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Comparison of LASSO, Ridge, and Elastic Net Regularization with Balanced Bagging Classifier

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Abstract
Predicting Drug-Induced Autoimmunity (DIA) is crucial in pharmaceutical safety assessment, as early identification of compounds with autoimmune risk can prevent adverse drug reactions and improve patient outcomes. Classification analysis often faces challenges when the number of predictor variables exceeds the number of observations or when high correlations among predictors lead to multicollinearity and overfitting. Regularization methods, such as Ridge Regression, Least Absolute Shrinkage and Selection Operator (LASSO), and Elastic-Net, help stabilize parameter estimation and improve model interpretability. This study focuses on building a binary classification model to predict the risk of DIA using 196 molecular descriptors derived from chemical compound structures. To address class imbalance in the response variable, the Balanced Bagging Classifier (BBC) is combined with regularized logistic regression models. Elastic Net + BBC outperforms other models with the highest accuracy (0.825), followed closely by LASSO + BBC and Ridge + BBC (both 0.816). This integration not only improves classification accuracy but also enhances generalization and the reliable detection of minority class instances, supporting the early identification of autoimmune risks in drug discovery.
Keywords: *Balanced Bagging Classifier, Binary Classification, Drug-Induced Autoimmunity, Feature Selection, Regularization*

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1. INTRODUCTION

Classification analysis often encounters challenges like high correlations among predictors or having more predictors than observations, which can lead to multicollinearity and overfitting. Regularization methods help address these issues by controlling coefficient estimates and improving model interpretability . Ridge Regression, LASSO, and Elastic-Net are among the most used regularization techniques.

The application of regularization to logistic regression has proven effective in various case studies within the healthcare field [1]. Previous research has demonstrated that this method offers advantages in leukemia data analysis, both in empirical data and simulation studies [2][3]. Another study applied LASSO logistic regression to identify factors associated with breast cancer risk from 29 variables, including dietary factors and previously established cancer risk factors [4]. Furthermore, the Elastic-Net logistic regression approach was employed to develop classification models and extract genetic signatures across various T-helper cell subsets and immune cell types [5]. Other research has revealed that LASSO and Ridge models tend to prioritize dependent variable categories with a dominant proportion in the training data [6].

In addition to challenges related to data dimensionality and correlations, class imbalance also poses a critical issue in classification analysis. Class imbalance occurs when certain classes are underrepresented in comparison to others. If the sample proportion falls below 35% of the total data, the dataset is classified as imbalanced [7]. Imbalanced class distributions in datasets can cause models to skew their predictions toward the majority class, thereby reducing accuracy for the minority class. To handle this challenge, methods such as the Balanced Bagging Classifier have been proposed. This method combines bootstrap sampling with classification models applied to adjusted subsets of data to ensure balance. In the context of school dropout risk prediction, this approach has proven to be the most effective method for handling imbalanced data and delivering superior classification performance compared to SMOTE and ADASYN [8]. The effectiveness of the Balanced Bagging Classifier has also been demonstrated in identifying the risk level of developing febrile neutropenia in cancer patients undergoing chemotherapy [9], highlighting the broad potential of this approach across diverse medical classification challenges.

Based on this background, this study focuses on developing a classification model to predict the risk of Drug-Induced Autoimmunity (DIA), an autoimmune condition triggered by the use of specific medications [10]. The classification model is developed using regularization approaches for logistic regression—namely LASSO, Ridge, and Elastic Net—which effectively address multicollinearity issues and select the most contributive predictor variables. A key challenge in the dataset is the severe class imbalance in the response variable, where the number of drugs known to induce DIA is significantly smaller than those with no known or confirmed association. To mitigate this, the Balanced Bagging Classifier method is employed, which integrates bootstrap sampling with classification algorithms applied to balanced data subsets. This approach not only enhances prediction accuracy for the minority class but also yields more stable models, thereby supporting early detection of potential drug-induced autoimmune reactions.

The novelty of this research lies in combining regularized logistic regression with ensemble-based balancing strategies to address both multicollinearity and class imbalance simultaneously. By integrating these methods, the study provides a more interpretable and robust framework compared to traditional machine learning techniques, while specifically targeting the underexplored area of drug-induced autoimmunity.

2. RESEARCH METHODOLOGY

2.1. Data

This study employs secondary data obtained from the UCI Machine Learning Repository. The dataset employed is the Drug-Induced Autoimmunity (DIA) Dataset, which contains molecular variables derived from chemical structure extraction using RDKit **[11]**. The dataset is publicly available and accessible via the Dataset DIA link.

2.2. Ridge Regression

Ridge Regression was selected for its ability to handle multicollinearity effectively by shrinking coefficient estimates, making it suitable for models with highly correlated predictors. This method was first introduced by Hoerl in 1962 to address the instability of estimators in Ordinary Least Squares (OLS) under conditions of high collinearity among independent variables **[12]**. This method operates similarly to OLS by minimizing the Residual Sum of Squares (RSS) in regression coefficient estimation, with the addition of an L_2 penalty term. The objective function can be expressed as shown in **Equation (1) [13]**.

$$\hat{\beta}_{Ridge} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 \tag{1}$$

The shrinkage parameter (λ) controls the magnitude of the penalty in Ridge Regression. This parameter determines the degree to which regression coefficients are shrunk toward zero. The larger the value of λ, the smaller the resulting regression coefficients **[14]**.

2.3. LASSO

The Least Absolute Shrinkage and Selection Operator (LASSO) was chosen for its strength in variable selection, allowing the model to enhance interpretability by reducing less important coefficients to zero. LASSO is a regression technique used to perform variable selection, enhancing prediction accuracy and model interpretability **[15]**. The LASSO coefficient estimates are obtained by minimizing the Residual Sum of Squares (RSS) with the addition of an L_1 penalty term, as expressed in **Equation (2)**.

$$\hat{\beta}_{LASSO} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| \tag{2}$$

The L_1 penalty in LASSO has the effect of shrinking some coefficient estimates to exactly zero when the shrinkage parameter (λ) is sufficiently large. This property enables LASSO to produce sparse models with fewer predictors, enhancing interpretability and simplifying the final model structure **[14]**.

2.4. Elastic-Net

Elastic-Net was used to combine the strengths of both Ridge and LASSO, making it particularly appropriate when facing datasets with many correlated predictors and a need for both regularization and variable selection. Elastic-Net is a regularization method introduced by Zou and Hastie in 2005 as a solution to certain limitations of the LASSO method. Elastic-Net combines the penalties of Ridge Regression and LASSO, enabling it to perform variable selection akin to LASSO while simultaneously addressing multicollinearity, as seen in Ridge Regression [16]. The combined L_1 and L_2 penalty terms in the minimization of the Residual Sum of Squares (RSS) are defined in **Equation (3)**.

$$\hat{\beta}_{elastic-net} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} \beta_j^2 \quad (3)$$

2.5. Regularization in Binary Logistic Regression

Binary logistic regression is a statistical method used to analyze the relationship between predictor variables and a response variable with two categories. This model calculates the probability that an observation is classified into either of the two groups [13]. The probability of an observation being classified into Class 1 is defined by the logistic function in **Equation (4)**.

$$p(x) = \frac{\exp\,(\beta_{k0} + \beta^T x)}{1 + \exp\,(\beta_0 + \beta^T x)} \quad (4)$$

In binary logistic regression, regularization is essential to avoid overfitting, particularly when the number of predictors is higher than the sample size or when there is high collinearity among predictors. Regularization is implemented by including a penalty term in the log-likelihood function, stabilizing parameter estimates and improving model interpretability [16]. The penalized estimation process is formalized in **Equation (5) [6]**.

$$\sum_{i=1}^{M} \log p_{ki}(x_i) - \lambda \left[\alpha \sum_{k=1}^{K} \sum_{j=1}^{p} |\beta_{kj}| + (1-\alpha) \sum_{k=1}^{K} \sum_{j=1}^{p} \beta_{kj}^2 \right] \quad (5)$$

The type of regularization applied in binary logistic regression is determined by the tuning parameter (α). If (α=0), the model reduces to Ridge Regression. If (α=1), the model becomes LASSO. If (0<α<1), the model employs Elastic-Net, which combines the penalties of LASSO and Ridge to address the limitations of each method.

2.6. Balanced Bagging Classifier

The Balanced Bagging Classifier is an extension of the bootstrap aggregating technique, an ensemble method that constructs multiple models on different bootstrap samples from the training dataset and aggregates their predictions to improve prediction stability and accuracy [17]. In the Balanced Bagging Classifier, under-sampling of the majority class is performed prior to model construction, ensuring that each base model is trained on a balanced subset of data during each iteration. This method enhances prediction performance for the minority class without compromising overall accuracy, while simultaneously mitigating base model variance and improving model generalizability [18].

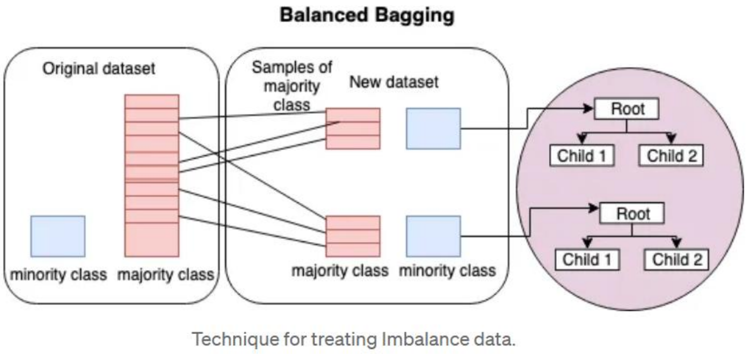

Figure 1. Balanced Bagging Concept [8]

2.7. Data Analysis Procedure

a. Data Exploration
   Data exploration involves examining the dataset structure, analyzing correlations among predictor variables, evaluating the class distribution of the response variable for classification, and identifying missing, duplicate, or invalid entries that require remediation.
b. Data Preprocessing
   During preprocessing, issues identified in the exploratory phase are addressed. This includes handling missing values, removing duplicates, and adjusting data types to ensure compatibility with subsequent analytical requirements.
c. Modelling
   Classification models are developed using regularization methods—LASSO, Ridge, and Elastic-Net—combined with Balanced Bagging aggregation. The analysis is implemented in R software (version 4.4.1) using the 'glmnet' package. Optimal regularization parameters are determined, and final predictions on the test data are derived from models trained with these parameters.
d. Model Performance Evaluation
   Model performance is assessed using classification accuracy metrics: accuracy, sensitivity, precision, and F1-Score. Additionally, the variables selected by each regularization method are compared to evaluate their interpretative consistency and relevance.

3. RESULTS AND DISCUSSION

3.1. Data Exploration

The dataset comprises 196 RDKit variables, which consist of molecular descriptors obtained from chemical compounds represented using the Simplified Molecular Input Line Entry System (SMILES). These descriptors encode information such as atom connectivity within molecules, charge distribution and electronic characteristics, physical surface area and molecular size, atom counts, presence of specific functional groups, lipophilic or hydrophilic tendencies, etc. All descriptors are numerical. A correlation analysis of these molecular descriptors revealed 252 variable pairs with high collinearity (Pearson correlation coefficient ($|r| > 0.8$). This strong inter-dependency among molecular descriptors indicates significant multicollinearity, which may compromise model stability and interpretability. To address this, regularization approaches were employed to automate variable selection, reduce model complexity, and retain predictive accuracy for Drug-Induced Autoimmunity (DIA) risk classification.

The molecular descriptors serve as predictor variables, while the response variable represents the risk of a drug inducing DIA. The class distribution of the response variable is illustrated in **Figure 2**.

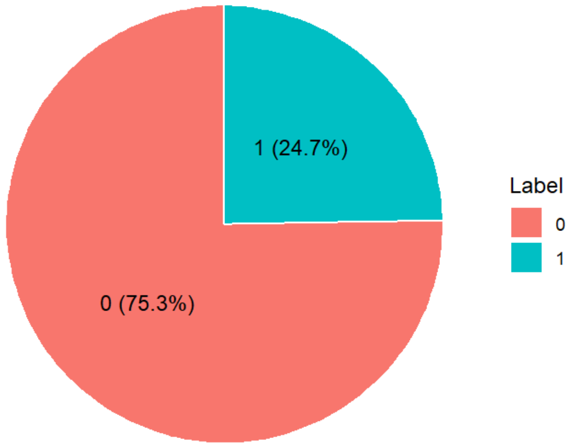

Figure 2. Autoimmune Toxicity Status

Drugs confirmed or documented to induce Drug-Induced Autoimmunity (DIA) constitute 24.7% of the total 477 observations in the dataset. The negative class (0), which includes drugs with no known association with DIA as well as drugs with unconfirmed risk, dominates the dataset (75.3%), indicating significant class imbalance. To address this imbalance, the Balanced Bagging Classifier (BBC) is applied during the modeling phase to ensure equitable learning across classes.

The dataset exhibited no missing values, ensuring completeness in the observational records. However, 19 variables contained duplicate entries, indicating redundant information that could introduce bias or overfitting if unaddressed. Additionally, one variable displayed constant values (zero variance), rendering it non-informative for predictive modeling. These redundant and non-contributing features were pruned during preprocessing to streamline the feature space and enhance model efficiency.

