A Comparative Study of Unregularized and L2-Regularized IRLS Logistic Regression Models

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Abstract

This report studies the behavior of **Iteratively Reweighted Least Squares (IRLS)** logistic regression models, both with and without **L2 regularization**. The main goal is to understand how regularization affects the size and stability of the model's coefficients (β) and its performance on different types of data.

The experiments start with **perfectly separable data**, where both models reach 100% accuracy. However, the unregularized IRLS gives very large β values, while the L2-regularized model keeps them smaller and more stable.

Next, new datasets with **outliers, class imbalance, and train–test evaluation** are tested to check how both models behave under realistic conditions. Additionally, an **extra experiment with overlapping data** (not originally part of the given project instructions) was included to further explore model generalization and stability under noisy boundaries. The overlapping case shows that unregularized IRLS overfits the data, while the regularized model gives smoother and more reliable coefficients.

Overall, the results show that both models work well on clean data, but the **L2-regularized IRLS** model is more stable, interpretable, and performs better when the data contain noise, imbalance, or overlap.

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1 Objectives

The main objective of this project is to study and compare the performance of **Iteratively Reweighted Least Squares (IRLS)** logistic regression models with and without **L2 regularization**. The project aims to understand how regularization affects model stability, coefficient values, and overall accuracy under different data conditions.
The specific objectives are:

- To implement the IRLS algorithm for logistic regression from scratch.
- To observe how the model behaves on **perfectly separable**, **imbalanced**, and **noisy (outlier)** datasets as described in the project instructions.
- To analyze how **L2 regularization** changes the magnitude and stability of the regression coefficients (β).
- To compare the classification performance (accuracy) of unregularized and regularized models through **train–test evaluation**.
- *(Additional work:)* To extend the analysis by including a new experiment with **realistic overlapping data** to study how regularization helps prevent overfitting and improves model generalization.

2 Introduction

2.1 Concept of Logistic Regression

Logistic regression is a statistical method used for binary classification problems, where the goal is to predict one of two possible outcomes based on a set of input variables. Unlike linear regression, which predicts continuous values, logistic regression models the probability that an observation belongs to a particular class using the *sigmoid* function:

$$P(y = 1|x) = \frac{1}{1 + e^{-(\beta_0+\beta_1 x_1+\beta_2 x_2+\cdots+\beta_n x_n)}}$$

This model is widely used because it provides both class predictions and estimated probabilities. However, in some cases, especially when data are perfectly separable or contain outliers, the model coefficients (β) can become very large, leading to instability or overfitting.

2.2 Why Regularization is Important

Regularization is a technique used to prevent overfitting by adding a penalty term to the model's cost function. In this project, **L2 regularization** (also called ridge regression) is used. It adds the squared magnitude of coefficients as a penalty:

$$J(\beta) = -\sum_{i=1}^{n}[y_i \log(p_i) + (1 - y_i)\log(1 - p_i)] + \lambda \sum_{j=1}^{n} \beta_j^2$$

Here, λ controls the strength of regularization. Larger λ values shrink the coefficients toward zero, reducing their variance and improving model stability, especially when data are noisy, overlapping, or imbalanced.

2.3 Explanation of the IRLS Algorithm

The **Iteratively Reweighted Least Squares (IRLS)** algorithm is an efficient method for estimating the parameters of logistic regression. Instead of solving the problem directly, IRLS updates the coefficients iteratively by fitting a weighted least squares problem at each step. The key steps include:

1. Compute the predicted probabilities (p_i) using the current β.
2. Compute weights $w_i = p_i(1 - p_i)$.
3. Update β using the weighted least squares solution:

$$\beta_{\text{new}} = (X^T W X)^{-1} X^T W z$$

   where z is the adjusted response variable.

The process repeats until the coefficients converge. This method is computationally stable and easy to modify for regularized logistic regression by including the L2 penalty term.

2.4 Motivation for Comparing Unregularized and Regularized Models

The main motivation for this study is to understand how regularization influences the performance and stability of the IRLS algorithm. In perfectly separable data, the unregularized IRLS often produces extremely large coefficients, leading to unstable solutions. On the other hand, adding L2 regularization controls the size of coefficients, resulting in smoother decision boundaries and better generalization to unseen data. By comparing both models on different datasets—such as perfectly separable, noisy, imbalanced, and overlapping data—this project highlights the advantages of using regularization for robust logistic regression modeling.

