Machine Learning 2023/2024 (2nd semester)

Master in Electrical and Computer Engineering

Department of Electrical and Computer Engineering

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Notebook #07: Classification (part 2)

k-Nearest Neighbor rule

Take a training set of pairs $\{(y_n, \mathbf{x}_n)\}_{n=1}^{N}$ for a M-class classification problem and let $k > 0$ be a given integer parameter. Given a sample/pattern $\mathbf{x}$, the k-nearest neighbor (k-NN) classification rule consists in assigning $\mathbf{x}$ to the class in which the majority of its k nearest training points belong to (according to a given metric).

Activity 1

Consider a set of data with two features from a representative data set of points of two classes (ω_1 and ω_2).

```
!wget -O dataset.csv.zip https://www.dropbox.com/s/evpwqery7uleqw1/data-set.csv.zip?dl=0 --quiet
!unzip dataset.csv.zip -d.
```

```
!unzip dataset.csv.zip -d.
```

```
Archive:  dataset.csv.zip
  inflating: ./data-set.csv
```

1.1. Extract the data from the data set.

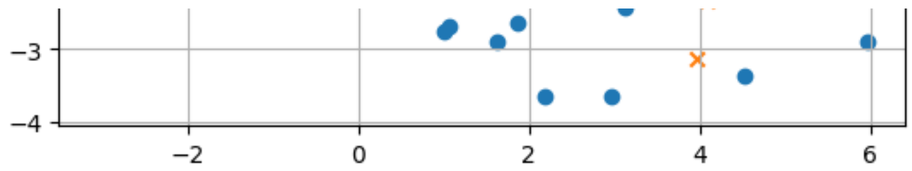
```
# Activity 1.1

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

# read data from file
df = pd.read_csv('data-set.csv')
npoints = df.values.shape[0]

print(df)
```

```
            X1        X2  label
0     0.641113  0.195007      1
1    -1.642258  2.807978      1
2     1.927658  0.569198      1
```

```
3    1.446395 -0.174693       1
4    3.048043  0.237330       2
..        ...       ...     ...
495  2.008408  1.898231       2
496  1.108552 -0.163538       1
497  1.068901  2.412580       2
498 -1.920007  2.571422       1
499  1.897878 -0.748237       1

[500 rows x 3 columns]
```

1.1. (cont) Plot the data from the data set.

```
# plot data
classData = df.values[:,2]
plt.figure()
plt.scatter(df.values[np.where(classData==1),0], df.values[np.where(classData==1),1], marker='o')
plt.scatter(df.values[np.where(classData==2),0], df.values[np.where(classData==2),1], marker='x')
plt.title('Training data')
plt.plot()
plt.grid()
plt.show()
```



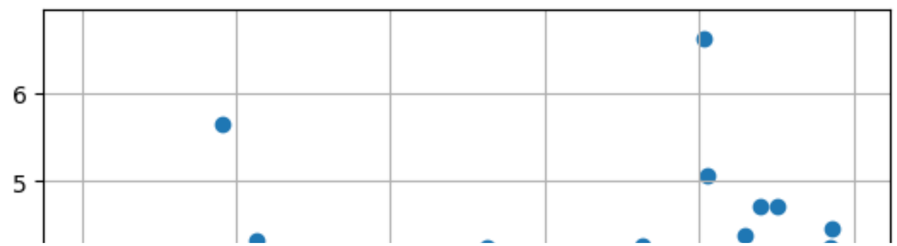
1.2 Given a pattern $\mathbf{x}$, define a function that computes the Euclidean distance to each point of the training data set.

