# 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.genfromtxt('dataset.txt', delimiter=',')[:,:]

# data = np.loadtxt('dataset.txt', delimiter=',')
print(data.shape)
print(data[0])
data[0,0] = 34.62365962451697
print(data[0])
# number of training data
n = data.shape[0]
print('Number of training data=',n)
```

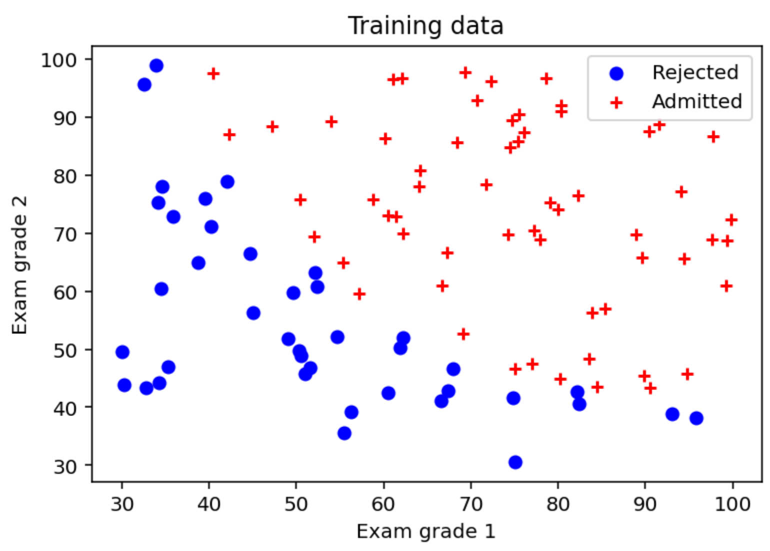
```
(100, 3)
[        nan 78.02469282  0.        ]
[34.62365962 78.02469282  0.        ]
Number of training data= 100
```

## 2. Explore the dataset distribution

Plot the training data points.

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

In [3]:
```
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(1)
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.title('Training data')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.show()
```



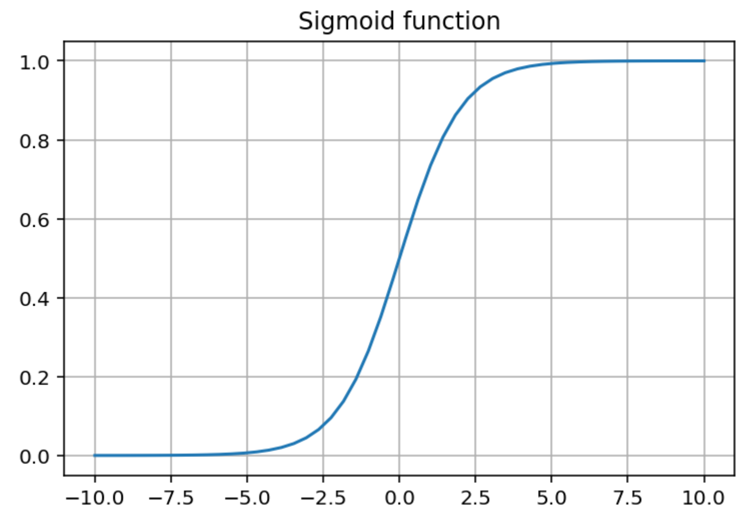

## 3. Sigmoid/logistic function

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

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

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

In [4]:
```
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:**

$$p_w(x) = \sigma(w_0 + w_1 x_{(1)} + w_2 x_{(2)}) = \sigma(w^T x)$$

**Implement the prediction function in a vectorised way as follows:**

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

Use the new function `sigmoid` .

In [5]:
```
# construct the data matrix X
n = data.shape[0]
X = np.ones([n, 3])
X[:,0] = 1
X[:,1] = x1
X[:,2] = x2

# parameters vector
w = np.array([-10,0.1,-0.2])[:,None]

# 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**

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

**Cross-Entropy**

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

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

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

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

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

where

$$p_w(x) = \sigma(Xw) = \begin{bmatrix} \sigma(w_0 + w_1 x_{1(1)} + w_2 x_{1(2)}) \\ \sigma(w_0 + w_1 x_{2(1)} + w_2 x_{2(2)}) \\ \vdots \\ \sigma(w_0 + w_1 x_{n(1)} + w_2 x_{n(2)}) \end{bmatrix} \quad \text{and} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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

In [6]:
```
def mse_loss(h_arr, label):  # mean square error
    diff = h_arr - label
    return np.dot(diff.T, diff) / len(label)

def ce_loss(h_arr, label):  # cross-entropy error

    return (np.dot(-label.T, np.log(h_arr)) - np.dot((1-label).T, np.log(1-h_arr))) / len(label)
y = data[:,2][:,None] # label
```

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

**Given the mean square loss**

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

The gradient is given by

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

**Given the cross-entropy loss**

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

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 [7]:

```
# loss function definition
def grad_mse(y_pred,y, X):
    n = len(y)
    tmp = np.multiply((y_pred - y), y_pred)
    tmp2 = np.multiply(tmp, (1-y_pred))
    grad = (np.dot(X.T, tmp2)*2) / n

    return grad

# loss function definition
def grad_ce(y_pred,y, X):
    n = len(y)
    grad = np.dot(X.T, (y_pred - y)*2) / n

    return grad

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

## 7. Implement the gradient descent algorithm

**Vectorized implementation for the mean square loss:**

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

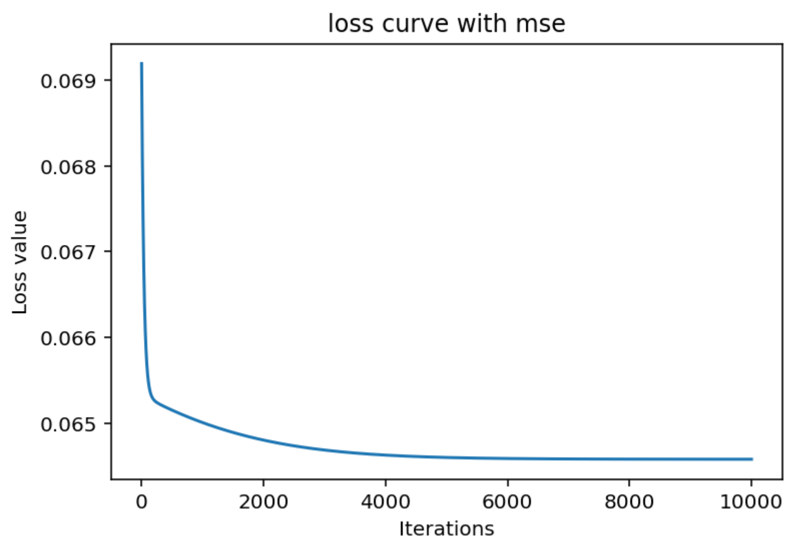
**Vectorized implementation for the cross-entropy loss:**

