

# Supervised Logistic Regression for Classification

---

## 0. Import library

```
In [1]: # Import libraries

# math library
import numpy as np

# visualization library
%matplotlib inline
from IPython.display import set_matplotlib_formats
set_matplotlib_formats('png2x', 'pdf')
import matplotlib.pyplot as plt

# machine learning library
from sklearn.linear_model import LogisticRegression

# 3d visualization
from mpl_toolkits.mplot3d import axes3d

# computational time
import time
```

## 1. Load dataset

---

The data features  $x_i = (x_{i(1)}, x_{i(2)})$  represent 2 exam grades  $x_{i(1)}$  and  $x_{i(2)}$  for each student  $i$ .

The data label  $y_i$  indicates if the student  $i$  was admitted (value is 1) or rejected (value is 0).

```
In [2]: # import data with numpy
data = np.loadtxt('dataset.txt', delimiter=',')

# number of training data
n = data.shape[0]
print('Number of training data=', n)
```

Number of training data= 100

## 2. Explore the dataset distribution

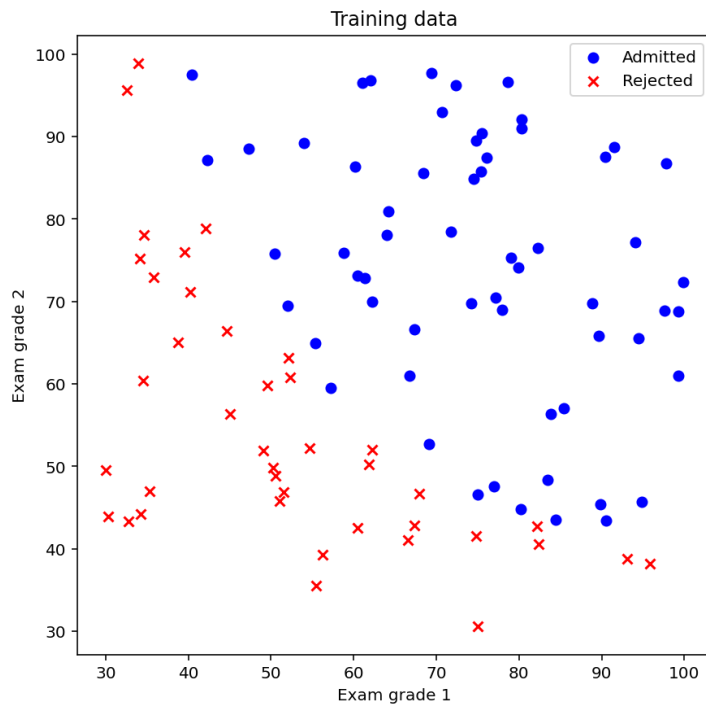
---

Plot the training data points.

You may use matplotlib function `scatter(x,y)` .

```
In [16]: x1 = data[:,0] # exam grade 1
x2 = data[:,1] # exam grade 2
idx_admit = (data[:,2]==1) # index of students who were admitted
idx_rejec = (data[:,2]==0) # index of students who were rejected

plt.figure(figsize = (7, 7))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.title('Training data')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.show()
```



### 3. Sigmoid/logistic function

$$\sigma(\eta) = \frac{1}{1 + \exp^{-\eta}}$$

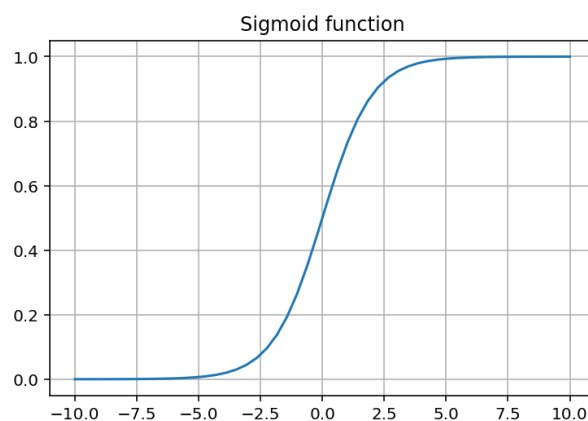
Define and plot the sigmoid function for values in [-10,10]:

You may use functions `np.exp`, `np.linspace`.

```
In [18]: def sigmoid(z):
          sigmoid_f = 1 / (1 + np.exp(-z))
          return sigmoid_f

          # plot
          x_values = np.linspace(-10,10)

          plt.figure(2)
          plt.plot(x_values,sigmoid(x_values))
          plt.title("Sigmoid function")
          plt.grid(True)
```



### 4. Define the prediction function for the classification

The prediction function is defined by:

$$p_w(x) = \sigma(w_0 + w_1x_{(1)} + w_2x_{(2)}) = \sigma(w^T x)$$

Implement the prediction function in a vectorised way as follows:

$$X = \begin{bmatrix} 1 & x_{1(1)} & x_{1(2)} \\ 1 & x_{2(1)} & x_{2(2)} \\ \vdots & & \\ 1 & x_{n(1)} & x_{n(2)} \end{bmatrix} \quad \text{and} \quad w = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} \Rightarrow$$

$$p_w(x) = \sigma(Xw) = \begin{bmatrix} \sigma(w_0 + w_1x_{1(1)} + w_2x_{1(2)}) \\ \sigma(w_0 + w_1x_{2(1)} + w_2x_{2(2)}) \\ \vdots \\ \sigma(w_0 + w_1x_{n(1)} + w_2x_{n(2)}) \end{bmatrix}$$

Use the new function `sigmoid`.

```
In [516]: # construct the data matrix X
n = x1.size
X = np.insert(np.append(np.array(x1).reshape(-1, 1),
                        np.array(x2).reshape(-1, 1), axis = 1), 0, 1, axis = 1)

# parameters vector
w = np.array([[ -5], [0.1], [0]])

# predictive function definition
def f_pred(X,w):

    p = sigmoid(np.dot(X, w))

    return p

y_pred = f_pred(X,w)
```

