
    from sklearn.pipeline import make_pipeline
    from sklearn.model_selection import train_test_split

# full data in correct form for sklearn
    Vfulldata = np.array(dataset.values[:,0]).reshape(-1,1) # reshape needed for s
    Ifulldata = np.array(dataset.values[:,1]).reshape(-1,1)

# split into training and test sets
```

```
In [5]: ## Question 1.1 - part 1 ##
       from pyomo.environ import *
       import pyomo.environ as pyo
       from pyomo.opt import SolverFactory
       import numpy as np
       import pandas as pd
       import matplotlib
       from matplotlib import pyplot as plt
       print('#############")
       print('Question 1.1 - part 1')
       print('############")
       print()
       dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
       dataset.head()
       V_f = dataset.values[:,0]
       I_f = dataset.values[:,1]
       # parameters
       N=len(I_f)
       model = ConcreteModel()
       # index
       model.I = range(N)
       # variables
       model.a = pyo.Var()
       model.b = pyo.Var()
       # objective function
       model.obj = Objective(expr=sum ( ( I_f[i] - ( model.a + model.b *V_f[i] ) )**2
       # define solver
       opt = pyo.SolverFactory('ipopt')
       opt.solve(model)
       # show results
       model.display()
       print()
       print('############")
       a=model.a.value
       b=model.b.value
       def I(V):
           I = a + b * V
           return I
       #### plot ####
       V=np.linspace(0.7,1.1,100)
```

```
I=I(V)
plt.figure()
plt.plot(V,I)
plt.plot(V_f , I_f)
plt.xlabel('Voltage, V')
plt.ylabel('Current, I')
plt.title('Diode I-V')
plt.legend(["Linear Regression", "Ground truth"], loc ="lower right")
plt.ylim((0,2.6))
plt.grid()
plt.show()
Question 1.1 - part 1
```

Model unknown

Variables:

a : Size=1, Index=None

Key : Lower : Value : Upper : Fixed : Stale : Domain None: None: -8.691267803430165: None: False: False: Reals

b : Size=1, Index=None

Key : Lower : Value : Upper : Fixed : Stale : Domain None: None: 10.714559790870089: None: False: False: Reals

Objectives:

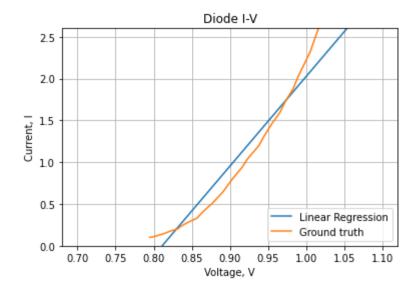
obj : Size=1, Index=None, Active=True

Key : Active : Value

True: 0.7726144097041545

Constraints:

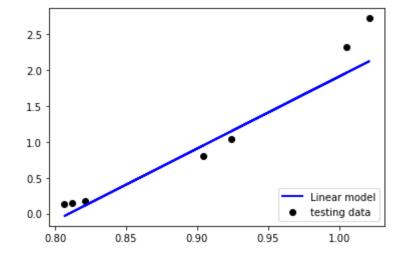
None



```
In [23]: ## Question 1.1 - part 2 ##
         import numpy as np
         import pandas as pd
         from sklearn import datasets, linear_model
         from sklearn.metrics import mean_squared_error, r2_score
         import matplotlib
         from matplotlib import pyplot as plt
         from sklearn.model_selection import train_test_split
         from sklearn.pipeline import make_pipeline
         print('############")
         print('Question 1.1 - part 2')
         print('############")
         print()
         # Load dataset
         dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
         dataset.head()
         V_f = dataset.values[:,0]
         I_f = dataset.values[:,1]
         # full data in correct form for sklearn (reshape needed for sklearn functions)
         Vfulldata = np.array(V_f).reshape(-1,1)
         Ifulldata = np.array(I_f).reshape(-1,1)
         # split into training and test sets
         V_train, V_test, I_train, I_test = train_test_split(Vfulldata, Ifulldata)
         print('number of training data for V is = ', len(V_train))
         print('number of training data for I is = ', len(I_train))
         print('number of testing data for V is = ', len(V_test))
         print('number of testing data for I is = ', len(I_test))
         print()
         # Create linear regression object
         regr = linear_model.LinearRegression()
         # Train the model using the training sets
         regr.fit(V_train, I_train)
         # Make predictions using the testing set
         I pred = regr.predict(V_test)
         # The coefficients
         print("Coefficients: \n \n", regr.coef_)
         print()
         # The mean squared error
         print("Mean squared error: %.2f" % mean_squared_error(I_test, I_pred))
         print()
         # Plot outputs
```

[[10.05248208]]

Mean squared error: 0.08



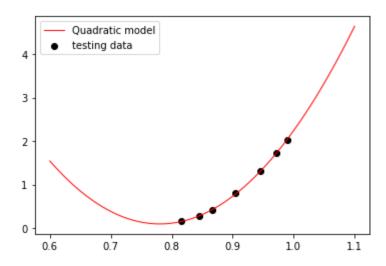
```
In [62]: ## Question 1.1 - part 3 ##
         import numpy as np
         import pandas as pd
         from sklearn import datasets, linear_model
         from sklearn.model_selection import train_test_split
         from sklearn.metrics import mean_squared_error, r2_score
         import matplotlib
         from matplotlib import pyplot as plt
         from sklearn.preprocessing import PolynomialFeatures
         from sklearn.linear_model import LinearRegression
         print('############")
         print('Question 1.1 - part 3')
         print('#############"")
         print()
         # Load dataset
         dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
         dataset.head()
         V_f = dataset.values[:,0]
         I_f = dataset.values[:,1]
         # full data in correct form for sklearn (reshape needed for sklearn functions)
         Vfulldata = np.array(V_f).reshape(-1,1)
         Ifulldata = np.array(I_f).reshape(-1,1)
         # split into training and test sets
         V_train, V_test, I_train, I_test = train_test_split(Vfulldata, Ifulldata)
         print('number of training data for V is = ', len(V_train))
         print('number of training data for I is = ', len(I_train))
         print('number of testing data for V is = ', len(V_test))
         print('number of testing data for I is = ', len(I_test))
         print()
         polynomial_features = PolynomialFeatures(degree = 2)
         Phi_V_train = polynomial_features.fit_transform(V_train)
         # Step 1: define and train a model
         model = LinearRegression()
         model.fit(Phi_V_train, I_train)
         #-----
         # Step 2: calculate coefficients and MSE
         Phi_V_test = polynomial_features.fit_transform(V_test)
         I_pred = model.predict(Phi_V_test)
```

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```
# The coefficients
print("Coefficients: \n \n", model.coef_)
# The mean squared error
print("Mean squared error for a model with M = 2 is = %7f" % mean_squared_erro
# Step 3: prediction
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
V = np.linspace(0.6, 1.1, 100)
V = np.array(V).reshape(-1,1)
Phi_V = polynomial_features.fit_transform(V)
I_pred = model.predict(Phi_V)
plt.plot(V, I_pred, color="red", linewidth=1)
plt.legend(["Quadratic model" , "testing data"], loc ="upper left")
plt.show()
Question 1.1 - part 3
number of training data for V is = 18
number of training data for I is = 18
number of testing data for V is = 7
number of testing data for I is = 7
Coefficients:
```

```
[[ 0.
              -69.44637406 44.49582398]]
```

Mean squared error for a model with M = 2 is = 0.000254



When the metaparameter (M) has a lower amount, by increasing that, the mean squared error (MSE) for the

testing data are reduced and the coefficients increase. However, we know that if the M is much bigger (for example, 8), the MSE will increase incredibly by increasing the M. This is because the overfitting happens. Thus, there is an optimal M to have the lowest MSE for the testing data.

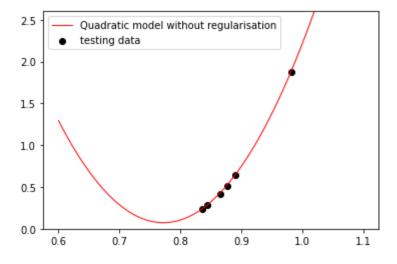
```
In []: from sklearn import linear_model
    reg = linear_model.Ridge(alpha=.5)
    reg.fit([[0, 0], [0, 0], [1, 1]], [0, .1, 1])
    Ridge(alpha=0.5)
    reg.coef_
    array([0.34545455, 0.34545455])
    reg.intercept_
```

```
In [6]: ## Question 1.1 - part 4 ##
        import numpy as np
        import pandas as pd
        from sklearn import datasets, linear_model
        from sklearn.model_selection import train_test_split
        from sklearn.metrics import mean_squared_error, r2_score
        import matplotlib
        from matplotlib import pyplot as plt
        from sklearn.preprocessing import PolynomialFeatures
        from sklearn.linear_model import LinearRegression
        print('############")
        print('Question 1.1 - part 4')
        print('#############"")
        print()
        # Load dataset
        dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
        dataset.head()
        V_f = dataset.values[:,0]
        I_f = dataset.values[:,1]
        # full data in correct form for sklearn (reshape needed for sklearn functions)
        Vfulldata = np.array(V_f).reshape(-1,1)
        Ifulldata = np.array(I_f).reshape(-1,1)
        # split into training and test sets
        V_train, V_test, I_train, I_test = train_test_split(Vfulldata, Ifulldata)
        print('number of training data for V is = ', len(V_train))
        print('number of training data for I is = ', len(I_train))
        print('number of testing data for V is = ', len(V_test))
        print('number of testing data for I is = ', len(I_test))
        print()
        polynomial_features = PolynomialFeatures(degree = 2)
        Phi_V_train = polynomial_features.fit_transform(V_train)
        # Step 1: define and train a model without regularisation
        model = LinearRegression()
        model.fit(Phi_V_train, I_train)
        #-----
        # Step 2: calculate coefficients and MSE
        Phi_V_test = polynomial_features.fit_transform(V_test)
        I_pred = model.predict(Phi_V_test)
```

```
# The coefficients
print("Coefficients: \n \n", model.coef_)
# The mean squared error
print("Mean squared error for a model without regularisation is = %.7f" % mean
MSE=np.zeros(shape = (2))
MSE[0] = (mean_squared_error(I_test, I_pred))
# Step 3: prediction
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
V = np.linspace(0.6, 1.1, 100)
V = np.array(V).reshape(-1,1)
Phi_V = polynomial_features.fit_transform(V)
I_pred = model.predict(Phi_V)
plt.plot(V, I_pred, color="red", linewidth=1)
plt.legend(["Quadratic model without regularisation" , "testing data"], loc ="
plt.ylim((0,2.6))
plt.show()
#-----
# Step 1: define and train a model with regularisation
polynomial features = PolynomialFeatures(degree = 2)
Phi_V_train = polynomial_features.fit_transform(V_train)
model_regularisation = linear_model.Ridge(alpha=0.5)
model_regularisation.fit(Phi_V_train, I_train)
#-----
# Step 2: calculate coefficients and MSE
Phi_V_test = polynomial_features.fit_transform(V_test)
I_pred_regularisation = model_regularisation.predict(Phi_V_test)
# The coefficients
print("Coefficients: \n \n", model_regularisation.coef_)
print()
# The mean squared error
print("Mean squared error for a model with regularisation is = %.7f" % mean_sq
print()
MSE[1] = (mean_squared_error(I_test, I_pred_regularisation))
# Step 3: prediction
```

```
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
V = np.linspace(-1,1.1,100)
V = np.array(V).reshape(-1,1)
Phi_V = polynomial_features.fit_transform(V)
I pred regularisation = model_regularisation.predict(Phi_V)
plt.plot(V, I_pred_regularisation, color="red", linewidth=1)
plt.legend(["Quadratic model with regularisation" , "testing data"], loc ="upp
plt.ylim((-2.3,2.6))
plt.show()
## plot MSE
fig = plt.figure()
ax = fig.add_axes([0,0,1,1])
Regularisation_mode = ['Without regularisation', 'With regularisation']
MSE_reg = [MSE[0], MSE[1]]
ax.bar(Regularisation_mode,MSE_reg)
plt.xlabel('Regularisation_mode', fontsize = 12)
plt.ylabel('MSE', fontsize = 12)
Question 1.1 - part 4
number of training data for V is = 18
number of training data for I is = 18
number of testing data for V is = 7
number of testing data for I is = 7
Coefficients:
[[
    0.
               -63.65816662 41.22203376]]
```