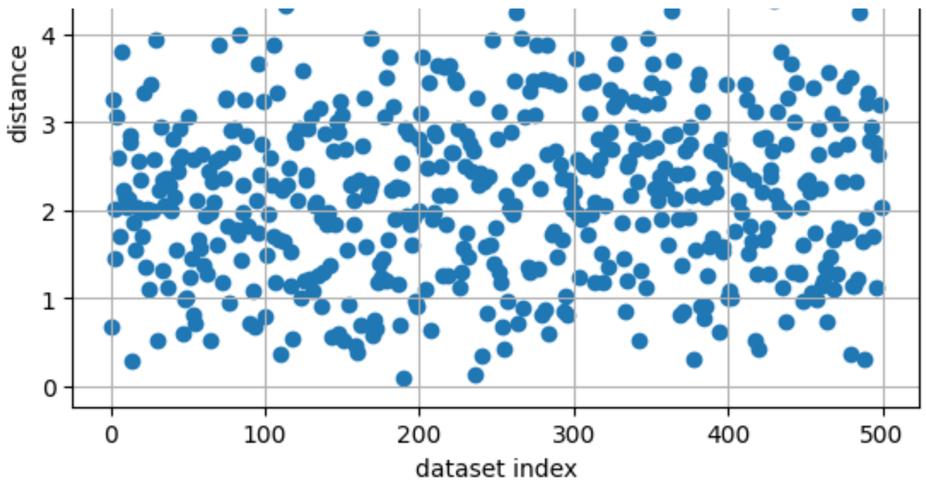
Test your function with the pattern $\mathbf{x} = (0, 0)^\top$ and plot the distances to the points of the dataset.

```
# Activity 1.2

def EuclideanDist(x, data):
  npoints = data.shape[0]
  distances = np.zeros(npoints)
  ''' to be completed
  for i in range(npoints) :
    distances[i] = ...
  '''
  return distances

x = [0,0]
dist = EuclideanDist(x,df.values)
plt.figure()
plt.scatter(range(df.values.shape[0]), dist, marker='o')
plt.plot()
plt.xlabel('dataset index')
plt.ylabel('distance')
plt.show()
```

```
# Activity 1.2 (solution)

def EuclideanDist(x, data):
  npoints = data.shape[0]
  distances = np.zeros(npoints)
  for i in range(npoints) :
```

```
    distances[i] = np.sqrt((x[0]-data[i,0])**2+(x[1]-data[i,1])**2)
  return distances

x = [0,0]
dist = EuclideanDist(x,df.values)
plt.figure()
plt.scatter(range(df.values.shape[0]), dist, marker='o')
plt.plot()
plt.xlabel('dataset index')
plt.ylabel('distance')
plt.grid()
plt.show()
```





1.3 Given an integer $k > 0$, a pattern, and a set of training points, define a function that classifies the pattern according to the k-NN rule.

Use your function to classify the pattern $\mathbf{x} = (0, 0)^\top$ according to the 7-NN rule.

```
# Activity 1.3

def kNN_classifier(k,x,data):
  npoints = data.shape[0]
  # compute distance to training points
  ''' to be completed
  dist = ...
  '''
  # sort along increasing distances
  ind = np.argsort(dist,axis=0)
  classes = data[:,2]
  classes_sorted = classes[ind]

  # determine class with more element in the k neighborhood
  c1 = 0
  c2 = 0
```

```
  ''' to be completed
  for i in range(k):
    if classes_sorted[i]==1 :
    ...
  '''
  if c1>c2:
    return 1
  else :
    return 2

x=[0,0]
k=7
print('class:',kNN_classifier(k,x,df.values))
```

```
# Activity 1.3 (solution)

def kNN_classifier(k,x,data):
  npoints = data.shape[0]
  # compute distance to training points
  dist = EuclideanDist(x,data)
  # sort along increasing distances
  ind = np.argsort(dist,axis=0)
  classes = data[:,2]
  classes_sorted = classes[ind]
  # determine class with more element in the k neighborhood
  c1 = 0
  c2 = 0
  for i in range(k):
    if classes_sorted[i]==1 :
      c1 +=1
    else :
      c2 +=1
  if c1>c2:
    return 1
  else :
    return 2

x=[0,0]
```

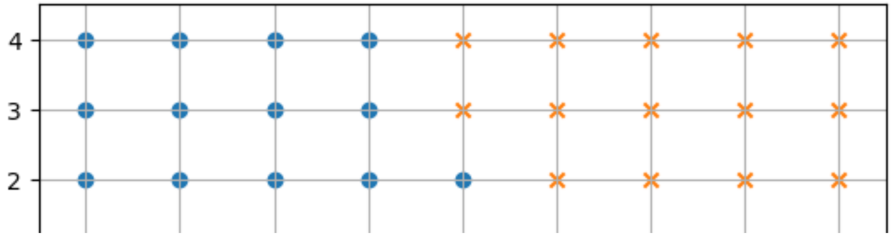
```
k=7
print('class:',kNN_classifier(k,x,df.values))
```