## 5. Define the classification loss function

### Mean Square Error

$$L(w) = \frac{1}{n} \sum_{i=1}^n (\sigma(w^T x_i) - y_i)^2$$

### Cross-Entropy

$$L(w) = \frac{1}{n} \sum_{i=1}^n (-y_i \log(\sigma(w^T x_i)) - (1 - y_i) \log(1 - \sigma(w^T x_i)))$$

The vectorized representation is for the mean square error is as follows:

$$L(w) = \frac{1}{n} (p_w(x) - y)^T (p_w(x) - y)$$

The vectorized representation is for the cross-entropy error is as follows:

$$L(w) = \frac{1}{n} (-y^T \log(p_w(x)) - (1 - y)^T \log(1 - p_w(x)))$$

where

$$p_w(x) = \sigma(Xw) = \begin{bmatrix} \sigma(w_0 + w_1x_{1(1)} + w_2x_{1(2)}) \\ \sigma(w_0 + w_1x_{2(1)} + w_2x_{2(2)}) \\ \vdots \\ \sigma(w_0 + w_1x_{n(1)} + w_2x_{n(2)}) \end{bmatrix} \quad \text{and} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

You may use numpy functions `.T` and `np.log`.

```
In [405]: # label = predict output
# h_arr = 정답 label
def mse_loss(label, h_arr): # mean square error
```

```

temp = label - h_arr
return np.mean(np.dot(temp.T, temp))

def ce_loss(label, h_arr): # cross-entropy error
    epsilon = 1e-5
    temp = np.dot(-(h_arr.T), np.log(label + epsilon)) - np.dot((1 - h_arr).T, np.log(1 - label + epsilon))
    return np.mean(temp)

```

## 6. Define the gradient of the classification loss function

Given the mean square loss

$$L(w) = \frac{1}{n} (p_w(x) - y)^T (p_w(x) - y)$$

The gradient is given by

$$\frac{\partial}{\partial w} L(w) = \frac{2}{n} X^T ((p_w(x) - y) \odot (p_w(x) \odot (1 - p_w(x))))$$

Given the cross-entropy loss

$$L(w) = \frac{1}{n} (-y^T \log(p_w(x)) - (1 - y)^T \log(1 - p_w(x)))$$

The gradient is given by

$$\frac{\partial}{\partial w} L(w) = \frac{2}{n} X^T (p_w(x) - y)$$

Implement the vectorized version of the gradient of the classification loss function

```

In [406]: # loss function of cross-entropy
def grad_loss_mse(y_pred, y):

    n = len(y)
    temp = (y_pred - y) * (y_pred * (1 - y_pred))
    loss = (2 * np.dot(X.T, temp)) / n

    return loss

# loss function of cross-entropy
def grad_loss_ce(y_pred, y):

    n = len(y)
    temp = y_pred - y
    loss = (2 * np.dot(X.T, temp)) / n

    return loss

# Test loss function
y = data[:, 2][:, None] # label
y_pred = f_pred(X, w) # prediction

gloss_mse = grad_loss_mse(y_pred, y)
gloss_ce = grad_loss_ce(y_pred, y)

```

## 7. Implement the gradient descent algorithm

Vectorized implementation for the mean square loss:

$$w^{k+1} = w^k - \tau \frac{2}{n} X^T ((p_w(x) - y) \odot (p_w(x) \odot (1 - p_w(x))))$$

Vectorized implementation for the cross-entropy loss:

$$w^{k+1} = w^k - \tau \frac{2}{n} X^T (p_w(x) - y)$$

Plot the loss values  $L(w^k)$  w.r.t. iteration  $k$  the number of iterations for the both loss functions.

```

In [407]: # gradient descent function definition
def grad_desc_mse(X, y , w_init=np.array([0,0,0])[:,None] ,tau=1e-4, max_iter=500):

    L_iters = np.zeros([max_iter]) # record the loss values
    w_iters = np.zeros([max_iter,2]) # record the loss values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations

        y_pred = f_pred(X, w) # linear prediction function
        grad_f = grad_loss_mse(y_pred,y) # gradient of the loss
        w = w - tau* grad_f # update rule of gradient descent
        L_iters[i] = mse_loss(y_pred,y) # save the current loss value
        w_iters[i,:] = w[0],w[1] # save the current w value

    return w, L_iters, w_iters

# run gradient descent algorithm
start = time.time()
w_init = np.array([-15, 0.1, 0.1])[:,None]
tau = 0.0001; max_iter = 1000
w_mse, L_iters, w_iters = grad_desc_mse(X,y,w_init,tau,max_iter)

print(w_mse)
print(L_iters[max_iter-1])

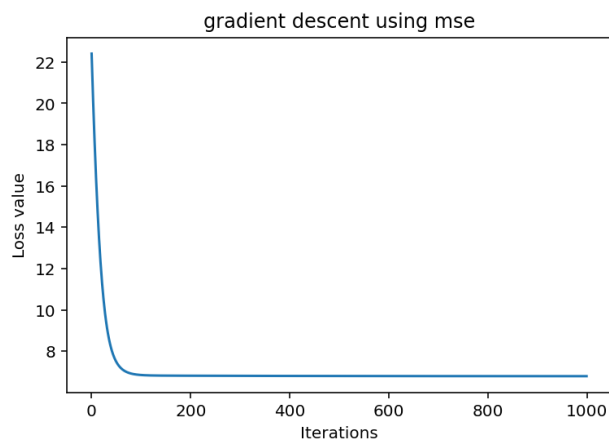
# plot
plt.figure(3)
plt.plot(L_iters)
plt.title('gradient descent using mse')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()