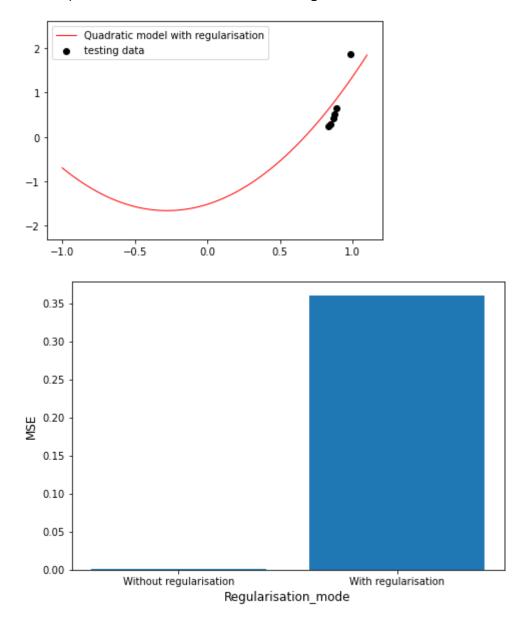
Mean squared error for a model without regularisation is = 0.0015304



Coefficients:

[[0. 1.02393278 1.84317483]]

Mean squared error for a model with regularisation is = 0.3605647



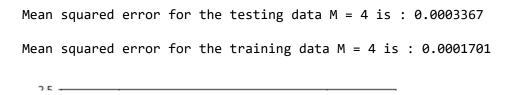
By adding the regularisation term, the coefficients are reduced incredibly. However, the MSE increases.

```
In [8]: ## Question 1.1 - part 5 ##
       import numpy as np
       import pandas as pd
       from sklearn import datasets, linear_model
       from sklearn.model_selection import train_test_split
       from sklearn.metrics import mean squared error, r2 score
       import matplotlib
       from matplotlib import pyplot as plt
       from sklearn.preprocessing import PolynomialFeatures
       from sklearn.linear_model import LinearRegression
       print('############")
        print('Question 1.1 - part 5')
       print('#############")
       print()
       # Load dataset
       dataset=pd.read_csv('files/diode_dataset.csv', names=['Vf', 'If'])
       dataset.head()
       V_f = dataset.values[:,0]
       I f = dataset.values[:,1]
       # full data in correct form for sklearn (reshape needed for sklearn functions)
       Vfulldata = np.array(V_f).reshape(-1,1)
       Ifulldata = np.array(I_f).reshape(-1,1)
       # split into training and test sets
       V_train, V_test, I_train, I_test = train_test_split(Vfulldata, Ifulldata)
       print('number of training data for V is = ', len(V_train))
       print('number of training data for I is = ', len(I_train))
       print('number of testing data for V is = ', len(V test))
       print('number of testing data for I is = ', len(I_test))
       print()
        # ----- M = 4 -----
       polynomial_features_4 = PolynomialFeatures(degree = 4)
       Phi_V_train_4 = polynomial_features_4.fit_transform(V_train)
       model_4 = LinearRegression()
       model_4.fit(Phi_V_train_4, I_train)
       Phi_V_test_4 = polynomial_features_4.fit_transform(V_test)
       I_pred_4_test = model_4.predict(Phi_V_test_4)
       I_pred_4_train = model_4.predict(Phi_V_train_4)
       # The coefficients
        print("Coefficients for M = 4 is : \n \n", model_4.coef_)
```

```
print()
# The mean squared error
print("Mean squared error for the testing data M = 4 is : %.7f" % mean squared
print()
print("Mean squared error for the training data M = 4 is : %.7f" % mean square
MSE test=np.zeros(shape = (4, 2))
MSE_train=np.zeros(shape = (4 , 2) )
MSE_test[0] = (4 , mean_squared_error(I_test, I_pred_4_test))
MSE_train[0] = (4 , mean_squared_error(I_train, I_pred_4_train))
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
V = np.linspace(0.6, 1.1, 100)
V = np.array(V).reshape(-1,1)
Phi_V_4 = polynomial_features_4.fit_transform(V)
I_pred_4 = model_4.predict(Phi_V_4)
plt.plot(V, I_pred_4, color="red", linewidth=1)
plt.legend(["M = 4 " , "testing data"], loc ="lower right")
plt.ylim((-0.5, 2.5))
plt.show()
\# ----- M = 6 -----
polynomial_features_6 = PolynomialFeatures(degree = 6)
Phi V train 6 = polynomial features 6.fit transform(V train)
model_6 = LinearRegression()
model_6.fit(Phi_V_train_6, I_train)
Phi_V_test_6 = polynomial_features_6.fit_transform(V_test)
I pred 6 test = model 6.predict(Phi V test 6)
I_pred_6_train = model_6.predict(Phi_V_train_6)
# The coefficients
print("Coefficients for M = 6 is : \n \n", model_6.coef_)
print()
# The mean squared error
print("Mean squared error for the testing data and M = 6 is : %.7f" % mean_squ
print()
print("Mean squared error for the training data and M = 6 is : %.7f" % mean_sq
print()
MSE_test[1] = (6 , mean_squared_error(I_test, I_pred_6_test))
MSE_train[1] = (6 , mean_squared_error(I_train, I_pred_6_train))
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
```

```
Phi_V_6 = polynomial_features_6.fit_transform(V)
I_pred_6 = model_6.predict(Phi_V_6)
plt.plot(V, I_pred_6, color="blue", linewidth=1)
plt.legend(["M = 6 " , "testing data"], loc ="lower right")
plt.ylim((-0.5, 2.5))
plt.show()
# ----- M = 8 -----
polynomial_features_8 = PolynomialFeatures(degree = 8)
Phi_V_train_8 = polynomial_features_8.fit_transform(V_train)
model_8 = LinearRegression()
model_8.fit(Phi_V_train_8, I_train)
Phi_V_test_8 = polynomial_features_8.fit_transform(V_test)
I_pred_8_test = model_8.predict(Phi_V_test_8)
I_pred_8_train = model_8.predict(Phi_V_train_8)
# The coefficients
print("Coefficients for M = 8 is : \n \n", model_8.coef_)
print()
# The mean squared error
print("Mean squared error for the testing data and M = 8 is : %.7f" % mean squ
print()
print("Mean squared error for the training data and M = 8 is : %.7f" % mean sq
print()
MSE_test[2] = (8 , mean_squared_error(I_test, I pred 8 test))
MSE_train[2] = (8 , mean_squared_error(I_train, I_pred_8_train))
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
Phi V 8 = polynomial features 8.fit transform(V)
I_pred_8 = model_8.predict(Phi_V_8)
plt.plot(V, I_pred_8, color="green", linewidth=1)
plt.legend(["M = 8 " , "testing data"], loc ="lower right")
plt.ylim((-0.5, 2.5))
plt.show()
# ------ M = 10 ------
polynomial_features_10 = PolynomialFeatures(degree = 10)
Phi_V_train_10 = polynomial_features_10.fit_transform(V_train)
model_10 = LinearRegression()
model_10.fit(Phi_V_train_10, I_train)
Phi_V_test_10 = polynomial_features_10.fit_transform(V_test)
I pred 10 test = model 10.predict(Phi V test 10)
```

```
I_pred_10_train = model_10.predict(Phi_V_train_10)
# The coefficients
print("Coefficients for M = 10 is : \n \n", model_10.coef_)
print()
# The mean squared error
print("Mean squared error for the testing data and M = 10 is : %.7f" % mean_sq
print()
print("Mean squared error for the training data and M = 10 is : %.7f" % mean_s
print()
MSE_test[3] = (10 , mean_squared_error(I_test, I_pred_10_test))
MSE_train[3] = (10 , mean_squared_error(I_train, I_pred_10_train))
# Plot outputs
plt.figure()
plt.scatter(V_test, I_test, color="black")
Phi_V_10 = polynomial_features_10.fit_transform(V)
I_pred_10 = model_10.predict(Phi_V_10)
plt.plot(V, I_pred_10, color="pink", linewidth=1)
plt.legend(["M = 10 " , "testing data"], loc ="upper left")
plt.ylim((-0.5, 2.5))
plt.show()
## plot MSE for the testing data
plt.figure()
x = MSE_test[:,0]
y = MSE_test[:,1]
plt.scatter(x , y, color="black")
plt.plot(x , y , color="red", linewidth=1)
## plot MSE for the training data
x = MSE_train[:,0]
y = MSE_train[:,1]
plt.scatter(x , y, color="green")
plt.plot(x , y , color="blue", linewidth=1)
plt.xlabel('M')
plt.legend(["MSE for the testing data", "MSE for the training data", "testing
plt.title('Impact of metaparameter (M) on MSE')
plt.show()
Question 1.1 - part 5
number of training data for V is = 18
number of training data for I is = 18
number of testing data for V is = 7
number of testing data for I is = 7
Coefficients for M = 4 is :
 [[
                 -2683.88820358 4432.55661942 -3264.43635148
    908.21906841]]
```



When the metaparameter (M) has a lower amount, by increasing that (M), the mean squared error (MSE) for the testing data are reduced and the coefficients increase. However, if the M is much bigger (for example, 8), the MSE for the testing data starts to increase. Thus, there is an optimal M to have the lowest MSE for the testing data.

But the MSE for the training data always are reduced by increasing the metaparameter M which is called overfitting.

Section 2: Clustering and Gaussian Mixtures

Unsupervised learning is all about data. We will use first the famous two moon data set to practice a little bit and digest some of the fundemental concepts. Since two moons data inherently has two clusters (each moon as a cluster), we can use this as a <u>ground truth (https://en.wikipedia.org/wiki/Ground_truth)</u>. In most real problems, we don't have this luxury of having the ground truth at hand!

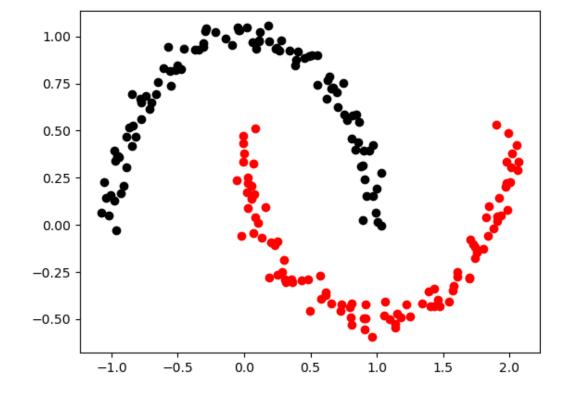
Note that Scikit Learn does not have its own global random state but uses the <u>numpy random state</u> (https://docs.scipy.org/doc/numpy-1.15.1/reference/generated/numpy.random.seed.html#numpy.random.seed) instead. See the code below.

Important Note on Random Number/Vector Generation

Each group has to use a different number seed (which is an arbitrary number as illustrated above) and groups cannot share seeds. The pseudo-randomness is used here to create diversity. Otherwise, if groups use the same seed, the results will be the same (opening the door to plagiarism) and significant number of points will be taken off! As a practical hint, you can use a modified-combination of your student numbers

```
In [4]: from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        # Set a random seed as you did in optimisation workshop by uncommenting the li
        #np.random.seed(Put here a group-specific number!)
        noisy_moons = datasets.make_moons(n_samples=200, noise=0.05)
        X = noisy_moons[0] # data points
        y = noisy_moons[1] # 0, 1 labels of class, 50 each - giving us the ground trut
        order_ind = np.argsort(y) # order labels, 50 each class
        X1 = X[order_ind[0:100]] # class 1
        X2 = X[order_ind[101:200]] # class 2
        # Plot data
        plt.figure()
        plt.scatter(X1[:,0], X1[:,1], color='black')
        plt.scatter(X2[:,0], X2[:,1], color='red')
```

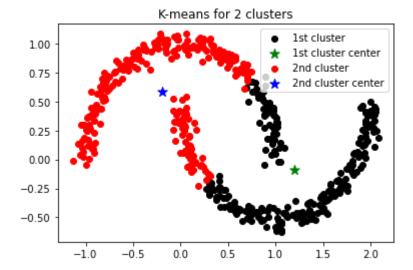
<IPython.core.display.Javascript object>



Question 2.1 [10%] K-means clustering

- 1. Use sklearn's k-means clustering algorithm to divide the two moon data given above (X) into two clusters. Plot the result and show the cluster centres that you found.
- 2. Experiment with different starting points (init='random') and number of clusters, e.g. 3, 4, 5. Write