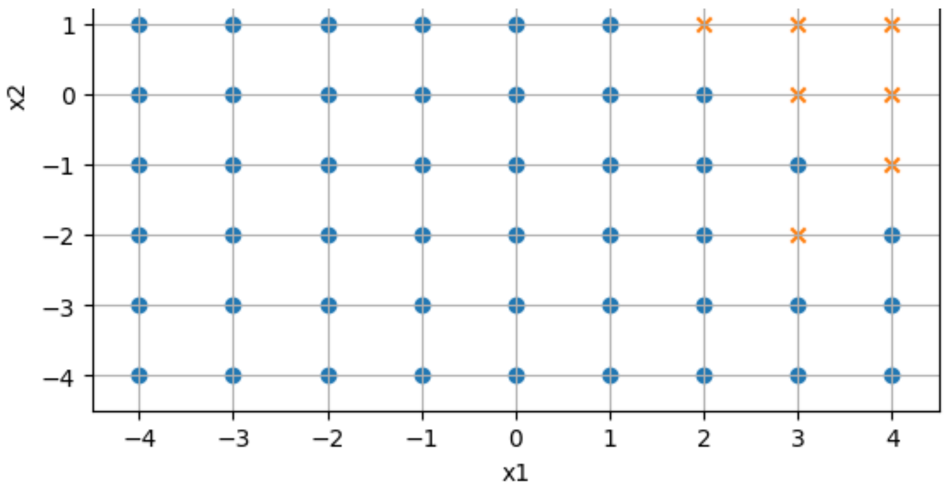
```
class: 1
```

1.4 Consider the set of points $\{(x_1, x_2) : x_1, x_2 \in \{-4, -3, -2, -1, 0, 1, 2, 3, 4\}\}$ and classify each of them according the 7-NN rule. Plot the results.

```
# Activity 1.4

# define grid of points to be classified
x1, x2 = np.meshgrid(np.arange(-4,5), np.arange(-4, 5))
X_plot = np.c_[x1.ravel(), x2.ravel()]


# classify each point of the grid
classification_kNN = []
''' to be completed
for i in range(X_plot.shape[0]):
  ...
'''

classification_kNN = np.array(classification_kNN)

# plot results
plt.figure()
plt.scatter(X_plot[np.where(classification_kNN==1),0], X_plot[np.where(classification_kNN==1),1], marker='o')
plt.scatter(X_plot[np.where(classification_kNN==2),0], X_plot[np.where(classification_kNN==2),1], marker='x')
plt.xlabel('x1')
plt.ylabel('x2')
plt.xlim(x1.min()-0.5, x1.max()+0.5)
plt.ylim(x2.min()-0.5, x2.max()+0.5)
plt.grid()
plt.show()
```

```
# Activity 1.4 (solution)

# define grid of points to be classified
x1, x2 = np.meshgrid(np.arange(-4,5), np.arange(-4, 5))
X_plot = np.c_[x1.ravel(), x2.ravel()]


# classify each point of the grid
classification_kNN = []
for i in range(X_plot.shape[0]):
  cl = kNN_classifier(7,X_plot[i], df.values)
  classification_kNN.append(cl)

classification_kNN = np.array(classification_kNN)

# plot results
plt.figure()
plt.scatter(X_plot[np.where(classification_kNN==1),0], X_plot[np.where(classification_kNN==1),1], marker='o')
plt.scatter(X_plot[np.where(classification_kNN==2),0], X_plot[np.where(classification_kNN==2),1], marker='x')
plt.xlabel('x1')
plt.ylabel('x2')
plt.xlim(x1.min()-0.5, x1.max()+0.5)
plt.ylim(x2.min()-0.5, x2.max()+0.5)
plt.grid()
plt.show()
```





Logistic regression (2-class case)

Consider two classes ω_1 and ω_2 and let

$$\ln \frac{P(\omega_1 \ \mathbf{x})}{P(\omega_2 \ \mathbf{x})} = \theta^\top \mathbf{x}.$$

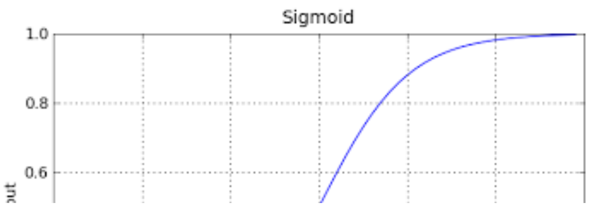
Noting that $P(\omega_1 \ \mathbf{x}) + P(\omega_2 \ \mathbf{x}) = 1$, and defining the threshold variable $t = \theta^\top \mathbf{x}$, we have

