Department of Electronic & Telecommunication Engineering, University of Moratuwa, Sri Lanka.

Learning from data and related challenges and classification

Walgampaya H.K.B. - 220675T

EN3150 - Pattern Recognition

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Contents

The Jupyter Notebook is available on GitHub
https://github.com/HimethW/Learning-from-data-and-related-challenges.git

1 Linear Regression

1) A set of data points (x_i, y_i) are known to form a line. The ordinary least squares(OLS) is performed on this dataset. The OLS minimizes a loss function which is defined as $\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$ with y_i and $\hat{y}_i$ are true and OLS outputs, respectively. The fitted OLS line and data points are shown in Figure 1. It is observed that the OLS fitted line is not aligned to majority of data points. What is the reason behind this?

The poor fitting of the OLS line with the data points is due to the presence of several outliers.
Reason:

- The loss function that is used in the OLS algorithm which is $\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$, is really sensitive towards outliers. This is because it takes the residual error between the predicted and true values(error) and squares it. as we can see, in the dataset there are several outliers and the error introduced from them is large. by squaring it, the impact of those outliers becomes even larger.
- So in order to minimize the loss, the OLS line is pulled towards the outliers as shown in the figure. This results in the OLS line not fitting with the majority of data points.

2) To reduce the impact of outliers, a modified loss function is introduced. It is given as $L = \frac{1}{N}\sum_{i=1}^{N} a_i\,(y_i - \hat{y}_i)^2$ There are two schemes proposed for setting a_i:

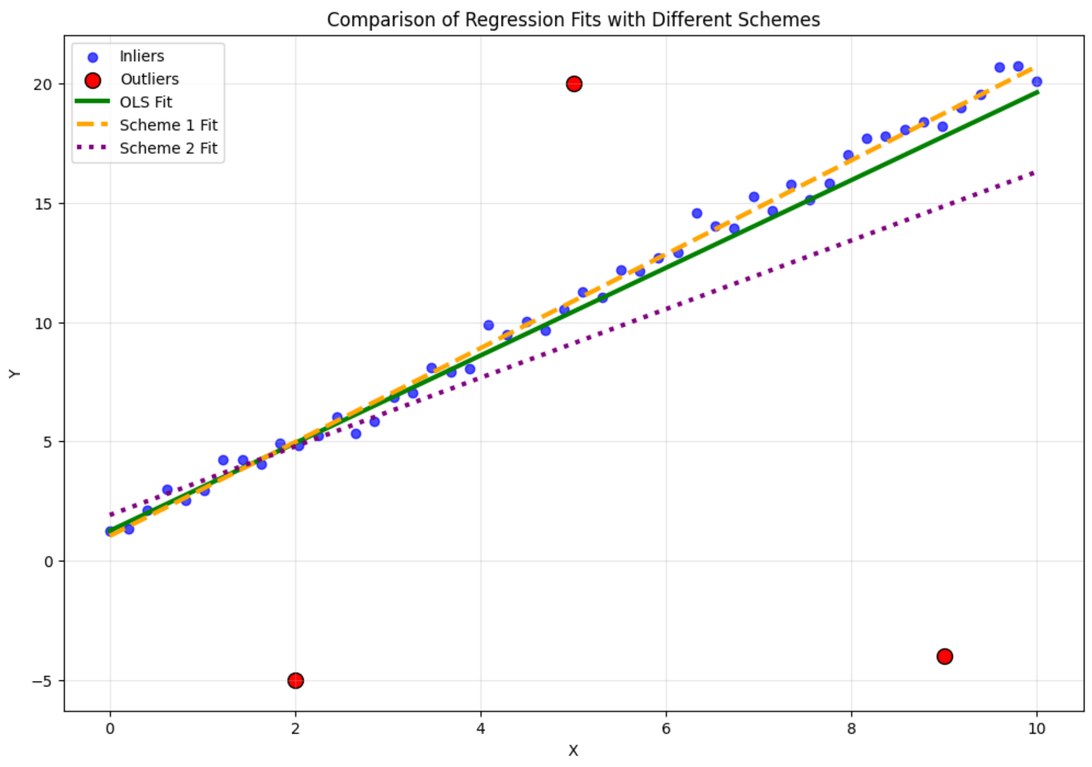
- **Scheme 1: For outliers $a_i = 0.01$ and for inliers $a_i = 1$,**
- **Scheme 2: For outliers $a_i = 5$ and for inliers $a_i = 1$.**

Under which scheme do you expect a better fitted line for inliers than the OLS fitted line in Figure 1. Justify your answer.

Let's consider a random dataset with several outliers and plot the OLS line using both schemes as well as with the original OLS algorithm

```python
np.random.seed(42)
n_inliers = 50
x_inliers = np.linspace(0, 10, n_inliers)

# y = 2*x + 1 + noise
y_inliers = 2 * x_inliers + 1 + np.random.normal(0, 0.5, n_inliers)

#Generate a few outliers
n_outliers = 3
x_outliers = np.array([2, 5, 9])
y_outliers = np.array([-5, 20, -4])

```

```python
#Combine into the full dataset. Last 3 elements are the outliers
X = np.concatenate([x_inliers, x_outliers]).reshape(-1, 1)
y = np.concatenate([y_inliers, y_outliers])

#Create the sample weights array for each scheme
# First 50 points are inliers (weight=1), last 3 are outliers
weights_scheme1 = np.ones(len(X))
weights_scheme1[-n_outliers:] = 0.01  # Downweight outliers

weights_scheme2 = np.ones(len(X))
weights_scheme2[-n_outliers:] = 5      # Overweight outliers

#Fit the models
#Standard OLS
model_ols = LinearRegression()
model_ols.fit(X, y)

#Scheme 1
model_scheme1 = LinearRegression()
model_scheme1.fit(X, y, sample_weight=weights_scheme1)

#Scheme 2
model_scheme2 = LinearRegression()
model_scheme2.fit(X, y, sample_weight=weights_scheme2)

#create x axis for plotting the models
x_plot = np.linspace(0, 10, 100).reshape(-1, 1)
y_plot_ols = model_ols.predict(x_plot)
y_plot_scheme1 = model_scheme1.predict(x_plot)
y_plot_scheme2 = model_scheme2.predict(x_plot)
```



A better fitted line for in-liners can be expected by using **Scheme 1:**
(For outliers $a_i = 0.01$ and for inliers $a_i = 1$)
Reason:

- The a_i value is used to determine how much weight we give to the error of the i^{th} data point.
- In scheme 1, by giving teh outliers a weight of 0.01, we are down-weighting there contribution by a factor of 100. This way we are able to neglect the large penalty they introduce. As for the inliers we are keeping the weight at 1, which is the normal value used in the original OLS algorithm so the inliner error contribution is not affected. This way we can get a better fit for the inliners. This can also be seen by the yellow dashed line in the above figure.
- In scheme 2, we overweight the outliers by giving them a larger weight than the inliers ($a_i = 5$). The outliers already give a large error term and by over weighting them, the outlier contribution increase even further. The model will now try more to fit the outliers than before, leading to the OLS line being more skewed towards the outliers. This can also be seen in the above figure using the purple dotted line.
- We can conclude that a better fit for the inliers can be expected by using **scheme 1**.

3) In brain image analysis (eg: fMRI), the brain is divided into multiple regions as show in Figure 2, each consisting of many voxels (pixels). A researcher wants to identify which brain regions are most predictive of a specific cognitive task. Why linear regression is not suitable algorithm for the above task?

- In this dataset, the number of features, which is the number of voxels can be very large (several hundreds of thousands). However, the number of observation that we can get will be very much lower than the number of features. So there can be many weight vectors that can be used to fit the regression line to our dataset, making it less generalized and unstable. This will lead to the model not working properly with new data.
- If linear regression is used, it will give a weight for each individual voxel. The resulting weight vector will be at the voxel level, making it hard to identify which region is most predictive (For example, some voxels in region 'A' will get a higher weight while some from the same region will get a lower weight). The goal is not to identify each voxel but to find out the region. Linear egression does not give a clear answer at the region level.

5) Which method (LASSO or group LASSO) is more appropriate in this setting, and why?

Method A: Standard LASSO

$$\min_w \left(\frac{1}{N} \sum_{i=1}^{N} (y_i - w^\top x_i)^2 \ + \ \lambda \|w\|_1 \right)$$

Method B: Group LASSO

$$\min_{w} \left(\frac{1}{N} \sum_{i=1}^{N} (y_i - w^\top x_i)^2 \; + \; \lambda \sum_{g=1}^{G} \|w_g\|_2 \right)$$

The best method is **Group Lasso**

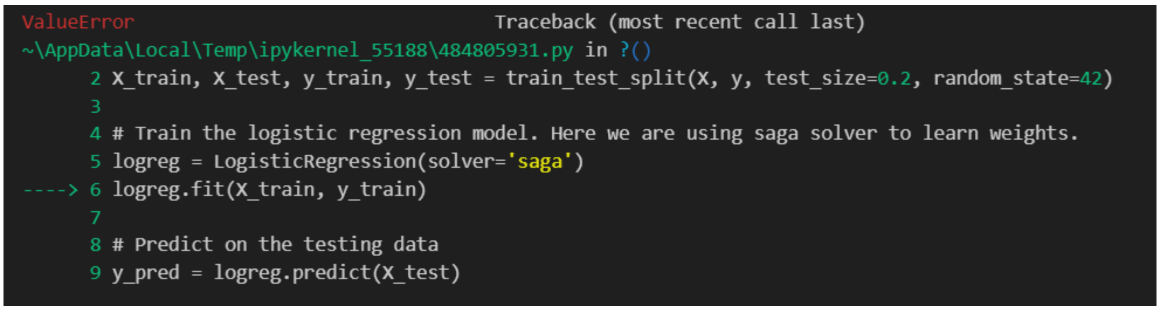
Reason:

- The Standard Lasso method adds a penalty term that is used to reduce large weights making the model more simple. This is done by the Lasso method taking the less important features and forcing their weight to be zero. The result is a sparse weight vector. However, this method removes features independently without caring about the regions. for example, some voxels from region 'A' might be kept as important while some voxels from the same region might be deemed unimportant.
- Group Lasso also has a penalty term but it is applied to entire groups rather than individual voxels. The L_2 norm $\|w_g\|_2$ measures the weight of the **w** vector for that entire group. So, as a result, it either keeps all the features in a particular group or deletes all the features in a group, instead of treating the voxels individually. If a region is predictive, all the voxels in that region is kept, providing a clear answer on which brain regions are most predictive.
- In conclusion we can say that Group Lasso is most suitable for the task.

2 Logistic regression

2) Now, use the code given in listing 2 to train a logistic regression model. Here, did you encounter any errors? If yes, what were they, and how would you go about resolving them ?

During training, the following error was encountered.
`ValueError: could not convert string to float: 'Adelie'`



```
ValueError                                Traceback (most recent call last)
~\AppData\Local\Temp\ipykernel_55188\484805931.py in ?()
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

      # Train the logistic regression model. Here we are using saga solver to learn weights.
      logreg = LogisticRegression(solver='saga')
----> logreg.fit(X_train, y_train)

      # Predict on the testing data
      y_pred = logreg.predict(X_test)
```

Figure 1: Encountered Error

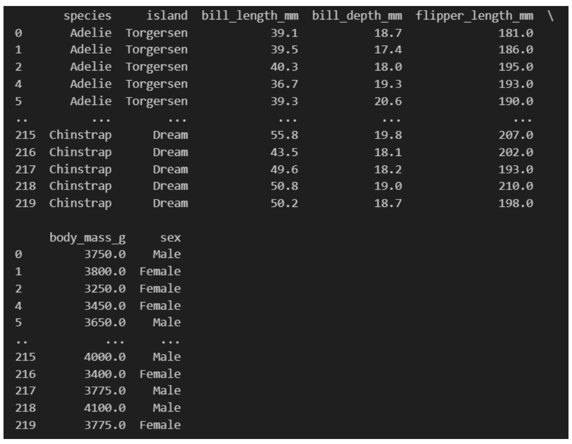
Reason:
The feature matrix X is taken after dropping the "class encoded" column from df_filterd. X still contains categorical columns such as Species, Island and Sex. However, the logistic

regression model in scikit-learn can only handle data with a numerical value so these features will result in a `ValueError` as shown above.

Solution:

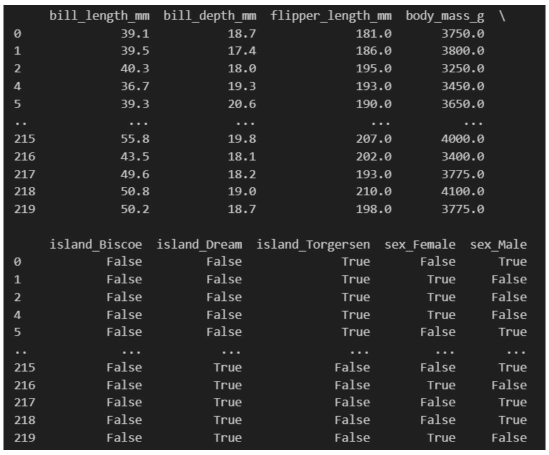
```python
#drop species column
X = X.drop(['species'], axis=1)

#encode the categorical colums using One-Hot encoding
X = pd.get_dummies(X, columns=['island', 'sex'])

# Split the data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
    random_state=42)

# Train the logistic regression model. Here we are using saga solver to
    learn weights.
logreg = LogisticRegression(solver='saga')
logreg.fit(X_train, y_train)

# Predict on the testing data
y_pred = logreg.predict(X_test)

# Evaluate the model
accuracy = accuracy_score(y_test, y_pred)
print("Accuracy:", accuracy)
print(logreg.coef_, logreg.intercept_)
```

- To get rid of the error, we need to encode the categorical columns.
- First remove the species colums as that is our target and not a feature.
  `X = X . drop (['species'] , axis =1)`
- Then use One-Hot encoding to convert 'island' and 'sex' to numbers.
  `X = pd.get_dummies(X, columns=['island', 'sex'])`



```
       species     island  bill_length_mm  bill_depth_mm  flipper_length_mm  \
0       Adelie  Torgersen            39.1           18.7              181.0
1       Adelie  Torgersen            39.5           17.4              186.0
2       Adelie  Torgersen            40.3           18.0              195.0
4       Adelie  Torgersen            36.7           19.3              193.0
5       Adelie  Torgersen            39.3           20.6              190.0
..         ...        ...             ...            ...                ...
215  Chinstrap      Dream            55.8           19.8              207.0
216  Chinstrap      Dream            43.5           18.1              202.0
217  Chinstrap      Dream            49.6           18.2              193.0
218  Chinstrap      Dream            50.8           19.0              210.0
219  Chinstrap      Dream            50.2           18.7              198.0

     body_mass_g     sex
0         3750.0    Male
1         3800.0  Female
2         3250.0  Female
4         3450.0  Female
5         3650.0    Male
..           ...     ...
215       4000.0    Male
216       3400.0  Female
217       3775.0    Male
218       4100.0    Male
219       3775.0  Female
```

Figure 2: Before encoding



```
     bill_length_mm  bill_depth_mm  flipper_length_mm  body_mass_g  \
0              39.1           18.7              181.0       3750.0
1              39.5           17.4              186.0       3800.0
2              40.3           18.0              195.0       3250.0
4              36.7           19.3              193.0       3450.0
5              39.3           20.6              190.0       3650.0
..              ...            ...                ...          ...
215            55.8           19.8              207.0       4000.0
216            43.5           18.1              202.0       3400.0
217            49.6           18.2              193.0       3775.0
218            50.8           19.0              210.0       4100.0
219            50.2           18.7              198.0       3775.0

     island_Biscoe  island_Dream  island_Torgersen  sex_Female  sex_Male
0            False         False              True       False      True
1            False         False              True        True     False
2            False         False              True        True     False
4            False         False              True        True     False
5            False         False              True       False      True
..             ...           ...               ...         ...       ...
215          False          True             False       False      True
216          False          True             False        True     False
217          False          True             False       False      True
218          False          True             False       False      True
219          False          True             False        True     False
```

Figure 3: After encoding

Result ⇒ `Accuracy:  0.5813953488372093`

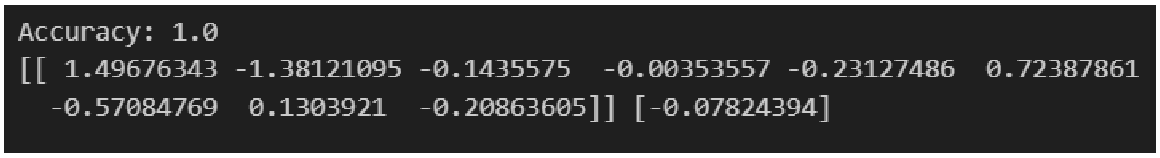
3) Why does the saga solver perform poorly?

- As mentioned above, the accuracy is about 0.581, which indicates poor performance. The main reason for this is that the "saga" solver is sensitive towards feature scaling.
- Our dataset has features that are on different scales. For example the mass is in thousands of grams while the bill length is around 40mm.
- The "saga" solver is based on stochastic gradient descent, so larger scales try to dominate the updating and learning process of the model. This will lead to poor performance and slow convergence.

4) Now change the solver to "liblinear" by using logreg = LogisticRegression(solver='liblinear'). What is the classification accuracy with this configuration?

Updated code:

```python
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
    random_state=42)
# Train the logistic regression model.
logreg = LogisticRegression(solver='liblinear')
logreg.fit(X_train, y_train)

# Predict on the testing data
y_pred = logreg.predict(X_test)

# Evaluate the model
accuracy = accuracy_score(y_test, y_pred)
print("Accuracy:", accuracy)
print(logreg.coef_, logreg.intercept_)
```



```
Accuracy: 1.0
[[ 1.49676343 -1.38121095 -0.1435575  -0.00353557 -0.23127486  0.72387861
  -0.57084769  0.1303921  -0.20863605]] [-0.07824394]
```

Figure 4: Accuracy when using liblinear solver

Result ⇒ `Accuracy: 1.0`

Solver	Accuracy
saga solver	0.5813953488372093
liblinear solver	1.0

5) Why does the "liblinear" solver perform better than "saga" solver?

- Our data is unscaled and the liblinear solver is better at handling unscaled data. This is because it internally used different optimization algorithms, making it more robust.
- Moreover, liblinear solver is optimized to handle small datasets (our dataset has only 9 features and 214 data items) making it more stable.

6) Explain why the model's accuracy (with saga solver) varies with different random state values ?

Random state value	Accuracy
10	0.6976744186046512
20	0.627906976744186
30	0.6744186046511628
42	0.5813953488372093
50	0.7674418604651163
60	0.6976744186046512
70	0.6744186046511628

Table 1: Accuracy comparison with different random state values

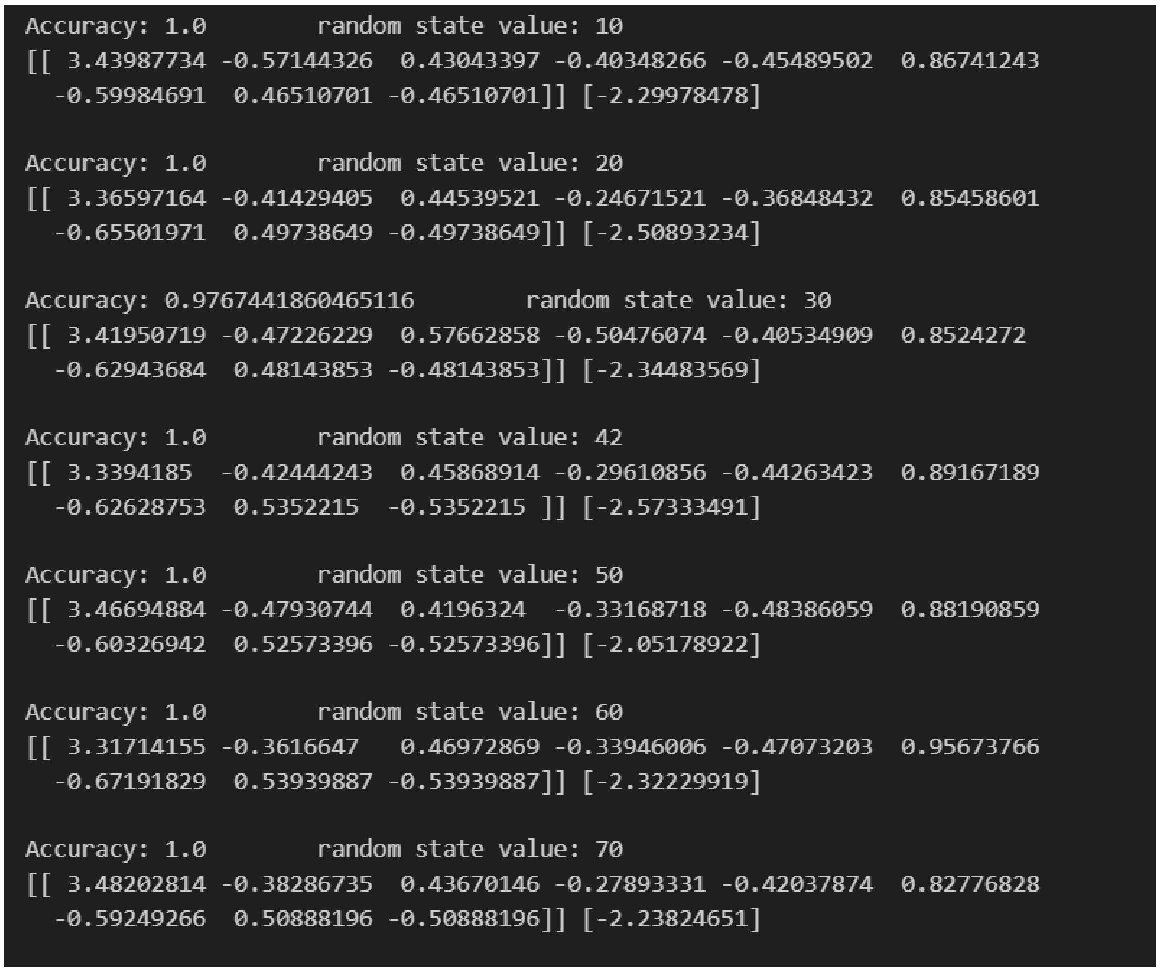
Reason:

- The saga solver uses the Stochastic gradient descent algorithm as mentioned above.
- So when the dataset is unscaled, the landscape where the gradient descent takes place becomes poorly shaped (very steep or narrow) and the starting point of the algorithm greatly affects the outcome. The random_state determines this starting point.
- Different random_states can cause the algorithm to converge to different local minima or even get stuck at some point, leading to different accuracy levels as shown in the above table

7) Compare the performance of the "liblinear" and "saga" solvers with feature scaling. If there is a significant difference in the accuracy with and without feature scaling, what is the reason for that. You may use Standard Scaler available in sklearn library.

- **saga solver with feature scaling**

```python
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()

random_state_vals = [10,20,30,42,50,60,70]
for rs in random_state_vals:
    # Split the data into training and testing sets
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size
    =0.2, random_state=rs)

    #scale the data
    X_train_scaled = scaler.fit_transform(X_train)
    X_test_scaled = scaler.transform(X_test)

    # Train the logistic regression model. Here we are using saga solver to learn weights.
    logreg = LogisticRegression(solver='saga')
    logreg.fit(X_train_scaled, y_train)

    # Predict on the testing data
    y_pred = logreg.predict(X_test_scaled)

    # Evaluate the model
    accuracy = accuracy_score(y_test, y_pred)
    print(f"Accuracy: {accuracy}        random state value: {rs}")
    print(logreg.coef_, logreg.intercept_)
    print()

```



```
Accuracy: 1.0        random state value: 10
[[ 3.43987734 -0.57144326  0.43043397 -0.40348266 -0.45489502  0.86741243
  -0.59984691  0.46510701 -0.46510701]] [-2.29978478]

Accuracy: 1.0        random state value: 20
[[ 3.36597164 -0.41429405  0.44539521 -0.24671521 -0.36848432  0.85458601
  -0.65501971  0.49738649 -0.49738649]] [-2.50893234]

Accuracy: 0.9767441860465116        random state value: 30
[[ 3.41950719 -0.47226229  0.57662858 -0.50476074 -0.40534909  0.8524272
  -0.62943684  0.48143853 -0.48143853]] [-2.34483569]

Accuracy: 1.0        random state value: 42
[[ 3.3394185  -0.42444243  0.45868914 -0.29610856 -0.44263423  0.89167189
  -0.62628753  0.5352215  -0.5352215 ]] [-2.57333491]

Accuracy: 1.0        random state value: 50
[[ 3.46694884 -0.47930744  0.4196324  -0.33168718 -0.48386059  0.88190859
  -0.60326942  0.52573396 -0.52573396]] [-2.05178922]

Accuracy: 1.0        random state value: 60
[[ 3.31714155 -0.3616647   0.46972869 -0.33946006 -0.47073203  0.95673766
  -0.67191829  0.53939887 -0.53939887]] [-2.32229919]

Accuracy: 1.0        random state value: 70
[[ 3.48202814 -0.38286735  0.43670146 -0.27893331 -0.42037874  0.82776828
  -0.59249266  0.50888196 -0.50888196]] [-2.23824651]
```

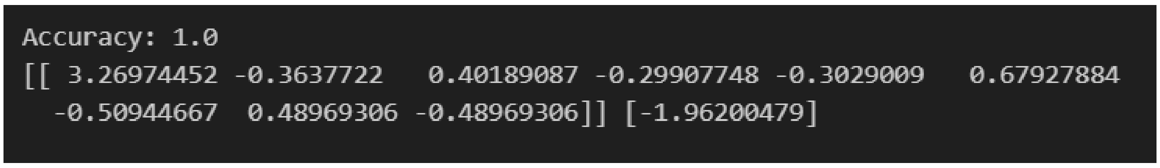
Figure 5: Accuracy of the saga solver after feature scaling

- As we can see the accuracy of the saga solver has improved significantly upto 1. Even after changing the random state, the accuracy did not decrease much(even when random_state = 30, the reduction in accuracy is insignificant) indicating that the model is stable. It has matched the accuracy of the liblinear solver.
- The reason for this is that after scaling, the dataset has a mean of 0 and a

standard deviation of 1. This gives a smooth landscape that is easier for the saga solver to perform stochastic gradient descent. It is no longer dominated by large scale features such as `body_mass` resulting in a optimal solution as shown above

- **liblinear solver with feature scaling**

```python
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size
    =0.2, random_state=42)

#scale the data
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

# Train the logistic regression model.
logreg = LogisticRegression(solver='liblinear')
logreg.fit(X_train_scaled, y_train)

# Predict on the testing data
y_pred = logreg.predict(X_test_scaled)

# Evaluate the model
accuracy = accuracy_score(y_test, y_pred)
print("Accuracy:", accuracy)
print(logreg.coef_, logreg.intercept_)

```



```
Accuracy: 1.0
[[ 3.26974452 -0.3637722   0.40189087 -0.29907748 -0.3029009   0.67927884
  -0.50944667  0.48969306 -0.48969306]] [-1.96200479]
```

Figure 6: Accuracy of the liblinear solver after feature scaling

  - As we can see the accuracy of the liblinear solver hasn't changed.
  - This is due to the liblinear solver being more robust towards unscaled small datasets. Even before scaling, it had found a optimal solution giving 100% accuracy.

8) Suppose you have a categorical feature with the categories 'red', 'blue', 'green', 'blue', 'green'. After encoding this feature using label encoding, you then apply a feature scaling method such as Standard Scaling or Min-Max Scaling. Is this approach correct? or not?. What do you propose

This approach is incorrect Reason:

- Label encoding assigns an integer value for the colours. For example `'red' = 0, 'blue' = 1, 'green' = 2`
- when we apply standard scaling or min-max scaling to this we are implying a mathematical order between colours (green is the highest and red is the lowest) even though

there is no such relation. This will lead to the model learning patterns that are not present.

- The correct method is to use One-Hot encoding. This represents the columns without introducing any order between categories. After encoding, scaling is not needed as the data is already on the binary scale (0 or 1).

Class label	**One-Hot encoding**
red	100
blue	010
green	001

Table 2: One-Hot encoding

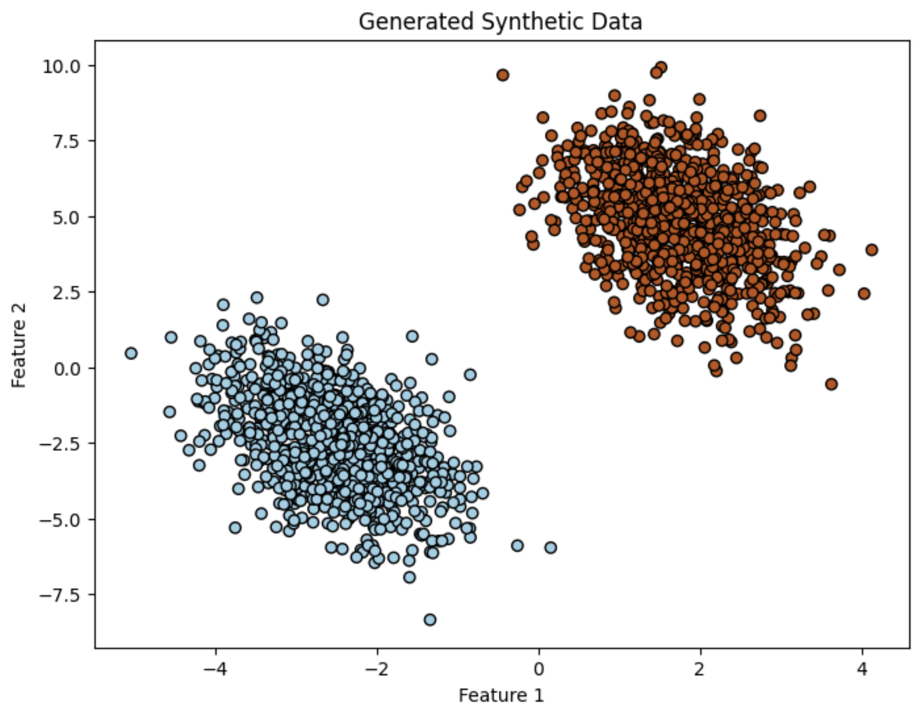
Data Sample	**Colour**
1	red
2	blue
3	green
4	blue
5	green

Table 3: Before encoding

Data Sample	**Is_red**	**Is_blue**	**Is_green**
1	1	0	0
2	0	1	0
3	0	0	1
4	0	1	0
5	0	0	1

Table 4: After One-Hot encoding

3 Logistic regression First/Second-Order Methods



2) Implement batch Gradient descent to update the weights for the given dataset over 20 iterations. State the method used to initialize the weights and reason for your selection

```
def sigmoid(z):
    #define the sigmoid function
    return 1 / (1 + np.exp(-z))

def loss_calc(y, y_hat):
    # Binary Cross-Entropy Loss
    return -np.mean(y * np.log(y_hat) + (1 - y) * np.log(1 - y_hat))

# Add a column of ones to X (bias term)
X_b = np.c_[np.ones((X.shape[0], 1)), X]  # X_b is now [1, feature1,
    feature2] with 2000 rows (2000x3 matrix)

n_in = X_b.shape[1]  # Number of input features including the bias term
limit = np.sqrt(6 / (n_in + 1)) #n_out is 1 for logistic regression(output
    features)

# Initialize weights from the Xavier Uniform distribution
w_ini = np.random.uniform(-limit, limit, size=(n_in, 1))
w_grad = w_ini      #this is a 3x1 matrix

 #make y a column vector
y = y.reshape(-1, 1)

```

```
learning_rate = 0.1
iterations = 20

# store the loss for plotting
loss_history_gradient = []

# Implement Batch Gradient Descent
for i in range(iterations):
    z = np.dot(X_b, w_grad)
    y_hat = sigmoid(z)      #this is a 2000x1 matrix

    # store the loss
    loss = loss_calc(y, y_hat)
    loss_history_gradient.append(loss)

    # Compute the gradients and update w
    gradient = np.dot(X_b.T, (y_hat - y)) / len(y)
    w_grad = w_grad - learning_rate * gradient

print("Final GD weights:\n", w_grad.ravel())
```

Result: `Final GD weights:  [0.08534997 0.78405749 0.5748131 ]`

Calculation explanation

- X_b is a new feature matrix with a column of 1 added to the front (bias term).
- The weight matrix w_{grad} is initialized.
- After that the learning rate and no. of iteration are defined.
- loss_history_gradient is an array used to store the loss values for plotting.
- z is the value we get when the weights aer used on the features. After that we get the predicted value $\hat{y}$ by passing z through a sigmoid function defined by sigmoid(z) $= \frac{1}{1+e^{-z}}$
- The loss is calculated using the Binary Cross Entropy Loss
- The the gradient was calculated using

$$\frac{\partial L}{\partial w_j} = \sum_{i=1}^{m} (\hat{y}_i - y_i)\, x_{j,i} \tag{1}$$

$$gradient = \frac{1}{m} X_b^\top (\hat{y} - y) \tag{2}$$

- The the new weights are calculated using $w_{grad} = w_{grad} - \alpha \times gradient$

Method used to initialize the weights:
The weights were initialized using the Xavier Uniform Initialization. It's taken using the following formula

$$w_{ini} \sim U(-limit, limit) \tag{3}$$

where,

$$limit = \sqrt{\frac{6}{n_{in} + n_{out}}} \tag{4}$$

n_{in} = number of input features (3 in this case with bias)
n_{out} = number of output units (1 in this case)

- Using this method we can avoid too small weights(vanishing gradients) and too large weights(exploding gradients).
- This formula ensures that when the number of input features are increased, the uniform distribution limits gets shrunk. So the initial guessing range also changes dynamically based on the inputs.
- An alternate would be zero initialization (simple). However, this is a symmetric starting point but the importance of different features are different. So it is not the best solution.

3) Specify the loss function you have used and state reason for your selection.

$$L = -\frac{1}{N}\sum_{i=1}^{N}(y_i log(\hat{y}_i) + (1 - y_i) log(1 - \hat{y}_i)) \tag{5}$$

The loss is calculated using the Binary Cross Entropy Loss. **Reason:**

- Our target variable is a binary value of 0 or 1. BCE is the best loss function for these type of applications as it uses log terms in the loss calculation and gives a heavy penalty if the prediction is wrong. This gives a strong gradient.
- On the other hand, MSE is used when the output is a continuous value. In that case, predicting a 0 as 1 is considered as a small error as they are close. But in classification, this is a major error and MSE does not give a heavy penalty. So MSE is not suitable.
- So we chose the Binary Cross Entropy Loss function.

4) Implement Newton's method to update the weights for the given dataset over 20 iterations

```python
# Initialize weights
w_newton = w_ini

loss_history_newton = []

# Newton's Method
for i in range(iterations):

    z = np.dot(X_b, w_newton)
    y_hat = sigmoid(z)


    loss = loss_calc(y, y_hat)
    loss_history_newton.append(loss)

    # Compute the gradient
    gradient = np.dot(X_b.T, (y_hat - y)) / len(y)

    # Compute the Hessian matrix
    R = np.diagflat(y_hat * (1 - y_hat))        # R is a diagonal matrix
    hessian = np.dot(X_b.T, np.dot(R, X_b)) / len(y)

    # Update the weights: w = w - H^{-1} * gradient
    w_newton = w_newton - np.dot(np.linalg.inv(hessian), gradient)

print("Final Newton's weights:\n", w_newton.ravel())
```

Calculation explanation

- Similar to before, first the weights are initialized.
- Then, for each iteration, the prediction $\hat{y}$ is calculated similar to before and the loss is calculated using the BCE.
- The gradient vector is then calculated using the previous algorithm.
- The weights are updated using the following formula

$$w_{newton} = w_{newton} - H^{-1}\nabla L \tag{6}$$

Where H is the hessian matrix of L

5) Plot the loss with respect to number of iterations for batch Gradient descent and Newton method's in a single plot. Comment on your results.

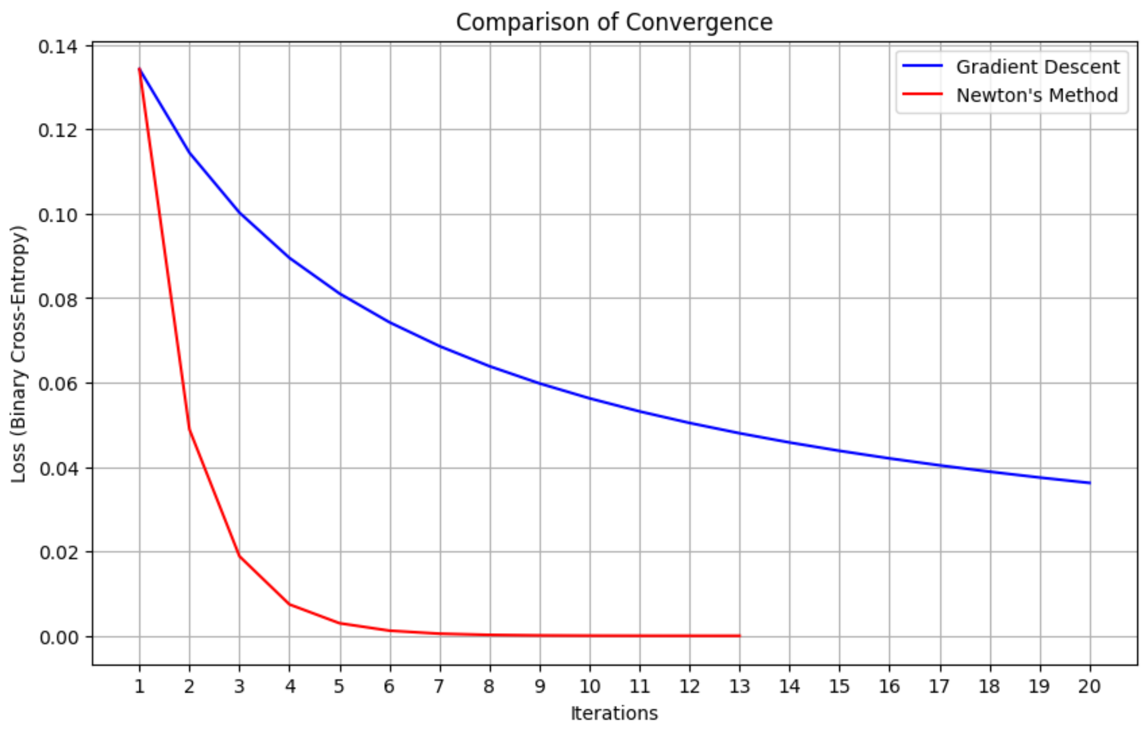


Figure 7: Loss comparison

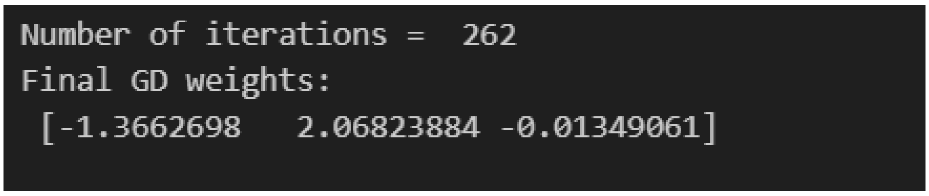
- It can be seen that the Newton's method converges much faster than the batch gradient descent. The loss of the Newtons method drops quickly while the loss of the gradient descent method decrease slowly.
- The reason for this is that the Newton's method is a second order method. It uses the Hessian matrix to get the curvature of the loss. This way, rather than following the steepest path towards the minima, it can get the exact step needed to get there. This results in quadratic convergence rather than the linear convergence shown in batch gradient descent.

6) Propose two approaches to decide number of iterations for Gradient descent and Newton's method.

1. **Provide a threshold to the gradient magnitude:**
   Rather than fixing the number of iterations, we can keep on updating the weights until the gradient of the loss has approached a specific threshold. When this happens we can decide that the algorithm has arrived at a local minima point where the slope is almost flat.

```python
# Add a column of ones to X (bias term)
X_b = np.c_[np.ones((X.shape[0], 1)), X]  # X_b is now [1, feature1,
    feature2] with 2000 rows (2000x3 matrix)

# Initialize starting weights to 0.
w_grad = w_ini      #this is a 3x1 matrix

 #make y a column vector
y = y.reshape(-1, 1)

learning_rate = 0.1
max_iterations = 1000
threshold = 0.05

# store the loss for plotting
loss_history_gradient = []

# Implement Batch Gradient Descent
for i in range(1,max_iterations+1):
    z = np.dot(X_b, w_grad)
    y_hat = sigmoid(z)      #this is a 2000x1 matrix

    # store the loss
    loss = loss_calc(y, y_hat)
    loss_history_gradient.append(loss)

    # Compute the gradients and update w
    gradient = np.dot(X_b.T, (y_hat - y)) / len(y)
    if(np.linalg.norm(gradient) < threshold):
      break
    w_grad = w_grad - learning_rate * gradient
print("Number of iterations = ",i-1)
print("Final GD weights:\n", w_grad.ravel())

```

   For the newtons Method also we can calculate the step value. The step is calculated using $H^{-1}gradient$. When this step size is very small we can stop the iterations since

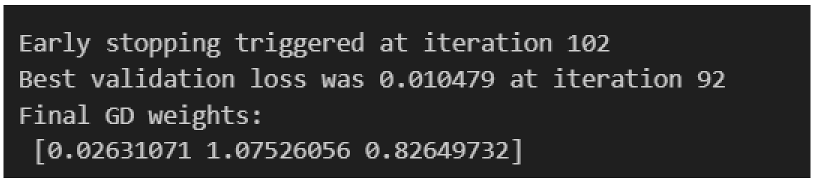


```
Number of iterations =  262
Final GD weights:
 [-1.3662698   2.06823884 -0.01349061]
```

the algorithm as reached a minimum point.

2. **Early stopping based on validation:**
   First, we can split the data into training and validation sets. Then after updating the weights in each iteration, calculate the loss for the validation set. Keep track of the best set of weights that gave the lowest loss for the validation set. At one point the loss for the validation set will start to increase while the training loss keeps on decreasing. This is when the models starts to overfit to the dataset. At this point revert the weights back to the previous weights, which gave the lowest loss. This way we can get the optimal number of iterations needed to train our model for generalized data

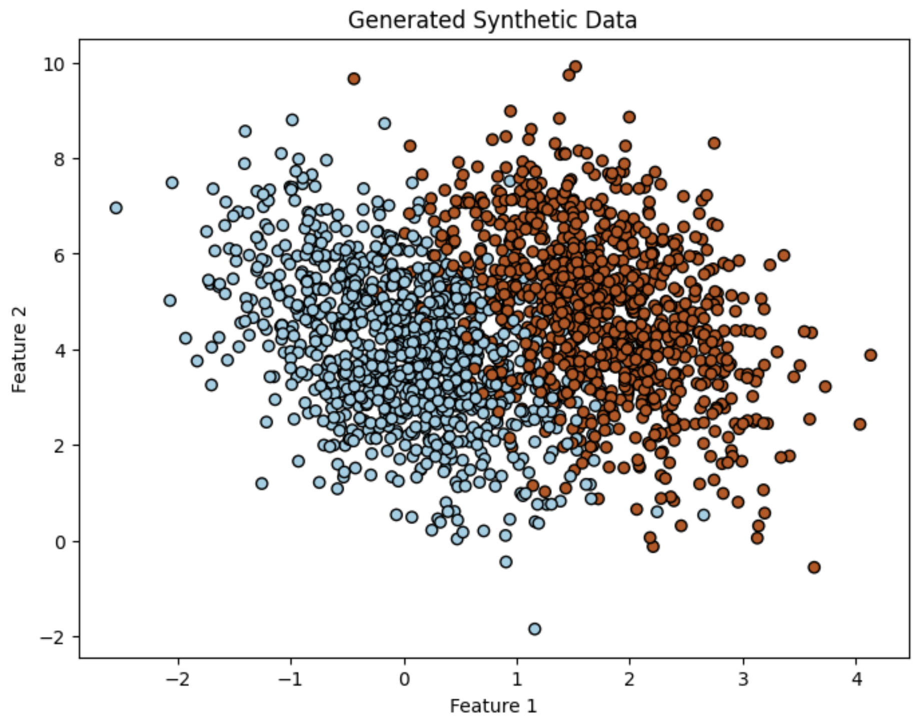
```python

#split the data
X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2,
    random_state=42, stratify=y)

X_train_b = np.c_[np.ones((X_train.shape[0], 1)), X_train]  # Training
    data with bias
X_val_b = np.c_[np.ones((X_val.shape[0], 1)), X_val]        #
    Validation data with bias


w_grad = w_ini # this is a 3x1 matrix

y_train = y_train.reshape(-1, 1)
y_val = y_val.reshape(-1, 1)

learning_rate = 0.1
max_iterations = 1000
no_improvement = 10          # How many iterations to wait after no
    improvement
tolerance = 0.001

best_val_loss = np.inf
best_weights = w_grad.copy() # Save a copy of the best weights
no_improvement_counter = 0     # Counter for how long we've waited
    without improvement

loss_history_gradient_3 = []
val_loss_history = [] # New list to track validation loss

# Batch Gradient Descent with Early Stopping
for i in range(max_iterations):
    # Use the training set to calculate gradient and update weights
    z_train = np.dot(X_train_b, w_grad)
    y_hat_train = sigmoid(z_train)

    train_loss = loss_calc(y_train, y_hat_train)
    loss_history_gradient_3.append(train_loss)

    gradient = np.dot(X_train_b.T, (y_hat_train - y_train)) / len(y_train)
    w_grad = w_grad - learning_rate * gradient

    # Use the validation dataset to checck the validation loss
    z_val = np.dot(X_val_b, w_grad)
    y_hat_val = sigmoid(z_val)
    current_val_loss = loss_calc(y_val, y_hat_val)
    val_loss_history.append(current_val_loss)

    if best_val_loss - current_val_loss > tolerance:
        best_val_loss = current_val_loss
        best_weights = w_grad.copy() # Save a copy of these best weights if the loss has reduced
        no_improvement_counter = 0          # Reset the counter
    else:
        # did not improve.
        no_improvement_counter += 1

    #check if there is no improvement for several iterations
    if no_improvement_counter >= no_improvement:
        print(f"\nEarly stopping triggered at iteration {i+1}")
        print(f"Best validation loss was {best_val_loss:.6f} at iteration {i+1 - no_improvement_counter}")
        # Revert our weights to the best ones we found
        w_grad = best_weights
        break
```



```
Early stopping triggered at iteration 102
Best validation loss was 0.010479 at iteration 92
Final GD weights:
 [0.02631071 1.07526056 0.82649732]
```

7) Suppose the centers in in listing 3 are changed to centers = [[2, 2], [5, 1.5]]. Use batch Gradient descent to update the weights for this new configuration. Analyze the convergence behavior of the algorithm with this updated data, and provide an explanation for convergence behavior

Now the centers are close together so there will be some overlapping between the classes.



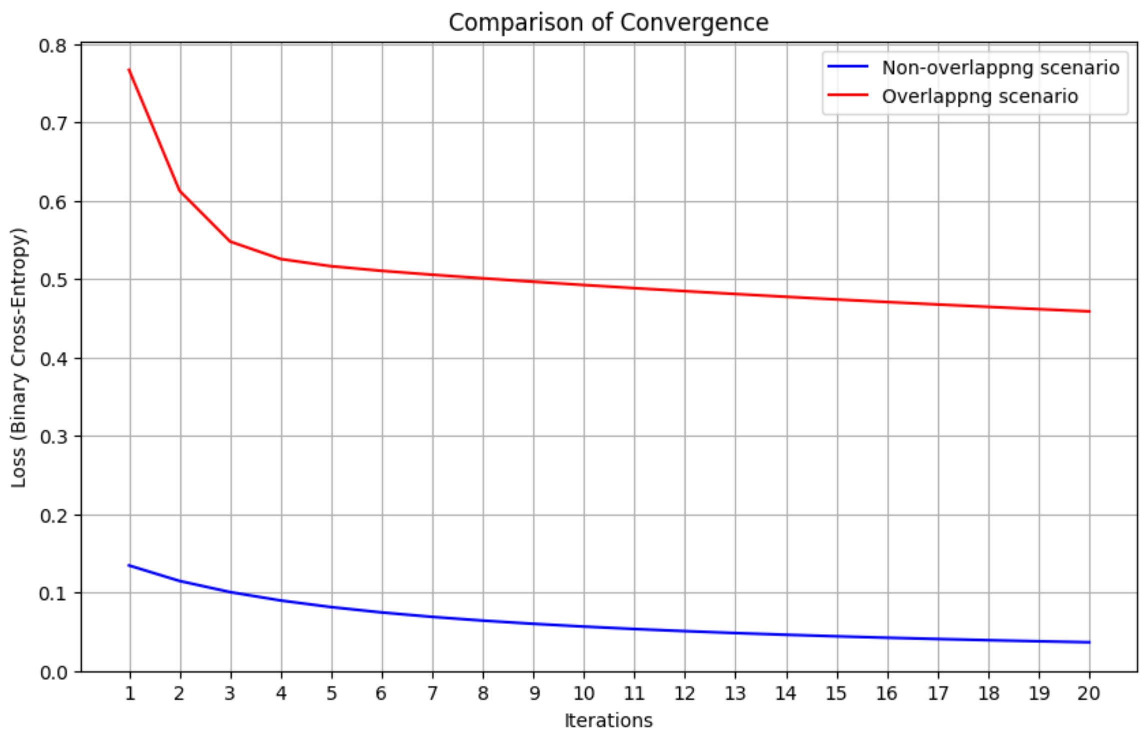
After using the batch gradient descent for 20 iterations, the following results were obtained.

Result: `Final GD weights:  [-0.06405436 0.8672853 -0.0861103 ]`

These were different from the previous results when using batch gradient descent on the non overlapping classes. The loss comparison is as follows.

Weights	**Non-overlapping Weights**	**Overlapping Weights**
w_0	0.08534997	-0.06405436
w_1	0.78405749	0.8672853
w_2	0.5748131	-0.0861103

Table 5: Weights after 20 iterations



- Previously the classes were far apart so we can find a line that separate them easily. But now there is no line that can perfectly separate them.
- Now the convergence is happening more slowly compared to the non overlapping classes scenario. The reason for this is that, in the overlapping region the model will be more uncertain and the predicted probability will be around 0.5.
- So, for uncertain points the gradient will be a smaller value resulting in the weight updates being smaller. Also the loss function can become more flat around the optimal solution reducing the gradient and slowing the convergence.
- Hence we can see that the convergence speed has significantly reduced.