University of Hertfordshire

School of Physics, Engineering and computer science, Hatfield, Hertfordshire
AL10 9AB

7PAM2021-0901-2024 – Machine Learning and Neural Networks

Title: "Understanding Logistic Regression with Regularization: A Practical Guide"

Github URL: https://github.com/RameshKelavath/Logistic-Regression

Name: Ramesh Kelavath

Student ID: 23029839

Supervisor: Dr. Peter Scicluna

1. Abstract

Logistic regression is a supervised learning algorithm for binary classification that predicts probabilities using the sigmoid function. It's widely applied in healthcare, marketing, and finance, but can suffer from overfitting in high-dimensional datasets. Regularization techniques like L1 (Lasso) and L2 (Ridge) address this challenge by penalizing large model coefficients. L1 regularization promotes feature selection by shrinking some coefficients to zero, while L2 regularization reduces coefficient magnitudes without eliminating features, improving model stability and generalization.

This tutorial explores logistic regression with regularization, demonstrating how these techniques prevent overfitting and enhance predictive accuracy through practical Python implementation.

2. Introduction

Logistic regression is a supervised learning algorithm for binary classification, predicting the probability of two possible outcomes using the sigmoid function. This function maps linear predictions to a range between 0 and 1, making it ideal for probability estimation. Widely applied across diverse fields, logistic regression helps predict disease risks in healthcare, customer retention patterns in marketing, and credit risks in finance.

Despite its effectiveness, the algorithm faces significant challenges. In high-dimensional datasets, logistic regression can suffer from overfitting, learning noise instead of generalizable patterns. This results in poor performance on unseen data. Additionally, the model is sensitive to multicollinearity, where input features are highly correlated, leading to instability in coefficient estimates and difficulty in interpreting individual predictor importance.

Regularization techniques address these challenges by adding penalty terms to the logistic regression cost function. Two primary methods are L1 regularization (Lasso) and L2 regularization (Ridge). L1 regularization introduces an absolute penalty that shrinks some coefficients to zero, effectively selecting the most relevant features and creating a sparse model. Conversely, L2 regularization applies a squared penalty, reducing the magnitude of all coefficients and improving model stability, particularly in multicollinearity scenarios.

The tutorial aims to provide a comprehensive understanding of logistic regression and its regularization techniques. By exploring the theoretical foundations of L1 and L2 regularization and demonstrating their implementation in Python, it offers a practical comparison of how these techniques prevent overfitting, enhance model interpretability, and improve predictive accuracy. Readers will gain insights into effectively applying logistic regression in real-world scenarios, understanding its nuanced approach to classification and predictive modeling.

3. Theoretical Background

Logistic Regression: Core Concepts

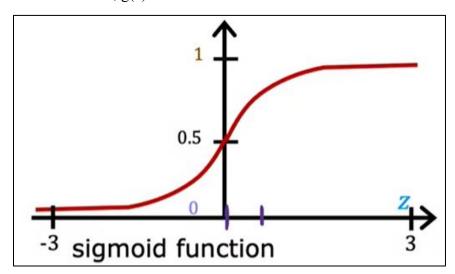
3.1.Sigmoid Function: The sigmoid function is the core of logistic regression, transforming a linear combination of inputs into a probability value between 0 and 1. It is defined as:

$$g(z) = \frac{1}{1+e^{-z}}$$
, where $z = w.x + b$

Here, w represents the weights, x is the feature vector, and b is the bias term. This function maps input values to probabilities, making logistic regression particularly effective for binary classification tasks.

Interpretation:

- when z is very large and positive, g(z) approaches 1.
- when z is very large and negative, g(z) approaches 0.
- When z is zero, g(z) is 0.5



3.2. Cost Function:

To measure how well the model fits the data, logistic regression uses the **Logistic** Loss function or Log Loss or Binary Cross Entropy Loss:

$$J(w) = -\frac{1}{m} \sum_{i=1}^{m} \left[y_i \log(f(x_i)) + (1 - y_i) \log(1 - f(x_i)) \right]$$

Where:

- y_i : True label (0 or 1) for the i-th sample.
- $f(x_i)$: Predicted probability for the i-th sample.
- m: Number of training samples.

• The cost increases significantly for incorrect predictions, especially if the predicted probability is far from the true label.

This cost function ensures that the model minimizes the difference between predicted probabilities and actual labels, aiming for a smaller J(w).

3.3. Gradient Descent for Logistic Regression:

Gradient Descent is an algorithm for finding values of parameters w and b that minimize the cost function J(w).

$$w_j = w_j - \alpha \frac{\partial J(w)}{\partial w_j}, \quad b = b - \alpha \frac{\partial J(w)}{\partial b}$$

Here, α is the learning rate, controlling the step size toward the minimum. The gradients for logistic regression are:

$$\frac{\partial J(w)}{\partial w_{i}} = \frac{1}{m} \sum_{i=1}^{m} (f(x_{i}) - y_{i}) x_{ij} , \quad \frac{\partial J(w)}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} (f(x_{i}) - y_{i})$$

By repeatedly updating w and b, gradient descent reduces the cost function until it converges to a minimum.