```

```

[[-14.99976342]
 [ 0.1266953 ]
 [ 0.11843229]]
6.78670445828824

```



```

In [418]: # gradient descent function definition
def grad_desc_ce(X, y , w_init=np.array([0,0,0])[:,None] ,tau=1e-4, max_iter=500):

    L_iters = np.zeros([max_iter]) # record the loss values
    w_iters = np.zeros([max_iter,2]) # record the loss values
    w = w_init # initialization

    for i in range(max_iter): # loop over the iterations

        y_pred = f_pred(X, w) # linear prediction function
        grad_f = grad_loss_ce(y_pred,y) # gradient of the loss
        w = w - tau* grad_f # update rule of gradient descent
        L_iters[i] = ce_loss(y_pred,y) # save the current loss value
        w_iters[i,:] = w[0],w[1] # save the current w value

    return w, L_iters, w_iters

# run gradient descent algorithm
start = time.time()
w_init = np.array([-20, 0.1, 0.02])[:,None]

```

```

tau = 0.0001; max_iter = 500
w_ce, L_iters, w_iters = grad_desc_ce(X,y,w_init,tau,max_iter)

print(w_ce)
print(L_iters[max_iter-1])

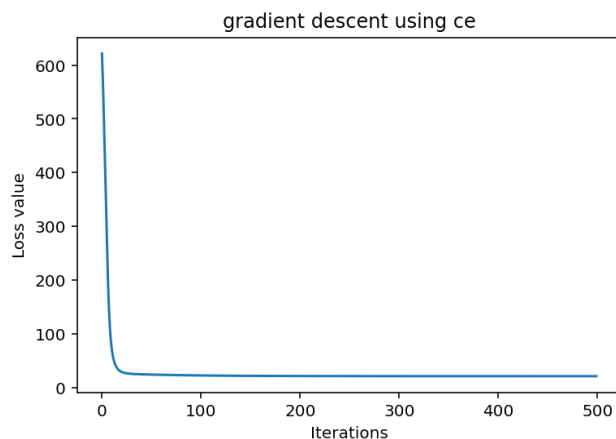
# plot
plt.figure(3)
plt.plot(L_iters)
plt.title('gradient descent using ce')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()

```

```

[[-19.99878008]
 [ 0.16564094]
 [ 0.15900519]]
20.830791631536393

```



## 8. Plot the decision boundary

The decision boundary is defined by all points

$$x = (x_{(1)}, x_{(2)}) \quad \text{such that} \quad p_w(x) = 0.5$$

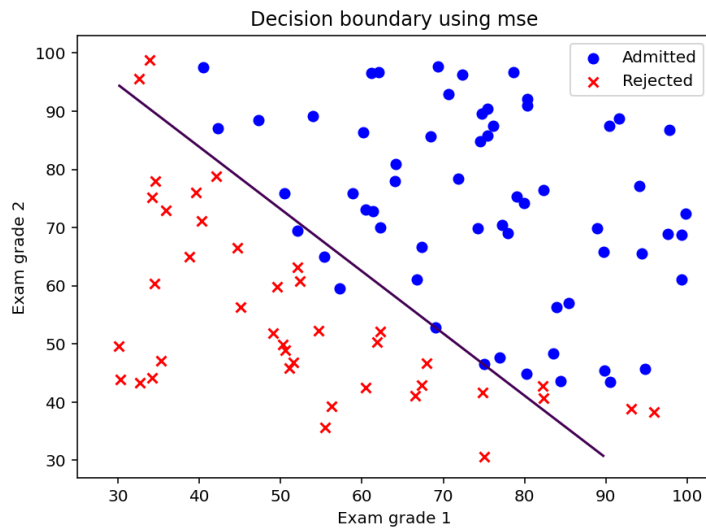
You may use numpy and matplotlib functions `np.meshgrid`, `np.linspace`, `reshape`, `contour`.

```

In [655]: # compute values p(x) for multiple data points x
x1_min, x1_max = X[:,1].min(), X[:,1].max() # min and max of grade 1
x2_min, x2_max = X[:,2].min(), X[:,2].max() # min and max of grade 2
xx1, xx2 = np.meshgrid(np.linspace(x1_min, x1_max), np.linspace(x2_min, x2_max)) # create meshgrid
X2 = np.ones([np.prod(xx1.shape),3])
X2[:,1] = xx1.reshape(-1)
X2[:,2] = xx2.reshape(-1)
p = f_pred(X2, w_mse)
p = p.reshape(50, -1)

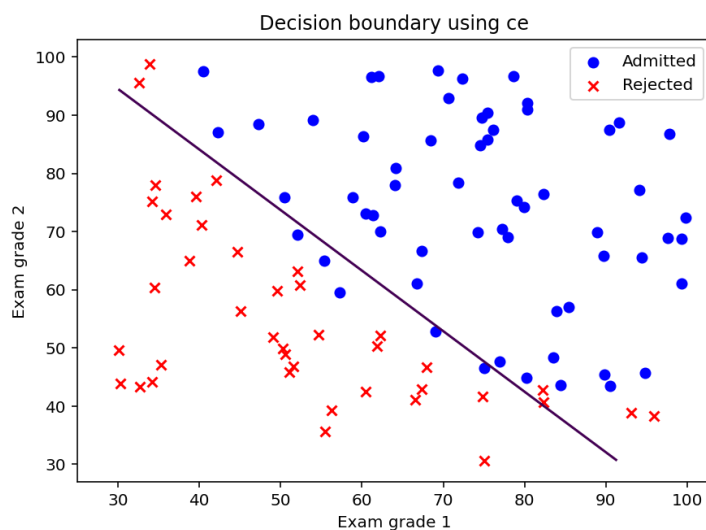
# plot
plt.figure(figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.contour(xx1, xx2, p, levels =[0.5])
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.title('Decision boundary using mse')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.show()

```



```
In [410]: p = f_pred(X2, w_ce)
p = p.reshape(50, -1)

# plot
plt.figure(figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.contour(xx1, xx2, p, levels =[0.5])
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.title('Decision boundary using ce')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.show()
```