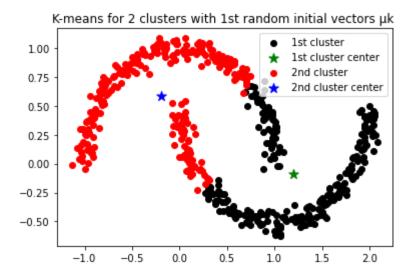
```
In [135]: ## Question 2.1 - part 1 ##
          print('#############"")
          print('Question 2.1 - part 1')
          print('############")
          print()
          from sklearn import cluster, datasets, mixture
          from sklearn.cluster import KMeans
          from sklearn.utils import shuffle
          from sklearn import decomposition
          from sklearn.mixture import GaussianMixture
          from sklearn import metrics
          import numpy as np
          from matplotlib import pyplot as plt
          from sklearn.cluster import KMeans
          random = np.random.seed(69007044)
          noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
          X = noisy_moons[0] # data points
          kmeans = KMeans(n_clusters=2, random_state=random).fit(X)
          label=kmeans.labels
          cluster0=[]
          cluster1=[]
          for count,item in enumerate(label):
             if item==0:
                 cluster0.append(X[count])
             elif item ==1:
                 cluster1.append(X[count])
          cluster0=np.array(cluster0)
          cluster1=np.array(cluster1)
          mean_cluster0 = np.mean(cluster0, axis=0)
          mean_cluster1 = np.mean(cluster1, axis=0)
          plt.scatter(cluster0[:,0], cluster0[:,1], color='black')
          plt.scatter(mean_cluster0[0], mean_cluster0[1], color='green' , s = 100 , mark
          plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
          plt.scatter(mean_cluster1[0], mean_cluster1[1], color='blue', s = 100, market
          plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluster"
          plt.title('K-means for 2 clusters')
```



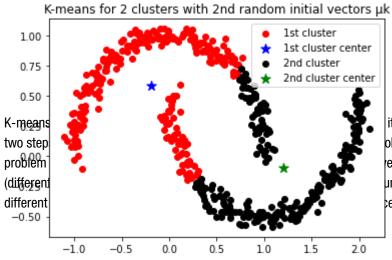
25 of 76

```
In [16]: ## Question 2.1 - part 2.a ( different starting points ) ##
         print('############")
         print('Question 2.1 - part 2.a ( different starting points )')
         print('#############")
         print()
         from sklearn import cluster, datasets, mixture
         from sklearn.cluster import KMeans
         from sklearn.utils import shuffle
         from sklearn import decomposition
         from sklearn.mixture import GaussianMixture
         from sklearn import metrics
         import numpy as np
         from matplotlib import pyplot as plt
         from sklearn.cluster import KMeans
         cost_function=[]
         random_1 = np.random.seed(69007044)
         noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
         X = noisy moons[0] # data points
         kmeans = KMeans(n_clusters=2, random_state=random_1).fit(X)
         label=kmeans.labels_
         cluster0=[]
         cluster1=[]
         for count,item in enumerate(label):
             if item==0:
                 cluster0.append(X[count])
             elif item ==1:
                 cluster1.append(X[count])
         cluster0=np.array(cluster0)
         cluster1=np.array(cluster1)
         mean_cluster0 = np.mean(cluster0, axis=0)
         mean_cluster1 = np.mean(cluster1, axis=0)
         plt.scatter(cluster0[:,0], cluster0[:,1], color='black')
         plt.scatter(mean_cluster0[0], mean_cluster0[1], color='green' , s = 100 , mark
         plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
         plt.scatter(mean_cluster1[0], mean_cluster1[1], color='blue' , s = 100 , marke
         plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluste
         plt.title('K-means for 2 clusters with 1st random initial vectors μk ')
         plt.show()
         random 2 = np.random.seed(70446900)
         print(random 2)
         noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
         X = noisy_moons[0] # data points
         kmeans = KMeans(n_clusters=2, random_state=random_2).fit(X)
```

```
label=kmeans.labels_
cluster0=[]
cluster1=[]
for count,item in enumerate(label):
    if item==0:
        cluster0.append(X[count])
    elif item ==1:
        cluster1.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
mean_cluster0 = np.mean(cluster0, axis=0)
mean cluster1 = np.mean(cluster1, axis=0)
plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
plt.scatter(mean_cluster0[0], mean_cluster0[1], color='blue', s = 100, marke
plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
plt.scatter(mean_cluster1[0], mean_cluster1[1], color='green' , s = 100 , mark
plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluste
plt.title('K-means for 2 clusters with 2nd random initial vectors μk')
```



None



its iterative method because both of its obal minimum because the optimization ectors μ k in the K-means method unction of the K-means method) result centers depend on the initial vectors μ k.

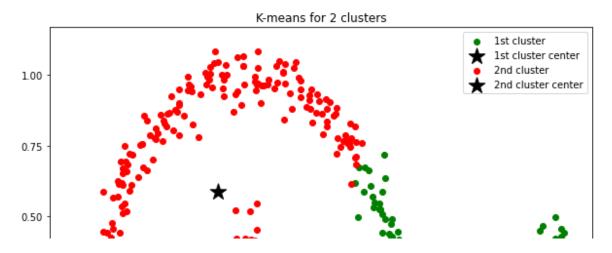
```
In [15]: ## Question 2.1 - part 2.b (different number of clusters) ##
        print('############")
        print('Question 2.1 - part 2.b (different number of clusters)')
        print('############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        cost_function=[]
        random = np.random.seed(69007044)
        noisy moons = datasets.make moons(n samples=500, noise=0.05)
        X = noisy_moons[0] # data points
        kmeans = KMeans(n_clusters=2, random_state=random).fit(X)
        label=kmeans.labels
        print('The cost function for K = 2 is = ' , abs(kmeans.score(X)))
        cost function.append(abs(kmeans.score(X)))
        cluster0=[]
        cluster1=[]
        for count,item in enumerate(label):
            if item == 0:
                cluster0.append(X[count])
            elif item == 1:
                cluster1.append(X[count])
        cluster0=np.array(cluster0)
        cluster1=np.array(cluster1)
        mean_cluster0 = np.mean(cluster0, axis=0)
        mean_cluster1 = np.mean(cluster1, axis=0)
        plt.figure(figsize=(10, 10))
        plt.scatter(cluster0[:,0], cluster0[:,1], color='green')
        plt.scatter(mean_cluster0[0], mean_cluster0[1], color='black' , s = 300 , mark
        plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
        plt.scatter(mean_cluster1[0], mean_cluster1[1], color='black' , s = 300 , mark
        plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluster"
        plt.title('K-means for 2 clusters')
        plt.show()
```

```
random = np.random.seed(69007044)
noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
X = noisy_moons[0] # data points
kmeans = KMeans(n_clusters=3, random_state=random).fit(X)
label=kmeans.labels_
print('The cost function for K = 3 is = ' , abs(kmeans.score(X)))
cost_function.append(abs(kmeans.score(X)))
cluster0=[]
cluster1=[]
cluster2=[]
for count,item in enumerate(label):
   if item == 0:
       cluster0.append(X[count])
   elif item == 1:
       cluster1.append(X[count])
   elif item == 2:
       cluster2.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
mean_cluster0 = np.mean(cluster0, axis=0)
mean_cluster1 = np.mean(cluster1, axis=0)
mean_cluster2 = np.mean(cluster2, axis=0)
#####
plt.figure(figsize=(10, 10))
plt.scatter(cluster0[:,0], cluster0[:,1], color='green')
plt.scatter(mean_cluster0[0], mean_cluster0[1], color='black' , s = 300 , mark
plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
plt.scatter(mean_cluster1[0], mean_cluster1[1], color='black' , s = 300 , mark
plt.scatter(cluster2[:,0], cluster2[:,1], color='blue')
plt.scatter(mean_cluster2[0], mean_cluster2[1], color='black' , s = 300 , mark
#####
plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluster"
plt.title('K-means for 3 clusters')
plt.show()
random = np.random.seed(69007044)
noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
X = noisy_moons[0] # data points
kmeans = KMeans(n_clusters=4, random_state=random).fit(X)
label=kmeans.labels_
```

```
print('The cost function for K = 4 is = ' , abs(kmeans.score(X)))
cost_function.append(abs(kmeans.score(X)))
cluster0=[]
cluster1=[]
cluster2=[]
cluster3=[]
for count,item in enumerate(label):
    if item == 0:
       cluster0.append(X[count])
   elif item == 1:
       cluster1.append(X[count])
   elif item == 2:
       cluster2.append(X[count])
   elif item == 3:
       cluster3.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
cluster3=np.array(cluster3)
mean_cluster0 = np.mean(cluster0, axis=0)
mean_cluster1 = np.mean(cluster1, axis=0)
mean_cluster2 = np.mean(cluster2, axis=0)
mean_cluster3 = np.mean(cluster3, axis=0)
#####
plt.figure(figsize=(10, 10))
plt.scatter(cluster0[:,0], cluster0[:,1], color='green')
plt.scatter(mean_cluster0[0], mean_cluster0[1], color='black' , s = 300 , mark
plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
plt.scatter(mean_cluster1[0], mean_cluster1[1], color='black' , s = 300 , mar
plt.scatter(cluster2[:,0], cluster2[:,1], color='blue')
plt.scatter(mean_cluster2[0], mean_cluster2[1], color='black' , s = 300 , mark
plt.scatter(cluster3[:,0], cluster3[:,1], color='orange')
plt.scatter(mean_cluster3[0], mean_cluster3[1], color='black' , s = 300 , mark
#####
plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluste
plt.title('K-means for 4 clusters')
plt.show()
random = np.random.seed(69007044)
noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
X = noisy_moons[0] # data points
kmeans = KMeans(n_clusters=5, random_state=random).fit(X)
label=kmeans.labels
print('The cost function for K = 5 is = ' , abs(kmeans.score(X)))
```

```
cost_function.append(abs(kmeans.score(X)))
cluster0=[]
cluster1=[]
cluster2=[]
cluster3=[]
cluster4=[]
for count,item in enumerate(label):
    if item == 0:
        cluster0.append(X[count])
   elif item == 1:
        cluster1.append(X[count])
    elif item == 2:
        cluster2.append(X[count])
   elif item == 3:
        cluster3.append(X[count])
   elif item == 4:
        cluster4.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
cluster3=np.array(cluster3)
cluster4=np.array(cluster4)
mean_cluster0 = np.mean(cluster0, axis=0)
mean_cluster1 = np.mean(cluster1, axis=0)
mean_cluster2 = np.mean(cluster2, axis=0)
mean_cluster3 = np.mean(cluster3, axis=0)
mean_cluster4 = np.mean(cluster4, axis=0)
plt.figure(figsize=(10, 10))
plt.scatter(cluster0[:,0], cluster0[:,1], color='green')
plt.scatter(mean_cluster0[0], mean_cluster0[1], color='black' , s = 300 , mark
plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
plt.scatter(mean_cluster1[0], mean_cluster1[1], color='black' , s = 300 , mark
plt.scatter(cluster2[:,0], cluster2[:,1], color='blue')
plt.scatter(mean_cluster2[0], mean_cluster2[1], color='black' , s = 300 , mark
plt.scatter(cluster3[:,0], cluster3[:,1], color='orange')
plt.scatter(mean_cluster3[0], mean_cluster3[1], color='black' , s = 300 , mark
plt.scatter(cluster4[:,0], cluster4[:,1], color='purple')
plt.scatter(mean_cluster4[0], mean_cluster4[1], color='black' , s = 300 , mark
plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluste
plt.title('K-means for 5 clusters')
plt.show()
plt.scatter([2,3,4,5], cost_function, color='green', s = 200 , marker='*')
```

The cost function for K = 2 is = 203.01346251785884



With increasing number of clusters (K), the cost function (J) is reduced because the centers of clusters are nearer to the data of their own cluster. But different number of clusters result different clusters. For example, if we want to assign the data points to 4 clusters, some data points are assigned to a cluster but those data points are not assigned to that cluster when we want to have 5 clusters.