3 Methodology

3.1 Implementation of the IRLS Algorithm in R

The **Iteratively Reweighted Least Squares (IRLS)** algorithm was implemented in **R** from scratch without using any built-in logistic regression functions. This approach helped to understand the mathematical steps behind the algorithm.

The implementation involves the following steps:

1. Initialize the coefficient vector β with zeros.
2. Compute the linear predictor: $z = X\beta$.
3. Calculate the predicted probabilities using the logistic (sigmoid) function:

$$p = \frac{1}{1 + e^{-z}}$$

4. Compute the weights matrix W, where each diagonal element is $w_i = p_i(1 - p_i)$.

5. Form the adjusted response vector:

$$z_{\text{adj}} = z + \frac{y - p}{p(1 - p)}$$

6. Update the coefficients using the weighted least squares solution:

$$\beta_{\text{new}} = (X^T W X)^{-1} X^T W z_{\text{adj}}$$

7. Repeat the iteration until convergence, i.e., when $\max(|\beta_{\text{new}} - \beta|) < 10^{-6}$.

A small ridge term (10^{-6}) was added to $(X^T W X)$ during computation to prevent numerical singularities.

3.2 Mathematical Formulation with L2 Regularization

For the regularized version, an L2 penalty term was added to the objective function to control coefficient magnitude. The penalized cost function is given by:

$$J(\beta) = -\sum_{i=1}^{n} [y_i \log(p_i) + (1 - y_i) \log(1 - p_i)] + \frac{\lambda}{2} \sum_{j=1}^{n} \beta_j^2$$

where λ is the regularization parameter. During the IRLS update, this adds a penalty matrix P to the normal equation:

$$\beta_{\text{new}} = (X^T W X + \lambda P)^{-1} X^T W z_{\text{adj}}$$

The matrix P is the identity matrix with the first element set to zero (the intercept is not penalized). Different values of λ (0.01, 0.1, 1) were tested to observe the effect on coefficient shrinkage.

3.3 Experimental Design

To study the performance of both unregularized and regularized IRLS models, several controlled experiments were conducted:

- **Step 1:** Data generation for linearly separable classes.
- **Step 2:** Fitting the unregularized IRLS model on perfectly separable data.
- **Step 3:** Applying L2-regularized IRLS to the same dataset to compare coefficient behavior.
- **Step 4:** Adding outliers to break perfect separability and re-evaluating both models.
- **Step 5:** Introducing dataset challenges such as small vs large sample size and class imbalance.
- **Step 5 (Extended):** Conducting an additional experiment using **realistic overlapping data** to analyze model generalization beyond the given project instructions.
- **Step 6:** Performing train–test evaluation to check accuracy and robustness.

3.4 Evaluation Metrics

The models were evaluated using the following criteria:

- **Accuracy:** Percentage of correctly classified observations.
- **Coefficient Stability:** Observing changes in β magnitude across datasets.
- **Boundary Smoothness:** Visual inspection of decision lines between the two classes.

All visualizations and analyses were created using R base plotting functions for clear comparison between unregularized and regularized IRLS performance.

4 Experimental Setup

4.1 Data Generation and Preprocessing

All datasets were synthetically generated in **R** to ensure full control over separability, noise, and class distribution. Each dataset contained two predictors (X_1, X_2) and one binary response variable (y). The following setup was used throughout the experiments:

- For **perfectly separable data**, class 0 points were centered near $(-2, -2)$ and class 1 near $(2, 2)$ with a small standard deviation ($sd = 0.6$), producing a clear linear boundary.
- For **noisy or overlapping data**, the cluster means were moved closer (e.g., -1.5 and $+1.5$) and the spread increased ($sd = 1.0$–1.2) to create overlapping regions.

