HW3 - Coding Assignment

In order to get full marks, your result should include:

- 1. Your code.
- 2. Optimal W^* and \boldsymbol{b}^* .
- 3. Training loss curve.
- 4. Plot of training data along with decision boundary.
- 5. Plot of test data along with decision boundary.
- 6. Test error.

7 (20 points) Softmax Classification

In Question 5, we derived the derivative of cross-entropy loss with respect to each entry of W and b of each class. We now want to extend the expressions to vector form and implement them to accomplish a gradient descent training process.

Assume $\mathbf{p} = (p_0, \dots, p_{K-1})^T \in \mathbb{R}^K$, $\mathbf{W} = (\mathbf{w}_0, \dots, \mathbf{w}_{K-1})^T \in \mathbb{R}^{K \times D}$ and $\mathbf{b} = (b_0, \dots, b_{K-1})^T \in \mathbb{R}^K$, the gradient of $\mathcal{L}_{\text{xent}}(\mathbf{x}, y; \mathbf{W}, \mathbf{b})$ with respect to the W and b is given by:

$$\frac{\partial \mathcal{L}_{\mathsf{xent}}(\mathbf{x}, y; \mathsf{W}, \mathbf{b})}{\partial \mathsf{W}} = (\mathbf{p} - \mathbf{y})\mathbf{x}^T, \qquad \frac{\partial \mathcal{L}_{\mathsf{xent}}(\mathbf{x}, y; \mathsf{W}, \mathbf{b})}{\partial \mathbf{b}} = \mathbf{p} - \mathbf{y}$$

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial \mathbf{W}} = \sum_{i} (\mathbf{p}^{(i)} - \mathbf{y}^{(i)}) \mathbf{x}^{(i)T}, \qquad \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial \mathbf{b}} = \sum_{i} (\mathbf{p}^{(i)} - \mathbf{y}^{(i)})$$

the W and **b** is given by: $\frac{\partial \mathcal{L}_{\text{xent}}(\mathbf{x}, y; \mathsf{W}, \mathbf{b})}{\partial \mathsf{W}} = (\mathbf{p} - \mathbf{y})\mathbf{x}^T, \qquad \frac{\partial \mathcal{L}_{\text{xent}}(\mathbf{x}, y; \mathsf{W}, \mathbf{b})}{\partial \mathbf{b}} = \mathbf{p} - \mathbf{y}$ and the gradient of $\mathcal{L}(\mathsf{W}, \mathbf{b})$ with respect to the W and **b** is given by: $\frac{\partial \mathcal{L}(\mathsf{W}, \mathbf{b})}{\partial \mathsf{W}} = \sum_i (\mathbf{p}^{(i)} - \mathbf{y}^{(i)})\mathbf{x}^{(i)^T}, \qquad \frac{\partial \mathcal{L}(\mathsf{W}, \mathbf{b})}{\partial \mathbf{b}} = \sum_i (\mathbf{p}^{(i)} - \mathbf{y}^{(i)})$ Furthermore, if we represent the training dataset in the matrix form: $\mathsf{X} = (\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(n-1)})^T \in \mathbb{R}^{n \times K}$, $\mathsf{Y} = (\mathbf{y}^{(0)}, \dots, \mathbf{y}^{(n-1)})^T \in \{0, 1\}^{n \times K}$ and $\mathsf{P} = (\mathbf{y}^{(0)}, \dots, \mathbf{y}^{(n-1)})^T \in \{0, 1\}^{n \times K}$ and

$$\mathsf{P} = (\mathbf{p}^{(0)}, \dots, \mathbf{p}^{(n-1)})^T \in \mathbb{R}^{n \times K}. \text{ Thus, the gradient of } \mathcal{L}(\mathsf{W}, \mathbf{b}) \text{ with respect to the W and } \mathbf{b} \text{ is given by:} \\ \frac{\partial \mathcal{L}(\mathsf{W}, \mathbf{b})}{\partial \mathsf{W}} = (\mathsf{P} - \mathsf{Y})^T \mathsf{X}, \qquad \frac{\partial \mathcal{L}(\mathsf{W}, \mathbf{b})}{\partial \mathbf{b}} = (\mathsf{P} - \mathsf{Y})^T \mathbf{1}$$
where $\mathbf{1} \in \mathbb{R}^n$ is a n -dim vector in which each entry is 1

where $1 \in \mathbb{R}^n$ is a *n*-dim vector in which each entry is 1.

Complete the sections marked with "your code" in the skeleton codes below.