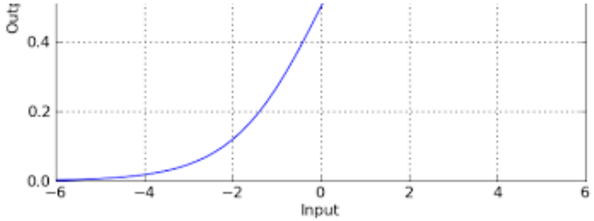
$$P(\omega_1 \ \mathbf{x}) = \sigma(t) \quad \text{and} \quad P(\omega_1 \ \mathbf{x}) = 1 - \sigma(t)$$

where

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$

is known as the **logistic sigmoid**.





The parameter θ is estimated using the **Maximum Likelihood method** applied to a set of training samples $\{(y_n, \mathbf{x}_n)\}_{n=1}^N$, where $y_n = 0$ if $\mathbf{x}_n \in \omega_1$ and $y_n = 1$ if $\mathbf{x}_n \in \omega_2$. The likelihood function is

$$P(y_1, \ldots, y_N \ \theta) = \prod_{n=1}^{N} \left(\sigma(\theta^\top \mathbf{x}_n)\right)^{y_n} \left(1 - \sigma(\theta^\top \mathbf{x}_n)\right)^{1-y_n}.$$

and the negative log-likelihood is then

$$L(\theta) = \sum_{n=1}^{N} \left(y_n \ln s_n + (1 - y_n) \ln(1 - s_n)\right)$$

where $s_n = \sigma(\theta^\top \mathbf{x}_n)$.

Minimization of $L(\theta)$ can be done using an iterative method such as the **gradient descent**.

Noting that

$$\frac{d\sigma(t)}{dt} = \sigma(t)(1 - \sigma(t)),$$

the gradient of the negative log-likelihood is

$$\nabla L(\theta) = \sum_{n=1}^{N} (s_n - y_n)\mathbf{x}_n = X^\top (s - y)$$

where

$$X^\top = [\mathbf{x}_1, \ldots, \mathbf{x}_N], \qquad s = [s_1, \ldots, s_N], \qquad y = [y_1, \ldots, y_N].$$

The gradient descent update scheme becomes

$$\theta^{(i+1)} = \theta^{(i)} - \eta_i X^\top \left(s^{(i)} - y\right)$$

where $\eta_i > 0$ is the learning rate

where $\eta > 0$ is the learning rate.

Activity 2

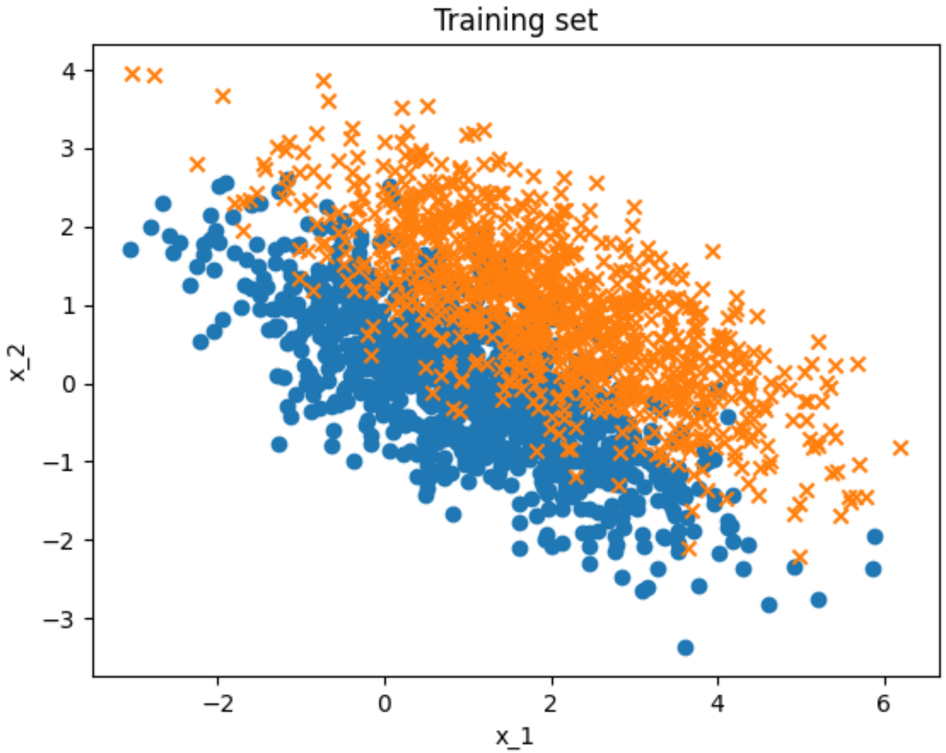
Consider a two-dimensional class problem with two classes (ω_0 and ω_1), characterized by Gaussian distributions with means $\mu_1 = (1, 0)^\top$ and $\mu_2 = (2, 1)^\top$, and covariances $\Sigma_1 = \Sigma_2 = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}$, respectively. Assume the classes are equiprobable.