Question 2.2 [15%] GMMs as density estimators

- Now use a Gaussian Mixture Model (GMM) for clustering the same two moon data. Try two clusters and plot your results. GMMs also provides you probabilities (of a sample belonging to a cluster). Print those of a few samples.
- Increase the number of components of your GMM model. What do you observe? Use a metric to choose the number of components in a principled way. Hint: check BIC (https://en.wikipedia.org/wiki/Bayesian_information_criterion) or AIC (https://en.wikipedia.org/wiki/Akaike_information_criterion)
- 3. It is maybe better to use GMM as a **generative model**! Generate 200 brand new samples from a trained GMM with your choice of parameters and plot your results. Discuss your findings!

```
In [2]: ## Question 2.2 - part 1 ##
        print('#############")
        print('Question 2.2 - part 1 ')
        print('############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        cost_function=[]
        random = np.random.seed(69007044)
        noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
        X = noisy_moons[0] # data points
        gm = GaussianMixture(n_components=2, random_state=0).fit(X)
        # print(qm.means )
        train_label=gm.predict(X)
        cluster0=[]
        cluster1=[]
        for count,item in enumerate(train_label):
            if item == 0:
                cluster0.append(X[count])
            elif item == 1:
                cluster1.append(X[count])
        cluster0=np.array(cluster0)
        cluster1=np.array(cluster1)
        mean_cluster0 = np.mean(cluster0, axis=0)
        mean_cluster1 = np.mean(cluster1, axis=0)
        # plt.show()
        plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
        plt.scatter(mean_cluster0[0], mean_cluster0[1], color='green' , marker='*')
        plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
        plt.scatter(mean_cluster1[0], mean_cluster1[1], color='blue' , marker='*')
        plt.legend(["1st cluster" , "1st cluster center" , "2nd cluster" , "2nd cluste
        plt.title('GMM for 2 clusters')
        data_1 = [0.87, 0.49]
        print('Data_1 is : ' , data_1)
        print('The probability of the blonging the data_1 to the cluster 1 is : ' , gm
        print('The probability of the blonging the data_1 to the cluster 2 is : '
        print('Thus, we can say that it blongs to the cluster : ' , 1 + gm.predict([da
        print()
        data_2 = [1.5, -0.5]
        print('Data_1 is : ' , data_2)
```

print('The probability of the blonging the data_2 to the cluster 1 is : ' , gm print('The probability of the blonging the data_2 to the cluster 2 is : ' , gm print('Thus, we can say that it blongs to the cluster : ' , 1 + gm.predict([da

Question 2.2 - part 1

Data 1 is : [0.87, 0.49]

The probability of the blonging the data_1 to the cluster 1 is : 0.52207961 35075607

The probability of the blonging the data_1 to the cluster 2 is : 0.47792038 64924395

Thus, we can say that it blongs to the cluster : 1

Data_1 is : [1.5, -0.5]

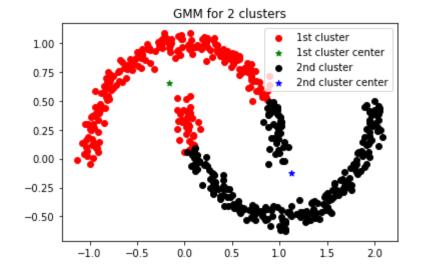
The probability of the blonging the data_2 to the cluster 1 is : 4.30093710

040551e-07

The probability of the blonging the data_2 to the cluster 2 is : 0.99999956

99062901

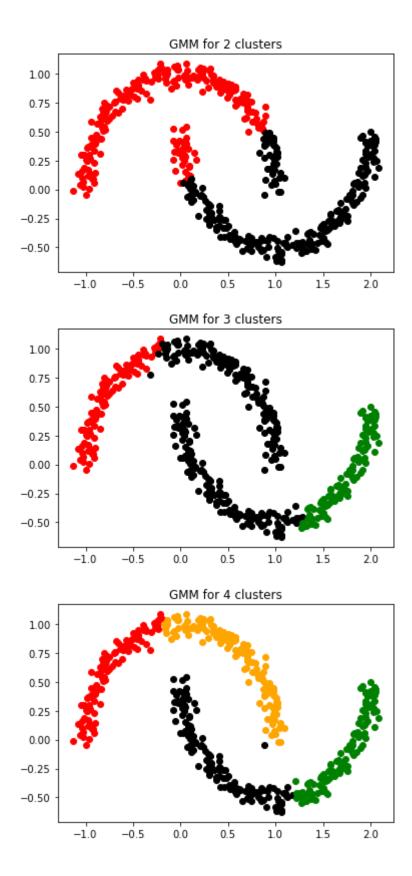
Thus, we can say that it blongs to the cluster : 2

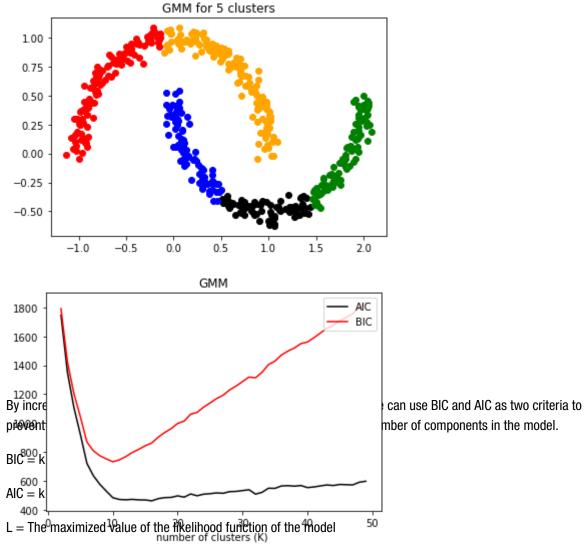


```
In [48]: ## Question 2.2 - part 2 ##
        print('############")
        print('Question 2.2 - part 2 ')
        print('#############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        random = np.random.seed(69007044)
        noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
        X = noisy_moons[0] # data points
        gm = GaussianMixture(n components=2, random state=0).fit(X)
        # print(gm.means_)
        train_label=gm.predict(X)
        cluster0=[]
        cluster1=[]
        for count,item in enumerate(train label):
           if item == 0:
               cluster0.append(X[count])
           elif item == 1:
               cluster1.append(X[count])
        cluster0=np.array(cluster0)
        cluster1=np.array(cluster1)
        plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
        plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
        plt.title('GMM for 2 clusters')
        plt.show()
        random = np.random.seed(69007044)
        noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
        X = noisy_moons[0] # data points
        gm = GaussianMixture(n_components=3, random_state=0).fit(X)
        # print(qm.means )
        train_label=gm.predict(X)
        cluster0=[]
        cluster1=[]
        cluster2=[]
        for count,item in enumerate(train label):
           if item == 0:
```

```
cluster0.append(X[count])
   elif item == 1:
       cluster1.append(X[count])
   elif item == 2:
       cluster2.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
plt.scatter(cluster2[:,0], cluster2[:,1], color='green')
plt.title('GMM for 3 clusters')
plt.show()
random = np.random.seed(69007044)
noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
X = noisy_moons[0] # data points
gm = GaussianMixture(n_components=4, random_state=0).fit(X)
# print(qm.means )
train_label=gm.predict(X)
cluster0=[]
cluster1=[]
cluster2=[]
cluster3=[]
for count,item in enumerate(train_label):
   if item == 0:
       cluster0.append(X[count])
   elif item == 1:
       cluster1.append(X[count])
   elif item == 2:
       cluster2.append(X[count])
   elif item == 3:
       cluster3.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
cluster3=np.array(cluster3)
plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
plt.scatter(cluster2[:,0], cluster2[:,1], color='green')
plt.scatter(cluster3[:,0], cluster3[:,1], color='orange')
plt.title('GMM for 4 clusters')
plt.show()
random = np.random.seed(69007044)
noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
X = noisy_moons[0] # data points
gm = GaussianMixture(n_components=5, random_state=0).fit(X)
train label=gm.predict(X)
```

```
cluster0=[]
cluster1=[]
cluster2=[]
cluster3=[]
cluster4=[]
for count,item in enumerate(train_label):
   if item == 0:
       cluster0.append(X[count])
   elif item == 1:
       cluster1.append(X[count])
   elif item == 2:
       cluster2.append(X[count])
   elif item == 3:
       cluster3.append(X[count])
   elif item == 4:
       cluster4.append(X[count])
cluster0=np.array(cluster0)
cluster1=np.array(cluster1)
cluster2=np.array(cluster2)
cluster3=np.array(cluster3)
cluster4=np.array(cluster4)
plt.scatter(cluster0[:,0], cluster0[:,1], color='red')
plt.scatter(cluster1[:,0], cluster1[:,1], color='black')
plt.scatter(cluster2[:,0], cluster2[:,1], color='green')
plt.scatter(cluster3[:,0], cluster3[:,1], color='orange')
plt.scatter(cluster4[:,0], cluster4[:,1], color='blue')
plt.title('GMM for 5 clusters')
plt.show()
aic metric=[]
bic_metric=[]
random = np.random.seed(69007044)
noisy moons = datasets.make moons(n samples=500, noise=0.05)
X = noisy_moons[0] # data points
for i in range(2,50):
   gm = GaussianMixture(n_components=i, random_state=0).fit(X)
   aic_metric.append(gm.aic(X))
   bic_metric.append(gm.bic(X))
plt.plot(range(2,50), aic_metric, color='black')
plt.plot(range(2,50), bic_metric, color='red')
plt.legend(["AIC" , "BIC"], loc ="upper right")
plt.xlabel('number of clusters (K) ')
plt.title('GMM')
Question 2.2 - part 2
```





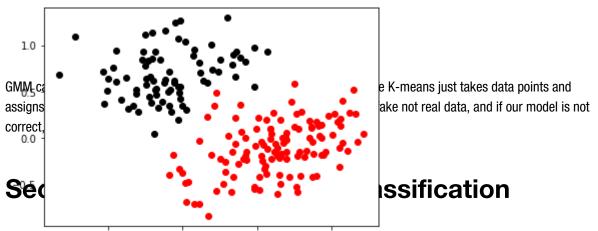
n = Number of data points

k =The number of components

As it can be seen, the penalty term is larger in BIC than in AIC.

The AIC tells us that around 10-15 is the best choice. However, the BIC suggests a simpler model with the number of components around 8-10.

```
In [1]: ## Question 2.2 - part 3 ##
        print('#############"")
        print('Question 2.2 - part 3 ')
        print('############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        cluster0=[]
        cluster1=[]
        random = np.random.seed(69007044)
        noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
        X = noisy_moons[0] # data points
        gm = GaussianMixture(n_components=2, random_state=random).fit(X)
        created_Data=gm.sample(200)
        for count,item in enumerate(created_Data[1]):
           if item == 0:
               cluster0.append(created_Data[0][count])
           elif item == 1:
               cluster1.append(created_Data[0][count])
        cluster0=np.array(cluster0)
        cluster1=np.array(cluster1)
        plt.scatter(cluster0[:,0], cluster0[:,1], color='black')
        plt.scatter(cluster1[:,0], cluster1[:,1], color='red')
        plt.show()
```



It is time to move beyond the toy data set. The next data set is still small and clean but is more interesting!

Example 3.1: Wireless Indoor Localization

The next data set shows the recorded signal strength from 7 different base stations at a smart phone. The phone is in one of the four rooms {1, 2, 3, 4}. The goal is to classify the location of the phone to one of the four rooms.

This <u>dataset (http://archive.ics.uci.edu/ml/datasets/Wireless+Indoor+Localization)</u> was used in the following publications:

- Jayant G Rohra, Boominathan Perumal, Swathi Jamjala Narayanan, Priya Thakur, and Rajen B Bhatt, 'User Localization in an Indoor Environment Using Fuzzy Hybrid of Particle Swarm Optimization & Gravitational Search Algorithm with Neural Networks', in Proceedings of Sixth International Conference on Soft Computing for Problem Solving, 2017, pp. 286-295.
- Rajen Bhatt, 'Fuzzy-Rough Approaches for Pattern Classification: Hybrid measures, Mathematical analysis, Feature selection algorithms, Decision tree algorithms, Neural learning, and Applications', Amazon Books

```
dataw = pd.read_csv('files/wifi_localization.csv', names=[f"s{i}" for i in ran
In [5]:
          dataw.head() # comment one to see the other
Out[5]:
                 s1
                      s2
                          s3
                                   s5
                                       s6
                                           s7
                                               Room Number
           1995
                 -59
                     -59
                         -48
                              -66
                                  -50
                                       -86
                                           -94
                                                            4
           1996
                 -59
                     -56
                         -50
                              -62
                                  -47
                                       -87
                                           -90
                                                            4
                                                            4
           1997
                 -62
                     -59
                         -46
                              -65
                                  -45
                                       -87
                                           -88
           1998
                          -52
                              -61
           1999
                -59
                     -50
                         -45
                              -60 -45
                                      -88
                                                            4
In [1]:
```

16000 (2000, 8)

```
In [6]: SRI = dataw.iloc[:,:7]
# a.shape
loc = dataw.iloc[:,7]-1
# loc.shape

# split into training and test sets
```