## 9. Comparison with Scikit-learn logistic regression algorithm with the gradient descent with the cross-entropy loss

You may use scikit-learn function `LogisticRegression(C=1e6)` .

```
In [702]: # run logistic regression with scikit-learn
start = time.time()
logreg_sklearn = LogisticRegression(C=1e6) # scikit-learn logistic regression
y = data[:,2][:,None]
logreg_sklearn.fit(X[:, 1:3], y.ravel()) # learn the model parameters

# compute loss value
w_sklearn = np.zeros([3,1])
w_sklearn[0,0] = logreg_sklearn.intercept_
w_sklearn[1:3,0] = logreg_sklearn.coef_

y_pred_sklearn = logreg_sklearn.predict(X[:, 1:3]).reshape(-1, 1)
```

```

loss_sklearn = ce_loss(y_pred_sklearn, y)

# plot
plt.figure(4,figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')

x1_min, x1_max = X[:,1].min(), X[:,1].max() # grade 1
x2_min, x2_max = X[:,2].min(), X[:,2].max() # grade 2

xx1, xx2 = np.meshgrid(np.linspace(x1_min, x1_max), np.linspace(x2_min, x2_max)) # create meshgrid

X2 = np.ones([np.prod(xx1.shape),3])
X2[:,1] = xx1.reshape(-1)
X2[:,2] = xx2.reshape(-1)

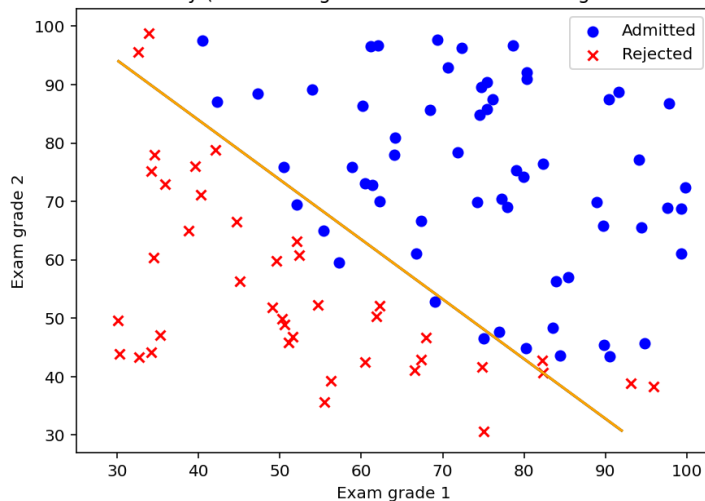
p = f_pred(X2, w_ce)
p = p.reshape(50, -1)
plt.contour(xx1, xx2, p, levels = [0.5], colors = ['black'])

p_sklearn = f_pred(X2, w_sklearn)
p_sklearn = p_sklearn.reshape(50, -1)
plt.contour(xx1, xx2, p_sklearn, levels = [0.5], colors = ['orange']);

plt.title('Decision boundary (black with gradient descent and orange with scikit-learn)')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.legend()
plt.show()

```

Decision boundary (black with gradient descent and orange with scikit-learn)



## 10. Plot the probability map

```

In [705]: num_a = 500
grid_x1 = np.linspace(20,110, num_a)
grid_x2 = np.linspace(20,110, num_a)

score_x1, score_x2 = np.meshgrid(grid_x1, grid_x2)

Z = np.zeros((len(grid_x1), len(grid_x2)))

for i in range(len(grid_x1)):
    for j in range(len(grid_x2)):
        temp_X = np.array([[1, 1, 1]])
        temp_X[0, 1] = grid_x1[i]
        temp_X[0, 2] = grid_x2[j]
        predict_prob = sigmoid(np.dot(temp_X, w_mse))
        Z[j, i] = predict_prob

# actual plotting example
fig = plt.figure(figsize=(10,10))

ax = fig.add_subplot(111)
ax.set_xlabel('Exam grade 1')
ax.set_ylabel('Exam grade 2')

```



```

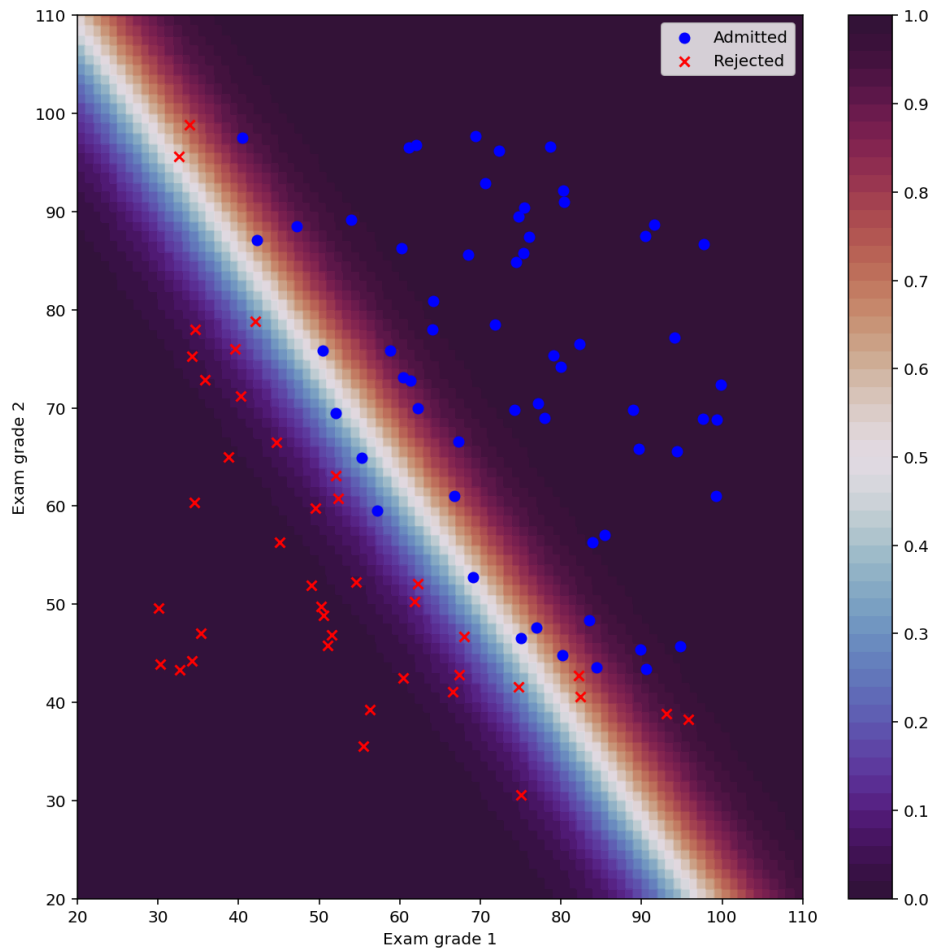
ax.set_xlim(20, 110)
ax.set_ylim(20, 110)

cf = ax.contourf(score_x1, score_x2, Z, cmap = 'twilight_shifted', levels = 50)
ax.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
ax.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
cbar = fig.colorbar(cf, ticks = [0.00, 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 1.00],)

cbar.update_ticks()

plt.legend()
plt.show()