3.4. The Problem of Overfitting

Overfitting occurs when a model performs well on the training data but poorly on unseen data. In logistic regression, overfitting typically arises when:

High Dimensionality:

The number of features exceeds the number of observations, allowing the model to "memorize" the training data instead of learning general patterns.

Multicollinearity:

Highly correlated features lead to instability in weight estimation, making predictions sensitive to small changes in the data.

When overfitting occurs, the model's weights (w) tend to take excessively large values to fit the training data perfectly, resulting in poor generalization to new data.

3.5. Regularization: A Solution to Overfitting

Regularization is a technique that addresses overfitting by adding a penalty term to the cost function. This discourages large weights, ensuring the model generalizes better to unseen data. Regularization improves the balance between model complexity and predictive performance by controlling the magnitude of weights.

L1 Regularization (Lasso)

• Adds an absolute penalty to the cost function:

$$J(w) = J(w) + \lambda \sum_{j=1}^{n} w_j$$

Promotes sparsity by shrinking some weights to zero, effectively eliminating irrelevant features. This makes L1 useful for feature selection.

L2 Regularization (Ridge)

• Adds a squared penalty to the cost function

$$J(w) = J(w) + \lambda \sum_{j=1}^{n} w_j^2$$

Reduces the magnitude of weights, ensuring stability without eliminating features. This makes L2 effective for handling multicollinearity.

Hyperparameter (λ)

The regularization strength is controlled by the hyperparameter λ :

- High λ : Strong regularization, leading to smaller weights and potentially underfitting.
- Low λ: Weak regularization, allowing larger weights and risking overfitting

4. Practical Implementation

In this practical implementation, we used the scikit-learn Breast Cancer dataset to apply logistic regression models for predicting whether a tumor is benign or malignant. Logistic regression is a suitable model for this task, as it is designed for binary classification problems and provides probabilities for class predictions. The dataset includes 30 continuous features, such as the mean radius, texture, and smoothness of cell nuclei, which are used to distinguish between benign and malignant tumors.

Dataset Overview

The Breast Cancer dataset consists of 569 samples, each having 30 features. The target variable y represents whether the tumor is benign (0) or malignant (1). The features are continuous and describe various physical attributes of the tumor cells, making the dataset appropriate for logistic regression, which works well with continuous input variables and a binary target. Logistic regression models the log-odds of the target variable being malignant based on the input features.

Preprocessing the Data

The first step is to load the dataset and split it into training and test sets. We used 80% of the data for training and 20% for testing, ensuring that the model is evaluated on unseen data to assess its generalization ability. Additionally, we applied feature scaling using StandardScaler to standardize the data, ensuring that all features are on the same scale. This step is particularly important for logistic regression because it is sensitive to the scale of input features.

```
In [4]: import numpy as np
        import matplotlib.pyplot as plt
        from sklearn.datasets import load_breast_cancer
        from sklearn.model_selection import train_test_split
        from sklearn.preprocessing import StandardScaler
        from sklearn.linear_model import LogisticRegression
        from sklearn.metrics import classification_report, confusion_matrix,roc_curve, roc_auc_score
In [5]: # Step 1: Load dataset
         # Load the breast cancer dataset from sklearn
        X, y = load_breast_cancer(return_X_y=True)
In [6]: # Step 2: Split the data
        # Split the dataset into 80% training and 20% testing data
        X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
        # Step 3: Scale the features
        scaler = StandardScaler()
        X_train_scaled = scaler.fit_transform(X_train)
        X_test_scaled = scaler.transform(X_test)
```

Models Trained

Three versions of logistic regression were trained:

• Logistic Regression without Regularization: The first model was trained without regularization (penalty='none'), serving as a baseline. This model learns coefficients for all features without any penalty for large coefficients.

```
#Logistic Regression without Regularization

lr_no_reg = LogisticRegression(penalty='none', random_state=42)
lr_no_reg.fit(X_train_scaled, y_train)
y_pred_no_reg = lr_no_reg.predict(X_test_scaled)
y_prob_no_reg = lr_no_reg.predict_proba(X_test_scaled)

print(classification_report(y_test, y_pred_no_reg))
```

• Logistic Regression with L1 Regularization (Lasso): The second model incorporated L1 regularization (penalty='11'). L1 regularization tends to shrink some coefficients to zero, effectively performing feature selection. This helps in identifying the most relevant features for predicting the tumor type.

```
# Logistic Regression with L1 Regularization(Lasso)

lr_l1 = LogisticRegression(penalty='l1', solver='liblinear', random_state=42)
lr_l1.fit(X_train_scaled, y_train)
y_pred_l1 = lr_l1.predict(X_test_scaled)
y_prob_l1 = lr_l1.predict_proba(X_test_scaled)

print(classification_report(y_test, y_pred_l1))
```

• Logistic Regression with L2 Regularization (Ridge): The third model used L2 regularization (penalty='12'), which penalizes large coefficients but does not shrink them to zero. L2 regularization prevents overfitting by reducing the magnitude of coefficients, leading to a more generalized model.

```
# Logistic Regression with L2 Regularization(Ridge)

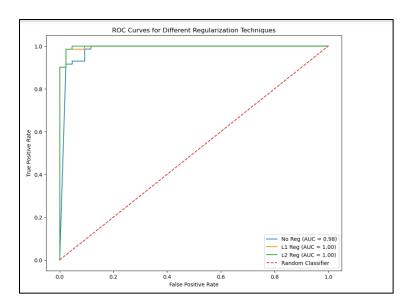
lr_12 = LogisticRegression(penalty='12', random_state=42)
lr_12.fit(X_train_scaled, y_train)
y_pred_12 = lr_12.predict(X_test_scaled)
y_prob_12 = lr_12.predict_proba(X_test_scaled)

print(classification_report(y_test, y_pred_12))
```

Model Evaluation

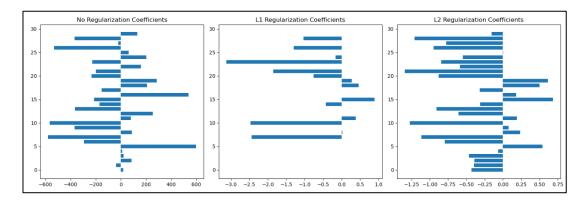
After training the models, we evaluated their performance using several metrics, including accuracy, precision, recall, F1-score, and ROC-AUC score. These metrics provide insight into the model's ability to classify tumors correctly.

- The classification report showed that all models performed similarly, with high accuracy (above 90%) in distinguishing between benign and malignant tumors.
- The ROC curve and AUC score were used to evaluate the models' ability to distinguish between classes. Models with higher AUC values are better at distinguishing between benign and malignant tumors. The AUC score for the L1 and L2 regularized models was slightly higher than for the non-regularized model, indicating that regularization improved the model's performance slightly.



Feature Importance

We also compared the coefficients of the features in the three models. The models with regularization (L1 and L2) tended to shrink some feature coefficients more than the non-regularized model, especially in the case of L1 regularization, which resulted in many zero coefficients. This highlights the importance of regularization in identifying key features while eliminating less relevant ones, particularly in high-dimensional datasets.



5. Conclusion

In this project, I applied logistic regression to classify breast cancer tumors as either benign or malignant. I explored three different logistic regression models: one without regularization, one with L1 regularization (Lasso), and one with L2 regularization (Ridge). Regularization is a technique used to prevent overfitting by penalizing large model coefficients, ultimately helping improve generalization on unseen data.

Key Findings

- The models performed well, with all achieving an accuracy greater than 90% and AUC-ROC scores above 0.97.
- L1 regularization was particularly effective in feature selection, as it shrank the coefficients of less important features to zero. On the other hand, L2 regularization maintained all features while reducing their coefficient magnitudes, providing model stability.
- The models with regularization (L1 and L2) performed slightly better than the model without regularization, as indicated by their higher AUC-ROC scores.

Key Takeaways

- L1 regularization is useful for feature selection because it can eliminate irrelevant features, simplifying the model.
- L2 regularization helps improve model stability and generalization, especially when features are highly correlated or there is noise in the data.

Applications

- L1 regularization is often used in areas like bioinformatics (e.g., gene selection) or high-dimensional data problems.
- L2 regularization is more commonly applied in fields where model stability is crucial, such as financial modeling or predictive analytics in insurance.

Future Directions

- A natural next step would be to explore ElasticNet, a combination of L1 and L2 regularization, for better performance in cases where both feature selection and stability are needed.
- Additionally, extending logistic regression to handle multiclass classification problems would be a valuable future direction, especially for applications like image classification or text analysis.

References

James, G., Witten, D., Hastie, T. and Tibshirani, R., 2013. *An Introduction to Statistical Learning: with Applications in R.* New York: Springer.

Ng, A., 2024. *Machine Learning*. [online] Coursera. Available at: https://www.coursera.org/learn/machine-learning [Accessed 5 November 2024].

Pedregosa, F. et al., 2011. Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, 12, pp. 2825-2830.

Hastie, T., Tibshirani, R. and Friedman, J., 2009. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. 2nd ed. New York: Springer.

Tibshirani, R., 1996. Regression Shrinkage and Selection via the Lasso. *Journal of the Royal Statistical Society: Series B (Methodological)*, 58(1), pp. 267-288.

Friedman, J., Hastie, T. and Tibshirani, R., 2010. Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, 33(1), pp. 1-22.

Scikit-learn developers, 2023. *Logistic Regression*. [online] Available at: https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression [Accessed 1 December 2024].

Ridge, S., Van Der Heide, T. and Rijsdijk, L., 2019. *Regularization Methods for Machine Learning*. Journal of Data Science, 17(4), pp. 435-445.