Question 3.1 [15%] Clustering-based classification

- Use k-means clustering on the training data to find the 4 cluster corresponding to the rooms. Then, test their quality using a <u>mutual information based score</u>. (https://scikit-learn.org/stable/modules /clustering.html#mutual-information-based-scores)
- 2. Conduct a <u>PCA analysis (https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html)</u> on the data with 2, 3, 4 features: find singular values, variance ratios, and plot in 2D or 3D (for 2 or 3 features). What is the number of features that balances information and complexity? Is there redundancy in data? Discuss.
- 3. Now, repeat k-means clustering with the PCA-transformed data. Do you see an improvement in scores? Why or why not? Discuss, based on your knowledge of PCA and k-means clustering.
- 4. What information does k-means ignore when used for classification? Is what we do a good classification method? What can you say about the complexity of the problem given?

```
In [7]: ## Question 3.1 - part 1 ##
       print('#############"")
       print('Question 3.1 - part 1 ')
       print('############")
       print()
       from sklearn import cluster, datasets, mixture
       from sklearn.cluster import KMeans
       from sklearn.utils import shuffle
       from sklearn import decomposition
       from sklearn.mixture import GaussianMixture
       from sklearn import metrics
       import numpy as np
       from matplotlib import pyplot as plt
       from sklearn.cluster import KMeans
       import pandas as pd
       dataset=pd.read_csv('files/wifi_localization.csv',header=None)
       X = dataset.values[:,0:7]
       Y = dataset.values[:,7]
       random = np.random.seed(69007044)
       kmeans = KMeans(n_clusters=4, random_state=random).fit(X)
       predict_label=kmeans.labels_
       print('K-means clustering quality is : ' , metrics.adjusted_mutual_info_score(
       Question 3.1 - part 1
       K-means clustering quality is: 0.8871530457012681
```

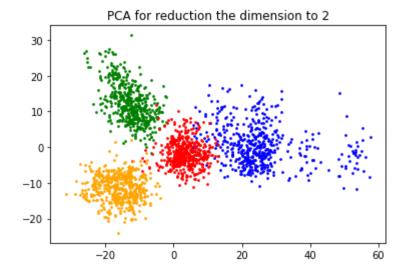
```
In [14]: ## Question 3.1 - part 2 ##
        print('#############"")
        print('Question 3.1 - part 2 ')
        print('#############")
        print()
        import numpy as np
        from sklearn.decomposition import PCA
        from sklearn import cluster, datasets, mixture
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from mpl_toolkits import mplot3d
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        import pandas as pd
        dataset=pd.read_csv('files/wifi_localization.csv',header=None)
        X = dataset.values[:,0:7]
        Y = dataset.values[:,7]
        random = np.random.seed(69007044)
        # print(X,Y)
        pca = PCA(n components=2,random state=random)
        pca.fit(X)
        print('variance ratio in the case of reduction the dimension to 2 : ',pca.expl
        print('singular values in the case of reduction the dimension to 2: ',pca.sin
        X PCA 2=pca.transform(X)
        class1=[]
        class2=[]
        class3=[]
        class4=[]
        for count,item in enumerate(Y):
            if item == 1:
                class1.append(X_PCA_2[count])
            elif item == 2:
                class2.append(X_PCA_2[count])
            elif item == 3:
                class3.append(X_PCA_2[count])
            elif item == 4:
                class4.append(X_PCA_2[count])
        class1=np.array(class1)
        class2=np.array(class2)
        class3=np.array(class3)
        class4=np.array(class4)
```

```
#####
plt.scatter(class1[:,0], class1[:,1], color='green',s=3)
plt.scatter(class2[:,0], class2[:,1], color='blue',s=3)
plt.scatter(class3[:,0], class3[:,1], color='red',s=3)
plt.scatter(class4[:,0], class4[:,1], color='orange',s=3)
plt.title('PCA for reduction the dimension to 2')
plt.show()
pca = PCA(n_components=3, random_state=random)
pca.fit(X)
print()
print()
print('variance ratio in the case of reduction the dimension to 3 : ',pca.expl
print('singular values in the case of reduction the dimension to 3 : ',pca.si
X_PCA_3=pca.transform(X)
class1=[]
class2=[]
class3=[]
class4=[]
for count,item in enumerate(Y):
   if item == 1:
       class1.append(X_PCA_3[count])
   elif item == 2:
       class2.append(X_PCA_3[count])
   elif item == 3:
       class3.append(X_PCA_3[count])
   elif item == 4:
       class4.append(X_PCA_3[count])
class1=np.array(class1)
class2=np.array(class2)
class3=np.array(class3)
class4=np.array(class4)
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(projection='3d')
ax.scatter(class1[:,0], class1[:,1], class1[:,2], color='green', s=3)
ax.scatter(class2[:,0], class2[:,1], class2[:,2], color='blue', s=3)
ax.scatter(class3[:,0], class3[:,1], class3[:,2], color='red', s=3)
ax.scatter(class4[:,0], class4[:,1], class4[:,2], color='orange', s=3)
plt.title('PCA for reduction the dimension to 3')
plt.show()
pca = PCA(n_components=4, random_state=random)
pca.fit(X)
print()
print()
print('variance ratio in the case of reduction the dimension to 4 : ',pca.expl
```

print('singular values in the case of reduction the dimension to 4 : ',pca.si Question 3.1 - part 2

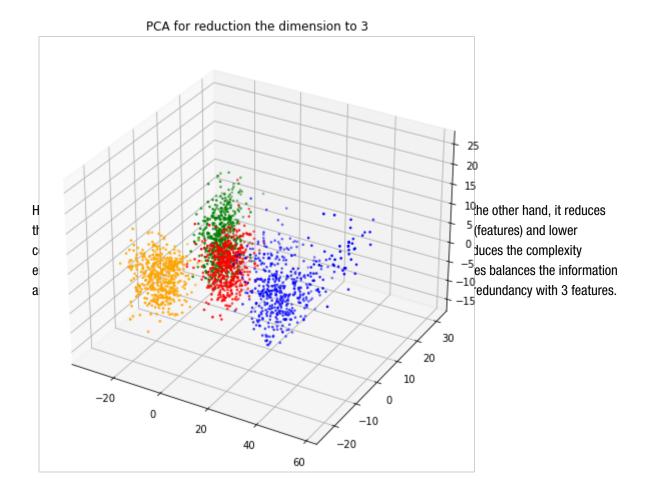
variance ratio in the case of reduction the dimension to 2 : [0.65587897 0. 19869441]

singular values in the case of reduction the dimension to 2: [782.99443538 430.96266874]



variance ratio in the case of reduction the dimension to 3 : [0.65587897 0. 19869441 0.04942925] singular values in the case of reduction the dimension to 3: [782.99443538

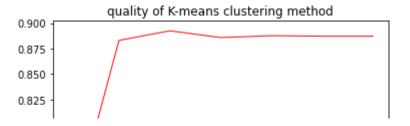
430.96266874 214.95069305]



variance ratio in the case of reduction the dimension to 4: [0.65587897 0. 19869441 0.04942925 0.03029916] singular values in the case of reduction the dimension to 4: [782.99443538 430.96266874 214.95069305 168.29148088]

```
In [7]: ## Question 3.1 - part 3 ##
        print('#############"")
        print('Question 3.1 - part 3 ')
        print('############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.decomposition import PCA
        from sklearn.cluster import KMeans
        from sklearn.utils import shuffle
        from sklearn import decomposition
        from sklearn.mixture import GaussianMixture
        from sklearn import metrics
        import numpy as np
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        import pandas as pd
        dataset=pd.read_csv('files/wifi_localization.csv',header=None)
        X = dataset.values[:,0:7]
        Y = dataset.values[:,7]
        random = np.random.seed(69007044)
        clustring_quality=[]
        for i in range(1,8):
            pca = PCA(n components=i, random state=random)
           pca.fit(X)
           X PCA = pca.transform(X)
            kmeans = KMeans(n_clusters=4, random_state=random).fit(X_PCA)
            predict_label = kmeans.labels_
            clustring_quality.append(metrics.adjusted_mutual_info_score(Y, predict_lab
        print(clustring_quality)
        plt.plot([1,2,3,4,5,6,7], clustring_quality, color="red", linewidth=1)
        plt.xlabel('number of features ')
        plt.title('quality of K-means clustering method')
        plt.show()
```

[0.6976979455768423, 0.8830470047992286, 0.8924347394577512, 0.8857863655611 705, 0.8876091219649462, 0.8871530457012681, 0.8871530457012681]



According to the above figure, quality of clustering with K-means method is high enough even for the lower features. Moreover, the quality is higher for 3 features because PCA decreases the complexity and redundancy. We have an improvement for the lower features because K-means method works better for the lower dimensionality. The PCA helps K-means because it reduces the dimension of the data points. That is why we have an improvement. However, when we conduct a PCA analysis on the data with 1 dimension, the clustering quality of K-means method decreases. This is because by having just one dimension of the data points, we lose much information.

K-means method is a clustering method and so it does not use the labels. Thus, when it is used for classification, it ignores the labels and that is why we should not use it for the classification.

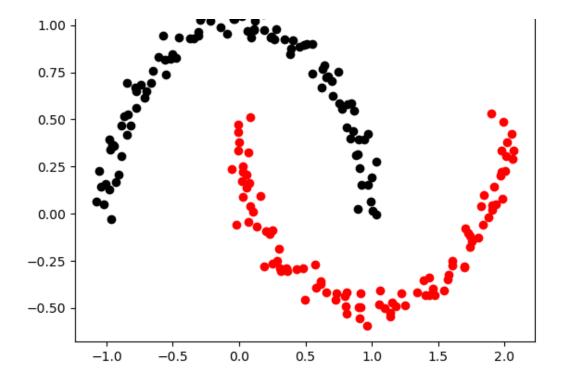
As professor said in the lectures, the classification is classification and the clustering is clustering. We could do better classification by using the classification methods than using the clustering ones. Naturally, we will suffer if we use the K-means for classification.

Section 4: Support Vector Machines (SVMs)

We have covered the theory of <u>SVMs (https://en.wikipedia.org/wiki/Support-vector_machine)</u> during the lectures. It is now time to see SVMs in action! It is appropriate to start with a noisy moon data set. We will use <u>sklearn.svm (https://scikit-learn.org/stable/modules/svm.html)</u> library.

```
In [7]: from sklearn import svm
        from sklearn.model_selection import GridSearchCV
        from sklearn import preprocessing
        from sklearn import metrics
        # helper function to visualise decision boundary, uses the svm model as input
        def plot_svc_decision_function(model, ax=None, plot_support=True):
            """Plot the decision function for a 2D SVC"""
            if ax is None:
                ax = plt.gca()
            xlim = ax.get_xlim()
            ylim = ax.get_ylim()
            # create grid to evaluate model
            x = np.linspace(xlim[0], xlim[1], 30)
            y = np.linspace(ylim[0], ylim[1
                                          1, 30)
            Y, X = np.meshgrid(y, x)
            xy = np.vstack([X.ravel(), Y.ravel()]).T
            P = model.decision_function(xy).reshape(X.shape)
            # plot decision boundary and margins
            ax.contour(X, Y, P, colors='k',
                       levels=[-1, 0, 1], alpha=0.5,
                       linestyles=['--', '-', '--'])
            # plot support vectors
            if plot_support:
                ax.scatter(model.support_vectors_[:, 0],
                           model.support_vectors_[:, 1],
                           s=300, linewidth=1, facecolors='none');
            ax.set_xlim(xlim)
            ax.set_ylim(ylim)
        # this is not necessary if you run it in the cell earlier...
        #np.random.seed(Put the same or different group specific number!)
        # Create a new moons data set
        new_moons = datasets.make_moons(n_samples=400, noise=0.15)
        Xm = new_moons[0] # data points
        ym = new_moons[1] # 0, 1 labels of class, 200 each - giving us the ground trut
        # Visualise the data set
        order_ind = np.argsort(ym) # order labels, 200 each class
        Xm1 = Xm[order_ind[0:200]] # class 1 - only for visualisation
        Xm2 = Xm[order_ind[201:400]] # class 2 - only for visualisation
        plt.figure()
        plt.scatter(X1[:,0], X1[:,1], color='black')
        plt.scatter(X2[:,0], X2[:,1], color='red')
```

<IPython.core.display.Javascript object>



Question 4.1 [20%] Binary SVM Classifiers

First divide the data (Xm, ym) to training and test sets using the default ratio. The range of data values is OK so you can skip data normalisation for this one.