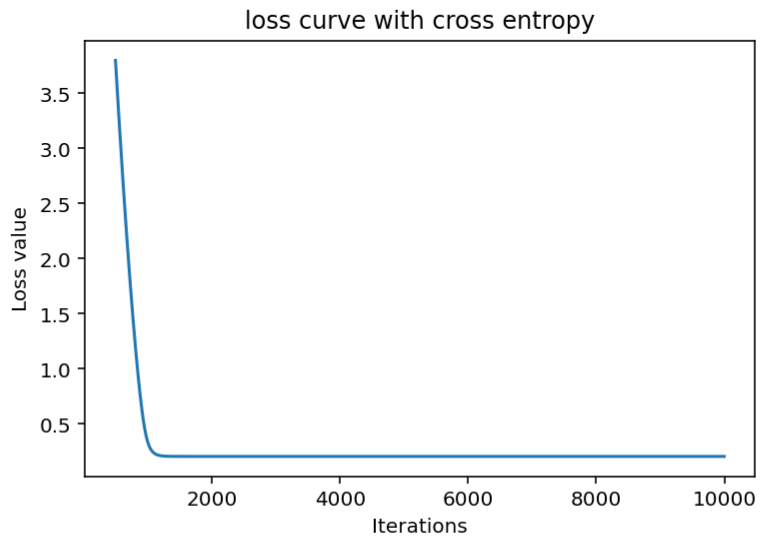
$$w^{k+1} = w^k - \tau\frac{2}{n}X^T(p_w(x) - y)$$

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

In [8]:
```
# 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,3]) # 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 predicition function
        grad_f = grad_mse(y_pred,y,X) # 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.reshape(1, len(w)) # save the current w value

    return w, L_iters, w_iters

# 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,3]) # 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 predicition function
        grad_f = grad_ce(y_pred,y,X) # 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.reshape(1, len(w)) # save the current w value

    return w, L_iters, w_iters

# run gradient descent algorithm
start = time.time()
w_init_mse = np.array([-25,0.2,0.2])[:,None]
w_init_ce = np.array([-22,-1,1])[:,None]
tau = 1e-4
max_iter = 10000
w_mse, L_iters_mse, w_iters_mse = grad_desc_mse(X,y,w_init_mse,tau,max_iter)
w_ce, L_iters_ce, w_iters_ce = grad_desc_ce(X,y,w_init_ce,tau,max_iter)

# plot
plt.figure(3)
plt.plot(L_iters_mse)
plt.title('loss curve with mse')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()

plt.figure(4)
plt.plot(L_iters_ce)
plt.title('loss curve with cross entropy')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()
```

```
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:7: RuntimeWarning: divide by zero encountered in log
  import sys
```



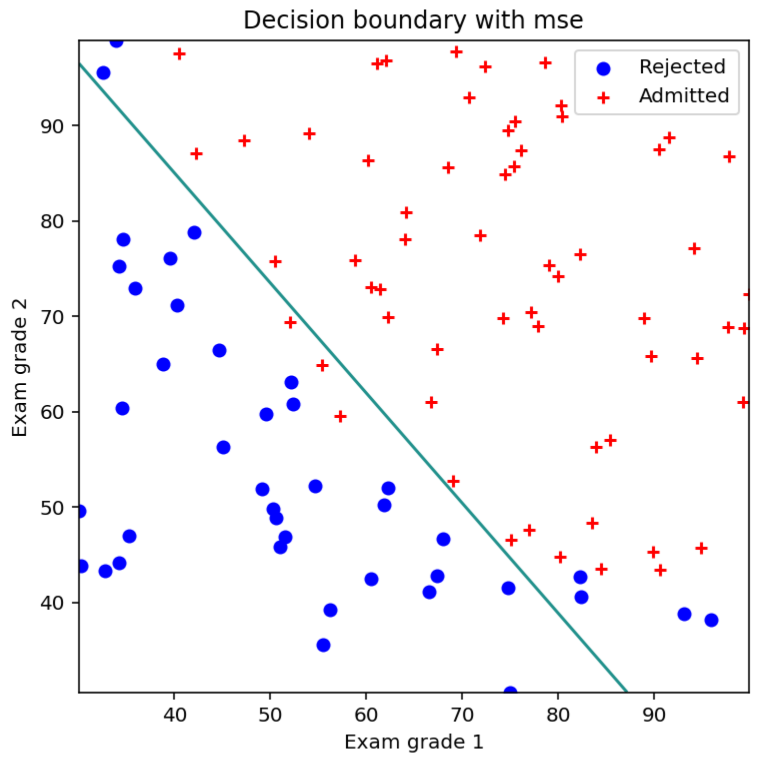

## 8. Plot the decision boundary

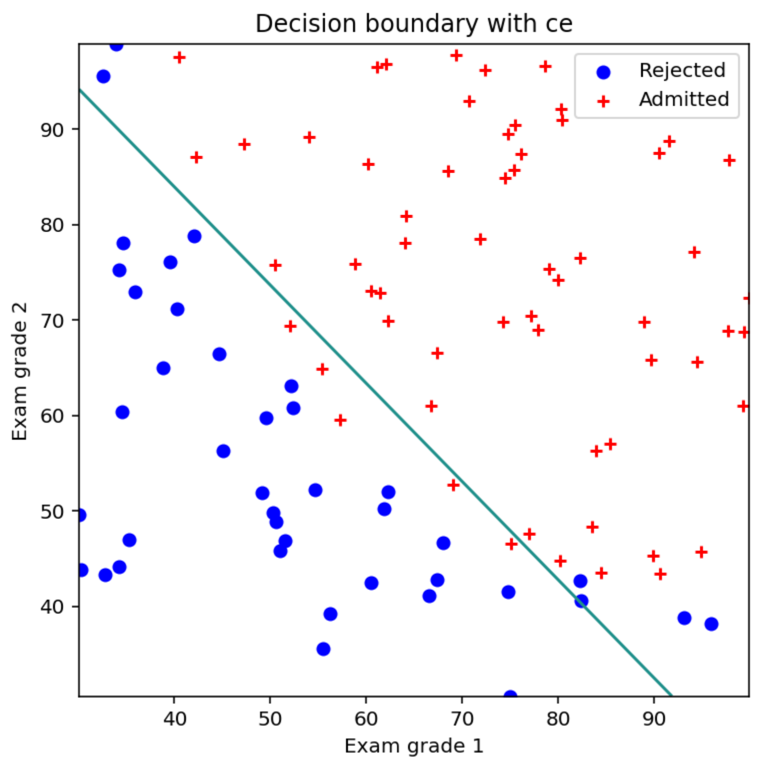
The decision boundary is defined by all points