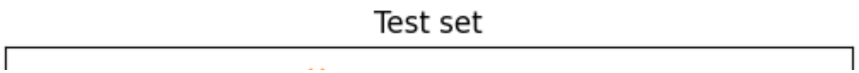
2.1 Obtain a training set $\mathcal{X}$ and a test set $\mathcal{X}_{\text{test}}$, each consisting of 1000 points from each class.

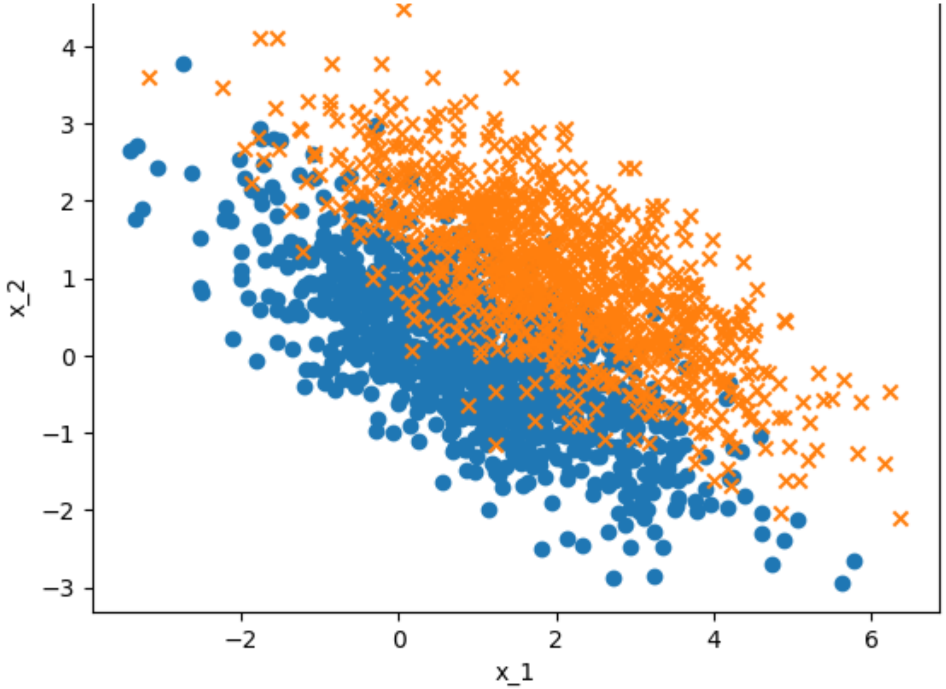
```
# Activity 2.1

import numpy as np
import matplotlib.pyplot as plt


# multivariate gaussian distribution
def gaussian(x, mean, cov):
    n = mean.size
    d = x-mean
    np.reshape(d,[n,1])
    exp_term = -0.5 * np.transpose(d) @ np.linalg.inv(cov) @ d
    f_term = 1.0/(np.sqrt( (2*np.pi)**n * np.linalg.det(cov)))
    pdf = f_term * np.exp(exp_term)
    return pdf


# to make sure we have always the same data
np.random.seed(10)

# Distribution for class 1
mu_1 = np.array([1,0])
```

```
mu_1 = np.array([1,0])
sigma_1 = np.array([[2,-1],[-1,1]])

# Distribution for class 2
mu_2 = np.array([2,1])
sigma_2 = np.array([[2,-1],[-1,1]])
#sigma_2 = np.array([[2,1],[1,1]])


# Generate training set
size_1 = 1000
size_2 = 1000
X_1 =  np.random.multivariate_normal(mu_1, sigma_1, size=size_1)
X_2 =  np.random.multivariate_normal(mu_2, sigma_2, size=size_2)

size_total = size_1+size_2
Y_1 = 0*np.ones((size_1,1))
Y_2 =   np.ones((size_2,1))

# put all data together
X = np.concatenate([X_1, X_2], axis=0)
Y = np.concatenate([Y_1, Y_2], axis=0)

# plot data points
plt.title('Training set')
plt.xlabel('x_1')
plt.ylabel('x_2')
# Class 1 (o)
plt.scatter(X_1[:,0], X_1[:,1], marker='o')
# Class 2 (x)
plt.scatter(X_2[:,0], X_2[:,1], marker='x')
plt.plot()
plt.show()

# Generate test set
Xtest_1 =  np.random.multivariate_normal(mu_1, sigma_1, size=size_1)
Xtest_2 =  np.random.multivariate_normal(mu_2, sigma_2, size=size_2)


# put all data together
Xtest = np.concatenate([Xtest_1, Xtest_2], axis=0)
Ytest = Y
```

```
Ytest = Y

# plot data points
plt.title('Test set')
plt.xlabel('x_1')
plt.ylabel('x_2')
# Class 0 (o)
plt.scatter(Xtest_1[:,0], Xtest_1[:,1], marker='o')
# Class 1 (x)
plt.scatter(Xtest_2[:,0], Xtest_2[:,1], marker='x')
plt.plot()
plt.show()

print(Xtest)
```