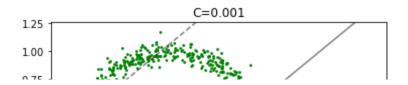
- 1. Try an <u>SVM classifier (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html)</u> with a linear kernel and different C parameters. Plot the test output and boundary. Discuss your observations and comment on linear separability of this data. Provide the precision, recall, and F-score metrics. *Hint:* see <u>sklearn.metrics (https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics)</u>, especially classification report (https://scikit-learn.org/stable/modules/generated
 - /sklearn.metrics.classification_report.html#sklearn.metrics.classification_report)
- 2. Next, use an RBF kernel (https://en.wikipedia.org/wiki/Radial_basis_function_kernel) and repeat the first part for different C and gamma parameters. Do you observe an improvement compared to the linear version (both visually and in terms of scores)? Discuss your results.
- 3. Perform a cross-validated grid-search over a parameter grid to find good C and gamma hyper-parameters. Plot the AUC (mean_train_AUC) vs gamma for the best C. Hint: check GridSearchCV (https://scikit-learn.org/stable/auto_examples/model_selection/plot_multi_metric_evaluation.html#sphx-glr-auto-examples-model-selection-plot-multi-metric-evaluation-py) and scoring parameter (https://scikit-learn.org/stable/modules/model_evaluation.html#scoring-parameter). Note that you should use semi-log plot!

```
In [1]: ## Question 4.1 - part 1 ##
       print('#############")
       print('Question 4.1 - part 1 ')
       print('############")
       print()
       from sklearn import cluster, datasets, mixture
       from sklearn.svm import LinearSVC,SVC
       from sklearn.metrics import classification_report
       import numpy as np
       from sklearn.model_selection import train_test_split
       from sklearn.metrics import precision_recall_fscore_support
       from matplotlib import pyplot as plt
       from sklearn.metrics import accuracy_score
       from sklearn.cluster import KMeans
       import pandas as pd
       random = np.random.seed(69007044)
       noisy_moons = datasets.make_moons(n_samples=5000, noise=0.05)
       X = noisy moons[0] # data points
       Y = noisy_moons[1] # data points
       X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.2, rando
       for c in [0.001,0.01,0.1,1,10]:
           clf = SVC(C=c,kernel='linear')
           clf.fit(X_train, y_train)
           predic_label=clf.predict(X_test)
           class0=[]
           class1=[]
           for count,item in enumerate(predic_label):
               if item == 0:
                  class0.append(X_test[count])
               elif item == 1:
                  class1.append(X_test[count])
           class0=np.array(class0)
           class1=np.array(class1)
           plt.scatter(class0[:,0], class0[:,1], color='green',s=3)
           plt.scatter(class1[:,0], class1[:,1], color='blue',s=3)
           print('############# report for c=%s ##############*/%c)
           target_names = ['class 0', 'class 1']
           print(classification_report(y_test, predic_label, target_names=target_name
           # print(precision_recall_fscore_support(y_test, predic_label))
```

```
ax=None
   plot_support=True
   if ax is None:
       ax = plt.gca()
   xlim = ax.get_xlim()
   ylim = ax.get_ylim()
   # create grid to evaluate model
   x = np.linspace(xlim[0], xlim[1], 30)
   y = np.linspace(ylim[0], ylim[1], 30)
   Y, X = np.meshgrid(y, x)
   xy = np.vstack([X.ravel(), Y.ravel()]).T
   P = clf.decision_function(xy).reshape(X.shape)
   # plot decision boundary and margins
   ax.contour(X, Y, P, colors='k',
             levels=[-1, 0, 1], alpha=0.5,
             linestyles=['--', '-', '--'])
   # plot support vectors
   if plot_support:
       ax.scatter(clf.support_vectors_[:, 0],
                 clf.support_vectors_[:, 1],
                 s=300, linewidth=1, facecolors='none');
   ax.set_xlim(xlim)
   ax.set_ylim(ylim)
   plt.title('C=%s'%c)
######################################
```

Question 4.1 - part 1

precision recall f1-score support class 0 0.86 0.84 0.85 515 class 1 0.84 0.86 0.85 485 0.85 1000 accuracy 0.85 0.85 macro avg 0.85 1000 weighted avg 0.85 0.85 0.85 1000



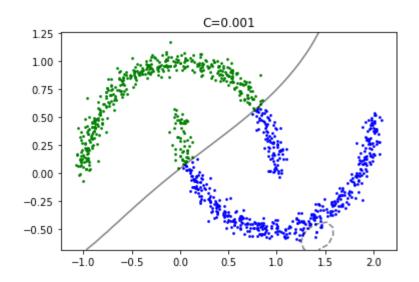
By increasing the C parameter in the linear kernel, the accuracy increases. However, this does not happen much for the C parameters greater than 0.1. I mean, the accuracy converges by increasing the C parameter and does not increase much for C>0.1. Also, the separability improvement in the linear kernel stops for the C>0.1.

```
In [10]: ## Question 4.1 - part 2.1 ##
        print('#############")
        print('Question 4.1 - part 2.1 ')
        print('############")
        print()
        from sklearn import cluster, datasets, mixture
        from sklearn.svm import LinearSVC,SVC
        from sklearn.metrics import classification_report
        import numpy as np
        from sklearn.model_selection import train_test_split
        from matplotlib import pyplot as plt
        from sklearn.cluster import KMeans
        import pandas as pd
        random = np.random.seed(69007044)
        noisy_moons = datasets.make_moons(n_samples=5000, noise=0.05)
        X = noisy_moons[0] # data points
        Y = noisy_moons[1] # data points
        X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.2, rando
        for c in [0.001,0.01,0.1,1,10]:
           clf = SVC(C=c,kernel='rbf',gamma='auto')
           clf.fit(X_train, y_train)
           predic_label=clf.predict(X_test)
           class0=[]
           class1=[]
           for count,item in enumerate(predic label):
               if item == 0:
                  class0.append(X_test[count])
               elif item == 1:
                  class1.append(X_test[count])
           class0=np.array(class0)
           class1=np.array(class1)
           plt.scatter(class0[:,0], class0[:,1], color='green',s=3)
           plt.scatter(class1[:,0], class1[:,1], color='blue',s=3)
           print('############## report for c=%s ###############"%c)
           target_names = ['class 0', 'class 1']
           print(classification_report(y_test, predic_label, target_names=target_name
           ax=None
           plot_support=True
```

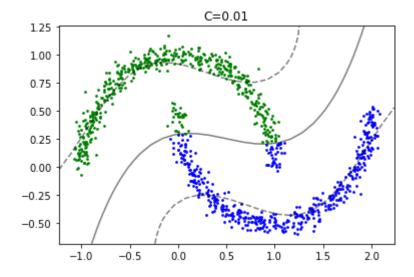
```
if ax is None:
    ax = plt.gca()
xlim = ax.get_xlim()
ylim = ax.get_ylim()
# create grid to evaluate model
x = np.linspace(xlim[0], xlim[1], 30)
y = np.linspace(ylim[0], ylim[1], 30)
Y, X = np.meshgrid(y, x)
xy = np.vstack([X.ravel(), Y.ravel()]).T
P = clf.decision_function(xy).reshape(X.shape)
# plot decision boundary and margins
ax.contour(X, Y, P, colors='k',
           levels=[-1, 0, 1], alpha=0.5,
           linestyles=['--', '-', '--'])
# plot support vectors
if plot_support:
    ax.scatter(clf.support_vectors_[:, 0],
               clf.support_vectors_[:, 1],
               s=300, linewidth=1, facecolors='none');
ax.set_xlim(xlim)
ax.set_ylim(ylim)
plt.title('C=%s'%c)
```

Question 4.1 - part 2.1

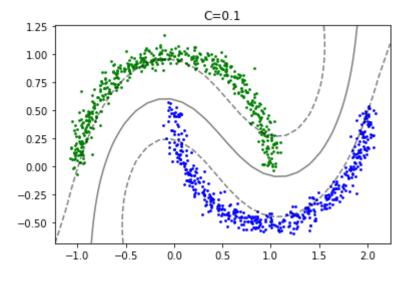
############	##### report	for c=0.0	0 <mark>01 ######</mark> ##	+###########
	precision	recall	f1-score	support
class 0	0.88	0.82	0.85	515
class 1	0.82	0.88	0.85	485
accuracy			0.85	1000
macro avg	0.85	0.85	0.85	1000
weighted avg	0.85	0 85	0 85	1000



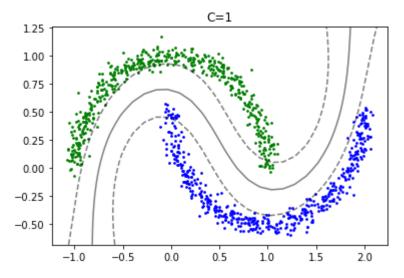
#############	##### report	for c=0.	01 #######	###########
	precision	recall	f1-score	support
class 0	0.94	0.93	0.94	515
class 1	0.93	0.94	0.93	485
accuracy			0.94	1000
macro avg	0.93	0.94	0.93	1000
weighted avg	0.94	0.94	0.94	1000



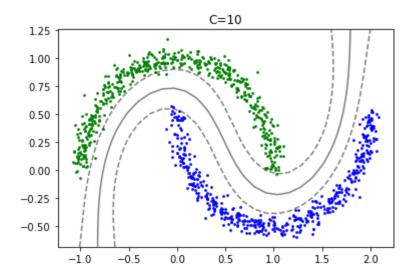
precision recall f1-score support class 0 1.00 1.00 1.00 515 class 1 1.00 1.00 1.00 485 1.00 1000 accuracy macro avg 1.00 1.00 1.00 1000 1.00 1.00 1.00 1000 weighted avg



class 0 class 1	1.00 1.00	1.00 1.00	1.00 1.00	515 485
accuracy			1.00	1000
macro avg	1.00	1.00	1.00	1000
weighted avg	1.00	1.00	1.00	1000



############	##### report precision		######## f1-score	
	precision	Lecam	11-Score	support
class 0	1.00	1.00	1.00	515
class 1	1.00	1.00	1.00	485
accuracy			1.00	1000
macro avg	1.00	1.00	1.00	1000
weighted avg	1.00	1.00	1.00	1000



By increasing the C parameter in the RBF kernel, the accuracy increases. However, this does not happen much for the C parameters greater than 0.01. I mean, the accuracy converges by increasing the C parameter and does not increase much for C>0.1. But the accuracy touches 1 and also, the separability of the data continues to be improved in RBF.

```
In [11]: ## Question 4.1 - part 2.2 ##
       print('#############")
       print('Question 4.1 - part 2.2 ')
       print('############")
       print()
       from sklearn import cluster, datasets, mixture
       from sklearn.svm import LinearSVC,SVC
       from sklearn.metrics import classification_report
       import numpy as np
       from sklearn.model_selection import train_test_split
       from matplotlib import pyplot as plt
       from sklearn.cluster import KMeans
       import pandas as pd
       random = np.random.seed(69007044)
       noisy_moons = datasets.make_moons(n_samples=5000, noise=0.05)
       X = noisy_moons[0] # data points
       Y = noisy_moons[1] # data points
       X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.2, rando
       for c in [0.001,0.01,0.1,1,10]:
          clf = SVC(C=c,kernel='linear')
          clf.fit(X_train, y_train)
          predic_label=clf.predict(X_test)
          class0=[]
          class1=[]
          for count,item in enumerate(predic label):
             if item == 0:
                 class0.append(X_test[count])
             elif item == 1:
                 class1.append(X_test[count])
          class0=np.array(class0)
          class1=np.array(class1)
          plt.subplot(1, 2, 1)
          plt.scatter(class0[:,0], class0[:,1], color='green',s=3)
          plt.scatter(class1[:,0], class1[:,1], color='blue',s=3)
          target_names = ['class 0', 'class 1']
          print(classification_report(y_test, predic_label, target_names=target_name
          ax=None
          plot_support=True
```

```
if ax is None:
   ax = plt.gca()
xlim = ax.get_xlim()
ylim = ax.get_ylim()
# create grid to evaluate model
x = np.linspace(xlim[0], xlim[1], 30)
y = np.linspace(ylim[0], ylim[1], 30)
Y, X = np.meshgrid(y, x)
xy = np.vstack([X.ravel(), Y.ravel()]).T
P = clf.decision_function(xy).reshape(X.shape)
# plot decision boundary and margins
ax.contour(X, Y, P, colors='k',
         levels=[-1, 0, 1], alpha=0.5,
         linestyles=['--', '-', '--'])
# plot support vectors
if plot_support:
   ax.scatter(clf.support_vectors_[:, 0],
            clf.support_vectors_[:, 1],
            s=300, linewidth=1, facecolors='none');
ax.set_xlim(xlim)
ax.set_ylim(ylim)
plt.title('C=%s'%c)
clf = SVC(C=c, kernel='rbf', gamma='auto')
clf.fit(X_train, y_train)
predic label = clf.predict(X test)
class0 = []
class1 = []
for count, item in enumerate(predic_label):
   if item == 0:
      class0.append(X_test[count])
   elif item == 1:
      class1.append(X_test[count])
class0 = np.array(class0)
class1 = np.array(class1)
plt.subplot(1, 2, 2)
plt.scatter(class0[:, 0], class0[:, 1], color='green', s=3)
plt.scatter(class1[:, 0], class1[:, 1], color='blue', s=3)
print('############## report rbf kernel for c=%s ############### %
target_names = ['class 0', 'class 1']
print(classification_report(y_test, predic_label, target_names=target_name
ax = None
plot_support = True
```