```



```

In [707]: num_a = 500
grid_x1 = np.linspace(20,110, num_a)
grid_x2 = np.linspace(20,110, num_a)

score_x1, score_x2 = np.meshgrid(grid_x1, grid_x2)

Z = np.zeros((len(grid_x1), len(grid_x2)))

for i in range(len(grid_x1)):
    for j in range(len(grid_x2)):
        temp_X = np.array([[1, 1, 1]])
        temp_X[0, 1] = grid_x1[i]
        temp_X[0, 2] = grid_x2[j]
        predict_prob = sigmoid(np.dot(temp_X, w_ce))
        Z[j, i] = predict_prob

# actual plotting example
fig = plt.figure(figsize=(10,10))

ax = fig.add_subplot(111)
ax.set_xlabel('Exam grade 1')
ax.set_ylabel('Exam grade 2')

ax.set_xlim(20, 110)
ax.set_ylim(20, 110)

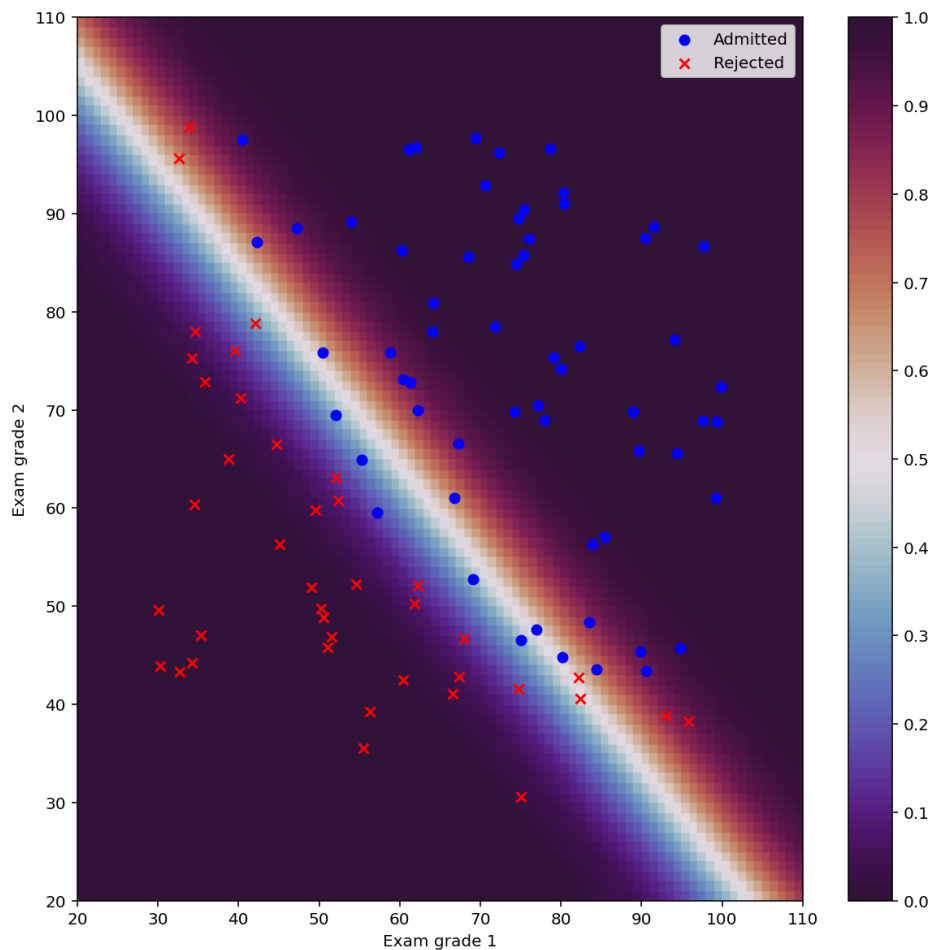
cf = ax.contourf(score_x1, score_x2, Z, cmap = 'twilight_shifted', levels = 100)
ax.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')