Load Data

```
In [1]: ▶ import numpy as np
            import matplotlib.pvplot as plt
            from sklearn import datasets
            # Load original Iris dataset.
            iris = datasets.load iris()
            old X = iris.data
            old_Y = iris.target
            # Create the modified Iris dataset.
                                  # We only use last 2 features.
            new_X = old_X[:,2:]
            new_Y = old_Y.reshape(-1,1)
                          np.vstack([new_X[:35], new_X[50:85], new_X[100:135]])
            Y_train = np.concatenate([new_Y[:35], new_Y[50:85], new_Y[100:135]])
                         np.vstack([new_X[35:50], new_X[85:100], new_X[135:]])
            X_test =
            Y_test = np.concatenate([new_Y[35:50], new_Y[85:100], new_Y[135:]])
            print(X_train.shape)
                                    # X_train.shape should be (105,2), which shows
                                   # 150 training points where each has 2 features.
            print(Y train.shape)
                                    # Y_train.shape should be (105,1) which shows 105
            print(np.unique(Y_train))# points where each point has label 0, 1 or 2.
            (105, 2)
            (105, 1)
            [0 1 2]
```

Visualization of Original Data

```
In [2]: ▶ import matplotlib as mpl
            from mpl_toolkits.mplot3d import Axes3D
            import math
            %config InlineBackend.figure_format = 'retina'
            %matplotlib inline
            from sklearn.utils import shuffle
            import scipy.io as sio
            plt.rcParams['figure.figsize'] = 8,8
```



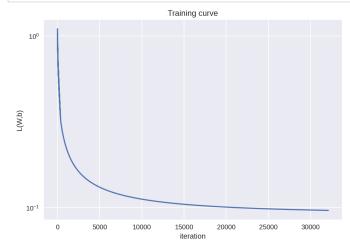
Training Procedure

```
"" Calculate the P (probability) matrix of softmax function.
               X: Feature matrix.
                                 Shape: [n,D].
               W: Weight matrix.
                                  Shape: [K,D].
                                  Shape: [K,1].
               b: Bias vector.
               Return the P matrix. Shape: [n,K].
               f
                        = W.dot(X.T) + b # Shape: [K,n].
                        = f - f.max(axis=0, keepdims=True)
               f
                                                         # Avoid the big number
               exp_f
                        = np.exp(f)
                                          # Shape: [K,n].
               sum_exp_f = exp_f.sum(axis=0, keepdims=True) # Shape: [1,n].
                        = (exp_f / sum_exp_f).T
               return P
```

```
def L_prime(X, Y, W, b):
    """ L'(W,b) function.
                  X: Feature matrix. Shape: [n,D].
                   Y: Label vector. Shape: [n,1].
                  W: Weight matrix. Shape: [K,D].
b: Bias vector. Shape: [K,1].
                  Return the gradients: dL/dW (Shape: [K,D]), dL/db (Shape: [K,1]).
                 # Get dimensions.
                  K, D = W.shape
                  n = X.shape[0]
                  # Generate the one-hot encoding form of Y.
                   Y_onehot = np.zeros((n, K))
                   for i in range(n):
                      Y_{onehot[i, Y[i]] = 1}
                  ## Get the P matrix.
                  P = softmax_P(X, W, b)
                                                                          # Shape: [K,1].
                  ## Calculate the gradients: dL/dW, dL/db.
                  dL_by_dW = np.dot((P - Y_onehot).T, X)
dL_by_db = np.dot((P - Y_onehot).T, np.ones((n,1)))
                                                                                                          # Shape: [K,D].
                  # Return the gradients.
                  return dL_by_dW, dL_by_db
In [29]: ► def L(X, Y, W, b):
""" L(W,b) function.
```

```
In [30]: | learning_rate = 0.0025
                                     # Number of iterations
# Number of classes.
              n_iter = 100000
              K = 3
              D = X_train.shape[1] # Number of feature dimensions
              W = np.zeros((K,D))
                                     # Weight matrix.
              b = np.zeros((K,1)) # Bias vector.
              # We will keep track of training loss over iterations.
              iterations = [0]
              L_list = [L(X_train, Y_train, W, b)]
              for i in range(n_iter):
                  ###### Begin your code ######
                  ## Calculate current gradients
                  gradient_W, gradient_b = L_prime(X_train, Y_train, W, b)
                  ## Perform gradient descent
                  W_new = W - learning_rate * gradient_W
b_new = b - learning_rate * gradient_b
                  ####### End your code #######
                  iterations.append(i+1)
                  L_list.append(L(X_train, Y_train, W_new, b_new))
                  \verb"norm" = np.abs(W_new-W).sum() + np.abs(b_new-b).sum() \\ \# \textit{L1-norm as jumping out criteria}.
                  if norm < 0.0005:
                      print("Gradient descent has converged after " + str(i) + " iterations.")
                  W = W_new
                  b = b_new
              print ('W matrix: \n' + str(W))
              print ('b vector: \n' + str(b))
              Gradient descent has converged after 32099 iterations.
              W matrix:
              [[-3.40416004 -6.62538814]
               [-0.25031952 -0.40788509]
               [ 3.65447956 7.03327322]]
              b vector:
              [[ 18.79108579]
                  6.29487369]
               [-25.08595948]]
```