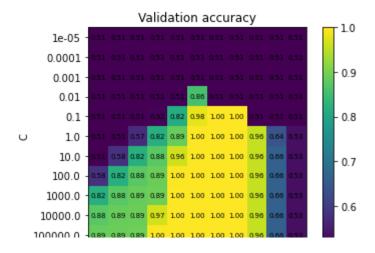
```
if ax is None:
      ax = plt.gca()
   xlim = ax.get_xlim()
   ylim = ax.get_ylim()
   # create grid to evaluate model
   x = np.linspace(xlim[0], xlim[1], 30)
   y = np.linspace(ylim[0], ylim[1], 30)
   Y, X = np.meshgrid(y, x)
   xy = np.vstack([X.ravel(), Y.ravel()]).T
   P = clf.decision_function(xy).reshape(X.shape)
   # plot decision boundary and margins
   ax.contour(X, Y, P, colors='k',
            levels=[-1, 0, 1], alpha=0.5,
            linestyles=['--', '-', '--'])
   # plot support vectors
   if plot_support:
      ax.scatter(clf.support_vectors_[:, 0],
               clf.support_vectors_[:, 1],
               s=300, linewidth=1, facecolors='none');
   ax.set_xlim(xlim)
   ax.set_ylim(ylim)
Question 4.1 - part 2.2
precision recall f1-score
                                     support
    class 0
               0.86
                                0.85
                       0.84
                                         515
    class 1
               0.84
                       0.86
                                0.85
                                         485
   accuracy
                                0.85
                                        1000
                       0.85
                                0.85
                                        1000
  macro avg
               0.85
                       0.85
weighted avg
               0.85
                               0.85
                                        1000
precision
                     recall f1-score
                                     support
    class 0
               0.88
                                         515
                       0.82
                                0.85
    class 1
               0.82
                       0.88
                                0.85
                                         485
```

Firstly, for the same C parameter, the accuracy of the RBF kernel is better than the linear kernel. Thus, the accuracy touches 1 in the RBF kernel.

Secondly, although when the accuracy is high in both linear and RBF kernels, it does not increase much by increasing the C parameter, the separability of the data continues to be improved in RBF. However, the improvement in the linear kernel stops. This is because the linear kernel is so simple kernel compared to the RBF kernel. This shows that the complexity in the RBF kernel helps it to learn better.

```
In [14]: ## Question 4.1 - part 3 ##
         print('#############")
         print('Question 4.1 - part 3 ')
         print('#############")
         print()
         import numpy as np
         import matplotlib.pyplot as plt
         from matplotlib.colors import Normalize
         from sklearn.svm import SVC
         from sklearn.preprocessing import StandardScaler
         from sklearn.datasets import load_iris
         from sklearn.model_selection import StratifiedShuffleSplit
         from sklearn.model_selection import GridSearchCV
         from sklearn import cluster, datasets, mixture
         from sklearn.svm import LinearSVC,SVC
         from sklearn.metrics import classification_report,accuracy_score
         import numpy as np
         from sklearn.model_selection import train_test_split
         from matplotlib import pyplot as plt
         from sklearn.cluster import KMeans
         import pandas as pd
         # dataset for grid search
         random = np.random.seed(69007044)
         noisy_moons = datasets.make_moons(n_samples=500, noise=0.05)
         X = noisy_moons[0] # data points
         Y = noisy_moons[1] # data points
         X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.2, rando
         C range = np.logspace(-5, 5, 11)
         gamma_range = np.logspace(-5, 5, 11)
         param_grid = dict(gamma=gamma_range, C=C_range)
         cv = StratifiedShuffleSplit(n_splits=5, test_size=0.2, random_state=random)
         grid = GridSearchCV(SVC(), param_grid=param_grid, cv=cv)
         grid.fit(X_train, y_train)
         print(
             "The best parameters are %s with a score of %0.2f"
             % (grid.best_params_, grid.best_score_)
         scores = grid.cv_results_["mean_test_score"].reshape(len(C_range), len(gamma_r
         plt.imshow(scores)
         plt.xlabel("gamma")
         plt.ylabel("C")
         plt.colorbar()
         plt.xticks(np.arange(len(gamma_range)), gamma_range, rotation=45)
         plt.yticks(np.arange(len(C_range)), C_range)
         plt.title("Validation accuracy")
```

The best parameters are {'C': 0.1, 'gamma': 10.0} with a score of 1.00



For the best amount of the C parameter (C=0.1) and by increasing the gamma parameter, the accuracy inreases at the first steps (until gamma = 10), then it decreases. Also, this is true for other amount of C parameter when it is higher than 0.01. But when the C<0.01, the gamma parameter cannot considerably have impact on the accuracy.

Moreover, for the fixed amount of the gamma parameter, the accuracy always increases by increasing the C parameter.

Section 5: Logistic Regression

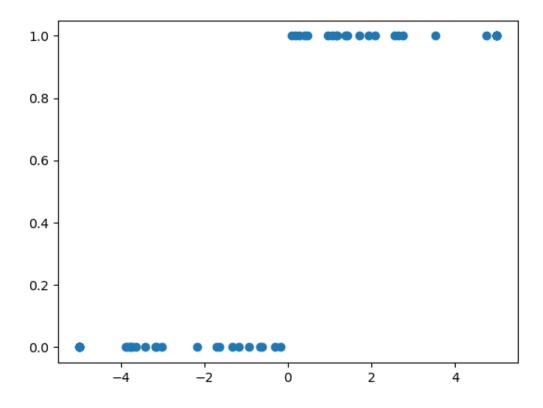
Logistic regression uses a linear statistical model. It measures the relationship between the categorical dependent variable and one or more independent variables by estimating probabilities using a logistic function. It is also used for classification. Let's start with a very simple example to **visualise the logistic function**.

```
In [8]: # Generate a toy dataset

toy_samples = 50
X_toy = np.linspace(-5, 5, toy_samples)
Xtoy_test = np.linspace(-5, 5, 200)
# gaussian noise added
X_toy = X_toy + 2*np.random.normal(size=toy_samples)
# upper, lower bound
X_toy = np.clip(X_toy,-5, 5).reshape(-1,1)
# create labels
y_toy = ((np.sign(X_toy)+1)/2.0).ravel()

# visualise
plt.figure()
plt.scatter(X_toy, y_toy)
```

<IPython.core.display.Javascript object>

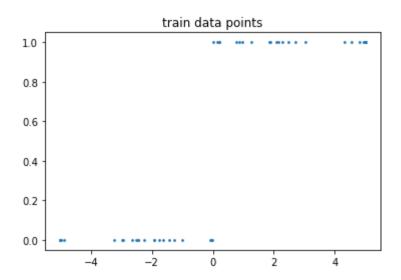


Question 5.1 [5%] Simple Logistic Regression (LR)

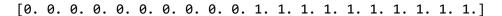
- Fit a logistic and linear regression model to the data (X_toy, y_toy). Find the logistic and linear model coefficients and bias (trained_model.coef_, trained_model.intercept_). Hint: check sklearn logistic regression (https://scikit-learn.org/stable/modules/generated /sklearn.linear_model.LogisticRegression.html).
- 2. Test your models on a simple test set (Xtoy_test) given above. Plot your results and discuss.

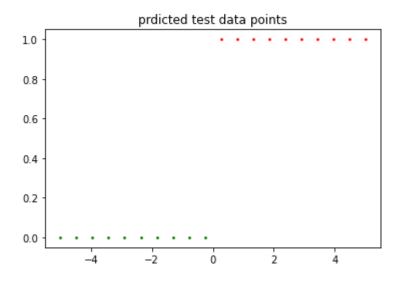
```
In [32]: ## Question 5.1 - part 1 & 2 ##
         print('############")
         print('Question 5.1 - part 1 & 2')
         print('############")
         print()
         import numpy as np
         from matplotlib import pyplot as plt
         from sklearn.linear model import LogisticRegression
         # import pandas as pd
         ###### part 1 #####
         toy_samples = 50
         X_toy = np.linspace(-5, 5, toy_samples)
         Xtoy_test = np.linspace(-5, 5,20)
         # gaussian noise added
         X_toy = X_toy + 2*np.random.normal(size=toy_samples)
         # upper, lower bound
         X_{toy} = np.clip(X_{toy}, -5, 5).reshape(-1,1)
         # create labels
         y_{toy} = ((np.sign(X_{toy})+1)/2.0).ravel()
         # visualise plt.figure() plt.scatter(X_toy, y_toy) plt.show()
         train_model = LogisticRegression(random_state=69007044).fit(X_toy,y_toy)
         # visualise
         plt.figure()
         plt.scatter(X_toy, y_toy,s=3)
         plt.title('train data points')
         plt.show()
         print('The linear model coefficient is : ' , train_model.coef_)
         print('The linear model bias is : ' , train_model.intercept_)
         print()
         ###### part 2 #####
         Xtoy_test = np.clip(Xtoy_test, -5, 5).reshape(-1,1)
         ytoy_test = ((np.sign(Xtoy_test)+1)/2.0).ravel()
         predict=train_model.predict(Xtoy_test)
         print (predict)
         class0=[]
         class1=[]
         for count,item in enumerate(predict):
             if item == 0:
                 class0.append(Xtoy_test[count])
             elif item == 1:
                 class1.append(Xtoy_test[count])
         class0=np.array(class0)
         class1=np.array(class1)
         # print(class0)
         #####
         plt.scatter(class0, np.zeros(len(class0)), color='green',s=3)
         plt.scatter(class1, np.ones(len(class1)), color='red',s=3)
```

```
plt.title('prdicted test data points')
```



The linear model coefficient is : [[1.86757118]] The linear model bias is : [0.19476885]





The red points are in the class 1 and the green ones are in the class 0. If a red point value was less than zero (in the left side of zero), the prediction would not be correct. Also, a green point value was greater than zero (in the right side of zero), the prediction would not be correct.

Thus, the prediction is correct because all predicted points are in the correct area.

Example 5.1: Electrical Grid Stability with Simulated Data

This simulated <u>dataset (http://archive.ics.uci.edu/ml/datasets/Electrical+Grid+Stability+Simulated+Data+)</u> is related to the local stability of a 4-node star system (where the electricity producer is in the center), which implements a decentralised Smart Grid Control concept.

Arzamasov, Vadim, Klemens Boehm, and Patrick Jochem. <u>'Towards Concise Models of Grid Stability.' (https://dbis.ipd.kit.edu/download/DSGC_simulations.pdf)</u> Communications, Control, and Computing Technologies for Smart Grids (SmartGridComm), 2018 IEEE International Conference on. IEEE, 2018

Note: In many engineering applications, such datasets can be generated through simulations (easy) or experimentation (harder). Different from classical ML applications, engineers often have a very good understanding of the underlying physical models, which gives a unique advantage. We will, however, keep it simple in this workshop and use the dataset as is.

Let's load and process the dataset.