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

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

In [9]:
```
# 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[:,0] = 1
X2[:,1] = xx1.reshape(-1)
X2[:,2] = xx2.reshape(-1)

p_mse = f_pred(X2, w_mse)
p_mse = p_mse.reshape(xx1.shape)
p_ce = f_pred(X2, w_ce)
p_ce = p_ce.reshape(xx1.shape[0], xx2.shape[0])

# plot
plt.figure(5,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.contour(xx1, xx2, p_mse, levels=1)
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.title('Decision boundary with mse')
plt.show()

plt.figure(6,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.contour(xx1, xx2, p_ce, levels=1)
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.title('Decision boundary with ce')
plt.show()
```



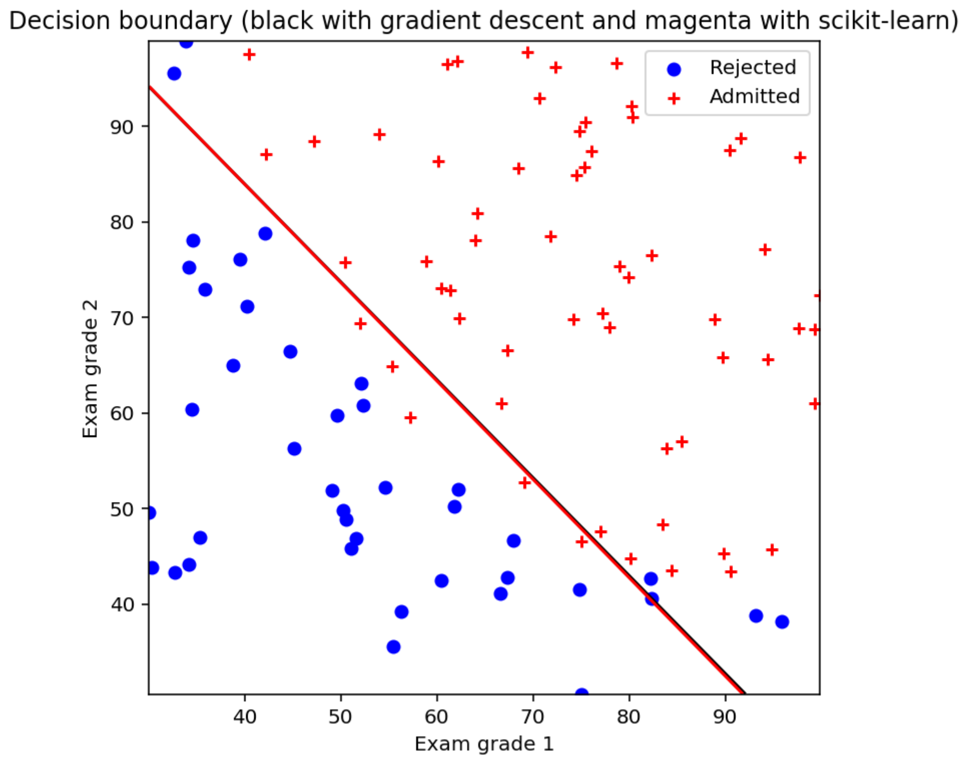




## 9. Comparison with Scikit-learn logistic regression algorithm with the gradient descent with the cross-entropy loss

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

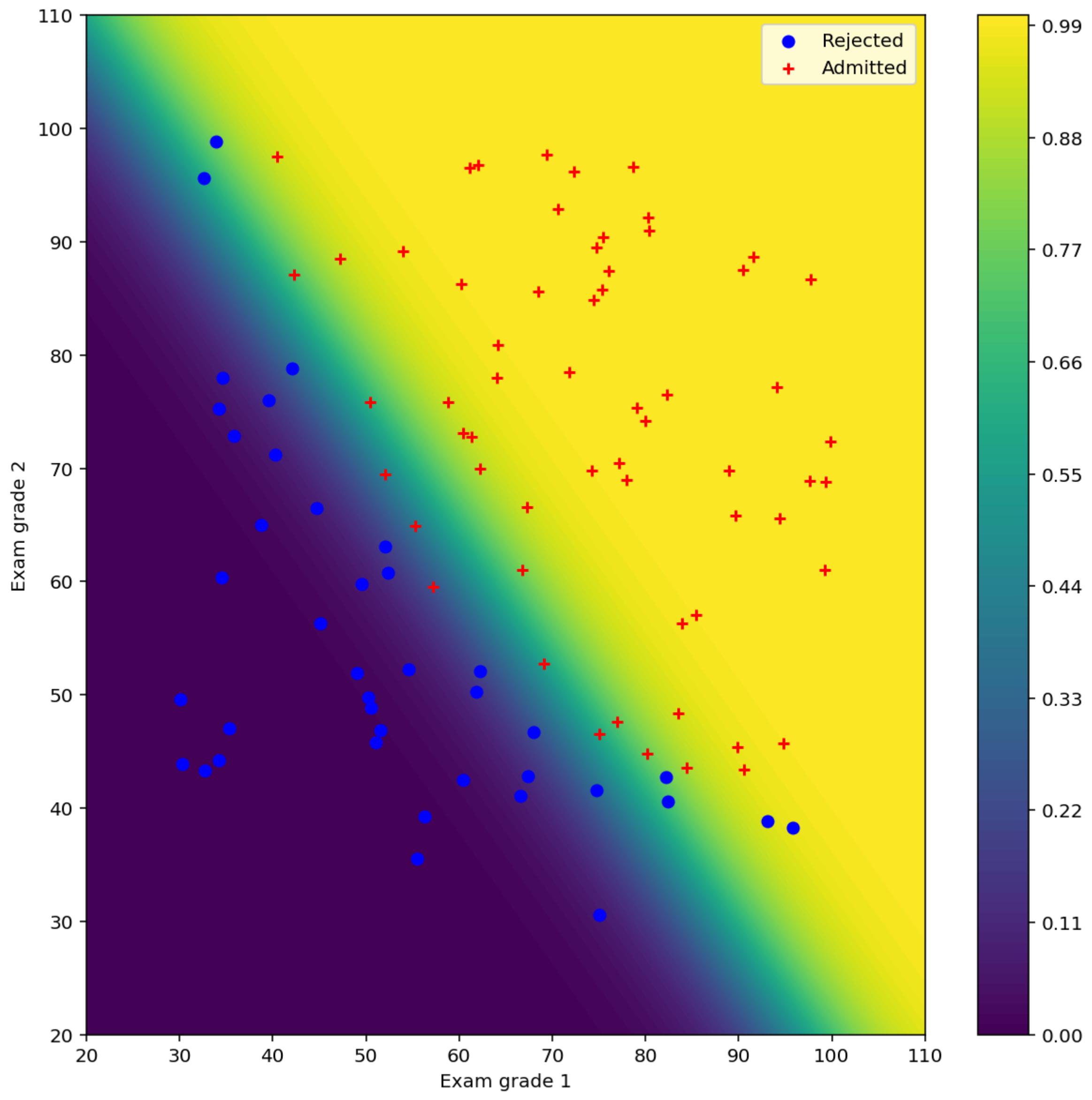
In [10]:
```
# run logistic regression with scikit-learn
start = time.time()
x_train = data[:,:2]
y = data[:,2][:,None]
logreg_sklearn = LogisticRegression()# scikit-learn logistic regression
logreg_sklearn.fit(x_train, y) # learn the model parameters
# compute loss value
w_sklearn = np.zeros([3,1])
w_sklearn[0,0] = logreg_sklearn.intercept_
w_sklearn[1:3,0] = logreg_sklearn.coef_[0]
# loss_sklearn = ce_loss()

# plot
plt.figure(4,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
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_sklearn)
p = p.reshape(50,50)
plt.contour(xx1, xx2, p, levels=1, colors='black' );
plt.contour(xx1, xx2, p_ce, levels=1, colors='red');

plt.title('Decision boundary (black with gradient descent and magenta with scikit-learn)')
plt.legend(loc=1)
plt.show()
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/utils/validation.py:760: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please chan
ge the shape of y to (n_samples, ), for example using ravel().
  y = column_or_1d(y, warn=True)
```