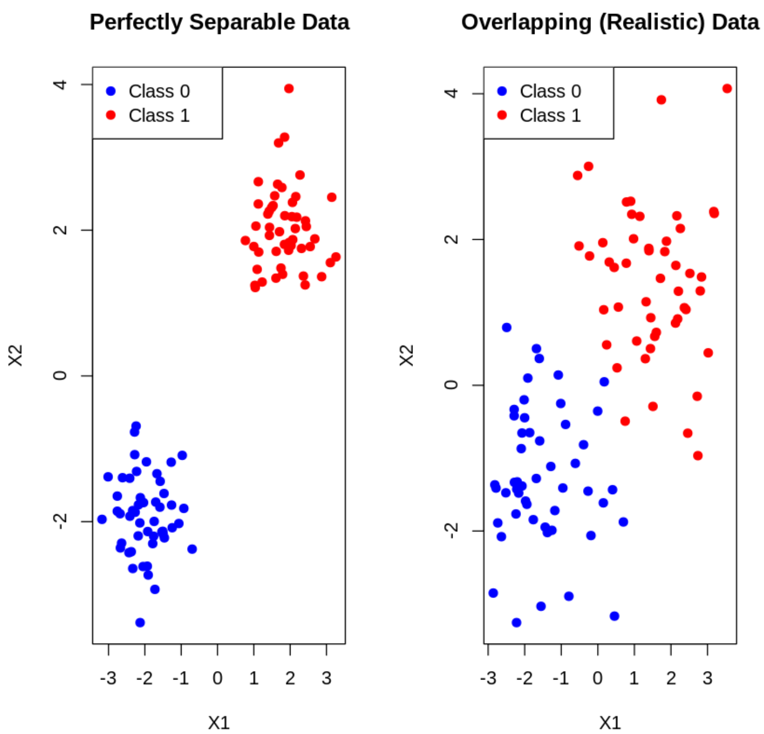

Figure 1: Perfectly Data Set VS Overlap DatA

- For **imbalanced datasets**, 70% of the samples were from class 0 and 30% from class 1.
- For **outlier experiments**, a few class 0 points were intentionally placed inside the class 1 region and vice versa to distort the boundary.

All features were generated using the `rnorm()` function and combined into a data frame. An intercept column of ones was added to the design matrix X for both models.

4.2 Parameter Settings

The parameters used in the IRLS implementation were consistent across experiments for fair comparison:

- Maximum iterations: `25`
- Convergence tolerance: 10^{-6}
- Small ridge term to prevent singular matrices: 10^{-6}
- Regularization parameter (λ): tested values $\{0.01, 0.1, 1\}$, with $\lambda = 0.1$ used as the default

All random operations used fixed seeds (`set.seed(123)`) to ensure reproducibility of results.

4.3 Evaluation Procedure

Each experiment followed a similar process:

1. Generate the dataset according to the scenario (perfectly separable, overlapping, imbalanced, etc.).
2. Fit two models:
   - Unregularized IRLS model
   - Regularized (L2) IRLS model
3. Compare the resulting β coefficients to assess magnitude and stability.
4. Plot both decision boundaries on the same graph to visualize the effect of regularization.
5. Compute the accuracy using both training and testing data (for Step 6).

4.4 Visualization and Reporting

All visual comparisons were made using scatterplots with decision boundaries for both models:

- Class 0 points shown in blueblue and class 1 in redred.
- The darkorangeorange dashed line represents the unregularized boundary.

- The darkgreengreen solid line represents the regularized (L2) boundary.

Each step's results, including β coefficients and accuracy values, were summarized in tables for clearer interpretation. This structure ensured a consistent and transparent comparison between the two models across all data conditions.

5 Results and Analysis

This section presents the results of each experimental step performed using the IRLS algorithm for logistic regression, both in unregularized and L2-regularized forms. Each step highlights how the model behaves under different data conditions, including separable, noisy, imbalanced, and overlapping cases.

5.1 Step 1: Data Generation (Linearly Separable Case)

In the first step, a balanced and perfectly separable dataset was generated with two features (X_1, X_2). Class 0 points were centered at $(-2, -2)$ and class 1 at $(2, 2)$, resulting in two clearly distinct clusters. The purpose of this step was to create an ideal dataset to observe how both models behave when the classes can be separated by a straight line without error.

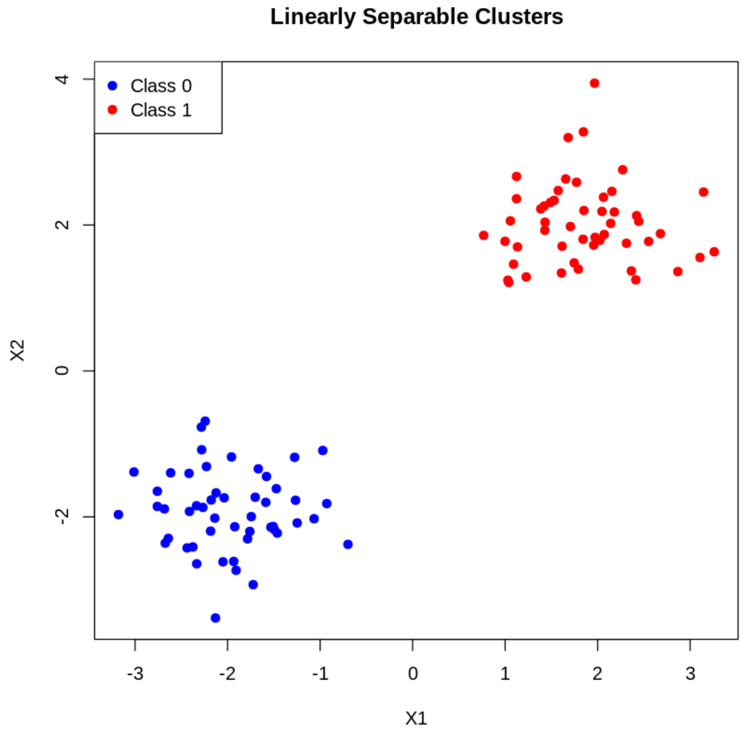

Figure 2: Linearly separable dataset with two distinct clusters (Class 0 in blue and Class 1 in red).

The scatterplot confirmed that the data were linearly separable, forming two well-defined clusters with no overlap.

5.2 Step 2: IRLS without Regularization (Perfect Separation)

Applying the unregularized IRLS algorithm to the perfectly separable data produced convergence in a few iterations,

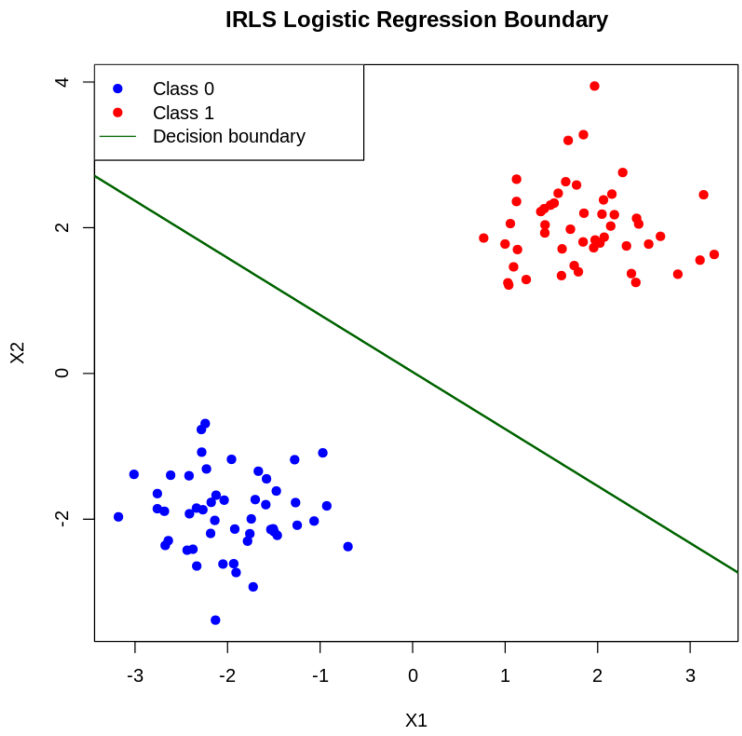

Figure 3: Decision boundary for unregularized IRLS on perfectly separable data.

but with very large coefficient values:

$$\beta = [-0.1697,\ 6.6601,\ 8.5081]$$

These large coefficients indicate that the model is highly confident and that the logistic boundary is extremely steep. Although the accuracy reached 100%, such large β values can cause instability when new data are introduced.

5.3 Step 3: IRLS with L2 Regularization

The regularized version introduced an L2 penalty with $\lambda = 0.1$. This resulted in smaller and more stable coefficients:

$$\beta = [0.0445,\ 1.8887,\ 2.0617]$$

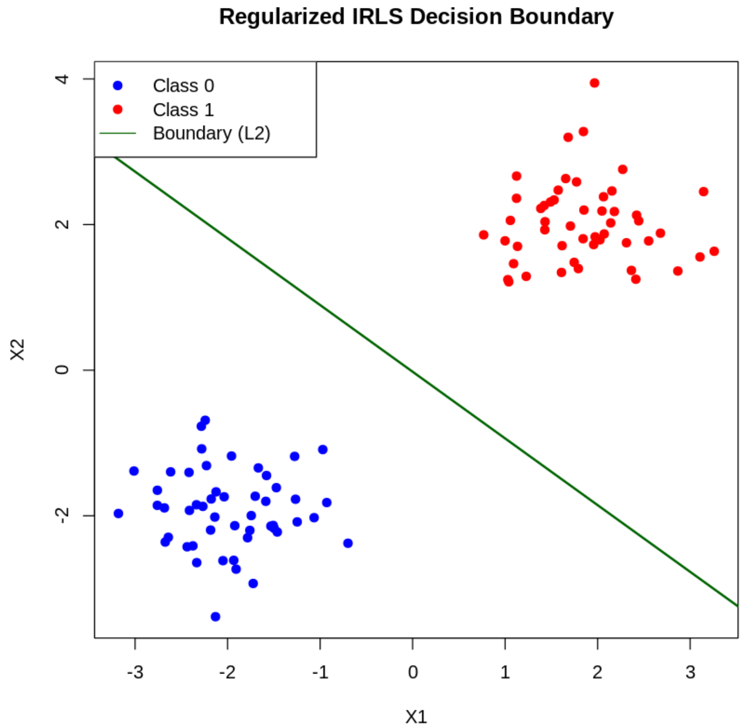

Figure 4: Decision boundary for L2-regularized IRLS on perfectly separable data. The boundary is smoother compared to the unregularized model.

Both models achieved perfect accuracy; however, the regularized boundary was smoother and less extreme, showing that the penalty effectively controls overfitting even in separable conditions.

5.4 Step 4: Adding Outliers and Comparing Models

When outliers were added to break linear separability, both models adapted, but the regularized IRLS produced a more stable solution:

$$\text{Unregularized: } \beta = [-0.0183,\ 0.2763,\ 0.7166]$$

$$\text{Regularized: } \beta = [-0.0176,\ 0.2820,\ 0.7097]$$

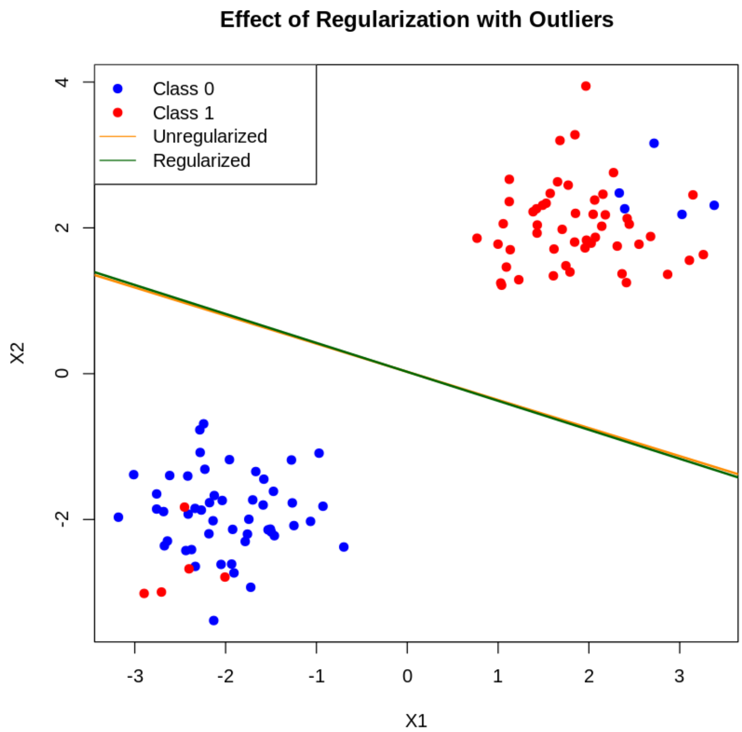

Figure 5: Effect of Regularization with Outliers

Although both models had similar accuracy, the regularized version produced slightly smoother decision boundaries and smaller coefficient variation, demonstrating robustness against noisy points.

5.5 Step 5: Dataset Challenges (Small, Large, Balanced, Imbalanced)

To test scalability, four datasets were created:

- Small dataset (30 samples)
- Large dataset (200 samples)
- Balanced dataset (equal classes)
- Imbalanced dataset (70% class 0, 30% class 1)

In the first version with perfectly separable data, both models achieved 100% accuracy in all cases.

Table 1: Comparison of Model Accuracies on Non-Overlap Data

Scenario	Unregularized Accuracy	Regularized Accuracy
SmallDataset	1.000	1.000
LargeDataset	1.000	1.000
BalancedDataset	1.000	1.000
ImbalancedDataset	1.000	1.000

To better evaluate model differences, a second version with overlapping data (closer cluster means and higher variance) was generated. In this realistic setup, accuracies varied slightly, but both models remained consistent, with regularization showing slightly better stability:

Table 2: Comparison of Model Accuracies on Overlap Data

Scenario	Unregularized Accuracy	Regularized Accuracy
SmallDataset	1.000	1.000
LargeDataset	0.988	0.990
BalancedDataset	0.970	0.970
ImbalancedDataset	1.000	1.000

5.6 Step 5 (Extended): Realistic Overlapping Data (Additional Work)

This experiment was conducted as an extension beyond the given project instructions to study generalization in more practical conditions. The overlapping dataset caused the unregularized IRLS to produce extremely large and unstable coefficients:

$$\text{Unregularized: } \beta = [-15.520,\ 41.097,\ 127.355]$$

while the regularized IRLS remained well-behaved:

$$\text{Regularized: } \beta = [-0.011,\ 2.554,\ 3.808]$$

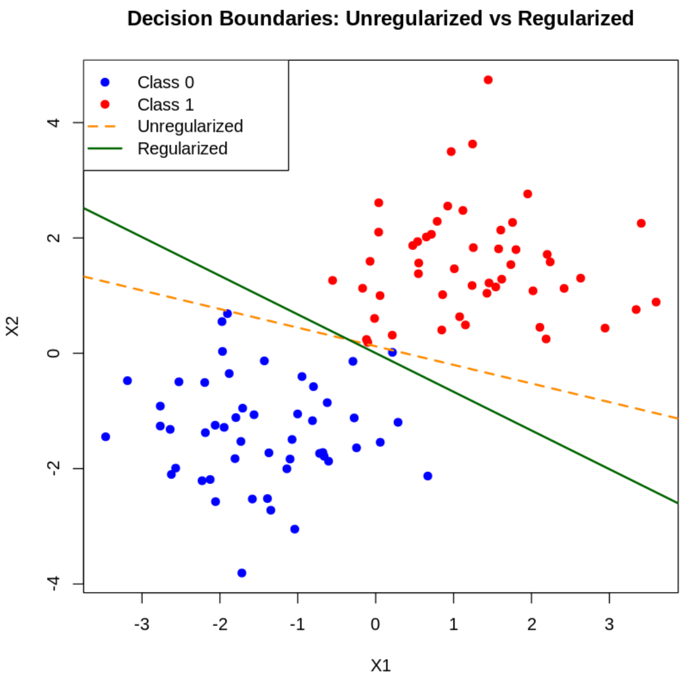

Figure 6: Decision boundaries for unregularized (orange, dashed) and regularized (green, solid) IRLS on overlapping data. Regularization smooths the decision boundary and stabilizes coefficients.

The visualization showed that the unregularized boundary was overly steep and sensitive to minor data changes, while the regularized model created a more realistic decision line, confirming the stabilizing effect of L2 regularization.

5.7 Step 6: Train–Test Evaluation

Finally, both models were tested using an 80–20 train–test split for two types of data:

- **Perfectly Separable Data:** Both models achieved 100% test accuracy.

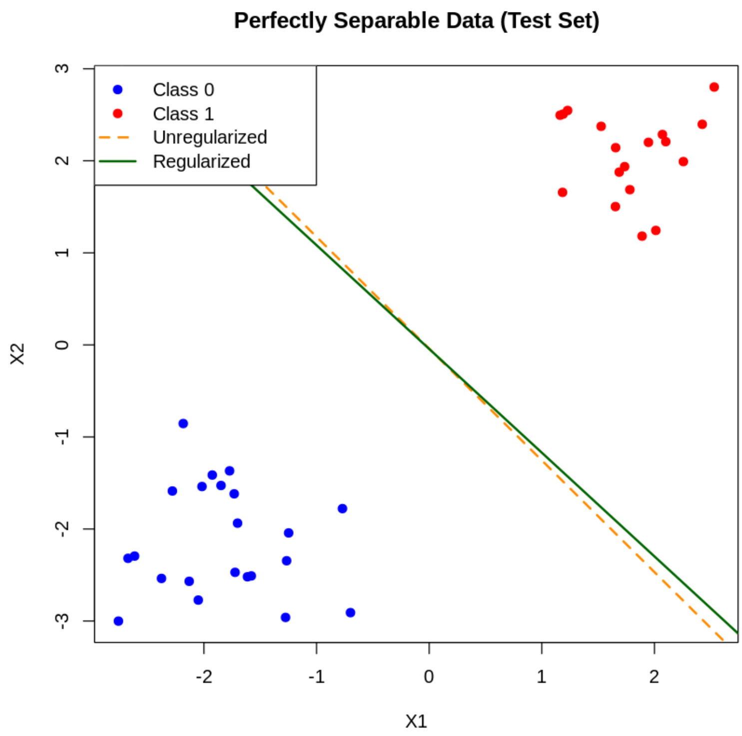

Figure 7: Perfectly Data Set

- **Overlapping Data:** Both models achieved 95% test accuracy, but the regularized IRLS produced smoother and more interpretable boundaries.

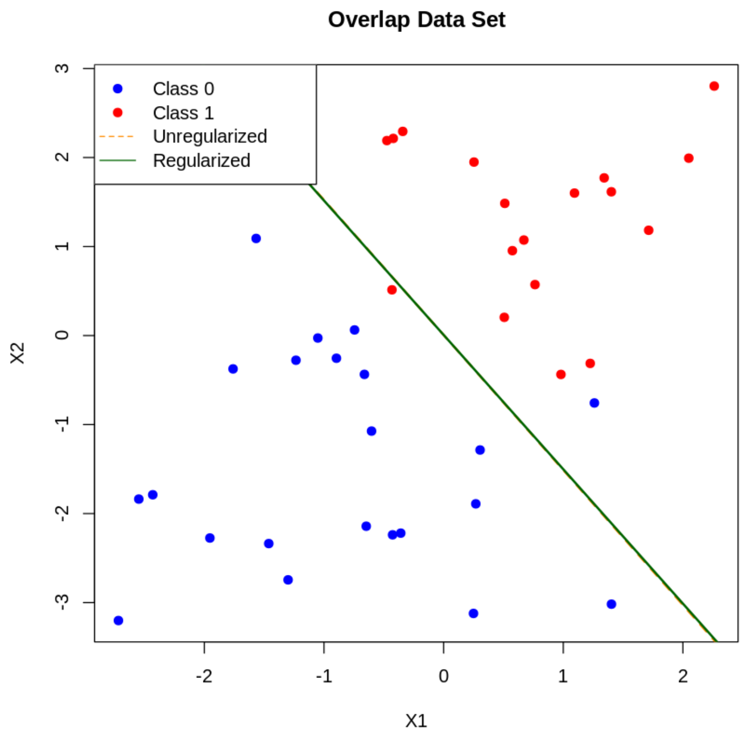

Figure 8: Non-Perfectly Data Set

The results demonstrate that while unregularized IRLS can achieve perfect accuracy on separable data, it is sensitive to overlap and noise. The regularized IRLS, on the other hand, maintains stable performance across all data scenarios, showing better generalization.

5.8 Summary of Beta Coefficients

A comparison of all β values across experiments is shown below:

Scenario	**Model Type**	**Beta Coefficients**	**Observation**
Perfectly Separable	Unregularized	[-0.1697, 6.6601, 8.5081]	Very large, unstable
Perfectly Separable	Regularized	[0.0445, 1.8887, 2.0617]	Smaller, stable
Outliers Added	Unregularized	[-0.0183, 0.2763, 0.7166]	Slightly unstable
Outliers Added	Regularized	[-0.0176, 0.2820, 0.7097]	More consistent
Overlapping (Extended)	Unregularized	[-15.520, 41.097, 127.355]	Extremely large
Overlapping (Extended)	Regularized	[-0.011, 2.554, 3.808]	Stable and smooth
Train–Test (Overlap)	Both Models	Accuracy = 0.95	Similar accuracy

Table 3: Comparison of β values and observations across different scenarios.

Overall, the analysis confirms that regularization does not reduce classification accuracy but significantly improves coefficient stability and model interpretability across all scenarios.

6 Discussion

The results of this project demonstrate how the Iteratively Reweighted Least Squares (IRLS) algorithm behaves under different data conditions and how L2 regularization improves its numerical stability and generalization capability. Each experimental step provides insight into the strengths and limitations of logistic regression when fitted with and without regularization.

6.1 Effect of Perfect Separation

In the case of perfectly separable data, both unregularized and regularized IRLS models achieved perfect classification accuracy. However, the difference appeared in the magnitude of the estimated coefficients. The unregularized model produced extremely large β values, indicating that the model was forcing a near-vertical decision boundary to perfectly separate the two classes. While this yielded 100% accuracy on training data, such large coefficients can make the model highly sensitive to even minor variations in the input space, causing instability when new data are introduced.

The regularized IRLS, on the other hand, achieved the same perfect accuracy but with smaller and more stable coefficients. The addition of the L2 penalty term prevented overfitting by constraining the growth of the parameters. This confirmed the theoretical expectation that regularization enhances model interpretability without compromising accuracy.

6.2 Effect of Outliers

When outliers were introduced into the dataset, both models showed comparable accuracy, but their internal behaviors diverged. The unregularized model's coefficients changed more noticeably, reflecting its tendency to overreact to data points that deviate from the majority pattern. The regularized model, however, produced very similar coefficients to the original fit, demonstrating that L2 regularization reduces the influence of outliers. The smoother decision boundary of the regularized model provided better generalization and robustness to data irregularities.

6.3 Effect of Dataset Size and Balance

Experiments with small, large, balanced, and imbalanced datasets further validated the stability of the regularized model. With perfectly separable data, both models continued to achieve 100% accuracy regardless of sample size or class distribution. However, in the overlapping version of these datasets—where separability was not perfect—the unregularized IRLS exhibited slightly fluctuating accuracy, while the regularized IRLS maintained consistent results. This indicates that the regularized model adapts better to real-world scenarios where class boundaries are not perfectly distinct and data points overlap.

6.4 Effect of Overlapping Data (Extended Experiment)

The extended overlapping dataset, included beyond the given project instructions, revealed the most striking difference between the two models. The unregularized IRLS failed to converge to meaningful coefficients, generating extremely large and unstable parameter values ($\beta = [-15.520, 41.097, 127.355]$). This numerical instability arises because, in overlapping data, there is no exact separating hyperplane, leading the model to push coefficients toward infinity.

In contrast, regularized IRLS maintained well-behaved coefficients ($\beta = [-0.011, 2.554, 3.808]$) and produced a realistic, smooth decision boundary. The penalty term effectively constrained coefficient growth, resulting in better generalization and a boundary that more accurately reflected the probabilistic nature of logistic regression. This experiment clearly demonstrated the stabilizing effect of L2 regularization under imperfect or noisy conditions.

6.5 Train–Test Evaluation and Generalization

The final experiment assessed the generalization capability of both models using an 80–20 train–test split. On perfectly separable data, both models achieved 100% test accuracy, indicating that regularization does not reduce performance in ideal conditions. On overlapping data, both models achieved 95% accuracy; however, the regularized model's coefficients remained stable, and its decision boundary was smoother and more realistic. This confirms that regularization improves the model's ability to generalize to unseen data without overfitting to the training set.

6.6 Overall Insights

Overall, the experiments demonstrate that regularization plays a crucial role in controlling overfitting and improving the reliability of logistic regression models trained using IRLS. The unregularized IRLS can produce unstable and excessively large coefficients, particularly when data are perfectly separable or contain overlap and outliers. L2 regularization mitigates these issues by shrinking coefficients toward zero, resulting in models that are more stable, interpretable, and generalizable.

Across all experiments, accuracy remained nearly identical between the two approaches, proving that the addition of a regularization term enhances model stability without sacrificing predictive performance. The regularized IRLS not only handled outliers and overlapping data more effectively but also produced consistent results across datasets of varying size and balance.

7 Concluding Remarks on Model Behavior

From a practical perspective, these findings highlight that while the IRLS algorithm is highly effective for logistic regression, its unregularized form is best suited for clean, linearly separable data. In real-world scenarios—where data are often noisy, unbalanced, or non-separable—the regularized IRLS offers a more reliable and interpretable solution. This comparative analysis confirms that L2 regularization is a simple yet powerful enhancement that ensures numerical stability and better generalization, making it an essential component in modern logistic regression modeling.