In [9]:	gri	iddata =	pd.rea	d_csv('	files/Da	ata_for_	_UCI_nam	ed.csv')				
Out[9]:		tau1	tau2	tau3	tau4	p1	p2	рЗ	p4	g1	g2	
	0	2.959060	3.079885	8.381025	9.780754	3.763085	-0.782604	-1.257395	-1.723086	0.650456	0.859578	0.
	1	9.304097	4.902524	3.047541	1.369357	5.067812	-1.940058	-1.872742	-1.255012	0.413441	0.862414	0.
	2	8.971707	8.848428	3.046479	1.214518	3.405158	-1.207456	-1.277210	-0.920492	0.163041	0.766689	0.
	3	0.716415	7.669600	4.486641	2.340563	3.963791	-1.027473	-1.938944	-0.997374	0.446209	0.976744	0.
	4	3.134112	7.608772	4.943759	9.857573	3.525811	-1.125531	-1.845975	-0.554305	0.797110	0.455450	0.
In [10]:	Xgr	rid = gr	iddata.	iloc[:,	0:13]							
	Xgr	rid = gr tau1	riddata. tau2	iloc[:,	0:13] tau4	p1	p2	р3	p4	g1	g2	
		• • • •	1/1		-	p1 3.763085	•	p3 -1.257395	p4 -1.723086	g1 0.650456	g2 0.859578	0.
		tau1	tau2	tau3	tau4	•	-0.782604	•	•			
<pre>In [10]: Out[10]:</pre>	0	tau1	tau2 3.079885	tau3 8.381025	tau4	3.763085 5.067812	-0.782604	-1.257395 -1.872742	-1.723086	0.650456	0.859578	0.
	0 1 2	tau1 2.959060 9.304097	tau2 3.079885 4.902524	tau3 8.381025 3.047541	tau4 9.780754 1.369357	3.763085 5.067812	-0.782604 -1.940058 -1.207456	-1.257395 -1.872742	-1.723086 -1.255012	0.650456 0.413441	0.859578 0.862414	0. 0.

```
In [11]: | ygrid = griddata.iloc[:, 13]
         # 0 if unstable and 1 if stable
         ygrid = [ 0 if x=='unstable' else 1 for x in ygrid]
         prepared data:
                               tau1
                                        tau2
                                                  tau3
                                                            tau4
                                                                        p1
                                                                                 р
         2
                 p3 \
          2.959060 3.079885 8.381025 9.780754 3.763085 -0.782604 -1.257395
         0
           9.304097 4.902524 3.047541 1.369357 5.067812 -1.940058 -1.872742
         1
           8.971707 8.848428 3.046479 1.214518 3.405158 -1.207456 -1.277210
         3 0.716415 7.669600 4.486641 2.340563 3.963791 -1.027473 -1.938944
         4 3.134112 7.608772 4.943759 9.857573 3.525811 -1.125531 -1.845975
                                                                stab
                 p4
                           g1
                                               g3
                                                        g4
                                     g2
         0 -1.723086  0.650456  0.859578  0.887445  0.958034  0.055347
         1 -1.255012 0.413441 0.862414 0.562139 0.781760 -0.005957
         2 -0.920492 0.163041 0.766689 0.839444 0.109853 0.003471
         3 -0.997374 0.446209 0.976744 0.929381 0.362718 0.028871
         4 -0.554305 0.797110 0.455450 0.656947 0.820923 0.049860
                                                                       [0, 1, 0, 0,
         0]
```

Question 5.2 [15%] Checking Grid Stability using Logistic Regression (LR)

Now, we can use the simulated dataset (Xgrid , ygrid) to check grid stability. We will use first logistic regression for this purpose. Unfortunately, it is not possible to directly visualise this dataset, so we have to use performance metrics.

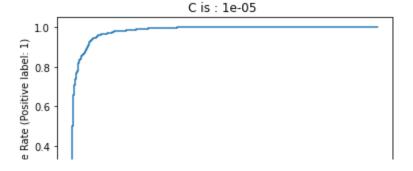
- Preprocess and normalise Xgrid using a <u>sklearn.preprocessing</u> (https://scikit-learn.org/stable /modules/classes.html#module-sklearn.preprocessing). You can use, for example, StandardScaler or MinMaxScaler.
- 2. Train a logistic regression model that classifies the grid as stable or not, based on input Xgrid. Don't forget to divide Xgrid into training and test sets. Quantify the performance of LR using standard metrics such as accuracy, precision, recall, and f1 score on the test set. Plot the ROC curve (https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics). How do these change w.r.t. parameter C (https://scikit-learn.org/stable/modules/linear model.html#logistic-regression)? Discuss your observations.
- 3. What are the coefficients of the LR that you trained? What do they tell you about the impact of independent input variables on the dependent output variable ygrid? Discuss. Hint: you can use statsmodels package (https://www.statsmodels.org) logistic regression to calculate p-values. Here is a nice tutorial (https://pythonguides.com/scikit-learn-logistic-regression/) on this. For further info, see e.g. this (http://www.r-tutor.com/elementary-statistics/logistic-regression/significance-test-logistic-regression) or this (http://blog.minitab.com/blog/adventures-in-statistics-2/how-to-interpret-regression-analysis-results-p-values-and-coefficients).
- 4. Use a nonlinear SVM, e.g. with rbf kernel, to solve the problem. Quantify the performance of SVM classifier and compare with LR one. Discuss your findings.

Answer as text here

```
In [33]: ## Question 5.2 - part 1 ##
       print('#############"")
       print('Question 5.2 - part 1')
       print('############")
       print()
       import pandas as pd
       from sklearn.preprocessing import StandardScaler
       griddata = pd.read_csv('files/Data_for_UCI_named.csv')
       griddata.head()
       Xgrid = griddata.iloc[:, 0:13]
       Xgrid.head()
       ygrid = griddata.iloc[:, 13]
       # 0 if unstable and 1 if stable
       ygrid = [ 0 if x=='unstable' else 1 for x in ygrid]
       scaler = StandardScaler()
       scaler.fit(Xgrid)
       print(scaler.transform(Xgrid))
       Question 5.2 - part 1
       [[-0.83537431 -0.79131661 1.14170354 ... 1.32162751 1.57902607
          1.07312049]
        [ 1.47829663 -0.12670487 -0.80311147 ... 0.13542358 0.93625569
         -0.58748693]
        -0.33209522]
        [-1.05234609 -0.87804866 1.28587062 ... -1.37001303 -1.38205402
         -1.28776846]
        [ 1.59768553 -0.45784646 -0.90902909 ... 1.32772953 1.06982944
          0.59749703
                   0.55855544 -0.32829064 ... -0.53325125 1.52285961
```

```
In [59]: ## Question 5.2 - part 2 ##
        print('#############")
        print('Question 5.2 - part 2')
        print('############")
        print()
        import numpy as np
        import pandas as pd
        from sklearn.model_selection import train_test_split
        from sklearn.preprocessing import StandardScaler
        from sklearn.metrics import precision_recall_fscore_support
        griddata = pd.read_csv('files/Data_for_UCI_named.csv')
        griddata.head()
        Xgrid = griddata.iloc[:, 0:13]
        Xgrid.head()
        ygrid = griddata.iloc[:, 13]
        # 0 if unstable and 1 if stable
        ygrid = [ 0 if x=='unstable' else 1 for x in ygrid]
        scaler = StandardScaler()
        scaler.fit(Xgrid)
        Xgrid = scaler.transform(Xgrid)
        # split into training and test sets
        X_train, X_test, y_train, y_test = train_test_split(Xgrid, ygrid)
        print('number of training data for X is = ', len(X_train))
        print('number of training data for y is = ', len(y_train))
        print('number of testing data for X is = ', len(X_test))
        print('number of testing data for y is = ', len(y_test))
        train_model = LogisticRegression(random_state=69007044).fit(X_train,y_train)
        y_predict=train_model.predict(X_test)
        accuracy =accuracy_score(y_test,y_predict)
        print('accuracy is : ' , accuracy)
        precision_recall_fscore_support(y_test, y_predict, average='micro')
        C_{range} = np.logspace(-5, 2, 8)
        for c in C_range:
            train_model = LogisticRegression(random_state=69007044,C=c).fit(X_train,y
            y_predict=train_model.predict(X_test)
            metrics.plot_roc_curve(train_model, X_test, y_test)
            plt.title('C is : %s ' %c)
         Question 5.2 - part 2
```


number of training data for X is = 7500 number of training data for y is = 7500 number of testing data for X is = 2500 number of testing data for y is = 2500 accuracy is : 0.9972



By increasing the C parameter, the AUC is improved and ROC becomes sharper which show the regularisation increases the accuracy.

```
In [81]: ## Question 5.2 - part 4 ##
         print('#############")
         print('Question 5.2 - part 4')
         print('############")
         print()
         from sklearn import cluster, datasets, mixture
         from sklearn.svm import LinearSVC,SVC
         from sklearn.metrics import classification_report
         import numpy as np
         from sklearn.model_selection import train_test_split
         from matplotlib import pyplot as plt
         from sklearn.cluster import KMeans
         import pandas as pd
         from sklearn.preprocessing import StandardScaler
         from sklearn.metrics import precision_recall_fscore_support
         griddata = pd.read_csv('files/Data_for_UCI_named.csv')
         griddata.head()
         Xgrid = griddata.iloc[:, 0:13]
         Xgrid.head()
         ygrid = griddata.iloc[:, 13]
         # 0 if unstable and 1 if stable
         ygrid = [ 0 if x=='unstable' else 1 for x in ygrid]
         scaler = StandardScaler()
         scaler.fit(Xgrid)
         Xgrid = scaler.transform(Xgrid)
         # split into training and test sets
         X_train, X_test, y_train, y_test = train_test_split(Xgrid, ygrid)
         print('number of training data for X is = ', len(X_train))
         print('number of training data for y is = ', len(y_train))
         print('number of testing data for X is = ', len(X_test))
         print('number of testing data for y is = ', len(y_test))
         range_C = np.logspace(-5, 5, 11)
         for c in range C:
             clf = SVC(C=c,kernel='rbf',gamma='auto')
             clf.fit(X_train, y_train)
             y_predict_svm=clf.predict(X_test)
             accuracy_svm =accuracy_score(y_test,y_predict_svm)
             train_model = LogisticRegression(random_state=69007044,C=c).fit(X_train,y
             y_predict_LR = train_model.predict(X_test)
             accuracy_LR = accuracy_score(y_test,y_predict_LR)
```

```
print('c is :' , c)
   print('accuracy for SVM is : ' , accuracy_svm)
   print('accuracy for LR is :' , accuracy_LR)
Question 5.2 - part 4
number of training data for X is = 7500
number of training data for y is = 7500
number of testing data for X is = 2500
number of testing data for y is = 2500
c is: 1e-05
accuracy for SVM is: 0.6424
accuracy for LR is: 0.6424
c is: 0.0001
accuracy for SVM is: 0.6424
accuracy for LR is: 0.7132
c is: 0.001
accuracy for SVM is: 0.6424
accuracy for LR is: 0.9372
c is: 0.01
accuracy for SVM is: 0.9424
accuracy for LR is: 0.9688
c is : 0.1
accuracy for SVM is : 0.9744
accuracy for LR is: 0.9896
c is: 1.0
accuracy for SVM is: 0.986
accuracy for LR is: 0.9964
c is : 10.0
accuracy for SVM is: 0.9844
accuracy for LR is: 0.9984
c is: 100.0
accuracy for SVM is: 0.982
accuracy for LR is: 0.9992
c is: 1000.0
accuracy for SVM is: 0.982
accuracy for LR is: 0.9996
c is: 10000.0
accuracy for SVM is: 0.982
accuracy for LR is: 0.9996
c is: 100000.0
accuracy for SVM is: 0.982
accuracy for LR is: 0.9996
```

The results show that LR always has higher accuracy than SVM.

Workshop Assessment Instructions

You should complete the workshop tasks and answer the questions within the allocated session! Submission deadline is the the end of second Week of the workshop. Please check Canvas for exact deadline!

It is mandatory to follow all of the submissions guidelines given below. Don't forget the Report submission information on top of this notebook!

- 1. The completed Jupyter notebook and its Pdf version (you can simply print-preview and then print as pdf from within your browser) should be uploaded to the right place in Canvas. It is your responsibility to follow the announcements! Late submissions will be penalised (up to 100% of the total mark depending on delay amount)!
- Filename should be "ELEN90088 Workshop W: StudentID1-StudentID2 of session Day-Time", where W refers to the workshop number, StudentID1-StudentID2 are your student numbers, Day-Time is your session day and time, e.g. Tue-14.
- 3. Answers to questions, simulation results and diagrams should be included in the Jupyter notebook as text, code, plots. If you don't know latex, you can write formulas/text to a paper by hand, scan it and then include as image within Markdown cells.
- Please submit your report individually. Partners can submit the same report.

Workshop Marking

- Each workshop has 10 points corresponding to 10% of the total subject mark. You will receive 3 points from the submitted report and 7 points from an individual oral examination.
- Individual oral quizzes will be scheduled within the next two weeks following the report submission. They will be during workshop hours. Therefore, it is important that you attend the workshops!
- The individual oral examination will assess your answers to workshop questions, what you have done in that workshop, and your knowledge of the subject material in association with the workshop.

Additional guidelines for your programs:

- Write modular code using functions.
- Properly indent your code. But Python forces you do that anyway ;)
- Heavily comment the code to describe your implementation and to show your understanding. No comments, no credit!
- Make the code your own! It is encouraged to find and get inspired by online examples but you should exactly
 understand, modify as needed, and explain your code via comments. If you resort to blind copy/paste, you
 will certainly not do well in the individual oral quizzes.