```

```
ax.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
cbar = fig.colorbar(cf, ticks = [0.00, 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 1.00])

cbar.update_ticks()

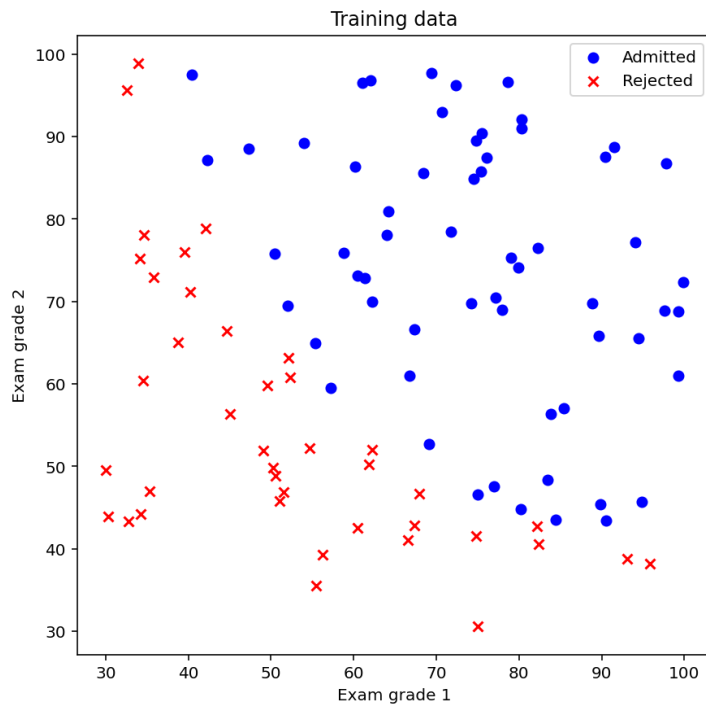
plt.legend()
plt.show()
```



## Output results

### 1. Plot the dataset in 2D cartesian coordinate system (1pt)

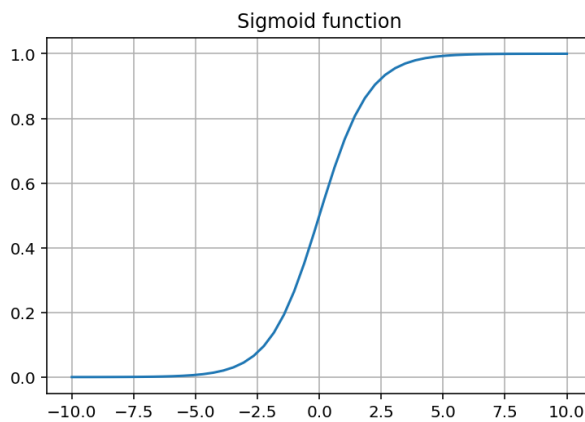
```
In [17]: plt.figure(figsize = (7, 7))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected' )
plt.title('Training data')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.show()
```



## 2. Plot the sigmoid function (1pt)

```
In [19]: # plot
x_values = np.linspace(-10,10)

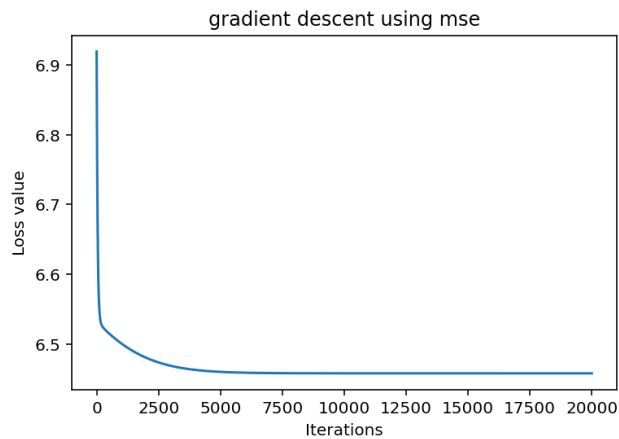
plt.figure(2)
plt.plot(x_values, sigmoid(x_values))
plt.title("Sigmoid function")
plt.grid(True)
```



## 3. Plot the loss curve in the course of gradient descent using the mean square error (2pt)

```
In [695]: start = time.time()
w_init = np.array([-25, 0.2, 0.2])[:,None]
tau = 0.0001; max_iter = 20000
w_mse, L_iters, w_iters = grad_desc_mse(X,y,w_init,tau,max_iter)

# plot
plt.figure(3)
plt.plot(L_iters)
plt.title('gradient descent using mse')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()
```

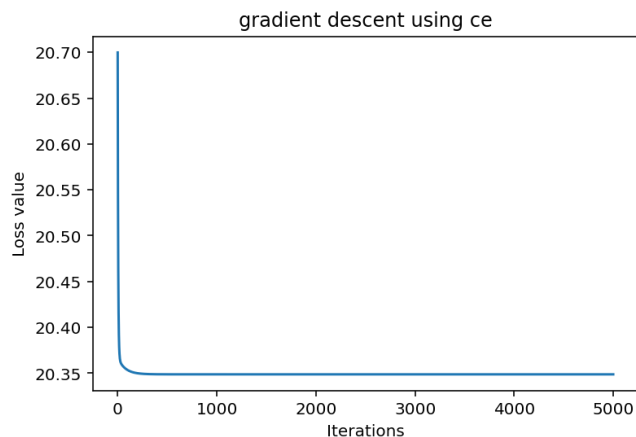


#### 4. Plot the loss curve in the course of gradient descent using the cross-entropy error (2pt)

```
In [694]: start = time.time()
w_init = np.array([-25, 0.2, 0.2])[:,None]

tau = 0.0001; max_iter = 5000
w_ce, L_iters, w_iters = grad_desc_ce(X,y,w_init,tau,max_iter)

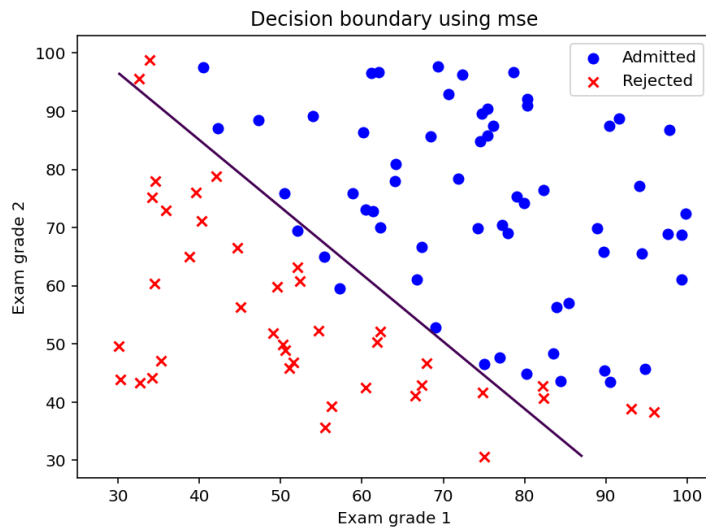
# plot
plt.figure(3)
plt.plot(L_iters)
plt.title('gradient descent using ce')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()
```