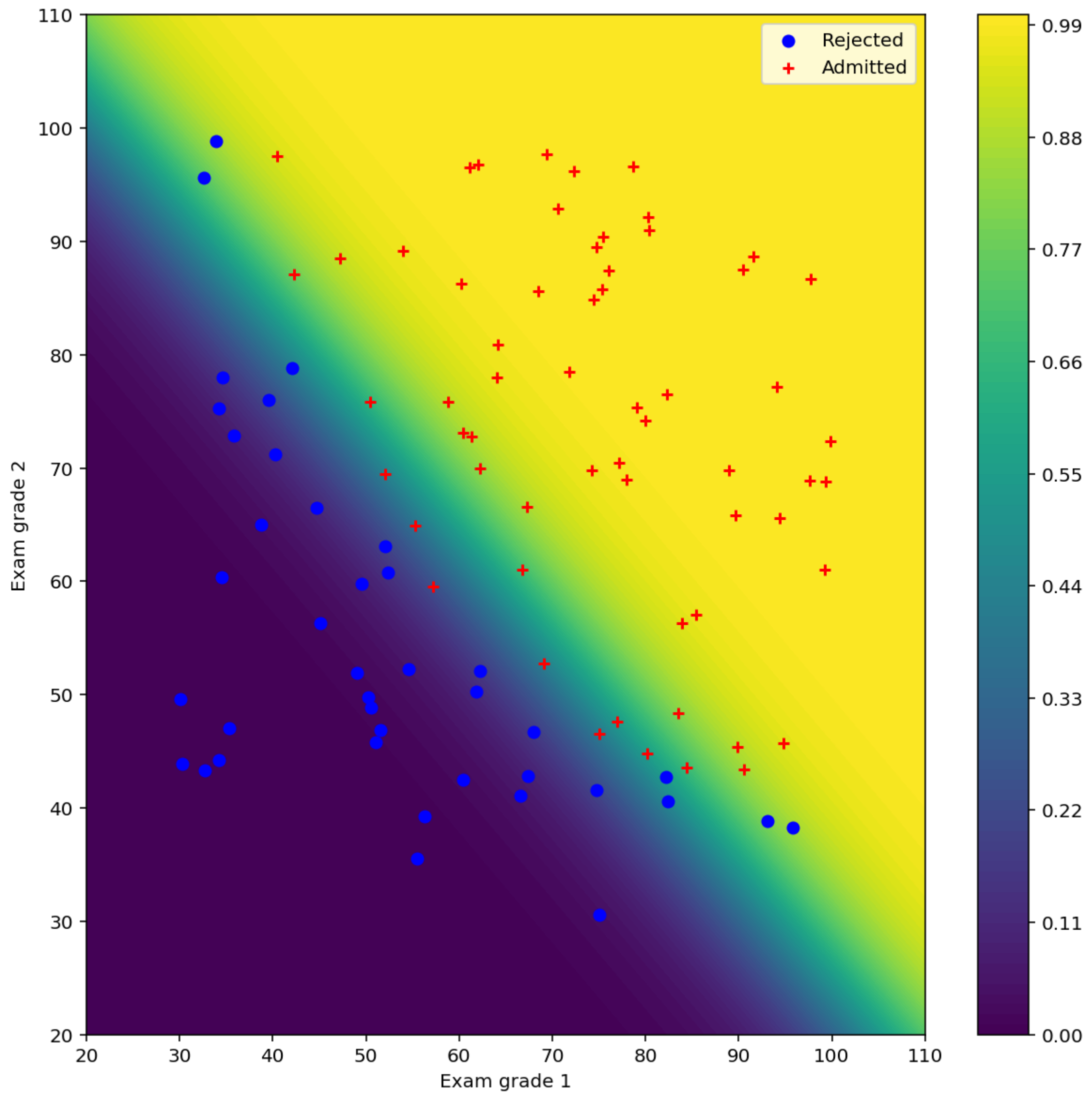



## 10. Plot the probability map

In [11]:
```
num_a = 110
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_mse = np.zeros([num_a, num_a])

for i in range(len(score_x1)):
    for j in range(len(score_x2)):

            predict_prob_mse = f_pred([1,grid_x1[i], grid_x2[j]], w_mse)
            Z_mse[j, i] = predict_prob_mse

            # actual plotting example

fig = plt.figure(figsize=(10,10))

ax1 = fig.add_subplot(111)
ax1.tick_params()
ax1.set_xlabel('Exam grade 1')
ax1.set_ylabel('Exam grade 2')

ax1.set_xlim(20, 110)
ax1.set_ylim(20, 110)
levels = np.linspace(0, 1, 101)
cf_mse = ax1.contourf(score_x1, score_x2, Z_mse, levels=levels)
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
cbar = fig.colorbar(cf_mse)
cbar.update_ticks()

plt.legend(loc=1)
plt.show()
```



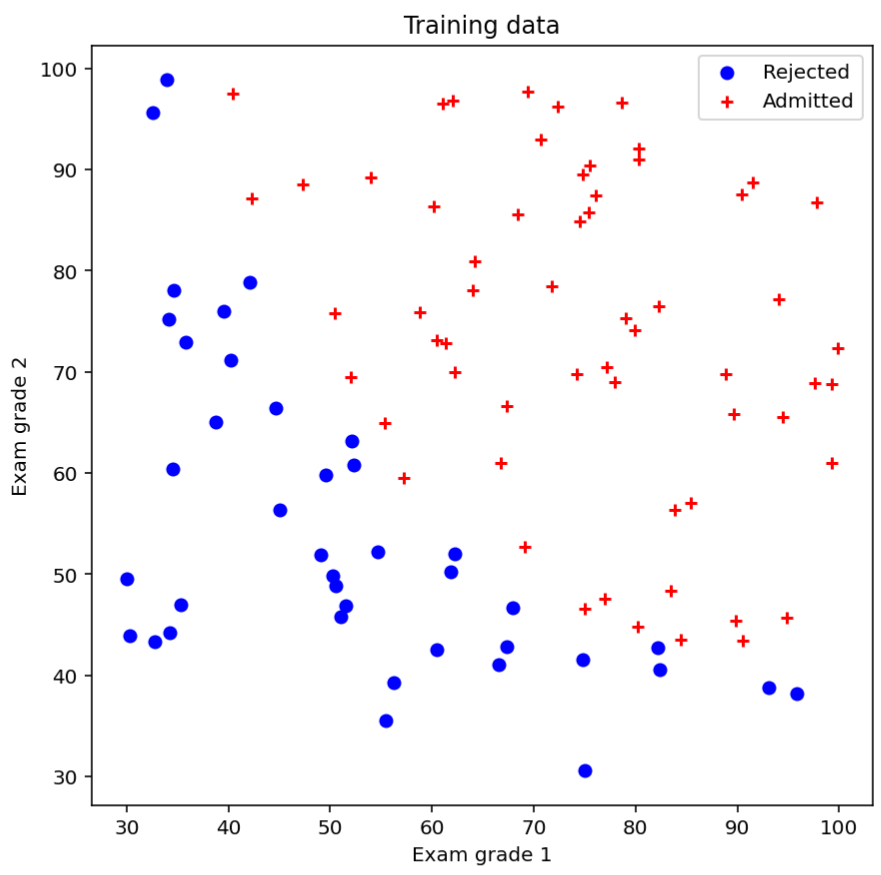
In [12]:
```
num_a = 110
grid_x1 = np.linspace(20,110,num_a)
grid_x2 = np.linspace(20,110,num_a)