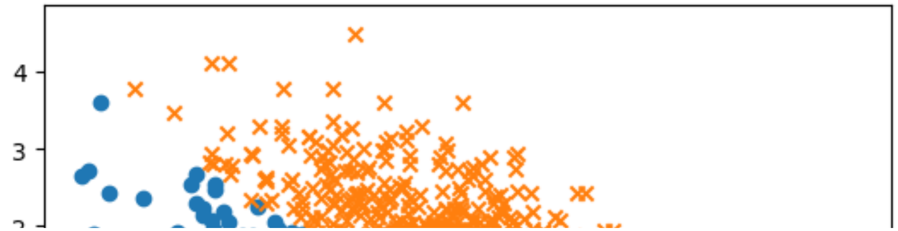

```
[[ 3.90333766 -1.73215595]
 [ 0.7655644   1.58256202]
 [-0.22752788  0.57822127]
 ...
 [-0.37384563  2.74388008]
 [ 1.46630906  0.9309507 ]
 [-1.77267106  4.12050268]]
```

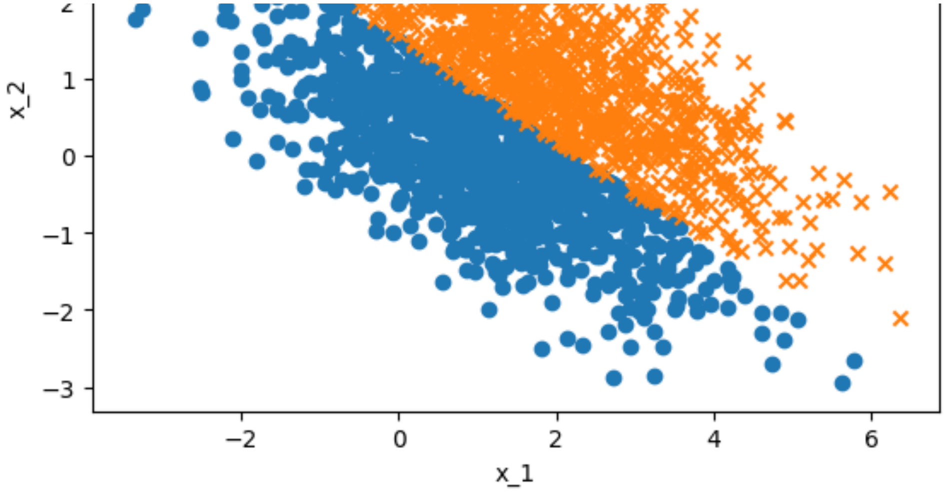
2.2 Classify the points in $\mathcal{X}_{\text{test}}$ using the Bayesian classification rule.

```
# Activity 2.2

# A priori probabilities
P_class1 = size_1/size_total
P_class2 = size_2/size_total

# classify each data point (Bayesian classification)
classification = []
''' to be completed
for i in range(size_total):
  prob_1 = P_class1 * gaussian(Xtest[i],mu_1,sigma_1)
  ...
'''

classification = np.array(classification)

# plot results
plt.figure()
plt.scatter(Xtest[np.where(classification==0),0], Xtest[np.where(classification==0),1], marker='o')
plt.scatter(Xtest[np.where(classification==1),0], Xtest[np.where(classification==1),1], marker='x')
plt.xlabel('x_1')
plt.ylabel('x_2')
plt.show()
```

```
# Activity 2.2 (solution)

# A priori probabilities
P_class1 = size_1/size_total
P_class2 = size_2/size_total

# classify each data point (Bayesian classification)
```

```
classification = []
for i in range(size_total):
  prob_1 = P_class1 * gaussian(Xtest[i],mu_1,sigma_1)
  prob_2 = P_class2 * gaussian(Xtest[i],mu_2,sigma_2)
  if prob_1 > prob_2 :
    classification.append(0)
  else :
    classification.append(1)

classification = np.array(classification)

# plot results
plt.figure()
plt.scatter(Xtest[np.where(classification==0),0], Xtest[np.where(classification==0),1], marker='o')
plt.scatter(Xtest[np.where(classification==1),0], Xtest[np.where(classification==1),1], marker='x')
plt.xlabel('x_1')
plt.ylabel('x_2')
plt.show()
```





