CSDS 391 Programming Assignment 2 Writeup

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Due On: December 4, 2020

Problem 1:

Problem 2:

(a)

The mean squared error is calculated using the following equation:

$$MSE = \frac{1}{n}\sum_n (Y_i - \hat{Y_i})^2$$

, where Y_i is the actual category of the ith item and $\hat{Y_i}$ is the predicted category by using our neural network.

The following codes compute the **mean squared error** for iris data. The parameter "data_vector" are the attributes we would like to take into account, it should be a dataframe of attributes. w_0, w_1, w_2 define the weights of neural network. The parameter "pattern_classes" is a dataframe of the category corresponding to the data_vectors. The **mean_square_error** makes use of the logistic non-linearity function in Problem 1.

```
# data vectors in dataframe, pattern classes in list
def mean_square_error(data_vectors, w0, w1, w2,
    pattern_classes):
    n = data_vectors.shape[0]
    data_vectors_list = data_vectors.values.tolist()
    pattern_classes_list = pattern_classes.tolist()
    temp_mse = 0
```

```
    for i in range(n):
        temp_mse = temp_mse + np.square(pattern_classes_list[
    i] - one_layer_network(w0, w1, w2, data_vectors_list[i
    ][0], data_vectors_list[i][1]))
    mse = temp_mse/n
    return mse
```

Listing 1: Mean Squared Error Calculation

(b)

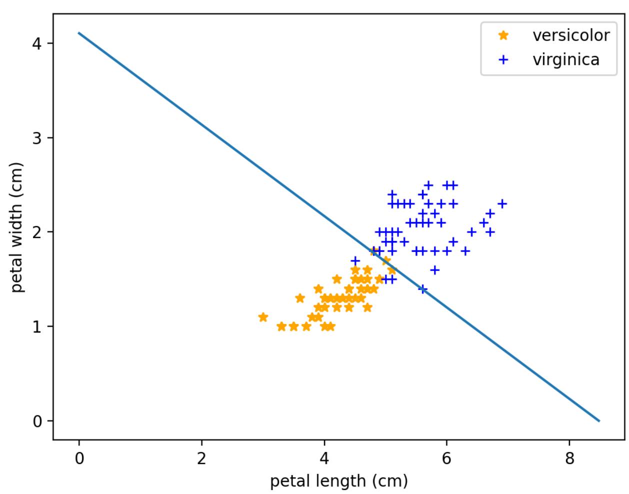
To plot the linear boundary, we find the x-intercept and y-intercept by using the following code:

```
plot([0,-w0/w1],[-w0/w2,0])
```

Listing 2: Plot Mean Squared Error

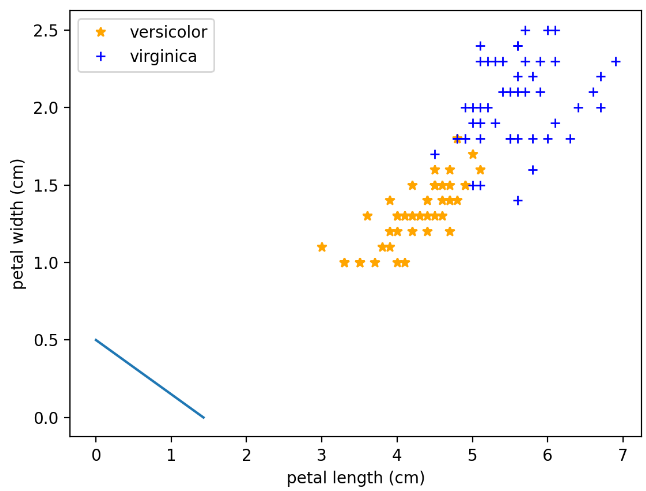
2.b.1

The first set of weights we've chosen is $[-3.9, 0.46, 0.95]$. The mean squared error we concluded is 0.13235245817007218. The following figure shows the linear boundary with our chosen set of weights. As we can tell from the graph, the linear boundary generally seperates the two categories of iris.



2.b.2

The second set of weights we've chosen is $[-1, 0.7, 2]$. The mean squared error we concluded is 0.48802189762271864. The following figure shows the linear boundary with our chosen set of weights. As we can tell from the graph, the linear boundary does not seperate these two categories at all.



(c)

To compute the gradient of the objective function, we need to take the derivative of the objective function. Assume $\mathbf{x}_i$ is the ith row with attribute petal length and petal width such that $x_i = [1, x_{i1}, x_{i2}]$(1 is placed here because w_0 requires 1 to be its coefficient). $\mathbf{w}$ is the set of weights for the attributes. The logistic function we get is:

$$\sigma(z) = \frac{1}{1+e^{-z}} = \frac{1}{1+e^{w \cdot x}}$$

Therefore, the mean squared function becomes:

$$MSE = \frac{1}{N} \sum_{i=1}^{n} (\sigma(w \cdot x_i) - y_i)^2$$

By taking the derivative of this objective function with respect to w_0, we have:

$$\frac{\partial MSE}{\partial w_0} = \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)\frac{\partial \sigma}{\partial w_0}$$
$$\frac{\partial MSE}{\partial w_0} = \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))\frac{\partial (w \cdot x)}{\partial w_0}$$
$$\frac{\partial MSE}{\partial w_0} = \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))$$

Similarly, by only changing the last derivative $\frac{\partial (w \cdot x)}{\partial w_0}$ to $\frac{\partial (w \cdot x)}{\partial w_1}$ and $\frac{\partial (w \cdot x)}{\partial w_2}$, we can compute the derivative of the objective function with respect to w_1 and w_2:

$$\frac{\partial MSE}{\partial w_1} = \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i1}$$
$$\frac{\partial MSE}{\partial w_2} = \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i2}$$

Therefore, the gradient of MSE is:

$$\nabla MSE = \begin{bmatrix} \frac{\partial MSE}{\partial w_0} \\ \\ \frac{\partial MSE}{\partial w_1} \\ \\ \frac{\partial MSE}{\partial w_2} \end{bmatrix} = \begin{bmatrix} \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i)) \\ \\ \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i1} \\ \\ \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i2} \end{bmatrix}$$

(d)

scalar form:

The scalar form of the gradient is computed in Problem 2 (c):

$$\nabla MSE = \begin{bmatrix} \frac{\partial MSE}{\partial w_0} \\ \\ \frac{\partial MSE}{\partial w_1} \\ \\ \frac{\partial MSE}{\partial w_2} \end{bmatrix} = \begin{bmatrix} \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i)) \\ \\ \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i1} \\ \\ \frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))x_{i2} \end{bmatrix}$$

vector form:

Let $X = \begin{bmatrix} x_{11}, x_{12}, 1 \\ \dots \\ x_{n1}, x_{n2}, 1 \end{bmatrix}$, which is a matrix represents the attributes(1 corresponds for bias). Since the term $\frac{2}{N}\sum_{i=1}^{N}(\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))$ is independent of the dimension j and common for $\frac{\partial MSE}{\partial w_0}$, $\frac{\partial MSE}{\partial w_1}$, and $\frac{\partial MSE}{\partial w_2}$, we can first express this term as $z_i = (\sigma(w \cdot x_i) - y_i)(1 - \sigma(w \cdot x_i))(\sigma(w \cdot x_i))$. The gradient of MSE becomes:

$$\nabla MSE = \frac{2}{m}\begin{bmatrix}\sum_{i=1}^{N} z_i \\ \sum_{i=1}^{N} z_i x_{i1} \\ \sum_{i=1}^{N} z_i x_{i2}\end{bmatrix} = \frac{2}{m}\begin{bmatrix}1, \dots, 1 \\ x_{11}, \dots, x_{n1} \\ x_{12}, \dots, x_{n2}\end{bmatrix}\begin{bmatrix}z_1 \\ \dots \\ z_n\end{bmatrix} = \frac{2}{m}\mathbf{X^T}\begin{bmatrix}z_1 \\ \dots \\ z_n\end{bmatrix}$$

Then, we attempt to expand the vector $z_i = \begin{bmatrix}z_1 \\ \dots \\ z_n\end{bmatrix}$:

$$z_i = \begin{bmatrix}(\sigma(\mathbf{w}\cdot\mathbf{x_1}) - y_1)(1-\sigma(\mathbf{w}\cdot\mathbf{x_1}))(\sigma(\mathbf{w}\cdot\mathbf{x_1})) \\ \dots \\ (\sigma(\mathbf{w}\cdot\mathbf{x_n}) - y_n)(1-\sigma(\mathbf{w}\cdot\mathbf{x_n}))(\sigma(\mathbf{w}\cdot\mathbf{x_n}))\end{bmatrix} =$$
$$\begin{bmatrix}\sigma(\mathbf{w}\cdot\mathbf{x_1}) - y_1 \\ \dots \\ \sigma(\mathbf{w}\cdot\mathbf{x_n}) - y_n\end{bmatrix} \star \begin{bmatrix}1-\sigma(\mathbf{w}\cdot\mathbf{x_1}) \\ \dots \\ 1-\sigma(\mathbf{w}\cdot\mathbf{x_n})\end{bmatrix} \star \begin{bmatrix}\sigma(\mathbf{w}\cdot\mathbf{x_1}) \\ \dots \\ \sigma(\mathbf{w}\cdot\mathbf{x_n})\end{bmatrix}$$

The $\star$ operation is defined as multiplying the ith row's elements. To simplify the expression, let $\sigma(\mathbf{Xw}) = \begin{bmatrix}\sigma(\mathbf{w^T x_1}) \\ \dots \\ \sigma(\mathbf{w^T x_n})\end{bmatrix}$. Thus, z_i can be expressed as $z_i = (\sigma(\mathbf{Xw}) - \mathbf{y}) \star (1 - \sigma(\mathbf{Xw})) \star \sigma(\mathbf{Xw})$. The vector form of gradient can be expressed as:

$$\nabla MSE = \frac{2}{m}\mathbf{X^T}(\sigma(\mathbf{Xw}) - \mathbf{y}) \star (\mathbf{1} - \sigma(\mathbf{Xw})) \star \sigma(\mathbf{Xw})$$

(e)

The code we used to calculate the gradient is as following:

```
def summed_gradient(x, w0, w1, w2, y):
    sigmoid_list = []
    n = len(x)
    error_list = []
    coefficient_list = []
    x = x.values.tolist()
    y = y.tolist()
    for i in range(len(x)):
        sigmoid_list.append(one_layer_network(w0, w1, w2, x[i][0], x[i][1]))
        error_list.append(sigmoid_list[i] - y[i])
        coefficient_list.append(error_list[i] * sigmoid_list[i] * (1 - sigmoid_list[i]))
```

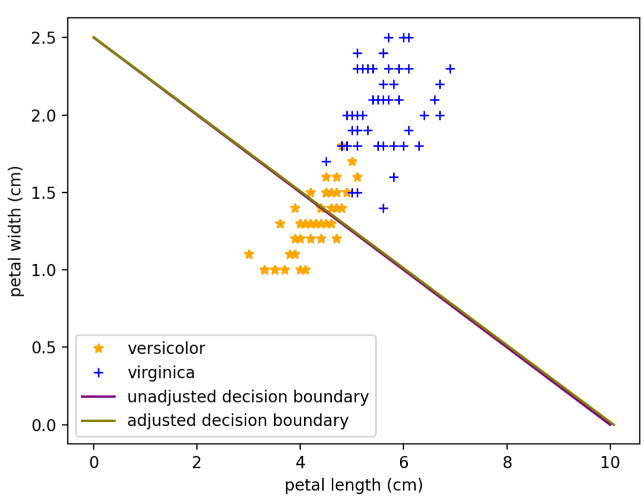
```python
    # number of rows = number of rows in data vectors, number of columns = number of columns in data vector + 1 since 1 for bias coefficient
    temp_matrix = np.ones((len(x), len(x[0]) + 1))
    temp_matrix[:, 1:] = x
    sum_term = np.zeros((len(x), len(x[0]) + 1))
    for i in range(len(coefficient_list)):
        sum_term[i] = (2/n) * temp_matrix[i] * coefficient_list[i]
    return np.sum(sum_term, axis = 0)
```

Listing 3: Calculate Gradient

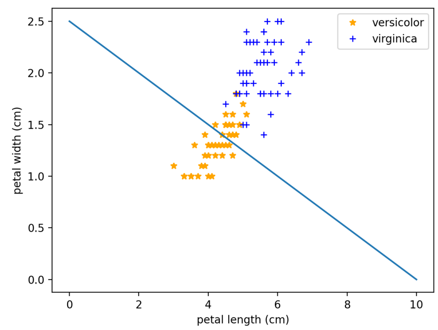
Let step size = 0.01. With the input weight $[w0, w1, w2] = [-5, 0.5, 2]$, we concluded the following table for the illustration of how the decision boundary changes for a small step:

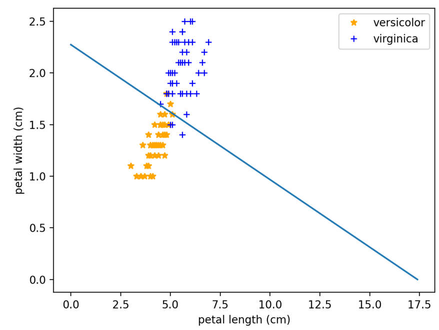
	old data	adjusted data
weights	[-5, 0.5, 2]	[-5.00080742 0.49665344 1.9989812]
MSE	0.48802189762271864	0.4879972995169846
decision boundary	m = -0.35, b = 0.5	m = -0.3497940478, b = 0.500093299

As we can tell from the table, the mean squared error reduced a little bit as we made a small step. To visualize the change of decision boundary, please refer to the following graph:



Since the small step is kind of hard to tell, we run this process for 10000 times in order to enlarge the difference. The following two graphs show the decision boundary before the adjustment and after the adjustment:





The code we used for this illustration is:

```
def illustrate_summed_gradient(x, w0, w1, w2, y):
    num_of_iter = []
    for i in range(10000):
        num_of_iter.append(i+1)
        temp1, temp2, temp3 = summed_gradient(x, w0, w1, w2,
  y)
        w0 = w0 - 0.01 * temp1
        w1 = w1 - 0.01 * temp2
        w2 = w2 - 0.01 * temp3
    plot([0,-w0/w1],[-w0/w2,0])
```

Listing 4: Illustration of the Change of Gradient

Problem 3:

(a)

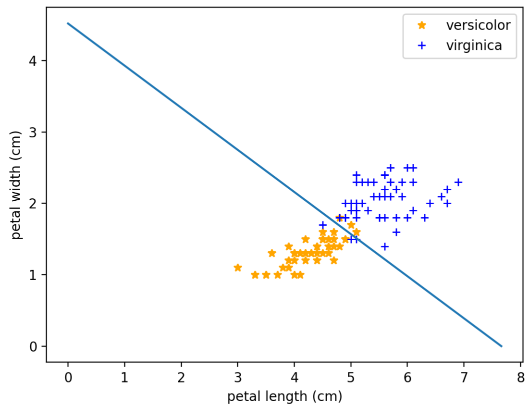
The code for gradient descent is as following:

```
def gradient_descent(a, b, x, w0, w1, w2, y):
    precision = 0.001 # mse we would like to reach
    max_iters = 20000 # max number of iterations
    iteration_counter = 0
    step_size = 0 # using armijo to update
    return_w = []
    current_w = [w0,w1,w2]
```

```
    current_mse = mean_square_error(x, w0, w1, w2, y)
    current_sum_g = summed_gradient(x, w0, w1, w2, y)
    improv_checker = 1 # check whether performed better
    # if current mse > the precision we defined and the number of iteration does not exceed the max iteration execute the gradient descent
    while mean_square_error(x, w0, w1, w2, y) > precision and iteration_counter < max_iters:
        if improv_checker > 0:
            return_w = current_w
        iteration_counter += 1
        temp0, temp1, temp2 = summed_gradient(x, w0, w1, w2, y)
        step_size = armijo_updating(a, b, x, y, w0, w1, w2)
        w0 = w0 -  step_size * temp0
        w1 = w1 -  step_size * temp1
        w2 = w2 - step_size * temp2
        current_w = [w0,w1,w2]
        next_mse = mean_square_error(x, w0, w1, w2, y)
        improv_checker = current_mse - next_mse
        current_mse = next_mse
        current_sum_g = summed_gradient(x, w0, w1, w2, y)
        print(w0, w1, w2, mean_square_error(x, w0, w1, w2, y))
        if improv_checker > 0:
            return_w = current_w
    plot([0,-w0/w1],[-w0/w2,0])
    print("MSE: ", mean_square_error(x, w0, w1, w2, y))
    return return_w
```

Listing 5: Gradient Descent

The basic idea is to specify a precision(in this case, mean squared error) and maximum number of iterations we would like to perform. We use the summed_gradient() function and the step size to update the weight in order to reduce the mse. The step size is a dynamic value obtained by using Armijo algorithm, which will be illustrated in section 3.d.
The following graph is a sample result using the gradient_descent() function on the example in section 2.b.2.:



(b)

(d)

The choice of gradient step size is important because if the step size is too large, the algorithm will not converge and jump around the minimum; if the step size is too small, the convergence will take place pretty slowly. Therefore, instead of using a constant step size, we decided to adjusted our step size while running the algorithm. To choose the step size, we used back-tracking inexact line search with Armijo rule(please refer to the article: Back-tracking with Armijo rule).

The basic idea is to start with a relatively large step size α_0 and subtract $\beta^k\alpha$ for $k = 1$ to n until a stopping condition(in this case, smaller than a predefined mse) is met. Choose the largest step size for α. The stopping step can be expressed as the following formula:

$$f(\mathbf{x} + \alpha\mathbf{d}) \leq f(\mathbf{x}) + \beta\alpha\nabla f(\mathbf{x})^T\mathbf{d}$$

, where f is the objective function, d is the descent direction, α and β are the parameters of Armijo algorithm. For the problem of iris dataset, we can rewrite the above function as following in order to update the step size:

$$f(\mathbf{w} - \alpha\nabla\mathbf{w}) \leq f(\mathbf{w}) - \beta\alpha\nabla f(\mathbf{x})^T f(\mathbf{x})$$

, where w is the weight. Since β is between 0 and 1, while the mean squared error converges to the minimum, the step size decreases.

The following code implements the Armijo algorithm:

```python
def armijo_updating(a, b, x, y, w0, w1, w2):
    step_size = a
    gradient = summed_gradient(x, w0, w1, w2, y)
    while mean_square_error(x, w0 - (step_size * gradient[0])
    , w1 - (step_size * gradient[1]), w2 - (step_size *
    gradient[2]), y) > mean_square_error(x, w0, w1, w2, y) -
    (0.5 * step_size * la.norm(gradient) ** 2):
        step_size = step_size * b
    return step_size
```

Listing 6: Armijo Updating Step Size

(e)