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

Z_ce = np.zeros([num_a, num_a])

for i in range(len(score_x1)):
    for j in range(len(score_x2)):

            predict_prob_ce = f_pred([1,grid_x1[j], grid_x2[i]], w_ce)
            Z_ce[j, i] = predict_prob_ce

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

ax2 = fig.add_subplot(111)
ax2.tick_params()
ax2.set_xlabel('Exam grade 1')
ax2.set_ylabel('Exam grade 2')

ax2.set_xlim(20, 110)
ax2.set_ylim(20, 110)


levels = np.linspace(0, 1, 101)
cf_ce = ax2.contourf(score_x1, score_x2, Z_ce, levels=levels)
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
cbar = fig.colorbar(cf_ce)
cbar.update_ticks()

plt.legend(loc=1)
plt.show()
```




# Output results

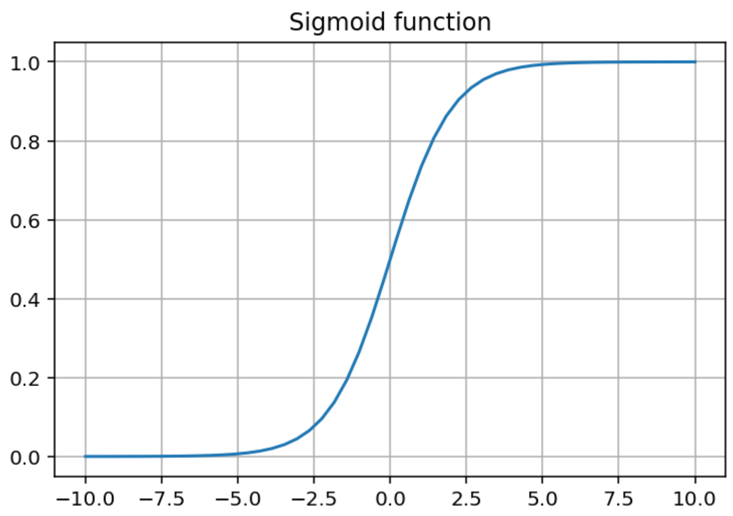
## 1. Plot the dataset in 2D cartesian coordinate system (1pt)

In [13]:
```
plt.figure(figsize=(7,7))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.title('Training data')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.show()
```