3.2. Data Preprocessing

The dataset was pre-partitioned into two parts: 80% used for training and 20% for testing. The SMILES variable (structural molecular representation) was removed, as its information was already comprehensively encoded in the numerical RDKit descriptors, which served as predictors in the modeling phase. Additionally, variables identified as duplicates during exploratory analysis and the constant variable were pruned to enhance computational efficiency and ensure robust predictive modeling.

3.3. Modelling

The classification models were developed using a two-stage approach for each regularization method. For LASSO Regression, variable selection was achieved by imposing an L_1 penalty on regression coefficients, shrinking non-contributing predictors to zero to produce a sparse model that mitigates overfitting. In contrast, Ridge Regression applied an L_2 penalty to the squared magnitude of coefficients, retaining all variables while stabilizing estimates under high multicollinearity. Elastic-Net, however, combined both L_1 and L_2 penalties, enabling simultaneous variable selection and multicollinearity handling, thereby addressing the limitations of each individual method. The optimal shrinkage parameter (λ) for each technique was determined through cross-validation.

The shrinkage parameter was determined through 10-fold cross-validation for each regularization method. A higher λ value corresponds to stronger coefficient penalties, simplifying the model by reducing its complexity. By selecting λ that minimizes the binomial deviance, the optimal model with the best predictive performance on the training data was identified. The cross-validation curve revealed that beyond the optimal λ point, the binomial deviance increases, indicating that excessive penalization degrades model performance. For LASSO regression, the optimal λ of 0.0187 achieved the best balance between model complexity and predictive accuracy. Ridge regression yielded an optimal λ of 0.1963, while Elastic-Net produced a λ of 0.0341, reflecting method-specific penalty levels to ensure accuracy and prevent overfitting.

Subsequently, the initial predictions from the regularized models were appended as additional variables to the training data, which were then used to train the Balanced Bagging Classifier (BBC). To address class imbalance, balanced subsets were created by under-sampling the majority class, and models were trained on each subset. This process utilized 50 bootstrap samples to enhance model stability and accuracy. The trained Balanced Bagging Classifier (BBC) was subsequently used on the test dataset, with predictions from the regularized models included as additional variables, following the same preprocessing procedures applied during training.

Table 1. Number of Coefficients for Each Model

Method	Number of Coefficients
Elastic-Net	52
LASSO	44
Ridge	176

As shown in **Table 1**, the Ridge model retained all 176 predictors, as its L_2 penalty shrinks coefficients but does not eliminate them. The LASSO model, using an L_1 penalty, reduced the model to 44 predictors by setting many coefficients exactly to zero. Elastic-Net, combining both penalties, retained 52 predictors—balancing between Ridge's retention and LASSO's sparsity. The number of non-zero coefficients reflects model complexity and the extent of variable selection.

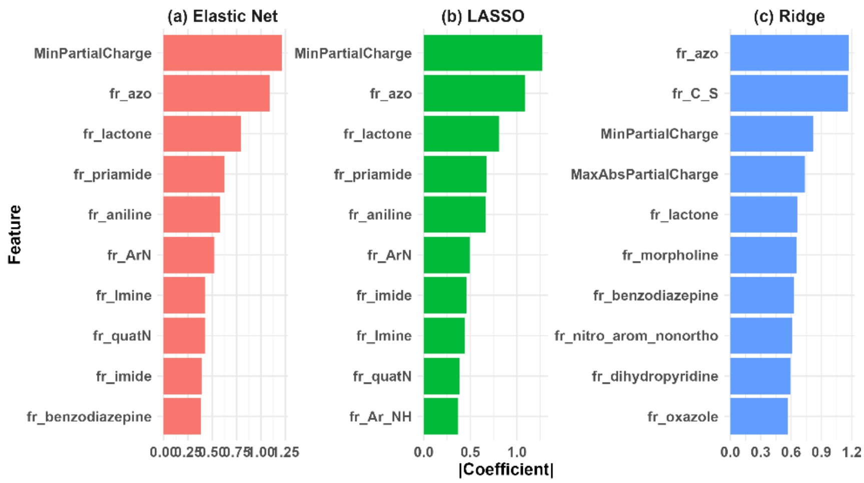

Figure 3. Feature Importance for Each Model (a) Elastic Net (b) LASSO (c) Ridge

Each model identifies the variables contributing most significantly to predictions based on the highest absolute coefficients. Both the Elastic-Net and LASSO models highlight `MinPartialCharge` as the most dominant variable, followed by `fr_azo` and `fr_lactone`, indicating similar patterns in their selection mechanisms despite differences in the total number of retained variables. The consistent prominence of variables such as `fr_priamide`, `fr_aniline`, and `fr_ArN` across both models further underscores their shared relevance in predicting Drug-Induced Autoimmunity (DIA). In contrast, the Ridge model, which retains all predictors, assigns weights to a broader set of variables. While `fr_azo` and `MinPartialCharge` remain influential, the inclusion of additional variables like `fr_C_S` and `MaxAbsPartialCharge` reflects Ridge's tendency to distribute importance across more features, including those excluded by LASSO and Elastic-Net during variable selection. This divergence highlights how regularization methods balance model interpretability against predictive stability.

3.4. Model Performance Evaluation

Final predictions from the modeling results using regularization methods combined with the Balanced Bagging Classifier were subsequently evaluated to assess the model's classification performance, as detailed in **Table 2**.

Table 2. **Model Performance Evaluation**

Model	Accuracy	Sensitivity	Precision	F1-Score
Elastic-Net + BBC	0.825	0.955	0.834	0.891
LASSO + BBC	0.816	0.944	0.833	0.885
Ridge + BBC	0.816	0.955	0.827	0.886

The evaluation results indicate that combining regularization methods with the Balanced Bagging Classifier (BBC) delivers strong overall classification performance. The Elastic-Net + BBC model achieved the highest accuracy (0.825) and F1-Score (0.891), indicating a well-balanced performance between sensitivity and precision. This suggests that the model is effective at correctly identifying positive cases while maintaining a relatively low rate of false positives. The LASSO + BBC model, although slightly lower in accuracy (0.816), achieved the highest precision (0.833), highlighting its strength in minimizing false positive predictions—particularly valuable in applications where misclassifying a negative instance as positive is costly. Meanwhile, the Ridge + BBC model matched LASSO in accuracy (0.816) but exhibited the highest sensitivity (0.955), making it the most effective in capturing true positive cases, which is critical when failing to detect a positive instance poses a higher risk.

Overall, the integration of regularization within the Balanced Bagging Classifier not only addresses data imbalance but also enhances model generalization. As a result, the model becomes more stable, adaptable to data variations, and delivers better predictive performance, particularly on imbalanced datasets. These findings support earlier research that identified the limitations of regularized models such as LASSO and Ridge, which tend to favor majority classes when applied to imbalanced data **[19][20]**. By embedding regularization within the Balanced Bagging framework, this study overcomes those limitations and demonstrates improved classification performance. This suggests that the synergy between regularization and ensemble techniques like Balanced Bagging Classifier can serve as a robust approach in domains where class imbalance is a critical challenge. The effectiveness of the Balanced Bagging Classifier observed in this study is consistent with the work of Barros et al. [8], who showed its superiority over SMOTE and ADASYN in predicting school dropout risks, and Bozcuk and Yildiz [9], Who applied it in the medical field for predicting febrile neutropenia. However, this study goes a step further by incorporating regularization into the ensemble process, resulting in a model that not only achieves balanced classification performance but also maintains interpretability and stability. These results highlight the potential of combining regularization with ensemble methods to build more generalizable predictive models, particularly in healthcare and other domains characterized by imbalanced data distributions.

4. CONCLUSION

Based on the analysis conducted, it can be concluded that the application of regularization methods combined with the Balanced Bagging Classifier (BBC) approach provides strong classification performance in modeling the risk of Drug-Induced Autoimmunity (DIA) on imbalanced data. The Elastic-Net + BBC model demonstrated the best overall performance with a high balance between precision and sensitivity, followed by the LASSO + BBC model, which excelled in precision, and the Ridge + BBC model, which was more sensitive to the positive class. The integration of regularization with Balanced Bagging Classifier has proven effective in enhancing the model's generalization ability and producing more accurate, stable, and adaptive predictions, particularly in binary classification contexts with imbalanced class distributions. This study highlights the potential for applying similar approaches in other predictive studies within the biomedical field.

AUTHOR CONTRIBUTIONS STATEMENT

First Author: Conceptualization, methodology, data curation, formal analysis, software, validation, visualization, writing–original draft. Second Author: Conceptualization, methodology, supervision, project administration, validation, writing–review & editing. Third Author: Conceptualization, methodology, resources, validation, writing–review & editing. Fourth Author: Conceptualization, methodology, supervision, project administration, writing–review & editing.

DATA AVAILABILITY

The data that support the findings of this study are openly available in the UCI Machine Learning Repository at https://archive.ics.uci.edu/dataset/1104/drug_induced_autoimmunity_prediction.

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