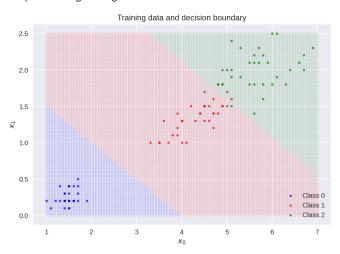
Training Loss Curve



Results on Training Data

```
In [32]: ▶ # Prepare for decision boundary.
              num = 100
              X0_plane_range = np.linspace(1,7,num)
              X1_plane_range = np.linspace(0,2.5,num)
              X0_plane, X1_plane = np.meshgrid(X0_plane_range, X1_plane_range)
              X_decision = np.stack([X0_plane.reshape(-1), X1_plane.reshape(-1)]).T
              P_{decision} = softmax_{P(X_{decision}, W, b)} # Shape: [n,K].
              yhat_decision = P_decision.argmax(axis=1).reshape(-1,1)
In [33]: ▶ # Training data points and decision boundary.
              plt.scatter(X_decision[yhat_decision[:,0]==0, 0],
                           X_decision[yhat_decision[:,0]==0, 1],
              marker='o', color='b', alpha=0.1, s=10)
plt.scatter(X_decision[yhat_decision[:,0]==1, 0],
                           X_decision[yhat_decision[:,0]==1, 1],
                           marker='o', color='r', alpha=0.1, s=10)
              plt.scatter(X_decision[yhat_decision[:,0]==2, 0],
                           X_decision[yhat_decision[:,0]==2, 1],
                           marker='o', color='g', alpha=0.1, s=10)
              plt.scatter(X_train[Y_train[:,0]==0, 0],
                           X_train[Y_train[:,0]==0, 1],
marker='o', color='b', alpha=0.7, s=10, label='Class 0')
              plt.scatter(X_train[Y_train[:,0]==1, 0],
                           X_train[Y_train[:,0]==1, 1],
                           marker='o', color='r', alpha=0.7, s=10, label='Class 1')
              plt.scatter(X_train[Y_train[:,0]==2, 0],
                           X_train[Y_train[:,0]==2, 1],
                           marker='o', color='g', alpha=0.7, s=10, label='Class 2')
              plt.xlabel('$x_0$')
              plt.ylabel('$x_1$')
plt.title('Training data and decision boundary')
              plt.legend(loc='lower right', fontsize=10)
```

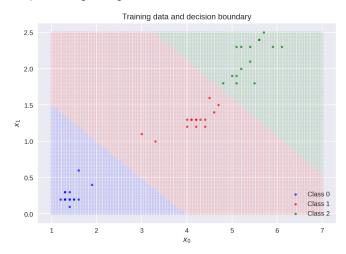
Out[33]: <matplotlib.legend.Legend at 0x7fb90a978460>



Results on Test Data

```
In [34]:
          ▶ # Test data points and decision boundary.
             plt.scatter(X_decision[yhat_decision[:,0]==0, 0],
                         X_decision[yhat_decision[:,0]==0, 1],
                         marker='o', color='b', alpha=0.1, s=10)
             plt.scatter(X_decision[yhat_decision[:,0]==1, 0],
                         X_decision[yhat_decision[:,0]==1, 1],
                         marker='o', color='r', alpha=0.1, s=10)
             plt.scatter(X_decision[yhat_decision[:,0]==2, 0],
                         X_{decision[yhat_decision[:,0]==2, 1],
                         marker='o', color='g', alpha=0.1, s=10)
             plt.scatter(X_test[Y_test[:,0]==0, 0],
                         X_test[Y_test[:,0]==0, 1],
                         marker='o', color='b', alpha=0.7, s=10, label='Class 0')
             plt.scatter(X_test[Y_test[:,0]==1, 0],
                         X_test[Y_test[:,0]==1, 1],
                         marker='o', color='r', alpha=0.7, s=10, label='Class 1')
             plt.scatter(X_test[Y_test[:,0]==2, 0],
                         X_test[Y_test[:,0]==2, 1],
                         marker='o', color='g', alpha=0.7, s=10, label='Class 2')
             plt.xlabel('$x_0$')
             plt.ylabel('$x_1$')
             plt.title('Training data and decision boundary')
             plt.legend(loc='lower right', fontsize=10)
```

Out[34]: <matplotlib.legend.Legend at 0x7fb90a51ba00>



```
In [35]: W # Calculate the test error.
P_test = softmax_P(X_test, W, b) # Shape: [n,K].
yhat_test = P_test.argmax(axis=1).reshape(-1,1)
test_error = 1 - np.sum(yhat_test == Y_test) / Y_test.shape[0]
print('Test error: {}'.format(test_error))
```

Test error: 0.0

8 (Extra Credit - 25 points) Feed-forward Neural Network for Classification

In this section, we will use the feed-forward network defined in Question 6, which is as follows

(You do **NOT** need to prove this sub-section, but understanding this sub-section can be beneficial to the programming part) Besides, in the gradient algorithm, we still need the \$\frac{\partial \mathcal{L}}{\partial \mat

- 1. \$\displaystyle\frac{\partial \mathcal{L}} {\partial \mathcal{L}}
- $2. $\displaystyle | frac{\hat{L}} {\mathbf L}} {\mathbf L} = \bigg(\frac{L}{\hbar} \right) \bigg(\frac{L}{\hbar} \right)$

Furthermore, assume $\hat{X} = (\mathbf{x}^{(0)}, ..., \mathbf{x}^{(0)}, ..., \mathbf{x}^{(0)}$

- $1. $\displaystyle \frac{\hat{L}_\text{mathbf}(y)} = \mathrm{frac}(\mu_{1}) (\mathbf(y)\displaystyle). $$$
- $2. $\displaystyle frac{partial \mathbb{L}_{text}{train}} {partial b_2} = \mathbb{1}^T \left(\mathbb{1}^T \right) ((\mathbf{partial primar}) $.$
- $3. $\displaystyle \frac{\hat{L}_\text{mathbf\{y\}\choose big}} \mathbb{E}_{\theta}(\mathbf\{p\}-\mathbb{F}_{\theta}) \displaystyle \frac{\hat{L}_\text{mathbf\{y\}\choose big}} \mathbb{E}_{\theta}.$
- 4. \$\displaystyle\frac{\partial \mathcal{L}_\text{\train}}{\partial \mathsf{W}_1} = \mathsf{X}^T\bigg(\big(\frac{\partial \mathcal{L}_\text{\train}}{\partial \mathsf{H}}\bigg)\$.
- 5. \$\displaystyle\frac{\partial \mathcal{L}_\text{train}} {\partial \mathcf{b}_1} = \bigg(\big(\frac{\partial \mathcal{L}_\text{train}}{\partial \mathcf{H}}\big)\circ \mathcf{H}}\\big)^T \mathcf{1}\$.

Complete the sections marked with "your code" in the skeleton codes below.

Load Data

```
In [36]: ▶ import numpy as np
             import matplotlib.pyplot as plt
             from sklearn import datasets
             # Load original Iris dataset.
             iris = datasets.load_iris()
             old_X = iris.data
             old_Y = iris.target
             # Create the modified Iris dataset.
             new_X = old_X[old_Y>0][:,2:]
                                                      # We only use last 2 features.
             new_Y = old_Y[old_Y>0].reshape(-1,1)
                                                     # Use class 1,2 and convert
             new_Y[new_Y==1] = -1
                                                      # them into class -1,1.
             new_Y[new_Y==2] = 1
             # Generate training set and test set.
                            np.vstack([new_X[:35],
                                                      new_X[50:85]]) # Shape: [70,2].
             Y_train = np.concatenate([new_Y[:35],
                                                      new_Y[50:85]]) # Shape: [70,1].
             X_{\text{test}} = \text{np.vstack}([\text{new}_X[35:50], \text{new}_X[85:100]]) # Shape: [30,2].
             Y_test = np.concatenate([new_Y[35:50], new_Y[85:100]]) # Shape: [30,1].
             print(X_train.shape)
                                       # X_train.shape should be (70,2), which shows
                                       # 70 training points where each has 2 features.
             print(Y train.shape)
                                       # Y_train.shape should be (70,1) which shows 70
             print(np.unique(Y_train))# points where each point has label -1, 1.
             (70, 2)
             (70, 1)
             [-1 1]
```

Visualization of Original Data

```
import matplotlib as mpl
from mpl_toolkits.mplot3d import Axes3D
import math
%config InlineBackend.figure_format = 'retina'
%matplotlib inline
from sklearn.utils import shuffle
import scipy.io as sio
plt.rcParams['figure.figsize'] = 8,8
```



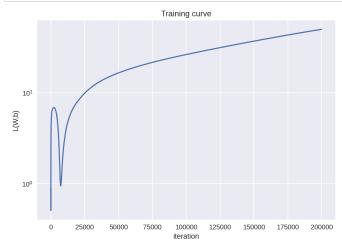
Training Procedure

```
In [40]: ► # Gradient of loss function: L'(W1, b1, W2, b2).
            def L_prime(X, Y, W1, b1, W2, b2):
    """ L'(W,b) function.
                X: Feature matrix.
                                      Shape: [n,2].
                Y: Label vector.
                                       Shape: [n,1].
                W1: Weight matrix W1. Shape: [2,3].
                b1: Bias vector b1. Shape: [3,1].
                W2: Weight matrix W2. Shape: [3,1].
                b2: Bias vector b2. Shape: [1,1].
                Return the gradients: dL/dW1 (Shape: [2,3]), dL/db1 (Shape: [3,1]),
                                     dL/dW2 (Shape: [3,1]), dL/db2 (Shape: [1,1]).
                # Get dimensions.
                n = X.shape[0]
                ###### Begin your code #####
                ## Calculate feed-forward values.
                H = sigmoid(np.dot(X, W1) + b1.T)
                                                             # Shape: [n, 3].
                # the derivative of the loss function with respect to the pre-activation value is Z2
                Z2 = np.dot(H, W2) + b2 # Shape: [n, 1].
                P = sigmoid(Z2)
                                          # Shape: [n, 1].
                ## Calculate the gradients: dL/dW1, dL/db1, dL/dW2, dL/db2. dL_by_dZ2 = (P - Y) * P * (1 - P)
                dL_by_dW2 = np.dot(H.T, dL_by_dZ2) # Shape: [3, 1].
                dL_by_db2 = np.sum(dL_by_dZ2, axis=0, keepdims=True) # Shape: [1, 1].
                dL_by_db1 = np.sum(dL_by_dH, axis=0, keepdims=True).T # Shape: [3, 1].
                ###### End your code #######
                # Return the gradients.
                return dL_by_dW1, dL_by_db1, dL_by_dW2, dL_by_db2
```

```
In [41]: M def L(X, Y, W1, b1, W2, b2):
                 """ L(W,b) function.
                X: Feature matrix.
                                       Shape: [n,2].
                Y: Label vector.
                                       Shape: [n,1].
                W1: Weight matrix W1. Shape: [2,3].
                b1: Bias vector b1.
                                      Shape: [3,1].
                W2: Weight matrix W2. Shape: [3,1].
                b2: Bias vector b2. Shape: [1,1].
                Return the loss.
                                      Shape: Scalar.
                # Get dimensions.
                n = X.shape[0]
                 ###### Begin your code #####
                 ## Calculate feed-forward values.
                H = sigmoid(np.dot(X, W1) + b1.T)
                                                                            # Shape: [n, 3].
                P = np.dot(H, W2) + b2
                                                                 # Shape: [n, 1].
                ## Get the Loss.
                 # Shape: Scalar.
                L = np.sum((Y - P)**2) / (2*n)
                 ###### End your code #######
                 return L
```

```
In [42]: ▶ ## The following codes might take a while to run, please be patient
             learning_rate = 0.0025
             n_{iter} = 200000
                                                     # Number of iterations
             np.random.seed(0)
             W1 = \text{np.random.randn}(2,3)/((2*3)**2) # Weight matrix 1.
             b1 = np.random.randn(3,1)/((3*1)**2)
                                                     # Bias vector 1.
             W2 = np.random.randn(3,1)/((3*1)**2)
                                                     # Weight matrix 2.
             b2 = np.random.randn(1,1)/((1*1)**2) # Bias vector 2.
             # We will keep track of training loss over iterations.
             iterations = [0]
             L_{list} = [L(X_{train}, Y_{train}, W1, b1, W2, b2)]
             for i in range(n_iter):
                 ###### Begin your code #####
                 ## Calculate current gradients
                 gradient_W1, gradient_b1, gradient_W2, gradient_b2 = L_prime(X_train, Y_train, W1, b1, W2, b2)
                 ## Perform gradient descent
                 W1_new = W1 - learning_rate * gradient_W1
                 b1_new = b1 - learning_rate * gradient_b1
                 W2_new = W2 - learning_rate * gradient_W2
b2_new = b2 - learning_rate * gradient_b2
                 ####### End your code #######
                 iterations.append(i+1)
                 L_list.append(L(X_train, Y_train, W1_new, b1_new, W2_new, b2_new))
                 # L1-norm of weight/bias changing.
                 norm = np.abs(W1_new-W1).sum() + np.abs(b1_new-b1).sum() + \
                         np.abs(W2_new-W2).sum() + np.abs(b2_new-b2).sum()
                 if i%40000 == 0 or i+1 == n iter:
                     print('i: {:6d} L: {:.3f} norm:{:.6f}'.format(i, L_list[-1], norm))
                 W1 = W1_new
                 b1 = b1 new
                 W2 = W2_new
                 b2 = b2_new
             print ('W1 matrix: \n' + str(W1))
             print ('b1 vector: \n' + str(b1))
             print ('W2 matrix: \n' + str(W2))
             print ('b2 vector: \n' + str(b2))
             i:
                     0 L: 0.845 norm:0.076396
             i: 40000 L: 14.265 norm:0.000295
             i: 80000 L: 22.565 norm:0.000176
             i: 120000 L: 30.378 norm:0.000159
             i: 160000 L: 39.464 norm:0.000162
             i: 199999 L: 50.016 norm:0.000161
             W1 matrix:
             [[ 0.30951536  0.32268003 -2.96626203]
              [ 0.42505523  0.48139955 -4.91518135]]
             b1 vector:
             [[-0.16274906]
              [-0.54433637]
              [23.11752175]]
             W2 matrix:
             [[ 3.85413823]
                4.08998147]
              [-24.4006325]]
             b2 vector:
             [[3.57411952]]
```

Training Loss Curve

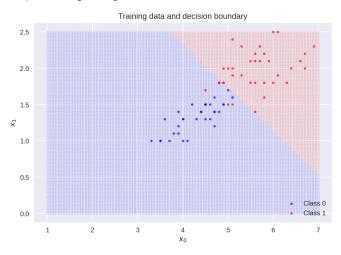


Results on Training Data

```
In [44]:  # Prepare for decision boundary.
    num = 100
    X0_plane_range = np.linspace(1,7,num)
    X1_plane_range = np.linspace(0,2.5,num)
    X0_plane, X1_plane = np.meshgrid(X0_plane_range, X1_plane_range)
    X_decision = np.stack([X0_plane.reshape(-1), X1_plane.reshape(-1)]).T

# Calculate feed-forward values.
    f_decision = sigmoid(X_decision.dot(W1)+b1.T).dot(W2)+b2.T # Shape: [n,1].
    yhat_decision = np.sign(f_decision)
```

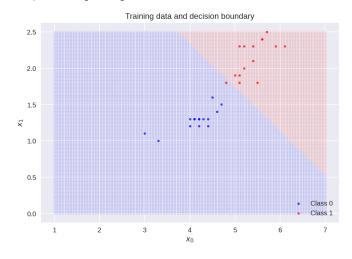
Out[45]: <matplotlib.legend.Legend at 0x7fb90b674b20>



Results on Test Data

```
In [46]: ▶ # Test data points and decision boundary.
            marker='o', color='b', alpha=0.1, s=10)
            plt.scatter(X_decision[yhat_decision[:,0]==1, 0],
                       X_decision[yhat_decision[:,0]==1, 1],
                       marker='o', color='r', alpha=0.1, s=10)
            plt.scatter(X_test[Y_test[:,0]==-1, 0],
                       X_test[Y_test[:,0]==-1, 1],
                       marker='o', color='b', alpha=0.7, s=10, label='Class 0')
            plt.scatter(X_test[Y_test[:,0]==1, 0],
                       X_test[Y_test[:,0]==1, 1],
                       marker='o', color='r', alpha=0.7, s=10, label='Class 1')
            plt.xlabel('$x_0$')
            plt.ylabel('$x_1$')
            plt.title('Training data and decision boundary')
            plt.legend(loc='lower right', fontsize=10)
```

Out[46]: <matplotlib.legend.Legend at 0x7fb90b907430>



Test error: 0.03333333333333333

In []: ▶