2.3 Perform logistic regression using the training set $\mathcal{X}$ to estimate the parameter vector θ. Classify the points in $\mathcal{X}_{\text{test}}$ using the estimated parameter.

Note: Use the gradient descent method and a learning parameter $\eta_i = 0.001$. *Stop iterations when* $\|\theta^{(i)} - \theta^{(i-1)}\|_\infty \leq 10^{-4}$.

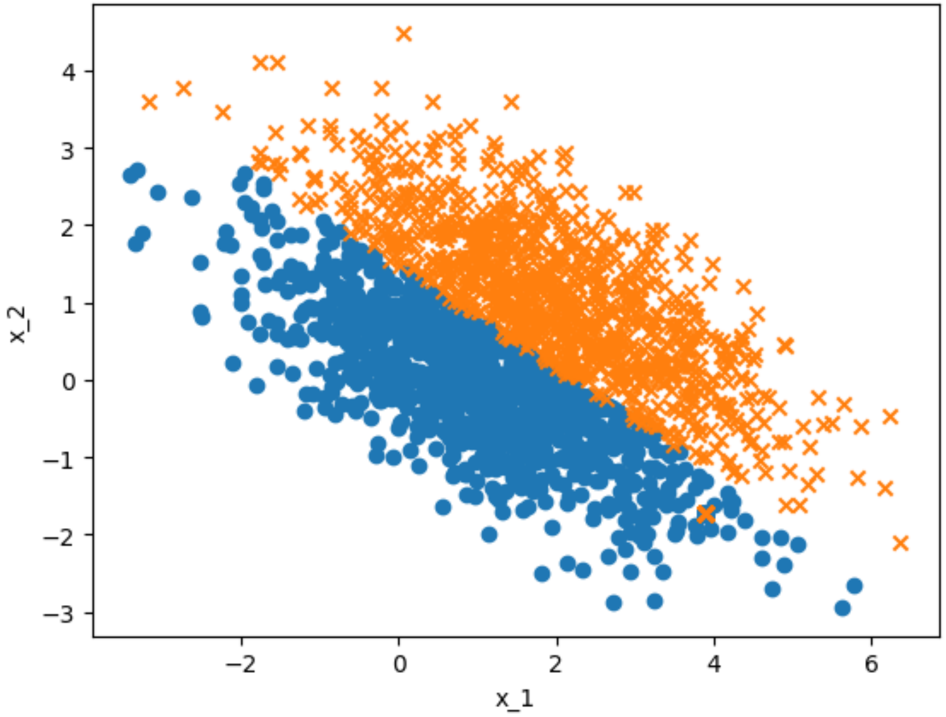
```
# Activity 2.3


# consider a 'bias' in the training set
Xones = np.concatenate([np.ones((X.shape[0],1)), X], axis=1)

theta_ini = np.array([[0, 0, 0]])
error_thres = 1e-4
eta = 0.001

theta = np.copy(theta_ini)
iter = 0
error=1

while error > error_thres :
  iter += 1
  theta_old = np.copy(theta)
  ''' to be completed
```

```
  s = ...
  theta = ...
  '''
  error = np.sum(np.abs(theta-theta_old))

print(iter,theta)

# consider a 'bias' in the test set
Xtest_ones = np.concatenate([np.ones((Xtest.shape[0],1)), Xtest], axis=1)

# apply the logistic function to the test set
stest = 1 / (1 + np.exp( -Xtest_ones @ np.transpose(theta)))

# plot results
plt.figure()
plt.scatter(Xtest[np.where(stest<0.5),0], Xtest[np.where(stest<0.5),1], marker='o')

plt.scatter(Xtest[np.where(stest>=0.5),0], Xtest[np.where(stest>=0.5),1], marker='x')
plt.xlabel('x_1')
plt.ylabel('x_2')
plt.show()
```

```
# Activity 2.3 (solution)

# consider a 'bias' in the training set
Xones = np.concatenate([np.ones((X.shape[0],1)), X], axis=1)

theta_ini = np.array([[0, 0, 0]])
error_thres = 1e-4
eta = 0.001

theta = np.copy(theta_ini)
iter = 0
error=1

while error > error_thres :
  iter += 1
  theta_old = np.copy(theta)
  s = 1 / (1 + np.exp(-Xones @ np.transpose(theta)))
  theta = theta - eta*np.transpose(s-Y) @ Xones
```

```
  error = np.sum(np.abs(theta-theta_old))

print(iter,theta)

# consider a 'bias' in the test set
Xtest_ones = np.concatenate([np.ones((Xtest.shape[0],1)), Xtest], axis=1)

# apply the logistic function to the test set
stest = 1 / (1 + np.exp( -Xtest_ones @ np.transpose(theta)))

# plot results
plt.figure()
plt.scatter(Xtest[np.where(stest<0.5),0], Xtest[np.where(stest<0.5),1], marker='o')
plt.scatter(Xtest[np.where(stest>=0.5),0], Xtest[np.where(stest>=0.5),1], marker='x')
plt.xlabel('x_1')
plt.ylabel('x_2')
plt.show()
```

```
430 [[-4.51054126  2.04295902  3.09073648]]
```



2.4 Compare the results obtained using the two methods (Bayesian and Logistic). Show the points that are not classified in the same way.

```
# Activity 2.4

for i in range(size_total) :
  if ''' insert condition ''' :
    print(Xtest[i],'Bayesian class is 0 and LOGREG class is 1')
  else :
    if ''' insert condition here ''' :
```

```
      print(Xtest[i],'Bayesian class is 1 and LOGREG class is 0')
```

```
# Activity 2.4 (solution)

for i in range(size_total) :
  if classification[i]==0 and stest[i]>=0.5 :
    print(Xtest[i],'Bayesian class is 0 and LOGREG class is 1')
  else :
    if classification[i]==1 and stest[i]<0.5 :
      print(Xtest[i],'Bayesian class is 1 and LOGREG class is 0')
```

```
[0.00625583 1.48614412] Bayesian class is 0 and LOGREG class is 1
[1.42882715 0.54059943] Bayesian class is 0 and LOGREG class is 1
[0.70162475 1.00998065] Bayesian class is 0 and LOGREG class is 1
[ 2.98732028 -0.5046536 ] Bayesian class is 0 and LOGREG class is 1
[2.0079877  0.15126916] Bayesian class is 0 and LOGREG class is 1
[1.39382859 0.55915643] Bayesian class is 0 and LOGREG class is 1
[-0.10735586  1.53792153] Bayesian class is 0 and LOGREG class is 1
```

```
[0.79926523 0.93949587] Bayesian class is 0 and LOGREG class is 1
[1.86923379 0.24758061] Bayesian class is 0 and LOGREG class is 1
[-0.62629824  1.90894693] Bayesian class is 0 and LOGREG class is 1
[2.10700705 0.06837522] Bayesian class is 0 and LOGREG class is 1
[0.64509714 1.06815318] Bayesian class is 0 and LOGREG class is 1
[ 3.47592831 -0.83496205] Bayesian class is 0 and LOGREG class is 1
[-1.18484877  2.25698004] Bayesian class is 0 and LOGREG class is 1
[1.3485946  0.58060223] Bayesian class is 0 and LOGREG class is 1
[1.30278357 0.61976907] Bayesian class is 0 and LOGREG class is 1
[-3.16478815  3.60350338] Bayesian class is 0 and LOGREG class is 1
```

2.5 Repeat the activity now considering that $\Sigma_2 = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}$.