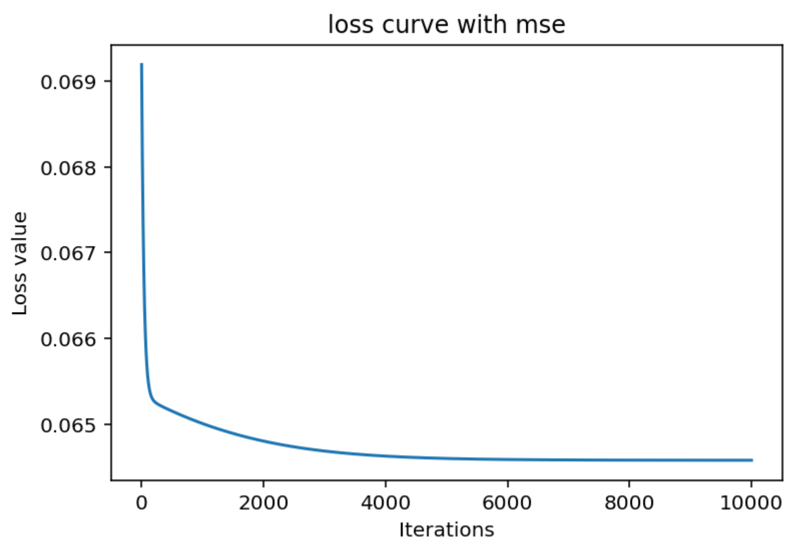

## 2. Plot the sigmoid function (1pt)

In [14]:
```
plt.figure(2)
plt.plot(x_values,sigmoid(x_values))
plt.title("Sigmoid function")
plt.grid(True)
```



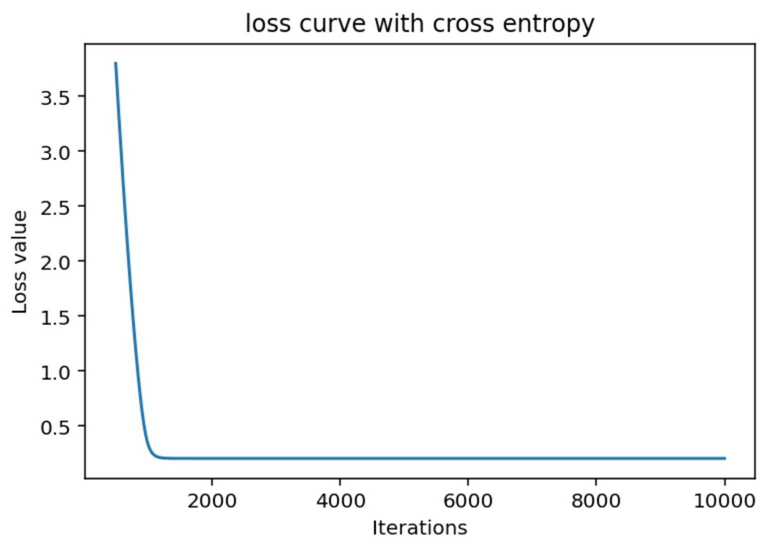

### 3. Plot the loss curve in the course of gradient descent using the mean square error (2pt)

In [15]:
```
plt.figure(3)
plt.plot(L_iters_mse)
plt.title('loss curve with mse')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()
```



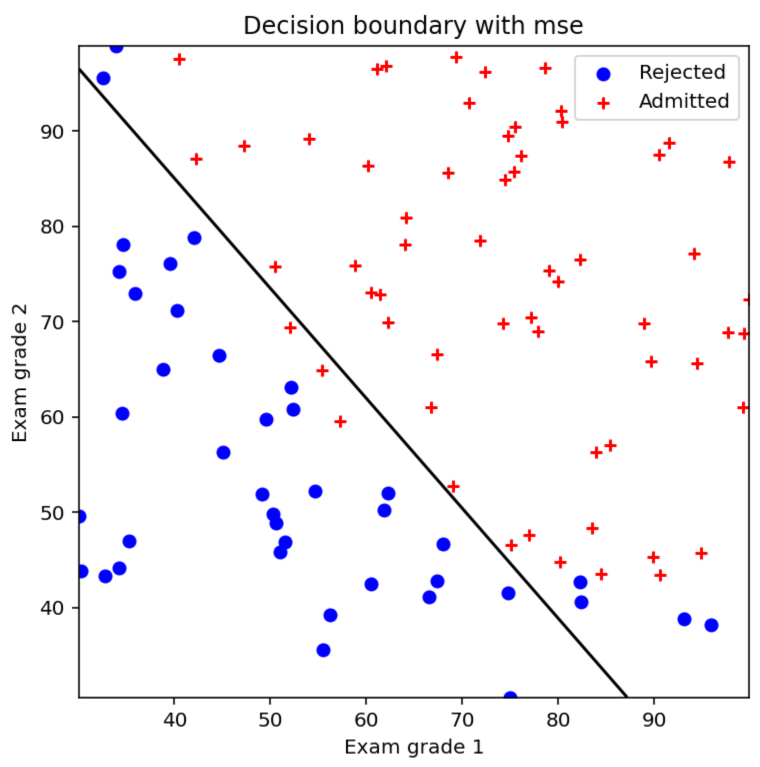

### 4. Plot the loss curve in the course of gradient descent using the cross-entropy error (2pt)

In [16]:
```
plt.figure(4)
plt.plot(L_iters_ce)
plt.title('loss curve with cross entropy')
plt.xlabel('Iterations')
plt.ylabel('Loss value')
plt.show()
```



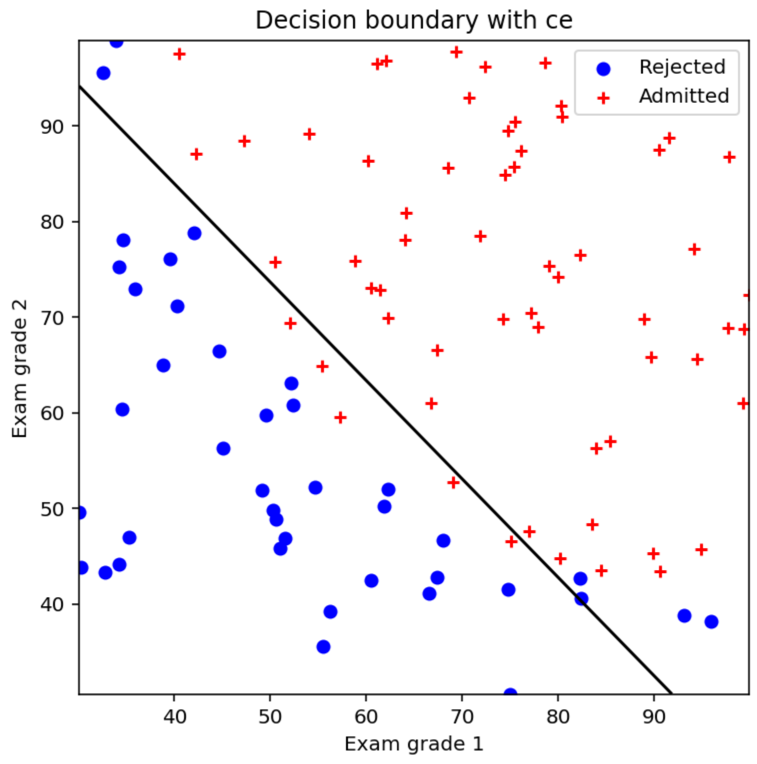

### 5. Plot the decision boundary using the mean square error (2pt)

In [17]:
```
plt.figure(5,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.contour(xx1, xx2, p_mse, levels=1, colors='black')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.title('Decision boundary with mse')
plt.show()
```



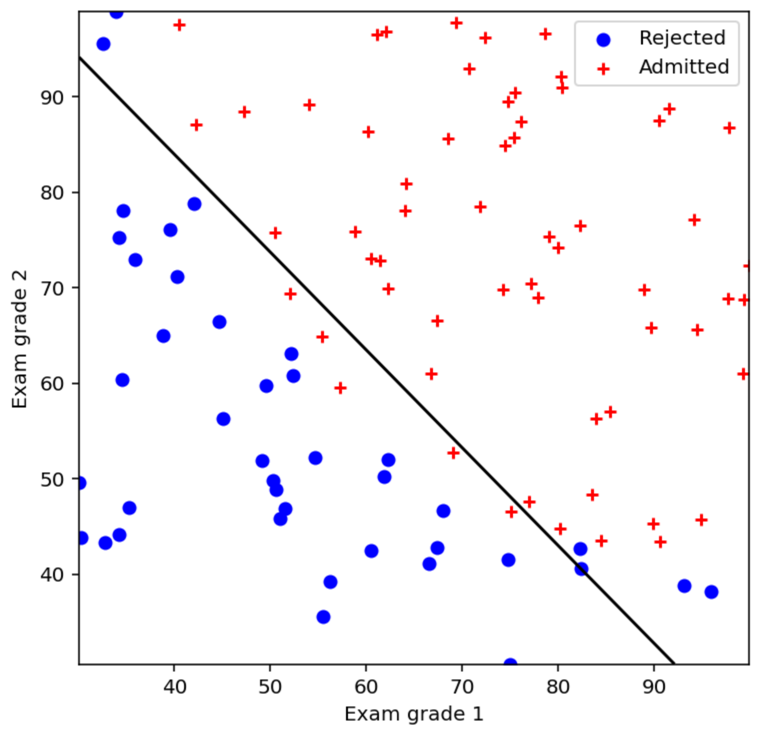

### 6. Plot the decision boundary using the cross-entropy error (2pt)

In [18]:
```
plt.figure(6,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.contour(xx1, xx2, p_ce, levels=1, colors='black')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.legend(loc=1)
plt.title('Decision boundary with ce')
plt.show()
```