#### 5. Plot the decision boundary using the mean square error (2pt)

```
In [696]: p = f_pred(X2, w_mse)
p = p.reshape(50, -1)

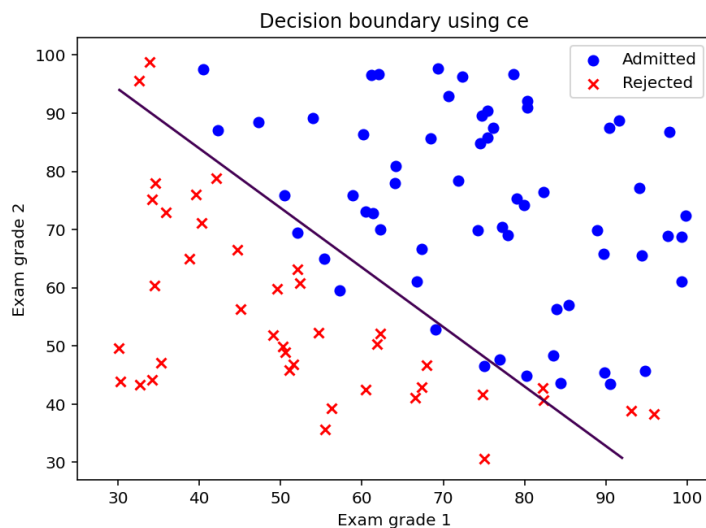
# plot
plt.figure(figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.contour(xx1, xx2, p, levels =[0.5])
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.title('Decision boundary using mse')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.show()
```



## 6. Plot the decision boundary using the cross-entropy error (2pt)

```
In [697]: p = f_pred(X2, w_ce)
p = p.reshape(50, -1)

# plot
plt.figure(figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.contour(xx1, xx2, p, levels = [0.5])
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc = 'upper right')
plt.title('Decision boundary using ce')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.show()
```



## 7. Plot the decision boundary using the Scikit-learn logistic regression algorithm (2pt)

```
In [698]: plt.figure(4,figsize=(7,5))
plt.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
plt.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')

x1_min, x1_max = X[:,1].min(), X[:,1].max() # grade 1
x2_min, x2_max = X[:,2].min(), X[:,2].max() # grade 2

xx1, xx2 = np.meshgrid(np.linspace(x1_min, x1_max), np.linspace(x2_min, x2_max)) # create meshgrid

X2 = np.ones([np.prod(xx1.shape),3])
X2[:,1] = xx1.reshape(-1)
```

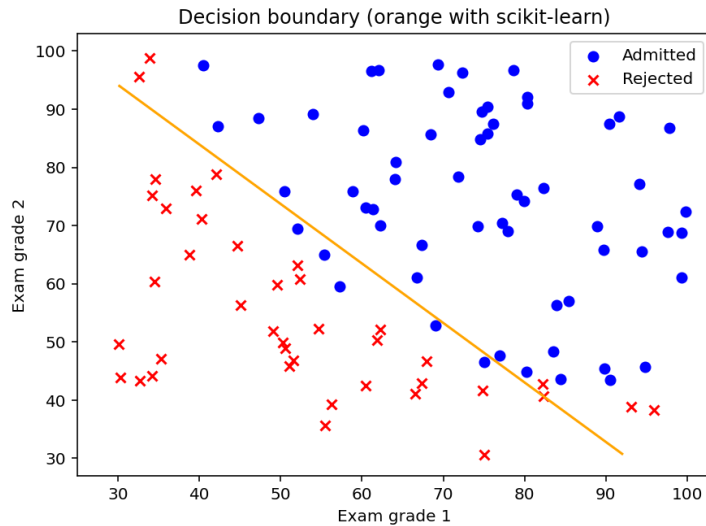
```

X2[:,2] = xx2.reshape(-1)

p_sklearn = f_pred(X2, w_sklearn)
p_sklearn = p_sklearn.reshape(50, -1)
plt.contour(xx1, xx2, p_sklearn, levels = [0.5], colors = ['orange']);

plt.title('Decision boundary (orange with scikit-learn)')
plt.xlim(25, 103)
plt.ylim(27, 103)
plt.legend()
plt.show()

```



## 8. Plot the probability map using the mean square error (2pt)

```

In [706]: # actual plotting example
fig = plt.figure(figsize=(10,10))

ax = fig.add_subplot(111)
ax.set_xlabel('Exam grade 1')
ax.set_ylabel('Exam grade 2')

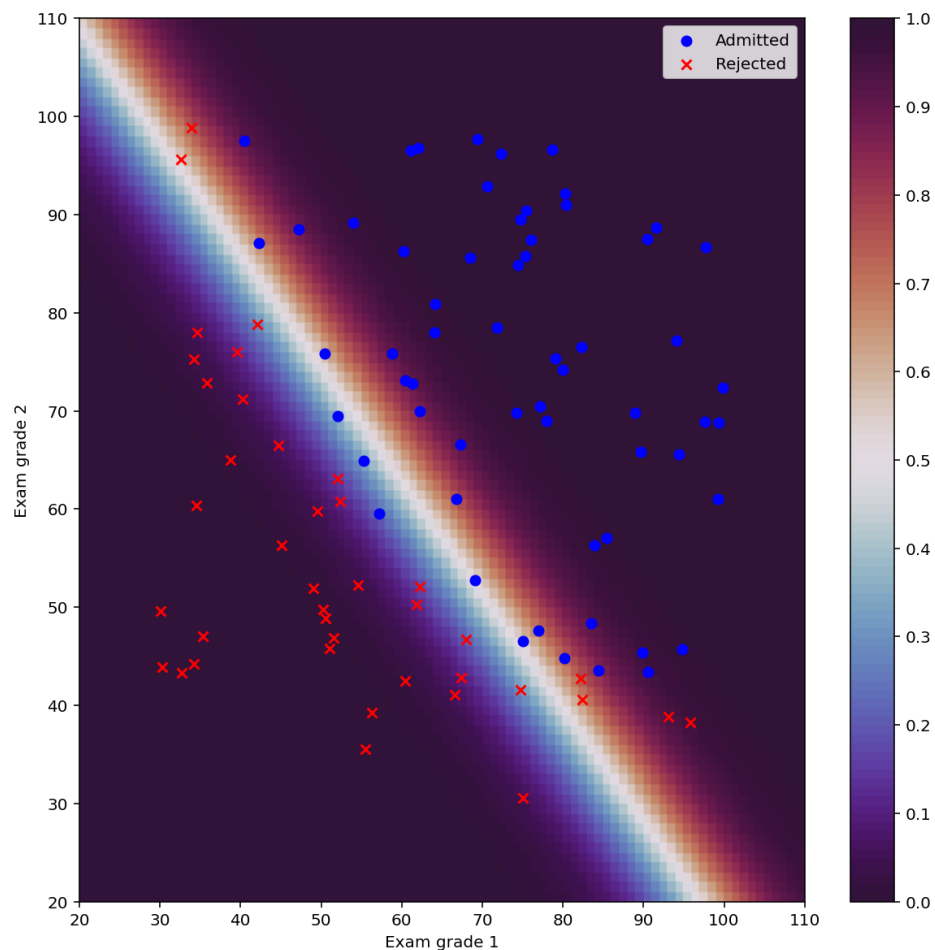
ax.set_xlim(20, 110)
ax.set_ylim(20, 110)

cf = ax.contourf(score_x1, score_x2, Z, cmap = 'twilight_shifted', levels = 100)
ax.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
ax.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
cbar = fig.colorbar(cf, ticks = [0.00, 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 1.00],)

cbar.update_ticks()

plt.legend()
plt.show()

```



## 9. Plot the probability map using the cross-entropy error (2pt)

```
In [708]: # actual plotting example
fig = plt.figure(figsize=(10,10))

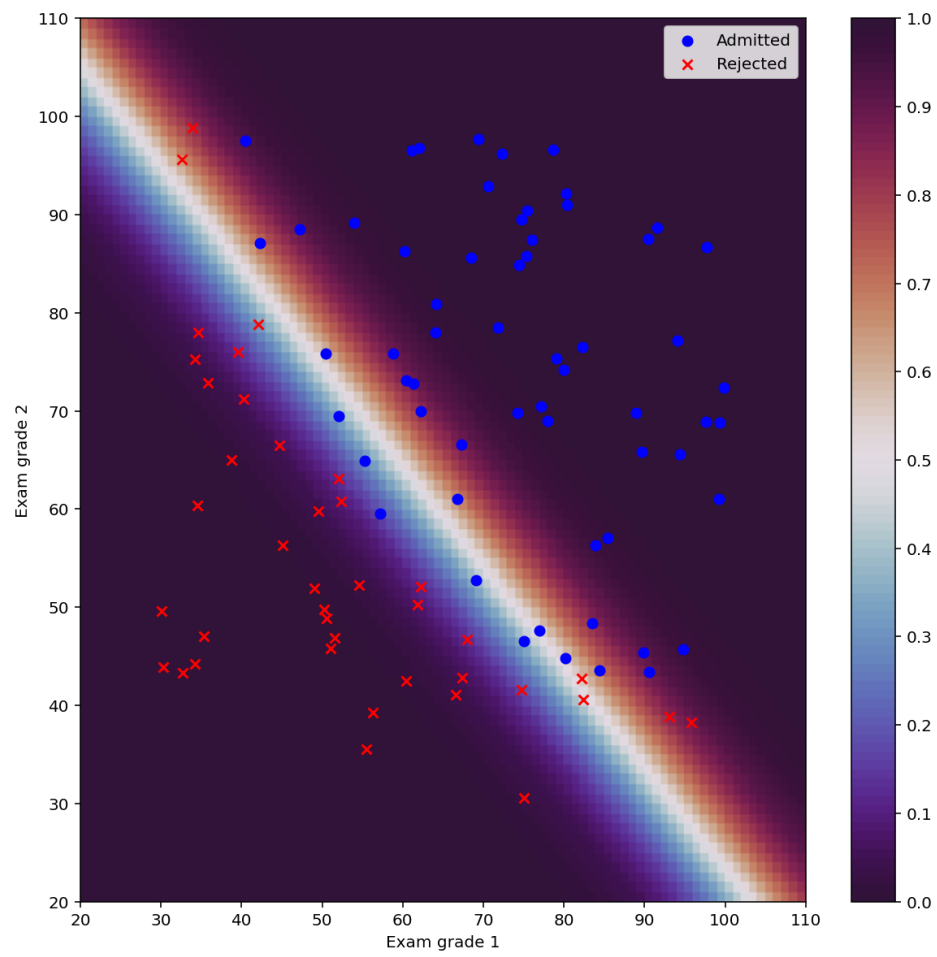
ax = fig.add_subplot(111)
ax.set_xlabel('Exam grade 1')
ax.set_ylabel('Exam grade 2')

ax.set_xlim(20, 110)
ax.set_ylim(20, 110)

cf = ax.contourf(score_x1, score_x2, Z, cmap = 'twilight_shifted', levels = 100)
ax.scatter(x1[idx_admit], x2[idx_admit], c = 'b', marker = 'o', label = 'Admitted')
ax.scatter(x1[idx_rejec], x2[idx_rejec], c = 'r', marker = 'x', label = 'Rejected')
cbar = fig.colorbar(cf, ticks = [0.00, 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 1.00])

cbar.update_ticks()

plt.legend()
plt.show()
```



In [ ]: