

PROJECT REPORT

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FINANCIAL DATA MINING

FINAL PROJECT

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Sunday 5^{th} May, 2024

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1 ABSTRACT

Variable selection is an important issue in regression. Typically, measurements are obtained for a large number of potential predictors in order to avoid missing an important link between a predictive factor and the outcome. This practice has only increased in recent years, as the low cost and easy implementation of automated methods for data collection and storage has led to an abundance of problems for which the number of variables is large in comparison to the sample size.

To reduce variability and obtain a more interpretable model, we often seek a smaller subset of important variables. However, searching through subsets of potential predictors for an adequate smaller model can be unstable [Breiman (1996)][1] and is computationally unfeasible even in modest dimensions.

To avoid these drawbacks, a number of penalized regression methods have been proposed in recent years that perform subset selection in a continuous fashion. Penalized regression procedures accomplish this by shrinking coefficients toward zero in addition to setting some coefficients exactly equal to zero (thereby selecting the remaining variables). The most popular penalized regression method is the lasso [Tibshirani (1996)][2]. Although the lasso has many attractive properties, the shrinkage introduced by the lasso results in significant bias toward 0 for large regression coefficients.

Other authors have proposed alternative penalties, designed to diminish this bias. Two such proposals are the Smoothly Clipped Absolute Deviation (SCAD) penalty [Fan and Li (2001)][3] and the Mimimax Concave Penalty [MCP; Zhang (2010)][4]. In proposing SCAD and MCP, their authors established that SCAD and MCP regression models have the so-called oracle property, meaning that, in the asymptotic sense, they perform as well as if the analyst had known in advance which coefficients were zero and which were nonzero.

2 INTRODUCTION

In numerous scientific disciplines, such as biology, the selection of appropriate variables for regression analysis is paramount. This involves identifying the most influential predictors from a plethora of variables to ensure accurate outcome predictions. To address this challenge, researchers have turned to nonconvex penalty functions like Smoothly Clipped Absolute Deviation (SCAD) and Minimax Concave Penalty (MCP) due to their *Oracle Property*.

The penalty functions for SCAD and MCP are nonconvex, which introduces numerical challenges in fitting these models. For the lasso, which does possess a convex penalty, least angle regression is a remarkably efficient method for computing an entire path of lasso solutions in the same order of time as a least squares fit. For nonconvex penalties, Zou and Li (2008)[5] have proposed making a local linear approximation (LLA) to the penalty, thereby yielding an objective function that can be optimized using the LARS algorithm.

More recently, coordinate descent algorithms for fitting lasso-penalized models have been shown to be competitive with the LARS algorithm, particularly in high dimensions [Friedman et al. (2007); Wu and Lange (2008)[6]; Friedman, Hastie and Tibshirani (2010)][7]. In the research paper, the application of Coordinate Descent Algorithms to SCAD and MCP regression models, for which the penalty is nonconvex is investigated. We will be going a step further and investigating the application of Stochastic Gradient Descent and Proximal Gradient Descent algorithms.

Methods for high-dimensional regression and variable selection have applications in many scientific fields, particularly those in high-throughput biomedical studies.

3 NON-CONVEX PENALTIES

Nonconvex penalties play a crucial role in regression by addressing the challenge of sparsity in coefficient estimates. Traditional convex penalties, such as the Lasso, tend to shrink all coefficients towards zero indiscriminately, potentially retaining variables that are not truly predictive. Nonconvex penalties, on the other hand, offer a more nuanced approach. By penalizing large coefficient values more heavily than small ones, they effectively encourage simpler models with fewer predictors. This mechanism promotes variable selection by driving less important coefficients towards zero, effectively excluding irrelevant predictors from the model.

The use of nonconvex penalties in regression is motivated by the desire to strike a balance between model complexity and predictive accuracy. In many real-world applications, especially those involving high-dimensional data, the number of potential predictors can far exceed the number of observations. This situation can lead to overfitting, where the model captures noise in the data rather than true underlying patterns. Nonconvex penalties help mitigate this risk by promoting sparsity in the coefficient estimates, thereby reducing the likelihood of overfitting and improving the generalization performance of the model.

Despite their advantages, nonconvex penalties also pose certain challenges. One such challenge is the computational complexity involved in optimizing models with these penalties, particularly when compared to models with convex penalties. Efficient optimization algorithms are required to fit models with nonconvex penalties effectively, ensuring that the computational burden remains manageable even for large-scale datasets.

In this project, we will delve into two prominent nonconvex penalties used in regression:

- Smoothly Clipped Absolute Deviation (SCAD)
- Minimax Concave Penalty (MCP)

We will explore their respective advantages and disadvantages, investigate their theoretical properties, and assess their performance in practical applications. By gaining a deeper understanding of these nonconvex penalties, we aim to provide insights into their suitability for various regression tasks and inform best practices for model selection and interpretation.

3.1 Smoothly Clipped Absolute Deviation (SCAD)

In the realm of regression analysis, the SCAD (Smoothly Clipped Absolute Deviation) penalty emerges as a powerful tool for addressing key challenges encountered with traditional methods. At its core, SCAD represents a departure from the linear penalty structures found in conventional techniques like the Lasso. Instead, it offers a nuanced approach, leveraging a specially designed penalty function that dynamically adjusts the severity of penalization based on the size of regression coefficients.

One of the primary motivations behind SCAD's development was to combat the tendency of traditional penalties to induce bias, particularly for large coefficient values. By incorporating a non-linear penalty function, SCAD introduces a level of adaptability that allows it to penalize large coefficients more aggressively while still maintaining desirable properties like continuity and thresholding.

The SCAD penalty function is characterized by its smooth, quadratic spline nature, featuring distinct knots that dictate the transition points between penalty regimes. This design ensures that the penalty is continuous and differentiable, facilitating efficient optimization procedures even in the presence of non-convexity.

Practically, the SCAD penalty serves two key purposes in regression analysis. Firstly, it encourages sparsity in the coefficient estimates by penalizing large coefficients more heavily, thereby promoting variable selection. Secondly, it helps mitigate bias associated with large coefficient values, leading to more accurate and interpretable models.

In high-dimensional settings, where the number of potential predictors exceeds the number of observations, SCAD offers a compelling solution. Its ability to simultaneously achieve variable selection and estimation makes it particularly well-suited for scenarios where model complexity needs to be carefully balanced against predictive accuracy.[8]

eds to be carefully balanced against predictive accuracy.[8]
The SCAD penalty function is as follows:
$$p(\beta) = \begin{cases} \frac{\lambda |\beta|^{2(a-1)}}{2a\lambda |\beta|^2 - \beta^2} - \frac{\lambda}{2} & \text{if } |\beta| \leq \lambda \\ \frac{2}{\lambda^2 (a+1)} & \text{if } \lambda < |\beta| \leq a\lambda \\ 0 & \text{otherwise} \end{cases}$$

3.2 Minimax Concave Penalty (MCP)

In the realm of regression analysis, the Minimax Concave Penalty (MCP) emerges as a formidable alternative to traditional methods like the Lasso and SCAD, offering less biased regression coefficients in sparse models. Introduced by Zhang in 2010, MCP serves as a potent tool for addressing the challenges associated with variable selection and estimation in high-dimensional datasets.

At its core, MCP operates by penalizing large regression coefficients while maintaining desirable properties like sparsity and unbiasedness. The penalty function of MCP is defined by a carefully crafted derivative that adjusts penalization based on the size of the coefficients, striking a balance between bias reduction and model complexity.

Mathematically, the MCP penalty function p() is expressed as follows:

$$p(\beta) = \begin{cases} \lambda |\beta| - \frac{2a\beta^2}{a\lambda^2} & \text{if } |\beta| \le a\lambda \\ 0 & \text{otherwise} \end{cases}$$

Where:

- β represents the coefficient estimates.
- $|\beta|$ denotes the absolute value of β .
- λ is the regularization parameter, controlling the strength of penalization.
- a is a parameter greater than 1, influencing the curvature of the penalty function.

Derivative of the Penalty Function:

$$p'(\beta) = \begin{cases} \operatorname{sgn}(\beta)(\lambda - a|\beta|) & \text{if } |\beta| \le a\lambda \\ 0 & \text{otherwise} \end{cases}$$

Where:

• $sgn(\beta)$ represents the sign of β .

One notable feature of MCP is its ability to minimize the maximum concavity among penalty functions satisfying certain conditions, making it the "most convex" choice within this framework. This property, along with its capability for unbiased variable selection, positions MCP as a valuable tool in regression analysis, particularly in scenarios with high-dimensional data and sparse models.

In comparison to SCAD, MCP offers a distinct approach to penalty imposition and coefficient estimation. While both methods aim to reduce bias in regression coefficients and promote sparsity, they differ in their penalty functions and underlying optimization mechanisms. MCP achieves its objectives by minimizing concavity and ensuring unbiasedness, thereby offering researchers an alternative avenue for tackling the complexities of modern regression analysis.

Overall, MCP represents a significant advancement in the field of variable selection regularization, offering researchers a powerful and flexible tool for addressing the challenges posed by high-dimensional datasets and sparse models.[9]

4 OPTIMIZATION ALGORITHMS

Optimization algorithms play a pivotal role in modern data analysis by facilitating efficient parameter estimation in regression models. Particularly, when dealing with nonconvex penalty functions like MCP and SCAD, specialized optimization techniques become essential for achieving accurate results in variable selection and model fitting.

In the context of regression analysis, the primary goal is to minimize a certain objective function that captures the discrepancy between the observed data and the model predictions. This function typically includes a term for the goodness-of-fit and a penalty term that penalizes complex models, promoting simplicity and sparsity in the final model.

For nonconvex penalty functions such as MCP and SCAD, traditional optimization methods may struggle due to the presence of multiple local minima and non-smoothness of the penalty functions. This is where tailored optimization algorithms come into play, offering efficient strategies for navigating the complex landscape of parameter space and finding the optimal solution.

The following three optimization techniques help in regression analysis:

- Stochastic Gradient Descent
- Proximal Gradient Descent
- Coordinate Gradient Descent

4.1 Stochastic Gradient Descent

Stochastic Gradient Descent (SGD) stands as a prominent iterative optimization method frequently utilized in machine learning tasks, particularly in scenarios where vast datasets and complex models are involved. Unlike traditional gradient descent algorithms that compute gradients based on the entire dataset, SGD updates model parameters incrementally using only one data point at each iteration.

This method offers several advantages over batch gradient descent, especially in the context of large-scale problems encountered in regression analysis with nonconvex penalty functions like MCP and SCAD. By processing individual data points rather than the entire dataset at once, SGD significantly reduces computation time and memory requirements, making it well-suited for handling massive datasets.

In essence, SGD operates by iteratively updating model parameters in the direction of the negative gradient of the objective function with respect to a single data point. This iterative approach allows SGD to navigate the parameter space more efficiently, ultimately converging to a local minimum while offering computational advantages, especially when dealing with high-dimensional data.

In the context of regression with nonconvex penalty functions like MCP and SCAD, SGD serves as a crucial optimization algorithm for efficiently minimizing the objective function and estimating model parameters. By incorporating SGD into the optimization procedure, researchers can expedite the process of fitting regression models, enabling faster convergence and improved scalability, particularly in scenarios involving large datasets and complex models.

$$\theta_{i+1} = \theta_i - \alpha \times \nabla_{\theta} J(\theta; x_j; y_j)$$

Where:

• θ represents the model parameters.

- α is the learning rate.
- $J(\theta; x_j; y_j)$ denotes the objective function evaluated with a single data point (x_j, y_j) .
- $\nabla_{\theta} J(\theta; x_j; y_j)$ is the gradient of the objective function with respect to the model parameters.

4.2 Proximal Gradient Descent

Proximal Gradient Descent (PGD) is a powerful optimization algorithm widely employed in machine learning and regression analysis, particularly when dealing with nonconvex penalty functions like MCP and SCAD. Unlike traditional gradient descent methods, PGD incorporates a proximal operator to handle non-smooth penalty terms efficiently.

PGD combines the advantages of gradient descent with the ability to handle non-smooth penalty functions, making it well-suited for sparse regression models where variable selection is crucial. By leveraging proximal operators, PGD can efficiently navigate the parameter space, leading to faster convergence and improved model estimation accuracy.

In the context of regression analysis with MCP and SCAD regularization, PGD offers several advantages over traditional optimization algorithms. Firstly, PGD allows for the incorporation of non-smooth penalty functions directly into the optimization process, enabling efficient variable selection and model fitting. Secondly, PGD can handle large-scale datasets and high-dimensional parameter spaces, making it suitable for complex regression problems encountered in practice.

Compared to Stochastic Gradient Descent (SGD), which updates model parameters based on individual data points, PGD takes a more direct approach by considering the entire dataset at each iteration. This allows PGD to exploit global information in the dataset, potentially leading to more stable convergence and improved model performance.

Specifically, PGD finds its utility in scenarios where accurate estimation of model parameters is essential, and variable selection plays a crucial role. In regression analysis with MCP and SCAD regularization, PGD facilitates the efficient estimation of sparse regression models while ensuring the stability and convergence of the optimization process.

$$\theta_{i+1} = \text{prox}_{\alpha\lambda}(\theta_i - \alpha \nabla J(\theta_i))$$

Where:

- θ represents the model parameters.
- α is the step size or learning rate.
- λ is the regularization parameter.
- $J(\theta)$ denotes the objective function.
- $\nabla J(\theta)$ is the gradient of the objective function.
- $\operatorname{prox}_{\alpha\lambda}(\cdot)$ denotes the proximal operator, which applies the soft-thresholding function with parameter $\alpha\lambda$.

4.3 Coordinate Gradient Descent

Coordinate Gradient Descent (CGD) stands out as a prominent optimization algorithm frequently employed in regression analysis, especially when dealing with nonconvex penalty functions like MCP and SCAD. Unlike traditional gradient descent methods that update all model parameters simultaneously, CGD updates one parameter at a time while keeping others fixed. This allows CGD to efficiently navigate the parameter space, particularly in high-dimensional settings.

In the context of regression with MCP and SCAD regularization, CGD offers several advantages over other optimization algorithms. Firstly, CGD is computationally efficient, especially when dealing with high-dimensional datasets, as it updates only one parameter at each iteration. This can lead to faster convergence and reduced computational complexity compared to methods that update all parameters simultaneously.

Furthermore, CGD can handle non-smooth penalty functions efficiently, making it well-suited for sparse regression models where variable selection is crucial. By updating parameters sequentially, CGD can effectively explore the parameter space and identify important predictors while disregarding irrelevant ones, thereby improving the interpretability and accuracy of the resulting regression model.

Compared to Proximal Gradient Descent (PGD), which incorporates a proximal operator to handle non-smooth penalty terms, CGD takes a different approach by updating parameters sequentially. While PGD may offer faster convergence in some cases, CGD can be more straightforward to implement and may exhibit better performance in certain scenarios, particularly when dealing with highly correlated predictors.

Additionally, unlike Stochastic Gradient Descent (SGD), which updates parameters based on individual data points, CGD considers the entire dataset at each iteration. This allows CGD to exploit global information in the dataset, potentially leading to more stable convergence and improved model performance, especially in scenarios with limited computational resources.

$$\theta_{i+1}^{(j)} = \text{prox}_{\alpha\lambda}(\theta_i^{(j)} - \alpha \frac{\partial \theta^{(j)}}{\partial J})$$

Where:

- θ represents the model parameters.
- α is the step size or learning rate.
- λ is the regularization parameter.
- $J(\theta)$ denotes the objective function.
- $\frac{\partial J}{\partial \theta^{(j)}}$ is the partial derivative of the objective function with respect to the j-th parameter.
- $\operatorname{prox}_{\alpha\lambda}(\cdot)$ denotes the proximal operator, which applies the soft-thresholding function with parameter $\alpha\lambda$.

5 DATASET

The Breast Cancer Wisconsin (Diagnostic) dataset, available through the UCI Machine Learning Repository, encompasses features extracted from digitized images of fine needle aspirates (FNA) of breast masses. These features play a crucial role in diagnosing breast cancer as malignant or benign.

The Key features are:

- ID number: Unique identifier for each instance in the dataset.
- Diagnosis: Indicates whether the breast mass is malignant (M) or benign (B).
- Mean Radius: Mean of distances from center to points on the perimeter of the nucleus.
- **Texture:** Standard deviation of gray-scale values in the nucleus.
- Perimeter: Perimeter of the nucleus.
- Area: Area of the nucleus.
- Smoothness: Local variation in radius lengths of the nucleus.
- Compactness: Measure of compactness calculated as (perimeter 2 /area) -1.0.
- Concavity: Severity of concave portions of the contour of the nucleus.
- Concave Points: Number of concave portions of the contour of the nucleus.
- **Symmetry:** Symmetry of the nucleus.
- Fractal Dimension: Measure of the complexity of the contour of the nucleus, known as "coastline approximation."

These features are computed based on the mean, standard error, and "worst" values, resulting in a total of 30 features per image. The dataset comprises 569 instances, with 357 benign and 212 malignant diagnoses.

	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	symmetry_mean	fractal_dimension_mean
0	М	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	0.07871
1	М	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	0.05667
2	М	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	0.05999
3	М	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	0.09744
4	М	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	0.05883

Figure 1: Mean Values

radius_se	texture_se	perimeter_se	area_se	smoothness_se	compactness_se	concavity_se	concave points_se	symmetry_se	fractal_dimension_se
1.0950	0.9053	8.589	153.40	0.006399	0.04904	0.05373	0.01587	0.03003	0.006193
0.5435	0.7339	3.398	74.08	0.005225	0.01308	0.01860	0.01340	0.01389	0.003532
0.7456	0.7869	4.585	94.03	0.006150	0.04006	0.03832	0.02058	0.02250	0.004571
0.4956	1.1560	3.445	27.23	0.009110	0.07458	0.05661	0.01867	0.05963	0.009208
0.7572	0.7813	5.438	94.44	0.011490	0.02461	0.05688	0.01885	0.01756	0.005115

Figure 2: Standard Error Values

radiu	s_worst	texture_worst	perimeter_worst	area_worst	smoothness_worst	compactness_worst	concavity_worst	concave points_worst	symmetry_worst	fractal_dimension_worst
	25.38	17.33	184.60	2019.0	0.1622	0.6656	0.7119	0.2654	0.4601	0.11890
	24.99	23.41	158.80	1956.0	0.1238	0.1866	0.2416	0.1860	0.2750	0.08902
	23.57	25.53	152.50	1709.0	0.1444	0.4245	0.4504	0.2430	0.3613	0.08758
	14.91	26.50	98.87	567.7	0.2098	0.8663	0.6869	0.2575	0.6638	0.17300
	22.54	16.67	152.20	1575.0	0.1374	0.2050	0.4000	0.1625	0.2364	0.07678

Figure 3: Worst Values

6 EXPLORATORY DATA ANALYSIS

Listing 1: Feature Data Types

6.1 Five Point Summary & Quantiles

	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	symmetry_mean	fractal_dimension_mean
count	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000 5
mean	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.088799	0.048919	0.181162	0.062798
std	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.079720	0.038803	0.027414	0.007060
min	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.000000	0.000000	0.106000	0.049960
25%	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.029560	0.020310	0.161900	0.057700
50%	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.061540	0.033500	0.179200	0.061540
75%	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.130700	0.074000	0.195700	0.066120
max	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.426800	0.201200	0.304000	0.097440

Figure 4: Metadata for Mean Parameters

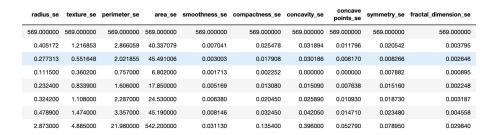


Figure 5: Metadata for Standard Error Parameters

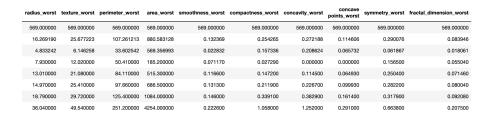


Figure 6: Metadata for worst parameters

6.2 Inferences and Visualizations

6.2.1 Distribution Analysis

- Count plot for diagnosis: Class distribution: 357 benign, 212 malignant
- Violin plot for Mean Parameters: One can seen that radius_mean, texture_mean, perimeter_mean, area_mean, compactness_mean, concavity_mean, concave points_mean have well-defined and separated means for the two classes of diagnosis, in comparison to, smoothness_mean, symmetry_mean, fractal_dimension_mean. This entails that the former variables are better classifiers as compared to the latter variables.

- Violin Plot for Standard Error Parameters: One can see that radius_se, perimeter_se, area_se, compactness_se, concavity_se, concave_points_se have well-defined and separated means for the two classes of diagnosis, in comparison to, smoothness_se, symmetry_se, fractal_dimension_se, texture_se. This entails that the former variables are better classifiers as compared to the latter variables.
- Violin Plot for Worst Parameters: One can see that radius_worst, texture_worst, perimeter_worst, area_worst, smoothness_worst, compactness_worst, concavity_worst, concave points_worst have well-defined and separated means for the two classes of diagnosis, in comparison to, symmetry_worst and fractal_dimension_worst. This entails that the former variables are better classifiers as compared to the latter variables.

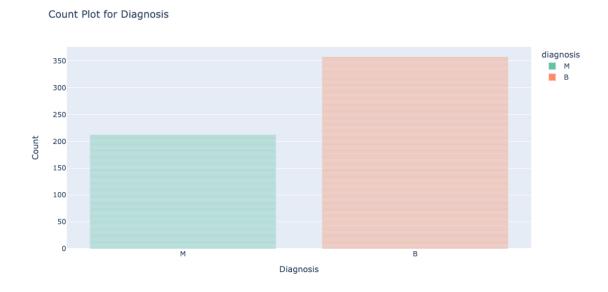


Figure 7: Count Plot For Diagnosis



Figure 8: Violin Plot for Mean Parameters

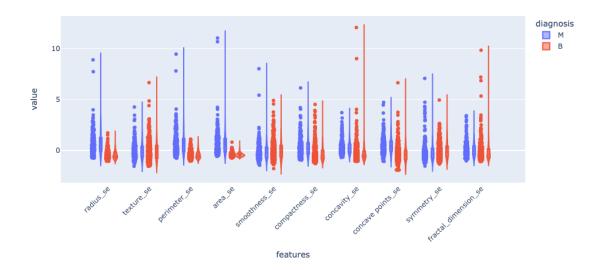


Figure 9: Violin Plot for Standard Error Parameters

Violin Plot for Third Ten Features

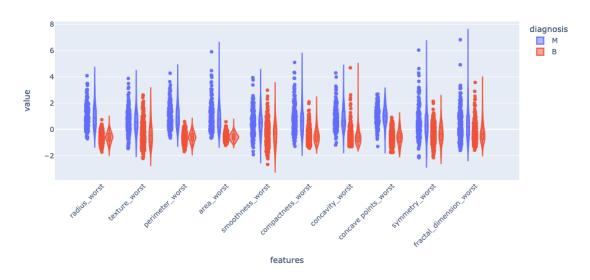


Figure 10: Violin Plot for Worst Parameters

6.2.2 Correlation Analysis

Correlation Heatmap

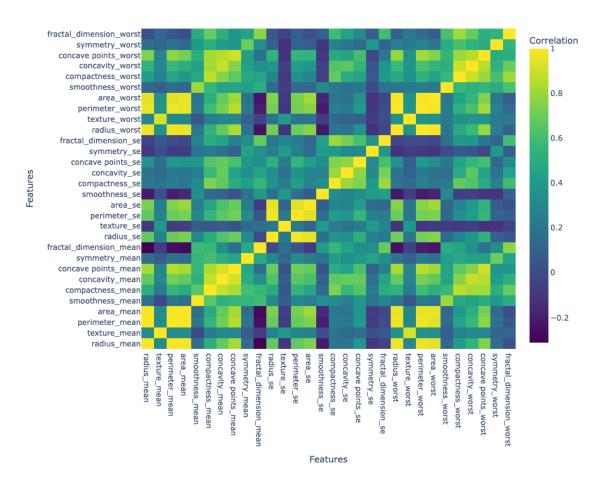


Figure 11: Correlation Heat Map

```
[('radius_mean', 'perimeter_mean'),('radius_mean', 'area_mean'),('radius_mean', 'radius_worst'),('radius_mean', 'perimeter_worst'),('radius_mean', 'area_mean'),('perimeter_mean', 'concave points_mean'),('perimeter_mean', 'radius_worst'),('perimeter_mean', 'perimeter_mean', 'perimeter_worst'),('area_mean', 'radius_worst'),('area_mean', 'perimeter_worst'),('area_mean', 'area_worst'), ('compactness_mean', 'concavity_mean'),('compactness_mean', 'concavity_mean', 'concave points_mean', 'concave points_mea
```

Listing 2: Pairs of variables with high correlation (above 0.85)

Correlation Matrix with High Correlation Pairs

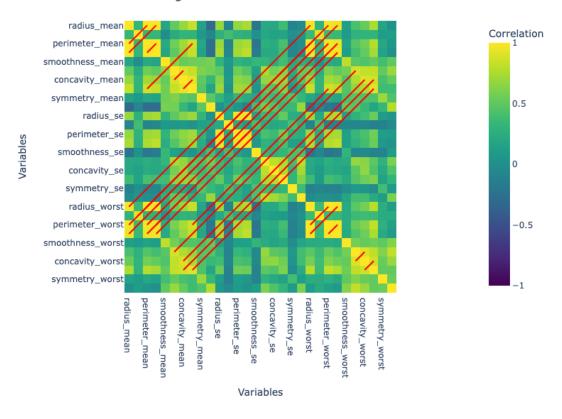


Figure 12: Correlation Matrix with Highly Correlated Pairs

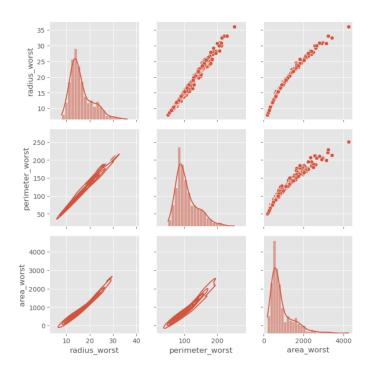


Figure 13: Correlation between Area worst, Perimeter worst, Radius worst

7 MINIMAX CONCAVE PENALTY

Accuracy: 0.9211 Classification Report:

Listing 3: Logistic Regression with MCP Penalty

Logistic Regression was performed with the MCP penalty included in the loss function to implement sparsity. The optimization method being used is the *Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS)* algorithm. A variant of this algorithm, that is, the L-BFGS-B was used as we are handling bound constraints in our loss function.

The α and γ values that control the strength and shape of the penalty function respectively, are by default set to 0.01 and 1.5 respectively. We will further optimize these parameters by hyper-parameter tuning.

recall f1-score



Figure 14: Classification Report for Logistic Regression with MCP Penalty

7.1 Hyperparameter Tuning

```
# Split the data into train and test sets
x_train, x_test, y_train, y_test = train_test_split(x_scaled, y, test_size=0.2, random_state=42)
             # Define the logistic loss function with MCP penalty def logistic_loss(w, X, y, alpha=0.01, gamma=1.5): # MCP parameters alpha and gamma
                           r = len(y)
yz = y * np.dot(X, w)
loss = np.sum(np.log1p(np.exp(-yz)))
reg = alpha * np.sum(np.sqrt(1 + (w / (gamma * alpha))**2) - 1)
return loss + reg
13
            initial_w = np.zeros(x_train.shape[1])
             # Define the optimization function
            # Define the optimization function

def optimize_model(params):
    alpha = params['alpha']
    gamma = params['gamma']
    result = minimize(logistic_loss, initial_w, args=(x_train, y_train, alpha, gamma), method='L-BFGS-B')
    optimal_w = result.x

    result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_result_resul
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                            y_pred = predict(x_test, optimal_w)
accuracy = accuracy_score(y_test, y_pred)
23
                             return accuracy, optimal_w
            # Define the parameter grid for hyperparameter tuning param_grid = {'alpha': [0.001, 0.01, 0.1], 'gamma': [1.0, 1.5, 2.0, 2.5, 3, 3.5, 4]}
            best_accuracy = 0
best_params = None
best_optimal_w = None
             # Perform hyperparameter tuning using ParameterGrid
for params in ParameterGrid(param_grid):
32
33
                            params in Parameterrid(param_grid):
accuracy, optimal_w = optimize_model(params)
print(f"Params: {params}, Accuracy: {accuracy:.4f}")
if accuracy > best_accuracy:
   best_accuracy = accuracy
   best_params = params
   best_optimal_w = optimal_w
                                            best_optimal_w = optimal_w
             print("Best Parameters:", best_params)
             print("Best Accuracy:", best_accuracy)
          # Predict using the best optimized coefficients
y_pred = predict(x_test, best_optimal_w)
```

Listing 4: Hyperparameter tuning for MCP Penalty

```
Params: {'alpha': 0.001, 'gamma': 1.0}, Accuracy: 0.9298
Params: {'alpha': 0.001, 'gamma': 1.5}, Accuracy: 0.9211
Params: {'alpha': 0.001, 'gamma': 2.0}, Accuracy: 0.9123
Params: {'alpha': 0.001, 'gamma': 2.5}, Accuracy: 0.9123
Params: {'alpha': 0.001, 'gamma': 3.5}, Accuracy: 0.9123
Params: {'alpha': 0.001, 'gamma': 3.5}, Accuracy: 0.9123
Params: {'alpha': 0.001, 'gamma': 4}, Accuracy: 0.9123
Params: {'alpha': 0.01, 'gamma': 1.0}, Accuracy: 0.9298
Params: {'alpha': 0.01, 'gamma': 1.5}, Accuracy: 0.9213
Params: {'alpha': 0.01, 'gamma': 2.0}, Accuracy: 0.9213
Params: {'alpha': 0.01, 'gamma': 2.5}, Accuracy: 0.9123
Params: {'alpha': 0.01, 'gamma': 3.5}, Accuracy: 0.9123
Params: {'alpha': 0.01, 'gamma': 3.5}, Accuracy: 0.9123
Params: {'alpha': 0.01, 'gamma': 3.5}, Accuracy: 0.9123
Params: {'alpha': 0.1, 'gamma': 1.0}, Accuracy: 0.9298
Params: {'alpha': 0.1, 'gamma': 1.5}, Accuracy: 0.9298
Params: {'alpha': 0.1, 'gamma': 1.5}, Accuracy: 0.9298
Params: {'alpha': 0.1, 'gamma': 2.5}, Accuracy: 0.9035
Params: {'alpha': 0.1, 'gamma': 3}, Accuracy: 0.9035
Params: {'alpha': 0.1, 'gamma': 3}, Accuracy: 0.9035
Params: {'alpha': 0.1, 'gamma': 3.5}, Accuracy: 0.9035
```

Figure 15: Parameter Grid Accuracy Comparision

Post hyper-parameter tuning we see that the α and γ values that gives us the best accuracy without the risk of over-penalizing the coefficients are 0.001 and 1.0 respectively. We will be using these values of α and γ to run the Coordinate Descent, Stochastic Gradient Descent, and the Proximal Gradient Descent algorithms.



Figure 16: Classification Report for Optimized parameters with MCP Penalty

7.2 Coordinate Descent with MCP Penalty

Listing 5: Coordinate Descent Optimization with MCP Penalty

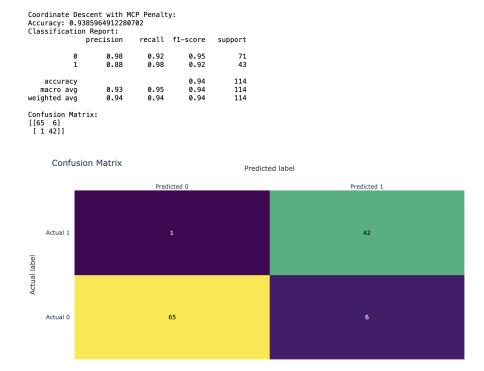


Figure 17: Classification Report for Coordinate Descent with MCP Penalty

7.3 Stochastic Gradient Descent with MCP Penalty

```
# Split the data into train and test sets
     x_train, x_test, y_train, y_test = train_test_split(x_scaled, y, test_size=0.2, random_state=42)
     # Define the logistic loss function with MCP penalty def logistic_loss(w, X, y, alpha=0.001, gamma=1): # MCP parameters alpha and gamma
    n = len(y)
yz = y * np.dot(X, w)
loss = np.sum(np.logip(np.exp(-yz)))
reg = alpha * np.sum(np.sqrt(1 + (w / (gamma * alpha))**2) - 1)
return loss + reg
# Stochastic Gradient Descent for MCP Penalty
10
11
     def stochastic_gradient_descent_mcp(X, y, alpha=0.001, gamma=1, max_iter=1000, tol=1e-5, learning_rate=0.01):#p
    n, d = X.shape
    w = np.zeros(d)
    f
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18
19
          yz = y_i * np.dot(X_i, w)
grad = -X_i * y_i / (1 + np.exp(yz))
w -= learning_rate * grad
w = np.sign(w) * np.maximum(0, np.abs(w) - alpha * gamma) / ((1 + alpha * gamma) * gamma)
\frac{20}{21}
22
23
24
                 if np.linalg.norm(grad) < tol:</pre>
26
     w_sgd_mcp = stochastic_gradient_descent_mcp(x_train, np.array(y_train))
def predict(X, w):#p
  logits = np.dot(X, w)
            return np.where(logits >= 0, 1, 0)
    y_pred_sgd_mcp = predict(x_test, w_sgd_mcp)
```

Listing 6: Stochastic Gradient Descent with MCP Penalty

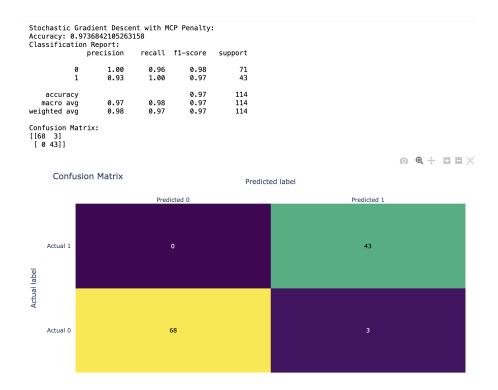


Figure 18: Classification Report for Stochastic Gradient Descent with MCP Penalty

7.4 Proximal Gradient Descent with MCP Penalty

Listing 7: Proximal Gradient Descent with MCP Penalty

Proximal Gradie Accuracy: 0.973			Penalty:		
ck to scroll output; doub P	le click to hide recision	recall	f1–score	support	
0 1	1.00 0.93	0.96 1.00	0.98 0.97	71 43	
accuracy macro avg weighted avg	0.97 0.98	0.98 0.97	0.97 0.97 0.97	114 114 114	
Confusion Matri [[68 3] [0 43]]	x:				
Confusio	n Matrix			Predi	icted label
		Predic	ted 0		Predicted 1
Actual 1		0			43
Actual label					
Actua					
Actual 0		68	3		3

Figure 19: Classification Report for Proximal Gradient Descent with MCP Penalty

Comparing the accuracy obtained from Coordinate Descent, Stochastic Gradient Descent, and Proximal Gradient Descent, applied on a loss function with the MCP penalty it was seen that the penalization has been very aggressive for the Stochastic Gradient and Proximal Gradient algorithms leading to over-fitting. Therefore, one conclude that Coordinate Descent algorithm works best for a loss function with an MCP penalty. This is in line with the conclusions being derived in the reference paper.

8 SMOOTHLY CLIPPED ABSOLUTE DEVIATION

Listing 8: Logistic Regression with SCAD Penalty

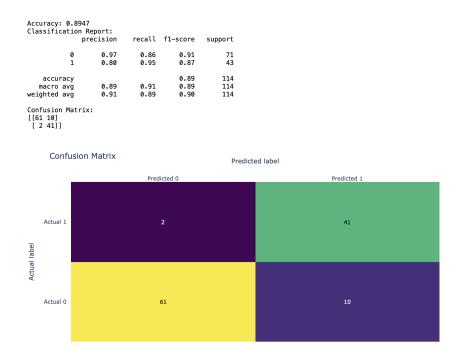


Figure 20: Classification Report for Logistic Regression with SCAD Penalty

Logistic Regression was performed with the SCAD penalty included in the loss function to implement sparsity. The optimization method being used is the *Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS)* algorithm. A variant of this algorithm, that is, the L-BFGS-B was used as we are handling bound constraints in our loss function.

The α and γ values that control the strength and shape of the penalty function respectively, are by default set to 0.01 and 3.7 respectively. We will further optimize these parameters by hyper-parameter tuning.

8.1 Hyperparameter Tuning

```
# Split the data into train and test sets
x_train, x_test, y_train, y_test = train_test_split(x_scaled, y, test_size=0.2, random_state=42)
     # Define the logistic loss function with SCAD penalty def logistic_loss(w, X, y, alpha=0.01, gamma=3.7): # SCAD parameters alpha and gamma
          n = len(y)
yz = y * np.dot(X, w)
loss = np.sum(np.log1p(np.exp(-yz)))
          reg = alpha * np.sum(np.where(np.abs(w) <= alpha, 0, np.where(np.abs(w) <= gamma * alpha, (gamma * alpha - np.abs(w)) / (gamma - 1), alpha / (gamma - 1))))
return loss + reg
12
    # Initialize coefficients
    initial_w = np.zeros(x_train.shape[1])
     # Predict using the optimized coefficients
def predict(X, w):
16
           logits = np.dot(X, w)
           return np.where(logits >= 0, 1, 0)
     # Define the optimization function
20
          alpha = params['alpha']
gamma = params['gamma']
result = minimize(logistic_loss, initial_w, args=(x_train, y_train, alpha, gamma), method='L-BFGS-B')
optimal_w = result.x
23
24
26
27
28
           y_pred = predict(x_test, optimal_w)
accuracy = accuracy_score(y_test, y_pred)
           return accuracy, optimal_w
    # Define the parameter grid for hyperparameter tuning
param_grid = {'alpha': [0.01, 0.1, 1.0], 'gamma': [2.0, 3.0, 3.7, 4.0]}
33
34
     best_accuracy = 0
best_params = None
     best_optimal_w = None
     # Perform hyperparameter tuning using ParameterGrid
     for params in ParameterGrid(param_grid):
    accuracy, optimal_w = optimize_model(params)
    print(f"Params: {params}, Accuracy: {accuracy:.4f}")
39
40
           if accuracy > best_accuracy:
   best_accuracy = accuracy
   best_params = params
   best_optimal_w = optimal_w
41
43
    print("Best Parameters:", best_params)
print("Best Accuracy:", best_accuracy)
     # Predict using the best optimized coefficients
49
50 y_pred = predict(x_test, best_optimal_w)
```

Listing 9: Hyperparameter tuning for SCAD Penalty

```
Params: {'alpha': 0.01, 'gamma': 2.0}, Accuracy: 0.8947
Params: {'alpha': 0.01, 'gamma': 3.0}, Accuracy: 0.8947
Params: {'alpha': 0.01, 'gamma': 3.7}, Accuracy: 0.8947
Params: {'alpha': 0.01, 'gamma': 4.0}, Accuracy: 0.8947
Params: {'alpha': 0.1, 'gamma': 2.0}, Accuracy: 0.8947
Params: {'alpha': 0.1, 'gamma': 3.0}, Accuracy: 0.8860
Params: {'alpha': 0.1, 'gamma': 3.7}, Accuracy: 0.8947
Params: {'alpha': 0.1, 'gamma': 3.7}, Accuracy: 0.8947
Params: {'alpha': 1.0, 'gamma': 2.0}, Accuracy: 0.9123
Params: {'alpha': 1.0, 'gamma': 3.0}, Accuracy: 0.9123
Params: {'alpha': 1.0, 'gamma': 4.0}, Accuracy: 0.9123
Params: {'alpha': 1.0, 'gamma': 4.0}, Accuracy: 0.9123
Best Parameters: {'alpha': 1.0, 'gamma': 2.0}
Best Accuracy: 0.9122807017543859
```

Figure 21: Parameter Grid for Accuracy Comparision for SCAD Penalty

Post hyper-parameter tuning we see that the α and γ values that gives us the best accuracy without the risk of over-penalizing the coefficients are 1.0 and 2.0 respectively. We will be using these values of α and γ to run the Coordinate Descent, Stochastic Gradient Descent, and the Proximal Gradient Descent algorithms.

Classificat	ion Repo	rt:			
	preci	.sion	recall	f1-score	support
	0	0.97	0.89	0.93	71
	1	0.84	0.95	0.89	43
accurac	:y			0.91	114
macro av	/g	0.90	0.92	0.91	114
weighted av	/g	0.92	0.91	0.91	114
Confusion M [[63 8] [2 41]]	latrix:				

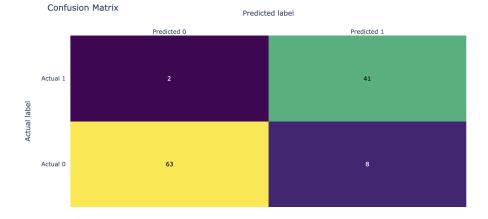


Figure 22: Classification Report for Optimized parameters with SCAD Penalty

8.2 Coordinate Descent with SCAD Penalty

```
# Split the data into train and test sets
      x_train, x_test, y_train, y_test = train_test_split(x_scaled, y, test_size=0.2, random_state=42)
      # Define the logistic loss function with SCAD penalty def logistic_loss(w, X, y, alpha=1, gamma=2): # SCAD parameters alpha and gamma
            logistic_loss(w, A, y, alpha 1, gamma 2, alpha 2, gamma 3, alpha 2, gamma 3, alpha 3, gamma 3, alpha 4, (gamma 1), alpha 4, (gamma 1))))

return loss + reg
10
11
     # Coordinate Descent
def coordinate_descent_scad(X, y, alpha=0.01, gamma=3.7, max_iter=1000, tol=1e-5):
             n, d = X.shape
w = np.zeros(d)
14
15
             w = np.zeros(d)
for _ in range(max_iter):
    w_prev = w.copy()
    for j in range(d):
        X_j = X[:, j]
        yz = y * np.dot(X, w)
        grad_j = -np.dot(X_j, y / (1 + np.exp(yz)))
        if w[j] == 0:
            w[j] = -grad_j * alpha / (1 + alpha)
16
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22
23
                     else:
    w[j] = np.sign(w[j]) * max(0, abs(grad_j) - alpha) / (1 + gamma)
if np.linalg.norm(w - w_prev) < tol:
24
25
26
      w_cd = coordinate_descent_scad(x_train, y_train)
     def predict(X, w):
    logits = np.dot(X, w)
     return np.where(logits >= 0, 1, 0)
y_pred_cd = predict(x_test, w_cd)
```

Listing 10: Coordinate Descent Optimization with SCAD Penalty



Figure 23: Classification Report for Coordinate Descent with SCAD Penalty

8.3 Stochastic Gradient Descent with SCAD Penalty

```
# Split the data into train and test sets
x_train, x_test, y_train, y_test = train_test_split(x_scaled, y, test_size=0.2, random_state=42)
      # Define the logistic loss function with SCAD penalty def logistic_loss(w, X, y, alpha=1, gamma=2): # SCAD parameters alpha and gamma
             logistic_loss(w, X, y, alpha=1, gamma=2): # SCAD parameters alpha and gamma
n = len(y)
yz = y * np.dot(X, w)
loss = np.sum(np.logip(np.exp(-yz)))
reg = alpha * np.sum(np.where(np.abs(w) <= alpha, 0, np.where(np.abs(w) <= gamma * alpha, (gamma * alpha - np.abs(w)) / (gamma - 1), alpha / (gamma - 1))))
return loss + reg</pre>
10
12
      # Stochastic Gradient Descent
      def stochastic_gradient_descent_scad(X, y, alpha=0.01, gamma=3.7, max_iter=1000, tol=1e-5, learning_rate=0.01):
    n, d = X.shape
              w = np.zeros(d)
for _ in range(max_iter):
    idx = np.random.permutation(n)
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17
18
19
20
21
                     idx = np.random.permutation(n)
for i in idx:
    X_i = X[i]
    y_i = y[i]
    yz = y_i * np.dot(X_i, w)
    grad = -X_i * y_i / (1 + np.exp(yz))
    w -= learning_rate * grad
    w = np.sign(w) * np.maximum(0, np.abs(w) - alpha / (1 + gamma))
if np.linalg.norm(grad) < tol:
    break</pre>
23
24
25
26
              return w
      w_sgd = stochastic_gradient_descent_scad(x_train, np.array(y_train))
      def predict(X, w):
   logits = np.dot(X, w)
29
      return np.where(logits >= 0, 1, 0)
y_pred_sgd = predict(x_test, w_sgd)
```

Listing 11: Stochastic Gradient Descent Optimization with SCAD Penalty

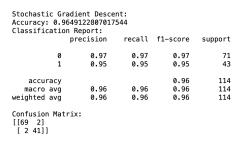




Figure 24: Classification Report for Stochastic Gradient Descent with SCAD Penalty

8.4 Proximal Gradient descent with SCAD Penalty

Listing 12: Proximal Gradient Descent Optimization with SCAD Penalty



Figure 25: Classification Report for Proximal Gradient Descent with SCAD Penalty

Comparing the accuracy obtained from Coordinate Descent, Stochastic Gradient Descent, and Proximal Gradient Descent, applied on a loss function with the SCAD penalty it was seen that Coordinate Gradient Descent outperforms the rest. Therefore, one conclude that Coordinate Descent algorithm works best for a loss function with an SCAD penalty. This is in line with the conclusions being derived in the reference paper.

9 BOOTSTRAPPING

Having established that the Coordinate Descent Algorithm works best with both the penalties MCP and SCAD, the durability of these models can be tested by bootstrapping across a number of samples. This can also help us determine which one of MCP and SCAD penalizes for sparsity better

```
# Define a function to calculate accuracy for a given set of parameters
   def get_accuracy(X_train, y_train, X_test, y_test, alpha, gamma):
    w_cd = coordinate_descent_mcp(X_train, y_train, alpha, gamma)
        y_pred_cd = predict(X_test, w_cd)
return accuracy_score(y_test, y_pred_cd)
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            X_boot, y_boot = X_train[indices], y_train.iloc[indices]
                                                                             # Use iloc for DataFrame indexing
            # Calculate accuracy on bootstrap sample
accuracy = get_accuracy(X_boot, y_boot, X_test, y_test, alpha, gamma)
             accuracies.append(accuracy)
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27
28
       # Calculate mean accuracy across samples
mean_accuracy = np.mean(accuracies)
        bias = mean_accuracy - get_accuracy(X_train, y_train, X_test, y_test, alpha, gamma)
variance = np.mean((accuracies - mean_accuracy) ** 2)
        return bias, variance, mean_accuracy
29
30
   alpha = 0.001
gamma = 1
```

Listing 13: Coordinate Descent with MCP - Bootstrapping

Attribute	10 samples	50 samples	100 samples	250 samples	500 samples
Bias	0.0018	-0.0144	-0.0122	-0.0165	-0.0147
Variance	0.0004	0.0010	0.0011	0.0011	0.0010
Mean Accuracy	0.9404	0.9242	0.9264	0.9221	0.9239

Table 1: MCP Bootstrap Attributes for 10,50,100,250,500 samples

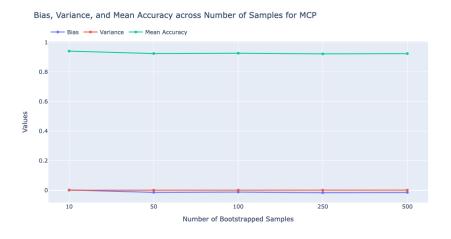


Figure 26: MCP Bootstrap Attributes Visualization

```
# Define a function to calculate accuracy for a given set of parameters
def get_accuracy(X_train, y_train, X_test, y_test, alpha, gamma):
    w_cd = coordinate_descent_scad(X_train, y_train, alpha, gamma)
    y_pred_cd = predict(X_test, w_cd)
                   turn accuracy_score(y_test, y_pred_cd)
      # Define a function to perform bootstrap sampling and calculate bias and variance def bootstrap_bias_variance(X_train, y_train, X_test, y_test, alpha, gamma, num_samples):
              accuracies = []
n_samples = len(X_train)
for _ in range(num_samples):
    # Generate bootstrap sample
    indices = np.random.choice(n_samples, size=n_samples, replace=True)
    X_boot, y_boot = X_train[indices], y_train.iloc[indices] # Use iloc for DataFrame indexing
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27
                      \begin{tabular}{lll} \# & Calculate & accuracy on bootstrap sample \\ accuracy = get\_accuracy(X\_boot, y\_boot, X\_test, y\_test, alpha, gamma) \\ accuracies.append(accuracy) \end{tabular}
              # Calculate mean accuracy across samples
mean_accuracy = np.mean(accuracies)
              # Calculate bias and variance
bias = mean_accuracy - get_accuracy(X_train, y_train, X_test, y_test, alpha, gamma)
variance = np.mean((accuracies - mean_accuracy) ** 2)
              return bias, variance, mean_accuracy
28
29
      # Example usage
     # Descript with SCAD - Bootstrapping
```

Listing 14: Coordinate Descent with SCAD - Bootstrapping

Attribute	10 samples	50 samples	100 samples	250 samples	500 samples
Bias	0.0526	0.0211	0.0232	0.0212	0.0209
Variance	0.0132	0.0116	0.0113	0.0099	0.0102
Mean Accuracy	0.1667	0.1351	0.1372	0.1352	0.1349

Table 2: SCAD Bootstrap Attributes for 10,50,100,250,500 samples

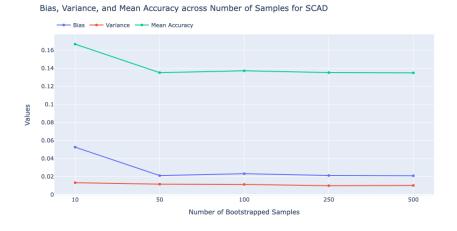


Figure 27: SCAD Bootstrap Attributes Visualization

10 CONCLUSION

Comparing the mean accuracies obtained with MCP and SCAD penalties in logistic regression, it becomes evident that the MCP penalty tends to yield sparser models compared to the SCAD penalty when utilizing the Coordinate Descent Algorithm for optimizing the loss function.

Primarily, the MCP penalty, characterized by its concave penalty function, offers a more pronounced regularization effect for smaller coefficients, effectively encouraging sparsity by pushing more coefficients to exactly zero. In contrast, while the SCAD penalty also promotes sparsity, its penalty function is smoother, resulting in a comparatively softer regularization, which may not aggressively push coefficients to zero, especially in scenarios where feature selection is crucial.

Moreover, the Coordinate Descent Algorithm, known for its efficiency in optimizing the logistic regression loss function, may align better with the optimization landscape induced by the MCP penalty. Its iterative nature, coupled with the specific characteristics of the MCP penalty function, allows for more effective exploration of the parameter space, leading to the identification of sparser models."

However, it's essential to note that the performance and sparsity-inducing capabilities of the penalties can also be influenced by factors such as dataset characteristics, feature correlations, and the magnitude of regularization. Nevertheless, in many cases, the combination of MCP penalty and Coordinate Descent Algorithm proves to be particularly adept at achieving both high accuracy and sparsity in logistic regression models. This confirms with what is derived in the paper referenced by us.

References

- [1] B. L., "Heuristics of instability and stabilization in model selection," Ann Statist, 1996.
- [2] T. R., "Regression shrinkage and selection via the lasso.," J Roy Statist Soc Ser B., 1996.
- [3] L. R. Fan J, "Variable selection via nonconcave penalized likelihood and its oracle properties," *J Amer Statist Assoc.*, 2001.
- [4] Z. CH, "Nearly unbiased variable selection under minimax concave penalty.," *Ann Statist.*, 2010.
- [5] L. R. Zou H, "One-step sparse estimates in nonconcave penalized likelihood models," *Ann Statist.*, 2008.
- [6] L. K. Wu TT, "Coordinate descent algorithms for lasso penalized regression.," Ann Apl Statist., 2008.
- [7] T. R. Friedman J Hastie T, "Regularization paths for generalized linear models via coordinate descent.," J Statist Softw, 2010.
- [8] J. H. Huiliang Xie, "Scad-penalized regression in high-dimensional partially linear models," *The Annals of Statistics*, vol. 31, p. 595, Mar. 2009.
- [9] A. A. S. K. Bahr kadhim Mohammed, "The minimax concave penalty (mcp) variable selection regularization method for regression discontinuity designs," *Department of Statistics, University of Al-Qadisiyah, Iraq*,