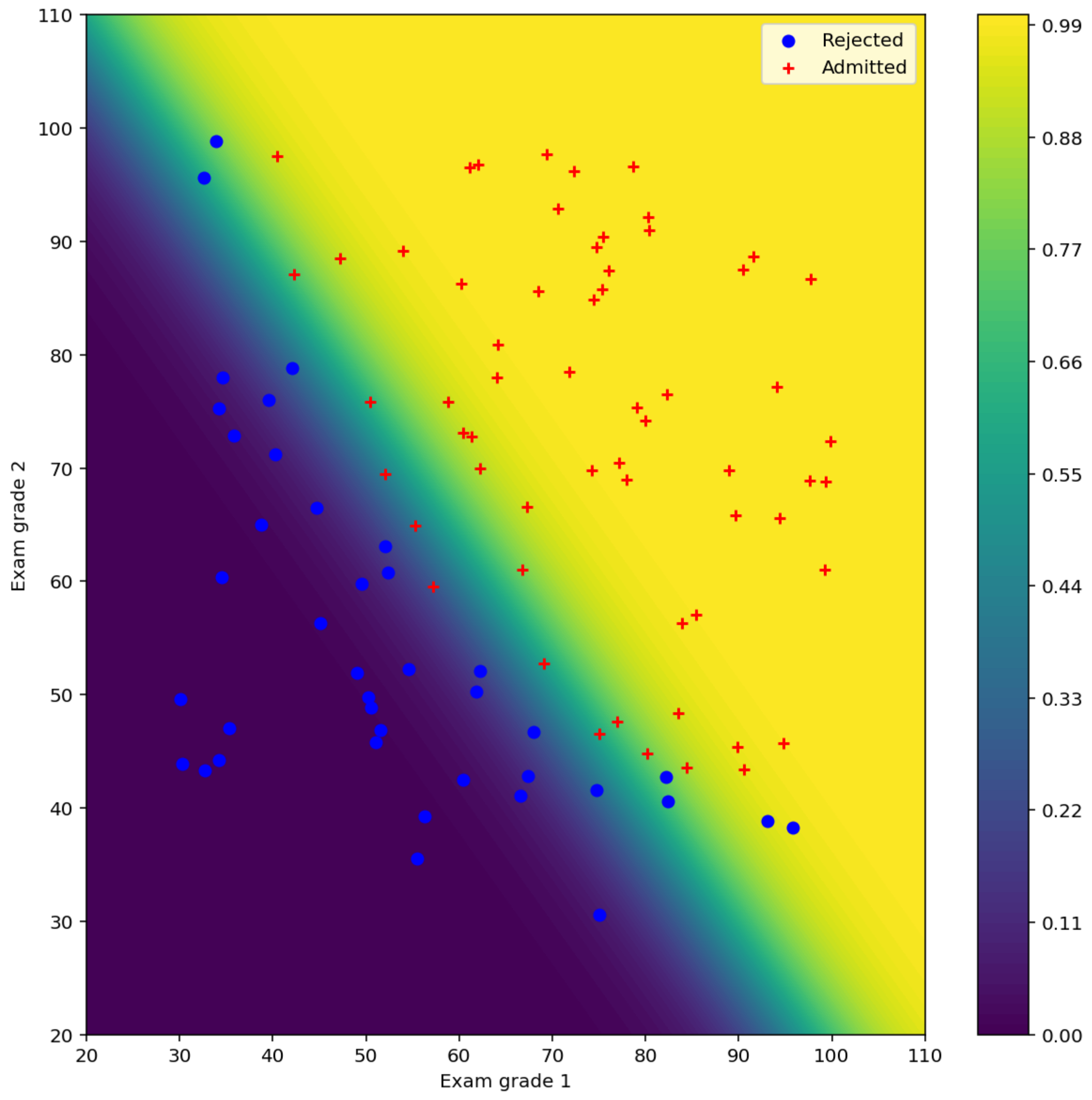

### 7. Plot the decision boundary using the Scikit-learn logistic regression algorithm (2pt)

In [19]:
```
plt.figure(4,figsize=(6,6))
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
plt.xlabel('Exam grade 1')
plt.ylabel('Exam grade 2')
plt.contour(xx1, xx2, p, levels=1, colors='black' );
plt.legend(loc=1)
plt.show()
```



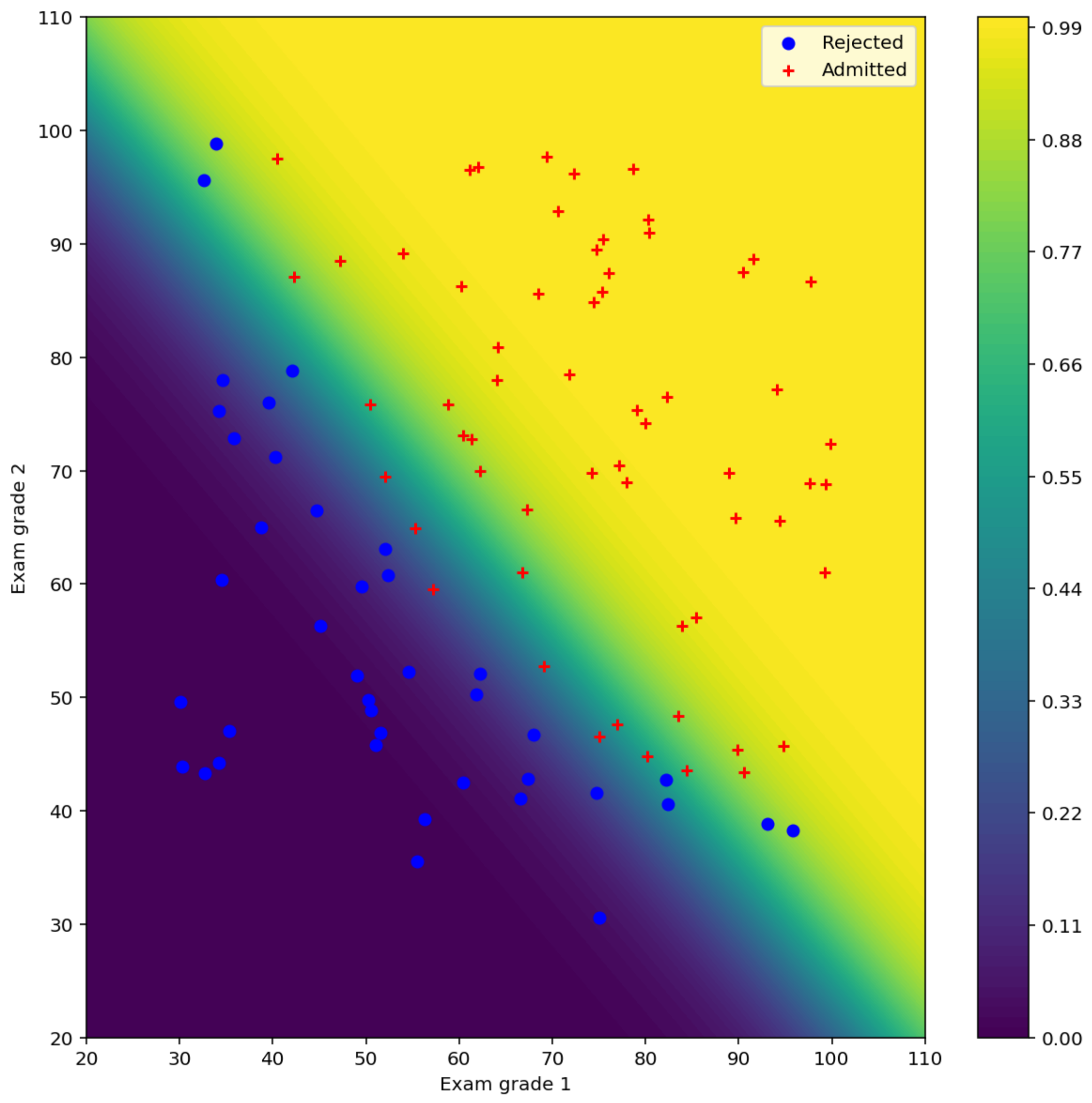

### 8. Plot the probability map using the mean square error (2pt)

In [20]:
```
fig = plt.figure(figsize=(10,10))

ax1 = fig.add_subplot(111)
ax1.tick_params()
ax1.set_xlabel('Exam grade 1')
ax1.set_ylabel('Exam grade 2')

ax1.set_xlim(20, 110)
ax1.set_ylim(20, 110)
levels = np.linspace(0, 1, 101)
cf_mse = ax1.contourf(score_x1, score_x2, Z_mse, levels=levels)
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
cbar = fig.colorbar(cf_mse)
cbar.update_ticks()

plt.legend(loc=1)
plt.show()
```




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

In [21]:
```
fig = plt.figure(figsize=(10,10))

ax2 = fig.add_subplot(111)
ax2.tick_params()
ax2.set_xlabel('Exam grade 1')
ax2.set_ylabel('Exam grade 2')

ax2.set_xlim(20, 110)
ax2.set_ylim(20, 110)


levels = np.linspace(0, 1, 101)
cf_ce = ax2.contourf(score_x1, score_x2, Z_ce, levels=levels)
plt.scatter(x1[idx_rejec], x2[idx_rejec], c='b', marker='o', label='Rejected')
plt.scatter(x1[idx_admit], x2[idx_admit], c='r', marker='+', label='Admitted')
cbar = fig.colorbar(cf_ce)
cbar.update_ticks()

plt.legend(loc=1)
plt.show()
```




In [21]: