## Exercie 1: Linear Decision Boundaries

### Part A

Lets load and important the iris data set

```
iris_data <- read.csv("./irisdata.csv")
summary(iris_data)
```

```
##   sepal_length    sepal_width     petal_length    petal_width
##  Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100
##  1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300
##  Median :5.800   Median :3.000   Median :4.350   Median :1.300
##  Mean   :5.843   Mean   :3.054   Mean   :3.759   Mean   :1.199
##  3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
##  Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
##        species
##  setosa    :50
##  versicolor:50
##  virginica :50
##
##
##
```

```
# Lets look at the head of the iris data set
head(iris_data)
```

```
##   sepal_length sepal_width petal_length petal_width species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         0.2  setosa
## 5          5.0         3.6          1.4         0.2  setosa
## 6          5.4         3.9          1.7         0.4  setosa
```

```
# Number of rows of the iris dataset (number of individual observations)
nrow(iris_data)
```

```
## [1] 150
```

```
# All of the columns are numeric except for the species column
# They are continuous because they correspond to length and width (except for species) # The species ar
sapply(iris_data, class)
```

```
## sepal_length  sepal_width petal_length  petal_width      species
##    "numeric"    "numeric"    "numeric"    "numeric"     "factor"
```

```
# The only categorical variable is species in this iris dataset
sapply(iris_data, class)
```

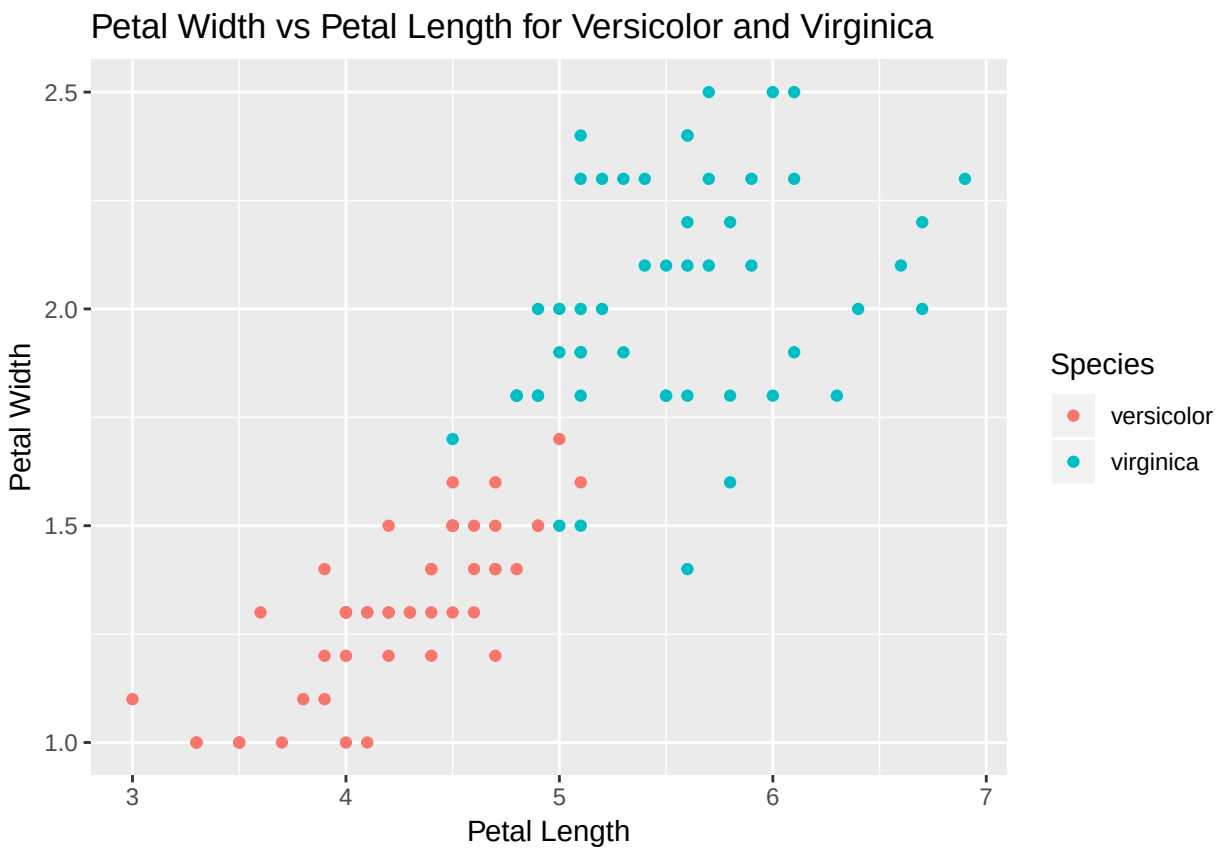
```
## sepal_length  sepal_width petal_length  petal_width      species
##    "numeric"    "numeric"    "numeric"    "numeric"     "factor"
```

From our observations it looks like there are 50 samples of three species: setosa, versicolor and virginica. Each of the samples has measurements of sepal length, sepal width and petal length.

Let's plot the second (versicolor) and third (virginica) iris classses:

```r
# Lets pick the 2nd and 3rd classes: versicolor and virginica and let's plot the subset
plot1 <- iris_data %>% filter(species %in% c('versicolor','virginica')) %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("Petal Width vs Petal Length for Versicolor and Virginica")

plot1
```




**Part B**

The following function will take in five inputs ($w_0$, $w_1$, $w_2$) which are constants that will be estimated later in this exercise and (x1, x2) which correspond to petal width and petal length. The output will return a value between a probability value between 0 and 1 where all values greater than or equal to 0.5 will correspond to the 3rd iris class (this class will be denoted by 1), and values below 0.5 to the 2nd iris class (this class will be denoted by 0).

```r
# inputs: c0, c1, c2, petal_width, petal_length
# outputs: value between 0 and 1 representing the probability

one_layer_neural_network <- function(w0, w1, w2, petal_length, petal_width) {

  # Linear function
  z <- w0 + w1*petal_length + w2*petal_width

  #result
  result <- 1/(1 + exp(-z))
```

```
  return (result)
}
```

### Part C

By playing around with the parameters, we select $w_0$ = -2.8, $w_1 = 0.25$ and $w_2 = 1$, which gives a decision boundary that separates the data decently (see below). The boundary that separates the data arises by noting the following:

Starting with the condition that a given iris flower is in class 1 (virginica):

$$\sigma(\mathbf{w}^T\mathbf{x}) \geq 0.5$$

where $\sigma$ is the logistic function, $\mathbf{w} = (w_0, w_1, w_2)$, and $\mathbf{x} = (1, x_1, x_2)$ ($x_1$ corresponds to petal length and $x_2$ corresponds to petal width). After a bit of manipulation, the above inequality implies the following:

$$\mathbf{w}^T\mathbf{x} \geq 0$$

Writing this out with our chosen values for the coefficients above gives us:

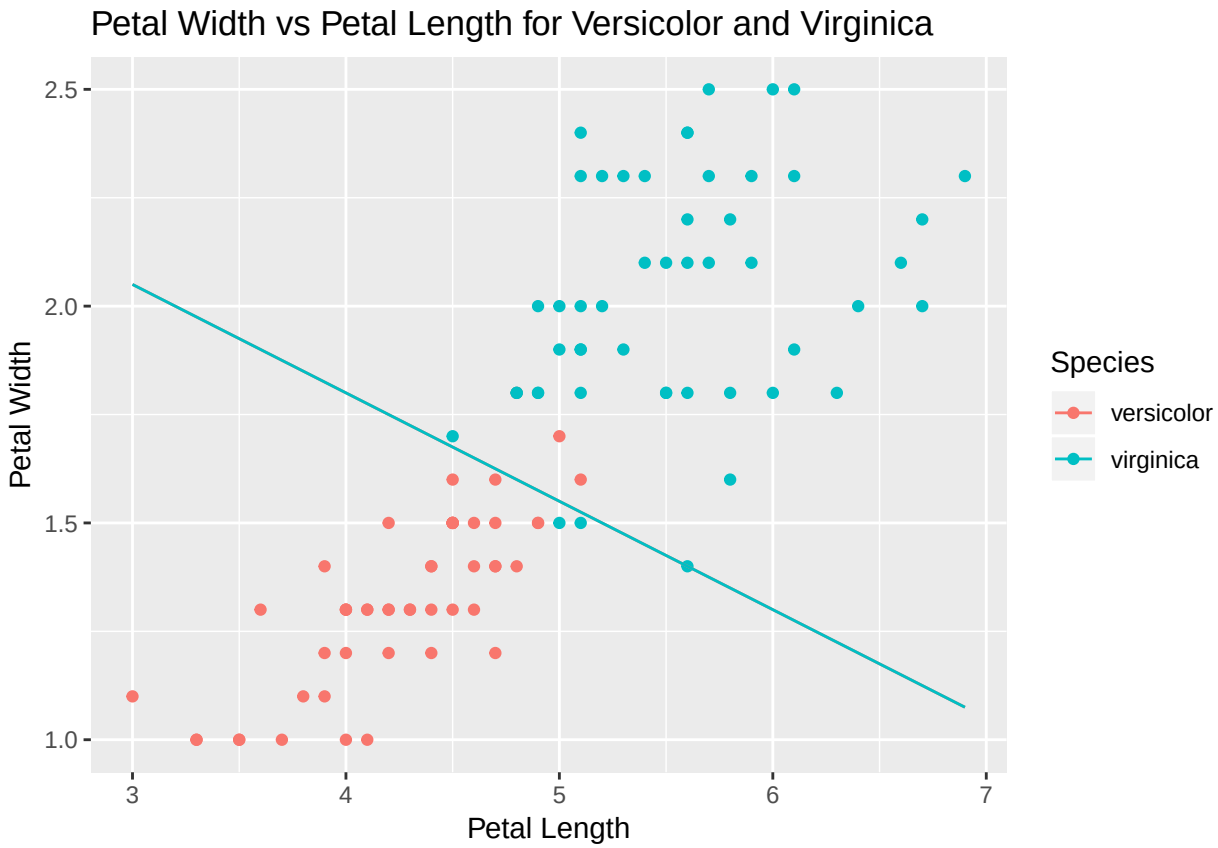
$$-2.8 + 0.25x_1 + x_2 \geq 0$$

Consequently, the decision boundary is given by the line $x_2 = 2.8 - 0.25x_1$ (above this line will be class 1 (virginica), and below this line will be class 0 (versicolor)). This result is plotted below:

```
z_function <- function(x) (2.8 + (-1/4)*x)

# Lets pick the 2nd and 3rd classes: versicolor and virginica and let's plot the subset
plot2 <- iris_data %>% filter(species %in% c('versicolor','virginica')) %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("Petal Width vs Petal Length for Versicolor and Virginica") + stat_function(fun = z_function)

plot2
```




**Part D**

```
# graph_data <- iris_data %>% filter(species %in% c('versicolor','virginica'))
#
# # We are going to use the plot 3D library to graph this
# x <- c(1,2,3,4,5,6,7,8,9,10)
# y <- c(1,2,3,4,5,6,7,8,9,10)
# z <- rep(0,10)
#
# for (i in 1:10)
# {
#   z[i]<-1/(1+exp(-(2.8 - 1/4*x[i] - y[i])))
# }
#
# p <- plot_ly(x = x, y = y, z = z) %>% add_surface()
# p
```

**Part E**

Now let's see how are function from Part B performs:

```
# Versicolor
data1 <- iris_data %>% filter (species == 'versicolor')

for (i in 1:50){
```

```
  if (one_layer_neural_network(-2.8, 0.25, 1, data1$petal_length[i], data1$petal_width[i]) < 0.5){
     resulting_flower <- "versicolor"

  } else {

    resulting_flower <- "virginica"
  }
  print(paste0("actual: versicolor, predicted: ", resulting_flower))
}
```

```
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
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## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
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## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: virginica"
## [1] "actual: versicolor, predicted: versicolor"
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## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: virginica"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
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## [1] "actual: versicolor, predicted: versicolor"
```

```
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
## [1] "actual: versicolor, predicted: versicolor"
```

```
# Virginica
data2 <- iris_data %>% filter (species == 'virginica')

for (j in 1:50){
  if (one_layer_neural_network(-2.8, 0.25, 1, data2$petal_length[j], data2$petal_width[j]) < 0.5){
     resulting_flower <- "versicolor"

  } else {
    resulting_flower <- "virginica"
  }
  print(paste0("actual: virginica, predicted: ", resulting_flower))
}
```

```
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
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## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: versicolor"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
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## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: versicolor"
```

```
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
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## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
## [1] "actual: virginica, predicted: virginica"
```

Results match to what we have seen in the graph above.

## Exercise 2: Neural Networks

### Part A

Mean squared error calculations. The inputs are in order: the data vectors (as the iris dataset that the petal length and petal width information is taken from), the parameters defining the neural network ($w_0$, $w_1$, $w_2$).

```
# Input feature vectors
X_data <- iris_data %>% filter(species %in% c("versicolor","virginica")) %>% select(petal_length, petal
# Pattern classes for each feature vector above
y_data <- iris_data %>%
  filter(species %in% c("versicolor","virginica")) %>%
  select(species) %>%
  mutate(label = ifelse(species == "versicolor", 0, 1)) %>%
  select(-species)

mean_squared_error <- function(X, y, w0, w1, w2) {

  # Outputs of neural network for each example
  NN_outputs <- rep(0,nrow(X))

  for (i in 1:nrow(X)){
    NN_outputs[i] = one_layer_neural_network(w0, w1, w2, X$petal_length[i], X$petal_width[i])
  }

  # Compute the differences between the NN outputs and the labels
  result = mean((NN_outputs - y$label)^2)

  # Return result
  return(result)
}
```

**Part B**

I have decided to look at three different values. First, I computed the mean square error of the original and got a mean square error of approximately 0.1489:

```
# Mean squared error for decision boundary we guessed above
paste0("Previous Mean Square Error: ", mean_squared_error(X_data, y_data, -2.8, 0.25, 1))
```

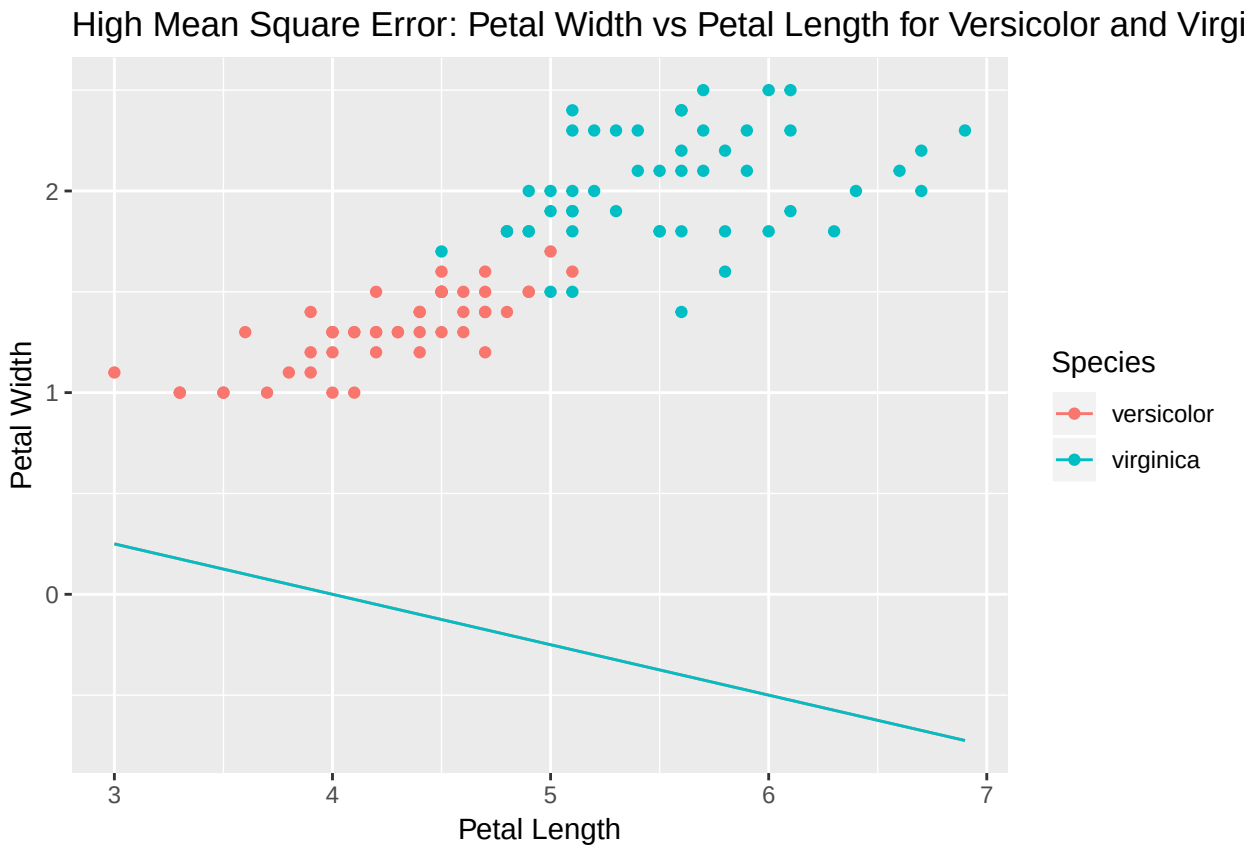
```
## [1] "Previous Mean Square Error: 0.148888121336409"
```

Then I made a completely incorrect estimate of the coefficients such that the boundary is not even touching any of the data points and got a much worse mean square error of 0.4401.

```
# High error
paste0("High Mean Square Error: ", mean_squared_error(X_data, y_data, 1, -0.25, -1))
```

```
## [1] "High Mean Square Error: 0.440092737113904"
```

```
z_function2 <- function(x) (1 - (0.25)*x)

plot3 <- iris_data %>% filter(species %in% c('versicolor','virginica')) %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("High Mean Square Error: Petal Width vs Petal Length for Versicolor and Virginica") +
  stat_function(fun = z_function2)

plot3
```

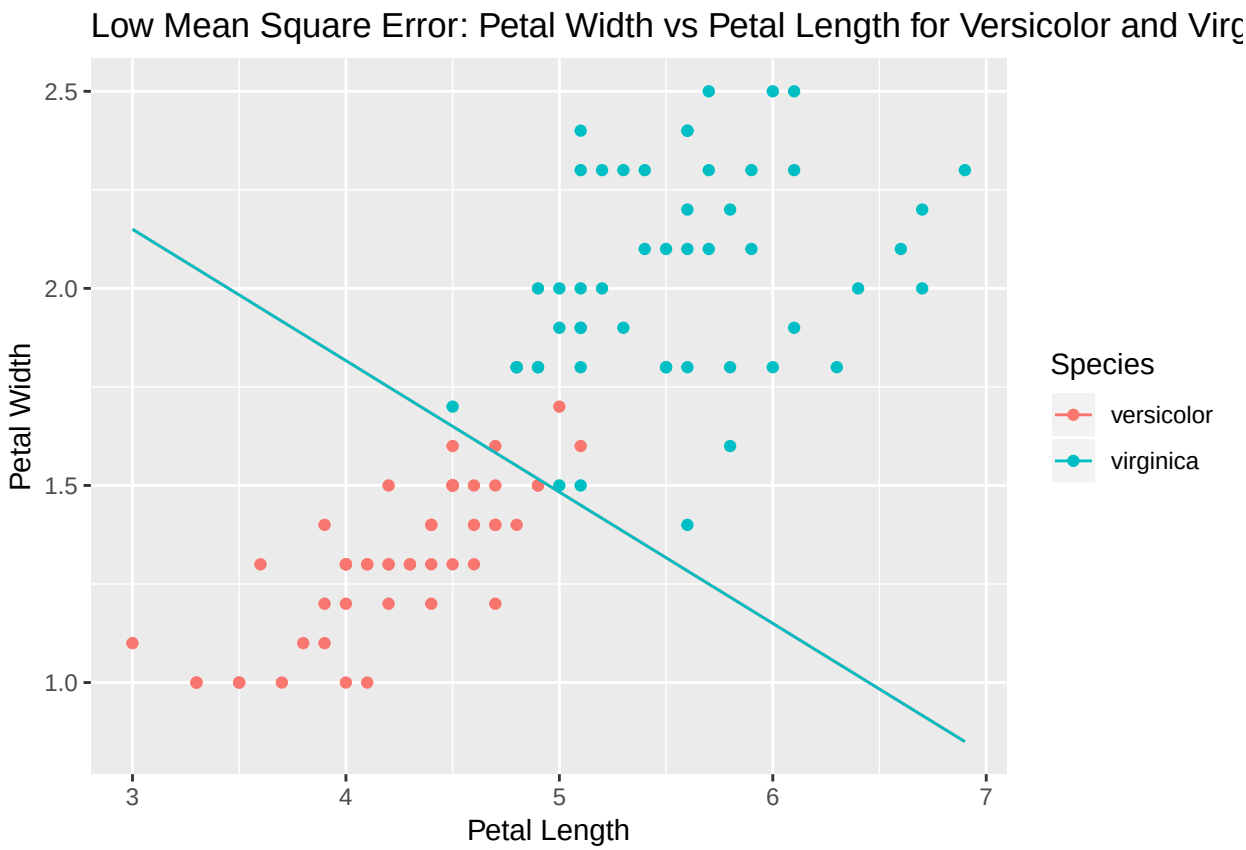



Finally, I found a slighly better boundary line that made only three points dislocated and decreased the mean square error slightly to 0.1423.

```r
# Low error
paste0("Low Mean Square Error: ", mean_squared_error(X_data, y_data, -3.15, 1/3, 1))
```

```
## [1] "Low Mean Square Error: 0.142297154674927"
```

```r
z_function3 <- function(x) (3.15 + (-1/3)*x)

plot4 <- iris_data %>% filter(species == 'versicolor' | species == 'virginica') %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("Low Mean Square Error: Petal Width vs Petal Length for Versicolor and Virginica") +
  stat_function(fun = z_function3)

plot4
```




**Part C**

Before we begin with the derivation, we will set up some notation for convenience. We will denote the number of examples in our data as $m$, which is this case is 100. Our data will be collected in the following matrix:

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} \\ \vdots & \vdots & \vdots \\ 1 & x_{m1} & x_{m2} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_m^T \end{bmatrix}$$

where $\mathbf{x}_1^T = \begin{bmatrix} 1 & x_{i1} & x_{i2} \end{bmatrix}$ is a single example with petal length $x_{i1}$ and petal width $x_{i2}$. We will also collect all the corresponding species/classes of these examples in a single vector $\mathbf{y}$ below:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

where $y_i$ is value (0 or 1) corresponding to the respective species of example $i$. We will also write the coefficients in a single vector $\mathbf{w}^T = \begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix}$. Also, once again, the logistic function is given by $\sigma(z) = (1 + \exp(-z))^{-1}$. With this notation set up, we write the mean squared error (MSE) as a function of the parameter vector as follows:

$$MSE(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} [\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i]^2$$

Noting that the derivative of the logistic function is $\sigma'(z) = \sigma(z)(1 - \sigma(z))$, we can compute the partial derivatives of the MSE with respect to each parameter ($w_0$, $w_1$, $w_2$) as follows:

$$\frac{\partial MSE}{\partial w_0} = \frac{2}{m} \sum_{i=1}^{m} [\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i] \frac{\partial \sigma(\mathbf{w}^T \mathbf{x}_i)}{\partial w_0} = \frac{2}{m} \sum_{i=1}^{m} [\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i][\sigma(\mathbf{w}^T \mathbf{x}_i)][1 - \sigma(\mathbf{w}^T \mathbf{x}_i)]$$

Similarly, we can write out the partials with respect to the other two parameters:

$$\frac{\partial MSE}{\partial w_1} = \frac{2}{m} \sum_{i=1}^{m} [\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i][\sigma(\mathbf{w}^T \mathbf{x}_i)][1 - \sigma(\mathbf{w}^T \mathbf{x}_i)] x_{i1}$$

$$\frac{\partial MSE}{\partial w_2} = \frac{2}{m} \sum_{i=1}^{m} [\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i][\sigma(\mathbf{w}^T \mathbf{x}_i)][1 - \sigma(\mathbf{w}^T \mathbf{x}_i)] x_{i2}$$

The $x_{i1}$ and $x_{i2}$ arises in the two results above because, for example, $\frac{\partial (\mathbf{w}^T \mathbf{x}_i)}{\partial w_1} = \frac{\partial}{\partial w_1}(w_0 + w_1 x_{i1} + w_2 x_{i2}) = x_{i1}$.

The combination of these three partial derivatives then gives the gradient of the MSE:

$$\nabla_{\mathbf{w}} MSE = \begin{bmatrix} \frac{\partial MSE}{\partial w_0} \\ \frac{\partial MSE}{\partial w_1} \\ \frac{\partial MSE}{\partial w_2} \end{bmatrix}$$

**Part D**

Now, having derived the scalar form of the result above, we will attempt to vectorize the result in a cleaner, convenient form.

$$\nabla_{\mathbf{w}} MSE = \frac{2}{m} X^T \left[ (\sigma(X\mathbf{w}) - \mathbf{y}) * \sigma(X\mathbf{w}) * (1 - \sigma(X\mathbf{w})) \right]$$

where $*$ indicates component-wise multiplication of vectors.

**Part E**

Let us write the code to computer the summed gradient for an ensemble of patterns. The algorithm goes as follows:

```
gradMSE <- function(X, y, w0, w1, w2) {
  dMSE_dw0 <- 0
  dMSE_dw1 <- 0
  dMSE_dw2 <- 0
  m = nrow(X)

  # Loop through all the examples in the input data
  for (i in 1:m){
    x_i1 = X$petal_length[i]
    x_i2 = X$petal_width[i]
    y_i = y$label[i]
    # Output of neural network for example i
    sigma = one_layer_neural_network(w0, w1, w2, x_i1, x_i2)

    # Append the contributions to the sums for each gradient component
    dMSE_dw0 <- dMSE_dw0 + (2/m)*(sigma - y_i)*(sigma)*(1 - sigma)*(1)
    dMSE_dw1 <- dMSE_dw1 + (2/m)*(sigma - y_i)*(sigma)*(1 - sigma)*(x_i1)
    dMSE_dw2 <- dMSE_dw2 + (2/m)*(sigma - y_i)*(sigma)*(1 - sigma)*(x_i2)
  }

  # Compile all components into a 3-dimensional vector
  gradient_result = c(dMSE_dw0, dMSE_dw1, dMSE_dw2)

  # Return result as a vector
  return(gradient_result)
}
```

In order to demonstrate how the gradient changes, we are going to run through the algorithm three times and and create three plots with the step size of 0.5.

```
# Initially constants are set to zero
W <- c(1, 1, 1)
print(W)
```

```
## [1] 1 1 1
```

```
print(paste("MSE Before Update:",mean_squared_error(X_data,y_data,W[1],W[2],W[3])))
```

```
## [1] "MSE Before Update: 0.498299605634765"
```

```
# We are going to iterate five times and print the respective plots
for (i in 1:10000){
  # Step size
  W <- W - (0.01)*gradMSE(X_data,y_data,W[1],W[2],W[3])
}

print(W)
```

```
## [1] -1.2396779 -0.3644774  1.9081652
```

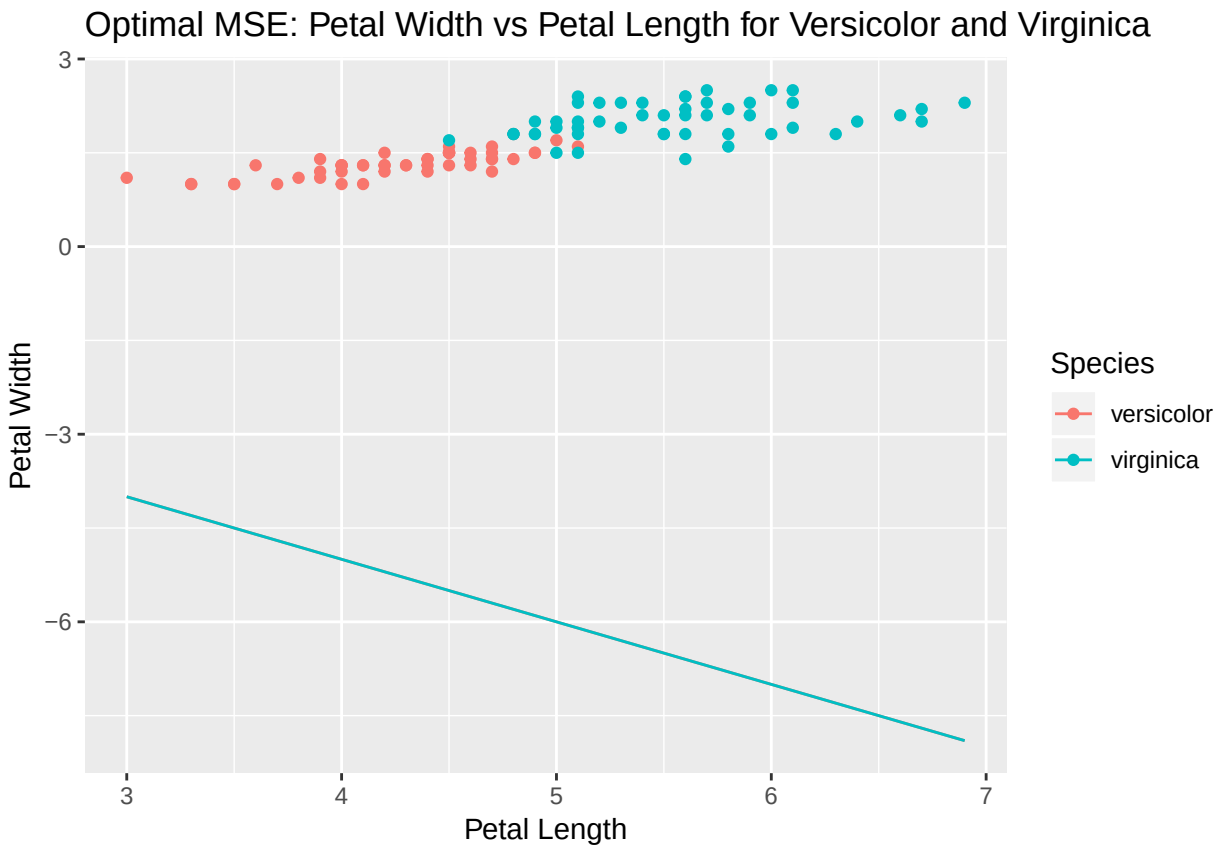
```
print(paste("MSE After Update:",mean_squared_error(X_data,y_data,W[1],W[2],W[3])))
```

```
## [1] "MSE After Update: 0.168168545747278"
```

The initial plot started with the value of the constants equal to w1 = 1, w2 = 1, w3 = 1.

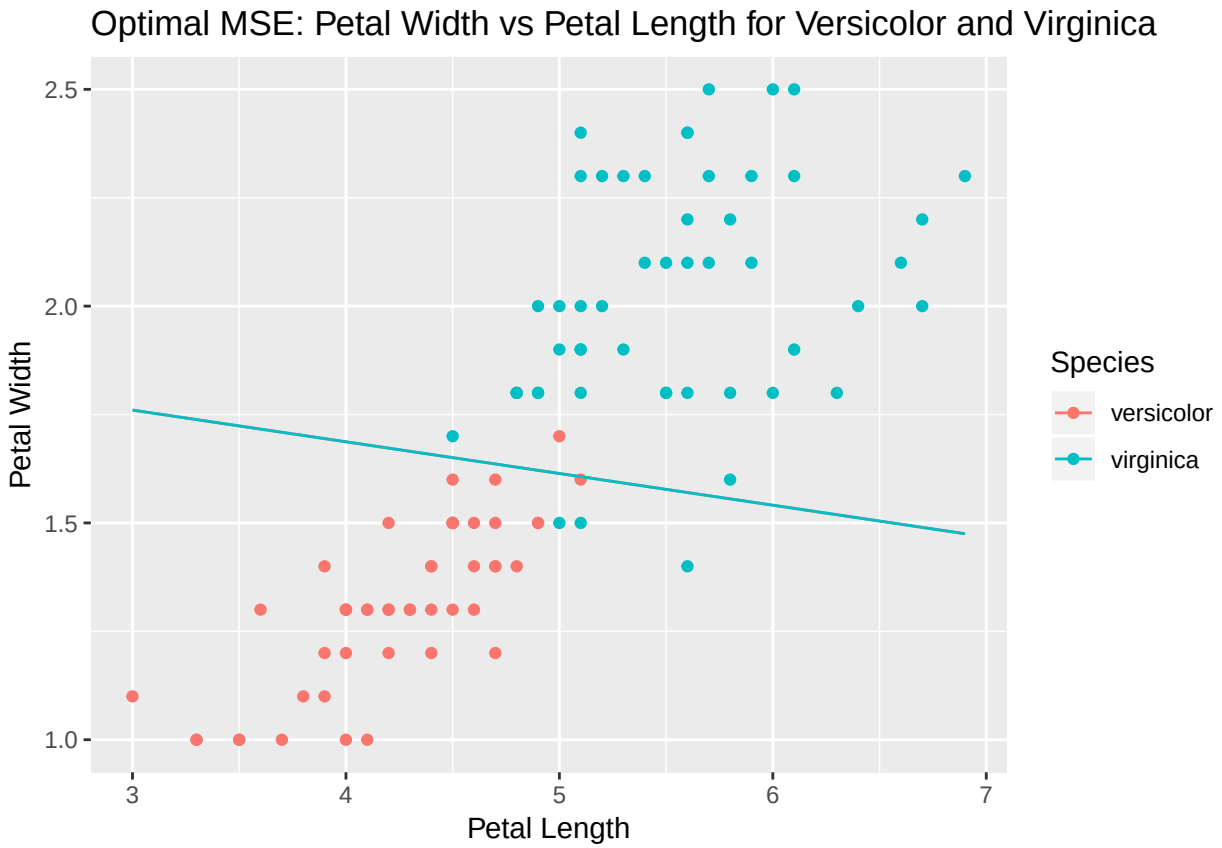
```
z_function4 <- function(x) ((-1) + (-1)*x)
```

```
plot5 <- iris_data %>% filter(species == 'versicolor' | species == 'virginica') %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("Optimal MSE: Petal Width vs Petal Length for Versicolor and Virginica") + stat_function(fun = z

plot5
```




After 10,000 iterations with the learning step size equal to 0.01 we get the following graph:

```
z_function5 <- function(x) ((4.3889725/2.2170461) + (-0.1621191/2.2170461)*x)

plot6 <- iris_data %>% filter(species == 'versicolor' | species == 'virginica') %>%
ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
ggtitle("Optimal MSE: Petal Width vs Petal Length for Versicolor and Virginica") + stat_function(fun = z

plot6
```




## Exercise 3: Learning a Decision Boundary Through Optimization

### Part A and Part B

Let us put everything together so we only have one method with the initial constants as an input as well as the gradient step size. We are also going to make both of our plotting functions inside our method directly.

```
optimizing <- function(w0, w1, w2, step_size, number_of_iterations) {

  W <- c(w0,w1,w2)

 mse <- c(0,number_of_iterations)
 iteration <- c(0, number_of_iterations)

  for (i in 1:number_of_iterations){
    mse[i] <- mean_squared_error(X_data, y_data, W[1], W[2], W[3])
    iteration[i] <- i
    W <- W - (step_size)*gradMSE(X_data,y_data,W[1],W[2],W[3])
  }

  # Make a new data frame to store results for the learning curve
  learning_curve_data <- cbind(mse, iteration)
  learning_curve_data <- as.data.frame(learning_curve_data)

  # Lets print the constants
  print(W)
```

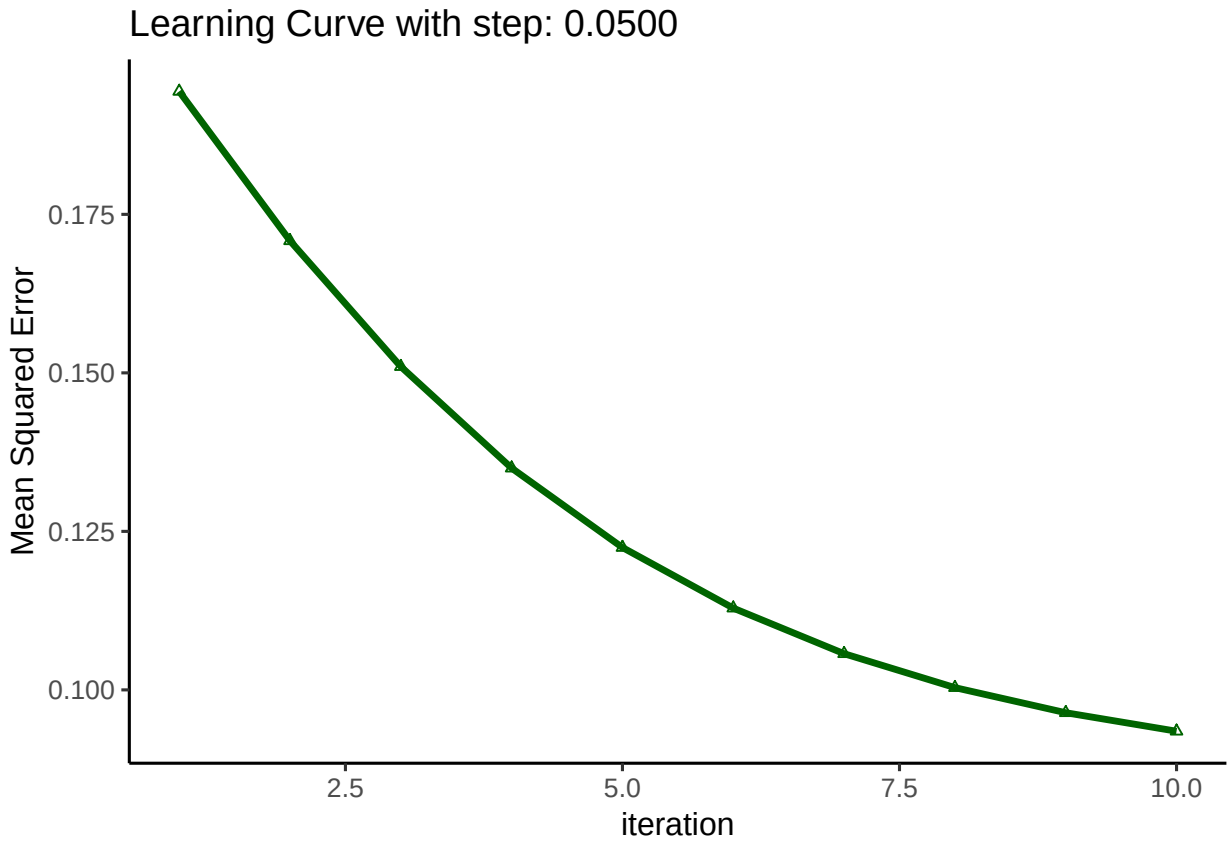
```
  # Lets print the MSE at this point as well
  print(paste("MSE: ",mean_squared_error(X_data,y_data,W[1],W[2],W[3])))

  optimizing_function <- function(x) ((-W[1]/W[3]) + (-W[2]/W[3])*x)

  # Current decision boundary location overlayed on the data
  optimizing_plot <- iris_data %>% filter(species == 'versicolor' | species == 'virginica') %>%
  ggplot(aes(x = petal_length, y = petal_width, color = species)) + geom_point() +
  labs(color = "Species") + xlab("Petal Length") + ylab("Petal Width") +
  ggtitle("Optimal MSE: Petal Width vs Petal Length for Versicolor and Virginica") +
     stat_function(fun = optimizing_function)

  optimizing_plot

  # Learning curve
  optimizing_curve <- ggplot(learning_curve_data, aes(x = iteration, y = mse)) +
  geom_point(size = 1.2, col = 'darkgreen', shape = 2) +
  geom_line(lwd = 1.2, col = 'darkgreen') + ylab('Mean Squared Error') +
  ggtitle(sprintf('Learning Curve with step: %0.4f', step_size)) +
  theme_classic(12)

  optimizing_curve
}
```

### Part C

We are going to test our function above with different (randomized) starting points.

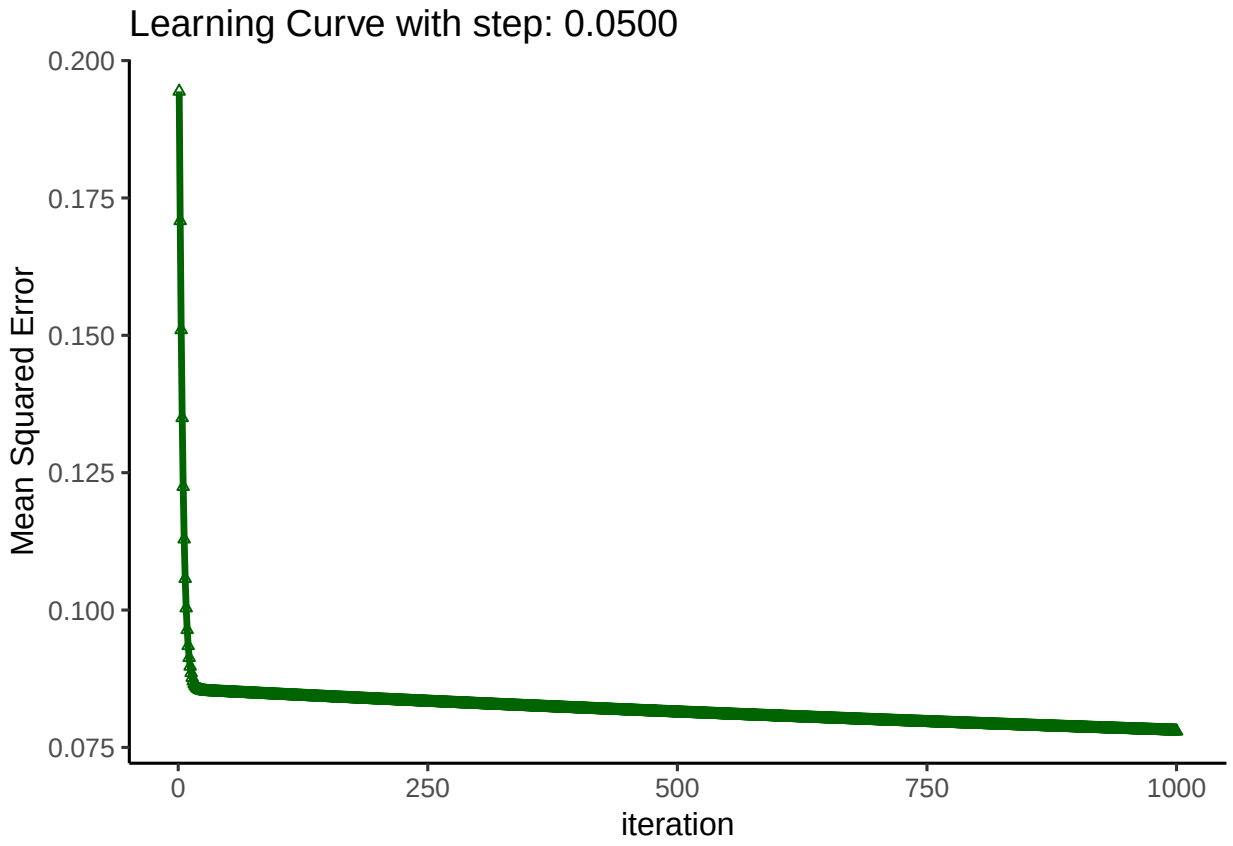
```
# Examples of function above
optimizing(-8,1,1, 0.05, 10)
```

```
## [1] -7.963988  1.202225  1.076713
## [1] "MSE:  0.0913312386594128"
```




```
optimizing(-8,1,1, 0.05, 1000)
```

```
## [1] -8.288184  1.164308  1.588009
## [1] "MSE:  0.0779416416297528"
```




**Part D**

The gradient step size was chosen by trial and error. If the gradient step size is too large, the algorithm will never converge and instead it will jump around the mimimum. If the gradient step size is too small, the algorithm will converge after a very long time. After experimenting with different types of learning rates, I decided on 0.005. This learning rate seemed to converge after a short time and at the same time did not get stuck on a local mimimum.

**Part E**

I have used two different checks for the stopping criteria. The first was based on a tolerance threshold for the minimum change in the gradients. If the gradients were not changing above a treshold set to 0.005 that the algorithm would stop. This stopping criterion is effective because the magnitude of the gradients is directly proportional to the error.

The second stopping measure was the number of iterations. When the gradient step is set too low it takes more iterations for the algoirthm to complete, than with a large gradient.