A review and recommendations on variable selection methods in regression models for binary data

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Abstract

The selection of essential variables in logistic regression is vital because of its extensive use in medical studies, finance, economics and related fields. In this paper, we explore four main typologies (test-based, penalty-based, screening-based, and tree-based) of frequentist variable selection methods in logistic regression setup. Primary objective of this work is to give a comprehensive overview of the existing literature for practitioners. Underlying assumptions and theory, along with the specifics of their implementations, are detailed as well. Next, we conduct a thorough simulation study to explore the performances of fifteen different methods in terms of variable selection, estimation of coefficients, prediction accuracy as well as time complexity under various settings. We take low, moderate and high dimensional setups and consider different correlation structures for the covariates. A real-life application, using a high-dimensional gene expression data, is also included in this study to further understand the efficacy and consistency of the methods. Finally, based on our findings in the simulated data and in the real data, we provide recommendations for practitioners on the choice of variable selection methods under various contexts.

Keywords: Logistic regression, Screening-based selection, Sparse models, Tree-based selection.

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1 Introduction

With the advancement of data collection mechanisms, there is a surge of enormous datasets in recent years. In the context of regression models, it typically introduces a large number of predictors, all of which may not be necessary to analyze or predict the outcome appropriately. In fact, large number of variables often increase the complexity without necessarily inducing a substantial improvement in the fit or the prediction accuracy. Naturally, it is preferable to model a data with a suitably chosen smaller set of predictors which allows better model interpretability, and in some cases, superior prediction accuracy. That is one of the first and foremost reasons why variable selection is essential. Our focus in this paper is specifically on the logistic regression models (LRM), which is one of the most used regression and classification algorithms for binary data. We aim to provide a comprehensive review of existing classical variable selection methods in such models.

The necessity of feature selection in LRM appears in a plethora of real-life applications from bioinformatics, medical research, finance, sports and other related fields. These research problems commonly consist of hundreds of predictors all of which may not be incorporated into the modeling structure. Gene expression data are the most popular examples in this regard (see Shevade and Keerthi [2003], Dara et al. [2017], Yang et al. [2018] for example). In another related study, Algamal and Lee [2015] focused on finding a smaller set of genes out of thousands that contribute the most in correctly classifying a tumor to be benign or malignant. Along a similar line, many medical studies (e.g. Liang et al. [2013], Wu et al. [2018], Bertoncelli et al. [2020]) aim to identify which factors out of hundreds increase the chance of a serious disease such as cerebral palsy, cancer, heart attack etc. In a finance-related application, Tian et al. [2015] used variable selection in logistic regression to model bankruptcy based on important micro-economic factors. Costa e Silva et al. [2017], on the other hand, analyzed the effects of important factors behind activity-related injuries in children and adolescents. Such applications are abound in literature, and they establish why variable selection methods are crucial in modeling binary data, especially for high dimensional cases where number of predictors is more than the number of sample observations.

The research on variable selection methods started around the 1960s. Since then, it has been rapidly growing. There has been a substantial amount of work in both linear and generalized linear models over the years. However, unlike linear models which have been reviewed thoroughly by several authors (e.g. Fan and Lv [2010], Heinze et al. [2018], Desboulets [2018], Epprecht et al. [2021]), to the best of our knowledge, a detailed review on variable selection methods in logistic regression setup has not been done till date. The study by Sanchez-Pinto et al. [2018] is perhaps the only work that includes considerable number of tree-based variable selection methods and compares them against three other popular approaches in a high-dimensional case. Speiser et al. [2019] did a limited study on the efficacy of different tree-based techniques used for predictive modeling. In another earlier paper, Zellner et al. [2004] compared the performances of stepwise selection procedures with the bagging method of Sauerbrei [1999]. Most recently, the performance of Smoothly Clipped Absolute Deviation (SCAD) and Adaptive Least Absolute Shrinkage and Selection operator (ALASSO) were evaluated by Arayeshgari et al. [2020] on a psychiatric distress dataset.

Evidently, there is an immense need of an extensive review of existing variable selection methods in LRM. To that end, our contribution in this paper is three-fold. First, we provide an in-depth discussion of many classical procedures which can be clearly categorized in four different types. Implementation details of these methods are also presented as necessary. Second, we conduct simulation studies in low, moderate and high-dimensional cases to understand the performance of specific algorithms under different assumptions. A high-dimensional real-life dataset is also used

in this aspect. Finally, acknowledging the fact that logistic regression is often used by machine learning practitioners as a classification problem for binary data, we evaluate both the inferential and the classification or prediction accuracy of all the methods in our study. We strongly believe that this comparative analysis would be helpful for a diverse class of practitioners.

Rest of the paper is structured in the following way. In Section 2, first we lay out the framework of the LRM and discuss the typology of variable selection procedures. Descriptions of different methods are provided next. Then, in Section 3, a detailed simulation study is presented to show the efficacy and comparison of fifteen methods. As a real-life application, we use a high-dimensional dataset from statistical genetics and discuss the results in Section 4. Finally, some recommendations and important concluding remarks are listed in Section 5.

2 Variable selection methods

2.1 Setup and typology of procedures

Before delving into the details of the variable selection methods, it is necessary to recall the structure of the LRM. In this setup, the response variable is always binary. If the outcome is a "success" (respectively, "failure"), we assign 1 (respectively, 0) as the value of the response variable. Let us use $Y = (y_1, y_2, \ldots, y_n)$ to denote the sample of response observations, which are assumed to depend on m number of covariates. For the ith sample observation, the vector of covariates is denoted by $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \ldots, x_{im})^\top$. The corresponding regression coefficients in the LRM are going to be denoted by $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_m)^\top$, and that is our primary parameter of interest. We shall use $\boldsymbol{X} = [\boldsymbol{x}_1 : \ldots : \boldsymbol{x}_n]^\top$ to denote the set of explanatory variables in the model. The order of the design matrix $\boldsymbol{X}$ is $n \times m$. Throughout this paper, n and m denote the number of observations and the total number of covariates respectively. Then, the LRM can be written using vector-matrix notations as

$$\text{logit}(Y \mid \boldsymbol{X}) = \boldsymbol{X}\boldsymbol{\beta}, \tag{2.1}$$

where $\text{logit}(Y \mid \boldsymbol{X})$ is used to denote the vector of logit transformation of y_i given $\boldsymbol{x}_i$ for $1 \leqslant i \leqslant n$, which is defined as

$$\text{logit}(y_i \mid \boldsymbol{x}_i) = \log \frac{P(y_i = 1 \mid \boldsymbol{x}_i)}{P(y_i = 0 \mid \boldsymbol{x}_i)}. \tag{2.2}$$

Writing the probability $P(y_i = 1 \mid \boldsymbol{x}_i)$ as π_i, we note that it can be expressed as $\pi_i = \frac{\exp\left(\boldsymbol{x}_i^\top \boldsymbol{\beta}\right)}{1 + \exp\left(\boldsymbol{x}_i^\top \boldsymbol{\beta}\right)}$. Since the complete likelihood for the binary data is

$$L(\boldsymbol{\beta}) = \prod_{i=1}^n \pi_i^{y_i} (1 - \pi_i)^{1-y_i}, \tag{2.3}$$

the log likelihood for the regression coefficients can be written as

$$\log L(\boldsymbol{\beta}) = \sum_{i=1}^n \left[y_i \left(\boldsymbol{x}_i^\top \boldsymbol{\beta} \right) - \log \left(1 + \exp \left(\boldsymbol{x}_i^\top \boldsymbol{\beta} \right) \right) \right]. \tag{2.4}$$

The method of iteratively reweighted least squares (IRLS) is typically used to find the maximum likelihood estimate of $\boldsymbol{\beta}$ in LRM (Green [1984]). However, the standard procedure would suffer if there is an issue of multicollinearity among the predictors. Especially, when m is large, it automatically increases the chances of both multicollinearity and overfitting. And in case of $m \geqslant n$, LRM fails to give a unique solution. Due to such issues, variable selection methods are needed.

In this paper, we are going to discuss the following four types of variable selection techniques:

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- Test-based methods,

- Penalty-based methods,

- Screening-based methods,

- Tree-based methods.

Arguably the most famous technique used by practitioners is the step-wise regression, which is a test-based method and was possibly the very first attempt at variable selection (Breaux [1967]). In such test-based approaches, each viable combination of input variables is considered to be a potential true model, and the selection is done based on some appropriate statistical measure such as p-values, adjusted R^2, Akaike Information Criterion (Akaike [1998]), Bayesian Information Criterion (Schwarz [1978]), Mallow's C_p (Mallows [1995]) etc. In the crudest possible way, such methods need to evaluate 2^m number of models if there are m number of regressors. Consequently, even for $m \geqslant$ 15, searching for the best model among these is computationally very expensive, and they become inconsistent in variable selection. Step-wise regression improves the computational efficiency to some extent, but by making a hard selection on every step, it makes choices that are locally optimal in each step but are suboptimal in general. The reader is referred to Hurvich and Tsai [1990], Steyerberg et al. [1999] and Whittingham et al. [2006] for more detailed criticism on variable selection inconsistency of this type of procedures. Because of the aforementioned shortcomings and considering the challenges in high-dimensional data, we are going to exclude these methods from our simulation study and are going to focus on the other three typologies.

Moving on to the second type, it is worth mention that the penalty-based methods are perhaps the most discussed techniques in the last decade. Following the seminal work on Least Absolute Shrinkage and Selection operator (LASSO) by Tibshirani [1996], these methods have been immensely popularized because of their nice properties in variable selection mechanism. In this typology of procedures, appropriate constraints are imposed on the regression coefficients' values through a penalty function. This introduces bias to reduce the variance. Penalty-based methods achieve sparsity by shrinking the near to zero values of the regression coefficients to precisely zero, thereby suggesting that those independent variables do not have any effect on the model. It is imperative to point out that the structure of the penalty functions has a significant impact on the number of variables selected and the amount of error in the regression coefficients. These methods are described in more detail in Section 2.2.

In case of screening-based methods, first a small number of variables are screened from the large number of predictors and then a smaller number of variables are selected using some penalty-based method or importance criteria. These methods are not particularly designed to do selection intrinsically but by ranking the importance of the variables. Screening-based methods are especially useful in an ultra high-dimensional setting where the number of variables grows with the number of observations (i.e. $m >> n$). Section 2.3 presents these methods in more detail.

One of the major disadvantages of the previous categories is that they heavily depend on the regularization parameters, which are not fixed and are calculated using cross-validation. Thus, they may fail to produce accurate and consistent results at times. In such situations, the fourth type of procedures i.e. the tree-based methods can be more useful. These methods utilize feature elimination characteristic embedded in random forests to select variables. In this work, we focus on five different tree-based approaches which are described in more detail in Section 2.4.

In Table 1, we list the variable selection methods from each of the four types. Corresponding references and suitable R packages (if available) are also listed there. Note that our focus for the rest of the paper would be on the fifteen methods of the last three categories. It is also worth

mention that there are several Bayesian methods and machine learning techniques that address the same problems, but we do not include them in this study and focus entirely on the aforementioned typologies.

Table 1: Variable selection methods along with relevant references and R packages.

Type	Name	Reference	R-package
Test-based	Forward / Backward / Step-wise Selection	Breaux [1967]	MASS
	Autometrics	Doornik et al. [2009]	gets
	GETS	Hendry and Krolzig [1999]	gets
Penalty-based	LASSO	Tibshirani [1996]	glmnet
	Adaptive LASSO (ALASSO)	Zou [2006]	glmnet
	SparseStep	van den Burg et al. [2017]	L0Learn
	ElasticNet	Zou and Hastie [2005]	glmnet
	Best Subset	Hazimeh and Mazumder [2020]	L0Learn
	Smoothly Clipped Absolute Deviation (SCAD)	Fan and Li [2001]	ncvreg
	Minimax Concave Penalty (MCP)	Zhang [2010]	ncvreg
Screening-based	Sure Independence Screening (SIS)	Fan and Lv [2008]	SIS
	Iterative Sure Independence Screening (ISIS)	Fan and Lv [2008]	SIS
	Stable Iterative Variable Selection (SIVS)	Mahmoudian et al. [2021]	SIVS
Tree-based	Boruta	Kursa et al. [2010]	Boruta
	Variable selection using random forests (VSURF)	Genuer et al. [2010]	VSURF
	Guided Regularized random forest (RRF)	Deng and Runger [2012]	RRF
	PIMP algorithm (PIMP)	Altmann et al. [2010]	vita
	The novel test approach (NTA)	Janitza et al. [2018]	vita

2.2 Penalty-based methods

There are mainly two types of penalties that are imposed on the objective function of variable selection problems. They are norm-based penalties and concave penalties. We present these in the two subsections below.

2.2.1 Norm based penalties

Vector norms are required to describe these models. Recall that the $\mathcal{L}_d$ norm ($d \geqslant 1$) for the n-dimensional vector $\boldsymbol{q} = (q_1, q_2, \ldots, q_n)^\top$ is defined as

$$\|\boldsymbol{q}\|_d = \left(\sum_{i=1}^{n} |q_i|^d \right)^{1/d}. \tag{2.5}$$

$\mathcal{L}_0$ norm is also defined, but in actuality it is not a norm. It is a cardinality function to represent the total number of non-zero elements in a vector. It is defined as

$$\|\boldsymbol{q}\|_0 = \# \{1 \leqslant i \leqslant n \mid q_i \neq 0\}, \tag{2.6}$$

where $\#$ is used to denote the cardinality of a set.

In this class of methods that leverage various norm-based penalties, the objective is to find the set of regression coefficients by minimizing an objective function that combines the negative log-likelihood and a constraint imposed on the regression coefficients. In general, these methods work around the following minimization problem:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \{-\log L(\boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|_\gamma^2\}. \tag{2.7}$$

Clearly, different degrees of the norm function would correspond to different algorithms. The three most popular methods, which take the form of eq. (2.7), are as follows.

$$\gamma = \begin{cases} 0 & \text{if it is SparseStep,} \\ 1 & \text{if it is LASSO,} \\ 2 & \text{if it is Ridge.} \end{cases} \tag{2.8}$$

We should recall that Frank and Friedman [1993] earlier proposed a more general bridge estimator where γ can be any nonnegative quantity, although an analytical solution was not developed in that work for any γ. Further note that the ridge regression (Hoerl and Kennard [1970]), which relies on the $\mathcal{L}_2$ penalty function, has an analytical solution, but is not sparse. So, it does not select variables but only does shrinkage. More generally, one can say that the use of $\mathcal{L}_\gamma$ norm selects variables when $0 \leqslant \gamma \leqslant 1$, but for $\gamma > 1$, it only shrinks. In a very recent paper by Wu [2021], ridge selection operator (RSO) and adaptive version of RSO (ARSO) were developed to propose a way to select variables through ridge regression for usual linear models. Its extension in the generalized linear model (GLM) seems possible, but a precise formulation is yet to be obtained, primarily due to the fact that the ridge penalized solution does not have a closed-form expression for GLM. In light of the above, the case of $\gamma > 1$ is not going to be a part of our discussion hereafter.

Turning attention to the SparseStep method (van den Burg et al. [2017]), observe that the $\mathcal{L}_0$ norm directly penalizes the number of nonzero coefficients and not their values, thereby inducing a high computational cost to search over the entire space. Subsequently, it makes SparseStep infeasible compared to others. LASSO regression is computationally faster and relies on the $\mathcal{L}_1$ norm to select variables by shrinking small coefficients exactly to zero. However, the results are biased even for large values of the coefficients (Zou [2006]). Moreover, if some of the variables are correlated, i.e. if they form a group, LASSO tends to select only one. And for high-dimensional problems where $m > n$, this method tends to select at most n variables, which is a major concern in practice (Efron et al. [2004]). To circumvent these limitations, Zou and Hastie [2005] proposed the method of ElasticNet, which is essentially a linear combination of ridge penalty and LASSO penalty. In this approach, the $\mathcal{L}_1$ penalty generates a sparse model, while the quadratic penalty removes the limitation of selecting at most n variables, encourages grouping effect and stabilizes the $\mathcal{L}_1$ regularization path. It also makes the loss function strongly convex and hence produces a unique estimate given by

$$\hat{\boldsymbol{\beta}}_{\text{ElasticNet}} = \arg\min_{\boldsymbol{\beta}} \left\{ -\log L(\boldsymbol{\beta}) + \lambda_1 \|\beta\|_1 + \lambda_2 \|\boldsymbol{\beta}\|_2^2 \right\}. \tag{2.9}$$

Another problem with LASSO, as pointed out by Meinshausen and Bühlmann [2006], is that it tends to select noise variables even for an optimally chosen tuning parameter (λ). Zou [2006] resolved it by developing an Adaptive LASSO (ALASSO) algorithm that enjoys the oracle property by utilizing the adaptive weights given to different coefficients. If $\boldsymbol{x} \circ \boldsymbol{y}$ represents the element-wise Hadamard product of two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, then the ALASSO estimate is given by

$$\hat{\boldsymbol{\beta}}_{\text{ALASSO}} = \arg\min_{\boldsymbol{\beta}} \left\{ -\log L(\boldsymbol{\beta}) + \lambda \|\boldsymbol{w} \circ \boldsymbol{\beta}\|_1 \right\}. \tag{2.10}$$

A pivotal issue with the above estimation problem is the initial choice of $\boldsymbol{w}$. Adaptive LASSO originally used MLE estimates as initial weights, but the assumption is invalid for high-dimensional data. Bühlmann and Van De Geer [2011] used LASSO estimates as initial weights, but since LASSO itself is biased and would produce zero coefficients for some variables, using it as weights may not be a perfect choice. Zou [2006] suggested using some unbiased estimate $\hat{\boldsymbol{\beta}}$ so that the ALASSO estimates can achieve oracle properties. As oracle property is an asymptotic guarantee when $n \to \infty$, it may not hold for a small sample size. In practice, the weights need not be exact, and one can get reasonable values of $\boldsymbol{w}$ from an initial estimate of $\boldsymbol{\beta}$, possibly from ordinary least squares, LASSO or ridge.

The aforementioned methods have been naturally extended to the GLM case. Refer to the work by Friedman et al. [2010] who formulated the theoretical development of a regularized path for such models via coordinate descent so that LASSO, ALASSO and ElasticNet can be applied in the LRM setup. An exciting application of ALASSO in LRM can be found in Cui et al. [2021] where they used this approach to select an important set of covariates for early diagnosis of Alzheimer's disease.

We close this subsection with another method that resolves an important limitation of the methods discussed above. Note that the above approaches either penalize the model size i.e. the number of non-zero coefficients (for example, SparseStep) or the size of the coefficients (for example, LASSO, ElasticNet etc.), but not both at the same time. Recently, Hazimeh and Mazumder [2020] proposed an extended family of $\mathcal{L}_0$ based estimators that are further regularized by $\mathcal{L}_q$ norm to avoid overfitting issues in both low and high signal-to-noise phenomena. They developed a fast algorithm to perform these sparse regularizations using coordinate descent and local combinatorial optimization algorithms. This approach is called the 'Best Subset' method and uses the estimate

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}}\{-\log L(\boldsymbol{\beta}) + \lambda_0 \|\boldsymbol{\beta}\|_0 + \lambda_q \|\boldsymbol{\beta}\|_q^q\}, \tag{2.11}$$

where $q \in \{1, 2\}$ depends on the type of desired additional regularization.

2.2.2 Concave penalties

In the second type of penalty-based methods, an appropriately chosen concave function $p_\lambda(\cdot)$ is used which leads to the general framework

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}}\{-\log L(\boldsymbol{\beta}) + p_\lambda(\boldsymbol{\beta})\}. \tag{2.12}$$

Non-negative garrotte by Breiman [1995] was one of the first methods to use non-convex penalties. If f_+ denotes the non-negative part of f, i.e. the quantity $\max\{f, 0\}$, then the concave penalty used in non-negative garrotte is given by

$$p_\lambda(\boldsymbol{\beta}) = n\lambda \sum_{j=1}^{m} \left(1 - \frac{\lambda}{\beta_j^2}\right)_+. \tag{2.13}$$

Due to variable selection inconsistency, the above method was rapidly disused. Fan and Li [2001] then proposed the Smoothly Clipped Absolute Deviation (SCAD) method and it is arguably the most prominent procedure in this typology. Recall that LASSO shrinks all the least square estimates by an identical amount of $\lambda/2$. If their absolute values are less than $\lambda/2$, they are shrunk to precisely zero. Because of this phenomenon, LASSO induces bias in estimating the larger values of beta estimates. SCAD penalty addresses this issue. For lower values of $\hat{\beta}_j$, the penalty is the same as LASSO, and it shrinks the coefficients to zero. For the value of $\hat{\beta}_j$ between λ and $\gamma\lambda$, the

penalty function smoothly transitions to quadratic and gradually relaxes the penalization rate. The penalty then remains constant for all the values of $\hat{\beta}_j$ larger than $\gamma\lambda$. Thus, in SCAD, eq. (2.12) uses

$$p_\lambda(\boldsymbol{\beta}) = \sum_{j=1}^{m} p(|\beta_j|; \lambda), \tag{2.14}$$

where, $p(t; \lambda)$ is the SCAD penalty indexed by a regularization parameter $\lambda \geqslant 0$ and is given by

$$p(t; \lambda) = \lambda \int_0^t \min\left\{1, \frac{(\gamma - x/\lambda)_+}{(\gamma - 1)}\right\} dx \tag{2.15}$$

for some $\gamma > 2$. In practice, one can choose different λ values for different β_j but we shall take the conventional approach of imposing same penalty on each regression coefficient.

Another concave penalty similar to SCAD is the Minimax Concave Penalty (MCP), proposed by Zhang [2010]. MCP also starts with the same penalization rate as LASSO but smoothly relaxes it to zero as the values of the regression coefficients increase. In contrast, in SCAD, this rate remains constant for a while and then decreases to zero. The penalty function corresponding to MCP is of the form of eq. (2.14), where

$$p(t; \lambda) = \lambda \int_0^t \left(1 - \frac{x}{\gamma\lambda}\right)_+ dx, \tag{2.16}$$

for appropriately chosen parameters λ and γ.

The tuning Parameter γ for SCAD or MCP (would be different for the two methods) controls the concavity of the penalty function. As $\gamma \to \infty$, both penalties converge to the $\mathcal{L}_1$ penalty, and the bias is minimised when γ is minimum. Still, the solution becomes unstable because there may exist multiple local minima of the loss function. Two applications of concave penalty-based methods in logistic regression can be found in Rezapur-Shahkolai et al. [2020] and Yan et al. [2011], whereas a comparative study between the two approaches can be found in Zhang [2007].

2.3   Screening-based methods

As mentioned in Section 2.1, penalty-based methods may fail in the case of ultra high dimensional data. Fan and Lv [2008] developed the Sure Independence Screening (SIS) method for such scenarios. Sure screening means that for large amount of data, after variable selection, the probability of all important variables surviving converges to 1. It filters out variables that have a weak correlation with the response. To put it mathematically, let $M_* = \{1 \leqslant i \leqslant m : \beta_i \neq 0\}$ be the true sparse model and let the non-sparsity size be $s = |M_*|$. Other $(m - s)$ variables can be correlated with the response via some linkage to the important variables in the model. If $\boldsymbol{w} = \boldsymbol{X}^\top \boldsymbol{Y}$ is a vector obtained by the component-wise regression where the matrix $\boldsymbol{X}$ and the vector $\boldsymbol{Y}$ are standardized such that each variable has mean 0 and variance 1, then $\boldsymbol{w}$ represents a vector of marginal correlations. Next, for $\nu \in (0, 1)$, arrange the elements of $\boldsymbol{w}$, i.e. the marginal correlations, in ascending order of magnitudes to get the sub-model

$$M_\nu = \{1 \leqslant i \leqslant m : |w_i| \text{ is among the first } [\nu n] \text{ largest of all } w_i\}.$$

It is a variable selection method based on correlation ranking of size $d = [\nu n] < n$. Observe that the computational cost is minimal, as this approach is just about multiplying a matrix of order $m \times n$ with a vector of $n \times 1$ and finding the largest $[n\nu]$ elements in it. After applying SIS to reduce the dimension from m to much smaller d, SCAD, ALASSO or any other variable selection technique can be used for further selection and estimation. The parameter d is typically selected

depending on the following algorithm to be performed after SIS. Overall, this method speeds up variable selection drastically and improves estimation accuracy in high-dimensional settings.

A caveat, however, is that SIS may fail to select some important variables. To overcome this problem, Iterative Sure Independence Screening (ISIS) has been introduced where a large scale variable screening is applied before a careful variable selection. Here, an SIS-based model selection is used first to select a primary set of variables, say A_1. Next, the residuals from regressing the response Y on the chosen set of variables in A_1 are treated as new responses and applied the same method as previous. The advantage of this iterative procedure is that, because the residuals are uncorrelated with the selected variables in A_1, it significantly weakens the possibility of choosing an unimportant variable that has a high correlation with Y through the chosen variables.

Stable iterative Variable Selection (SIVS), proposed by Mahmoudian et al. [2021], is another screening-based method for variable selection. SIVS works in five steps. It starts with removing the redundant features and standardizing the columns. Then, a predefined number of models are created using cross-validation. Based on the results, variable importance score (VIMP) is calculated such that the variables selected by most models and those who have a major contribution in predicting the outcome get a higher score. The variables with a VIMP score of zero are directly eliminated in the next step. Other variables with low VIMP scores are also eliminated following a suitable cutoff criteria discussed in the original paper.

Before moving on to the tree-based methods, we want to briefly mention two other methods which are beneficial for variable selection in linear models but are not yet completely developed for the GLM case. First of the two, Covariance Assisted Screening and Estimation (CASE) (Ke et al. [2014]) is a two-step screening-based method that deals with the case where the signals (non-zero coordinates of $\boldsymbol{\beta}$) are sparse as well as weak (absolute value of the non-zero coefficients are small). The two steps are patching and screening (PS) and patching and estimation (PE). In the PS step, a sequential χ^2 test is used to look for candidates in each signal island of a graph of strong dependence. In the PE step, penalized likelihood is used to re-investigate each candidate in the hope to solve the problem of false positives. The problem with CASE is to find an appropriate filtering method to sparsify the non-sparse variance-covariance matrix.

Ke and Yang [2017] proposed another method for variable ranking, known as Factor Adjusted Covariate Assisted Ranking (FA-CAR). In the FA step, the authors advocated for the use of principal component analysis (PCA) to sparsify the covariance matrix when the variables are strongly correlated. The CAR step exploits the sparse covariance matrix for the ranking of variables. Note that the concept of using PCA to sparsify the covariance matrix is similar to CASE, where suitable linear filtering was used, but the two methods have a different objective. FA-CAR's primary goal is to rank the variables, which are crucial in many statistical analyses. Variable selection can be done via appropriate thresholds as a by-product of the variable rankings.

2.4 Tree-based methods

Recall that the determination of the regularization parameters in penalty-based or screening-based methods is done through cross-validation, which sometimes results in inconsistency in variable selection. In such cases, tree-based methods are beneficial as they do not rely upon any such parameter and achieve good results even in the presence of missing data, outliers etc. Let us start this section with a brief background on decision trees as they are the building blocks of various tree-based methods.

The decision tree is a supervised machine learning algorithm with the tree's structure. Each internal node represents different features, each branch exhibits a decision rule, and each leaf represents an outcome. Random forest is an ensemble of decision trees (Breiman [2001]), and the

outcome depends on the decision tree outcomes through a majority rule in case of classification. Feature selection is an inherent part of random forest and is carried out by ranking the features according to some importance scores. Now depending on how a random forest grows, there are different types of variable selection methods.

Boruta algorithm (Kursa et al. [2010]) is perhaps one of the most famous and widely used tree-based methods for variable selection. In this method, a wrapper is built around the random forest classifier that iteratively compares the importance of the variables with that of randomly shuffled original ones (shadow variables). The algorithm selects a feature with higher importance than the maximum importance score of all shadow variables. These shadow variables are recreated in each iteration, and the algorithm stops when only the essential variables are left in the test. Naik and Mohan [2019] utilized Boruta in finding out the appropriate feature set for a stock prediction problem. Hallmark and Dong [2020], meanwhile, leveraged this algorithm to work on roadway safety models in an LRM setup.

Variable selection using Random Forest (VSURF) proposed by Genuer et al. [2010] is also popular and uses the mechanism embedded in the random forest to select variables. It works in a two-step approach. The features are ranked according to their Variable Importance (VI) score in the first step, and features with lower VI are eliminated. The threshold value is estimated from the standard deviation of VI scores of the useless variables. In the next interpretation step, a nested random forest is created using the variables that survived in the previous step. Subsequently, variables with the lowest out of bag errors are selected. For the prediction step, a further subset of variables is obtained by constructing an ascending number of random forests and implementing test criteria for selecting variables. VSURF has been used extensively in medical research. For example, Ganggayah et al. [2019] used it to find important factors affecting the survival rate of breast cancer, while Yin et al. [2019] utilized it in the prognosis of endometrioid endometrial adenocarcinoma disease using gene expression and clinical trials data. Another interesting application of different flavor can be found in Virdi et al. [2019] who deployed VSURF and LASSO to select a small set of variables and modelled mechanical properties of investment casting.

In an attempt to select the features more efficiently with the help of a regularization step over a general random forest, Deng and Runger [2012] developed regularized random forest. In the regularization step, selecting a new feature for splitting is penalized if the information gain is similar to the features used in previous splits. However, many features may have the same Gini information at leaf nodes because of its selection mechanism, and unimportant variables can be falsely selected for low sample sizes. To resolve this problem, Deng and Runger [2013] further proposed an improved version called the guided regularized random forest (RRF), where importance scores from normal random forests are used to guide the feature selection in the regularized random forest algorithm. In a binary data setting, Adam et al. [2017] applied this technique for feature selection and classification in early detection of phaeosphaeria leaf spot infestations in maize crops. These methods were also used by Sylvester et al. [2018] to select important panels from large scale nucleotide polymorphisms (SNP) panels for fine-scale population assignment.

As a final piece of this section, we discuss two other tree-based methods that resolve one particular drawback of the feature importance scores used in random forests, namely that they are biased towards features with many factors. It may result in the selection of unimportant variables. In order to overcome this, Altmann et al. [2010] proposed a novel method (PIMP) to estimate the distribution of importance scores based on repeated permutations of the response variable. The p-values of observed importance provide a corrected measure of feature importance. Interestingly, though PIMP rectifies certain issues of random forest-based approaches and is tractable for the low dimensional cases, it becomes computationally infeasible when the number of features is very high. Motivated by this limitation, Janitza et al. [2018] proposed a novel testing approach (NTA) based

on the cross-validated technique of permutation importance measures. Nembrini et al. [2020] used a modified version of NTA to select a subset of variables relevant to the willingness to pay for risky lifestyles. NTA was also used by Sun and Zhao [2020] to determine an important set of genes in the diagnosis of lung cancer.

3 Simulation study

3.1 Setups and implementation details

In our simulation study, we aim to compare the variable selection parsimony and predictive accuracy for the methods mentioned in the previous section. Six different setups are considered to mimic a wide range of problems encountered in real life. Throughout this section, keeping up with the earlier notations, we use n, m and p to denote the number of sample observations, the total number of covariates and the number of important covariates, respectively. The simulation frameworks are summarized in Table 2 and relevant discussions are provided next.

Table 2: Simulation setups used in this paper. Here, n is the sample size, m is the total number of covariates, p is the number of important covariates, and X_i stands for the ith covariate.

n	m	p	Correlation between covariates
	10	3	
100	100	5	Independent
	1000	10	
	10	3	
100	100	5	$\text{Corr}(X_i, X_j) = 0.5^{|i-j|}$
	1000	10	

We follow the usual logistic regression framework as in eq. (2.1). First step is to generate synthetic observations for m number of covariates (X_i) to constitute the $n \times m$ data matrix $\boldsymbol{X}$. To that end, two different correlation structures are utilized in our simulation. In the first case, we use an ideal assumption of independence across all covariates. In the second case, following Hazimeh and Mazumder [2020], an exponential hierarchical correlation structure is adopted. In particular, we assume that the correlation between the ith and the jth regressor is of the form $\rho^{|i-j|}$. For this simulation, we shall use $\rho = 0.5$ in all experiments. This indicates moderate correlation between nearby covariates, and negligible correlation amongst far apart covariates. Now, each row of the design matrix is simulated as a random observation from an appropriately chosen (based on desired correlation structure) m-dimensional zero-mean multivariate normal distribution.

For each correlation structure, we simulate $n = 100$ observations with the number of predictor variables m varying in the set $\{10, 100, 1000\}$. Observe that these choices represent low dimensional, moderate dimensional and high dimensional data, respectively. In these three cases, the number of important variables are chosen as $p \in \{3, 5, 10\}$, respectively. Now, to simulate the $m \times 1$ parameter vector $\boldsymbol{\beta}$, we randomly pick the p indexes that represent the important regressors. These coefficients are generated using the formula $Z + (0.5)\mathbb{I}\{Z > 0\} - (0.5)\mathbb{I}\{Z \leqslant 0\}$, where Z is a random observation from a normal distribution. Note that it ensures the condition $|\beta_j| \geqslant 0.5$ for all important coefficients β_j, and thereby avoids the cases of weak signals. Other $(m - p)$ coefficients are set to be zero and imply unimportant variables.

To assess and compare the performances of the competing variable selection methods, we repeat each experiment 100 times and evaluate the average accuracy across those repetitions.

A brief account of the implementation details for all the methods is warranted at this point. We use the R package "glmnet" by Friedman et al. [2010] to perform LASSO, ALASSO and ElasticNet. The first two methods are performed in default settings. The weights used for regression coefficients ($\boldsymbol{\beta}$) in ALASSO are taken as reciprocals of the absolute values of their ridge regression estimates. For ElasticNet, we use five-fold cross-validation technique to find the optimal values of α and λ parameters using the "caret" package (Kuhn [2021]). SparseStep and Best Subset method are implemented using the "L0Learn" package (Hazimeh et al. [2021]). In the case of the former, a five-fold cross-validation technique is used to determine the optimal values of λ and γ parameters, following which $\mathcal{L}_0$ penalty is applied to find the sparse estimates. Similarly, in the Best Subset method, we use the combination of $\mathcal{L}_0$ and $\mathcal{L}_2$ penalties in the loss argument. The methods that rely on concave penalties are executed using the R package "ncvreg" (Breheny and Huang [2011]). Here, the λ parameter is determined using ten-fold cross-validation.

Turn attention to the screening-based methods next. For SIS and ISIS, we use the default settings in the "SIS" package (Saldana and Feng [2018]). SIVS is carried out using the "sivs" package (Mahmoudian et al. [2021]). To screen important variables, the "strictness" argument is set to be 0.5, as in our settings, the number of important variables is assumed to be quite low. For real data analysis, we would try out different strictness levels and choose what is optimal. As suggested by the authors in the corresponding vignette, this argument is dependent on the problem at hand.

In all of the tree-based methods, we use "randomForest" (Liaw and Wiener [2002]) to grow the trees. Then, to conduct the Boruta algorithm, the "Boruta" package from Kursa et al. [2010] is utilized. Next, for VSURF, variables are selected in three steps. Features that survive after the interpretation step are taken to be determined by the algorithm. While implementing it through the "VSURF" package (Genuer et al. [2019]), the number of trees in each forest is set to 500. RRF is implemented via "RRF" (Deng and Runger [2012]), where we set γ as 0.5 to derive the coefficients of regularization. Finally, PIMP and NTA are carried out using the "vita" package (Celik [2015]). Features with p-values less than 0.05 in both the methods would be considered to be selected.

All the codes are run in RStudio Version 1.3.1093, equipped with R version 4.0.3, on a laptop with 8GB RAM and an 8-core AMD processor. Barring the specifications above, other arguments in all the packages are used in the default settings. It is also worth mentioning that all the functions are run on a single core without parallelization, allowing us to compare the computational times aptly.

3.2 Evaluation metrics

In the simulation study, we use ten different metrics to evaluate the performance of various methods. As we pointed out before, our objective is to assess the parsimony and correctness of the variable selection methods and their accuracy in estimation and prediction.

In order to address the first aspect above, we find the number of selected variables in each iteration and calculate the average across all iterations. It helps us to identify if a method performs well in selecting the correct number of important covariates. However, the correct number of covariates does not necessarily imply the correct set of covariates. We compute the average proportions of important and unimportant variables selected to analyse this particular property. A good procedure is expected to attain a near-correct selected number of variables. Further, the percentage of important variables selected should be close to 100%, while the same for the unimportant variables is expected to be close to zero. To define these quantities mathematically, let $\hat{\beta}_j$

and β_j (for $1 \leqslant j \leqslant m$) be the estimated and the true coefficients. We use $\hat{\boldsymbol{\beta}}$ and $\boldsymbol{\beta}$ to denote the corresponding vectors. Then, the aforementioned quantities are defined as

$$
\begin{aligned}
\text{Selected} &= \left\| \hat{\boldsymbol{\beta}} \right\|_0, \\
\text{Imp\%} &= \frac{\#\left\{ 1 \leqslant j \leqslant m : \hat{\beta}_j \neq 0, \beta_j \neq 0 \right\}}{\#\left\{ 1 \leqslant j \leqslant m : \beta_j \neq 0 \right\}}, \\
\text{Unimp\%} &= \frac{\#\left\{ 1 \leqslant j \leqslant m : \hat{\beta}_j \neq 0, \beta_j = 0 \right\}}{\#\left\{ 1 \leqslant j \leqslant m : \beta_j = 0 \right\}}.
\end{aligned}
\tag{3.1}
$$

For comparing the estimation performance of these methods, we use two different measures, which are remarkably popular in statistical literature (Chai and Draxler [2014]). These are mean squared error (MSE) and mean absolute error (MAE). Because tree-based methods are not typically used for estimation purposes, we calculate these errors only for the other typologies. The formal definitions of these measures are provided below.

$$
\text{MSE} = \frac{1}{n} \sum_{j=1}^{m} (\beta_j - \hat{\beta}_j)^2, \ \text{MAE} = \frac{1}{n} \sum_{j=1}^{m} \left| \beta_j - \hat{\beta}_j \right|.
\tag{3.2}
$$

For assessing the prediction accuracy of different methods, in each experiment, the data is divided into a training set and a test set, the latter being denoted as S_{te}. We fit each method to the training set and use that to predict the probability distribution for the observations in S_{te}. Below, $\hat{\pi}_i$ denotes the predicted probability of success for the ith event in the test set.

Now, to evaluate the prediction performance, we first compute the empirical accuracy as the percentage of overall correct predictions where success is predicted by ($\hat{\pi}_i > 0.5$). Next, we calculate the precision and the recall. The first one measures the accuracy of positives classified by the method, whereas recall measures the ability of a method to classify positives correctly. Both have their advantages in judging the prediction accuracy of a method. These measures lie between 0 and 1, and higher values are preferred. If TP, FP, and FN denote the true positives, the false positives and the false negatives respectively, then the above three quantities are defined as follows:

$$
\text{Accuracy} = 100 \left(\frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{TN} + \text{FN}} \right), \ \text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \ \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}.
\tag{3.3}
$$

Evidently, the above measures give an idea of the classification abilities of the method. However, they cannot provide an adequate idea of the predictive accuracy in the LRM setup where not only the predicted category, but also the predictive distribution is crucial (Czado et al. [2009]). To tackle this aspect, we use the Brier score (Brier [1950]) and show the closeness of the predicted probability distribution to the observed outcome. It is a proper scoring rule and is defined as

$$
\text{Brier} = \frac{1}{|S_{\text{te}}|} \sum_{i \in S_{\text{te}}} (y_i - \hat{\pi}_i)^2.
\tag{3.4}
$$

We also compute the average time taken by each variable selection method in each iteration under different settings. Computational time is always a pivotal metric in such studies, for a time-consuming method can turn out to be an infeasible choice in high-dimensional cases.

3.3 Simulation results

We start with a quick look at three important metrics (selected number of variables, MSE and prediction accuracy) for all the methods in all setups (Table 3). For the sake of brevity, detailed results on all other metrics are deferred to the Appendix. Below, we briefly discuss the results under the low and moderate dimensional setup and then focus on the high-dimensional case in more detail.

Table 3: Three important performance metrics for all the methods under different simulation setups

| | Independent case | | | | | | | | |
| Setup | $n = 100, m = 10, p = 3$ | | | $n = 100, m = 100, p = 5$ | | | $n = 100, m = 1000, p = 10$ | | |
Method	Selected	MSE	Accuracy	Selected	MSE	Accuracy	Selected	MSE	Accuracy
LASSO	6.43	0.763	83.30	20.55	0.210	82.90	25.61	0.070	73.40
ALASSO	3.91	0.485	83.90	13.82	0.142	81.90	30.20	0.061	72.70
SparseStep	2.54	0.650	84.00	2.43	0.168	80.70	1.64	0.064	70.90
ElasticNet	6.33	3.208	82.30	20.73	0.357	78.20	56.44	0.078	69.90
Best Subset	3.67	0.473	84.15	4.57	0.158	80.80	4.41	0.068	72.10
SCAD	3.08	8.289	84.35	10.35	0.574	82.90	19.79	0.065	75.10
MCP	3.47	0.514	84.65	5.91	0.158	82.50	8.59	0.067	74.80
SIS	3.09	8.556	83.60	3.32	0.171	80.00	3.80	0.063	71.00
ISIS	2.71	8.556	83.60	3.86	0.166	82.20	4.00	0.301	71.80
SIVS	2.71	0.974	84.56	4.21	0.242	82.90	4.16	0.070	74.60
Boruta	2.86		81.70	5.51		74.95	8.90		60.45
VSURF	2.96		81.28	7.14		75.90	26.47		65.20
RRF	3.33		80.97	3.66		76.57	6.50		62.00
PIMP	2.44		80.55	7.53		75.55	77.82		59.90
NTA	3.43		80.37	12.36		74.60	78.84		61.10
	Correlated case								
Setup	$n = 100, m = 10, p = 3$			$n = 100, m = 100, p = 5$			$n = 100, m = 1000, p = 10$		
Method	Selected	MSE	Accuracy	Selected	MSE	Accuracy	Selected	MSE	Accuracy
LASSO	5.91	0.549	82.60	16.79	0.220	81.65	26.33	0.070	75.30
ALASSO	3.75	0.442	83.75	12.72	0.148	81.75	29.50	0.058	73.55
SparseStep	2.35	1.757	83.05	2.45	0.151	82.75	1.66	0.062	71.35
ElasticNet	6.95	19.651	81.65	17.63	0.430	78.55	80.19	0.070	69.45
Best Subset	3.51	0.543	83.10	4.10	0.172	82.80	5.10	0.067	72.25
SCAD	3.20	0.672	82.45	8.83	0.150	83.20	19.10	0.062	75.00
MCP	2.78	0.657	82.80	5.25	0.144	83.65	7.99	0.065	74.65
SIS	2.45	24.431	82.05	2.60	0.178	79.20	3.59	0.061	72.95
ISIS	2.45	24.431	82.05	3.72	3.453	81.85	4.00	0.052	73.70
SIVS	2.90	1.002	83.75	3.94	0.239	82.60	4.26	0.068	74.30
Boruta	3.90		78.40	6.87		74.20	10.24		67.40
VSURF	3.33		79.06	6.43		76.25	24.22		66.65
RRF	3.84		78.94	3.96		72.96	5.19		68.75
PIMP	2.88		78.62	8.70		75.10	81.04		64.85
NTA	4.79		78.58	14.51		74.20	82.59		63.75

Table 3 demonstrates that all the methods are performing relatively well in terms of selection and prediction when the number of observations is much higher than the number of predictors (low

dimensional case). It is also seen that, as the number of variable increases, the overall selection performance decreases for all the methods. Interestingly, the performances of the methods in terms of the number of selected variables are not significantly different in correlated and uncorrelated setups. However, some variability can be seen in the values of Imp% and Unimp%. One possible explanation is that, for correlated case, if two variables are significantly correlated and only one of them is important, then few methods fail to make the correct choice.

Furthermore, we notice that LASSO and ElasticNet tend to select more number of variables than the rest (see Table A1 in the Appendix). Even if it ensures good accuracy in selecting the important variables, the percentage of unimportant variables selected also increases and is approximately 50% in the low dimensional case. However, this particular tendency of selecting more variables does not necessarily affect the prediction accuracy. We see that all penalty-based methods and screening-based methods achieve more than 80% accuracy on an average. For the tree-based methods, the accuracy drops slightly under 80% in the correlated structure, although they commonly select correct number of variables in this setup. Another interesting observation is that the MSE in estimating the coefficients is quite high for ElasticNet, SCAD, SIS and ISIS. Thus, even if their selection patterns or the accuracy measures are good, the estimates are unreliable. Upon close inspection, we observed that in few of the iterations, SCAD, SIS and ISIS estimate high values of the regression coefficients for some variables, thereby increasing average MSE for these methods.

We observe similar kind of results for moderate dimensional setup too. Table 3 shows that when the number of observations is equal to the number of predictors, tree-based methods perform inferior to other methods in terms of prediction accuracy. Figure A4 (see Appendix) also displays that median brier score of tree-based methods are generally more than other penalty-based and screening-based methods, only exception being the ElasticNet which registers higher brier score than other penalty-based approaches. Looking at the selection metrics, one can notice that SCAD, LASSO, ALASSO and ElasticNet typically select many irrelevant variables, albeit the prediction accuracy is good for all but ElasticNet. On the other hand, Best Subset, MCP, SIVS and Boruta are found to be the best methods in terms of variable selection performances. Not only they select appropriate set of variables, but the MSE of the estimated coefficients and brier scores are also lower for them.
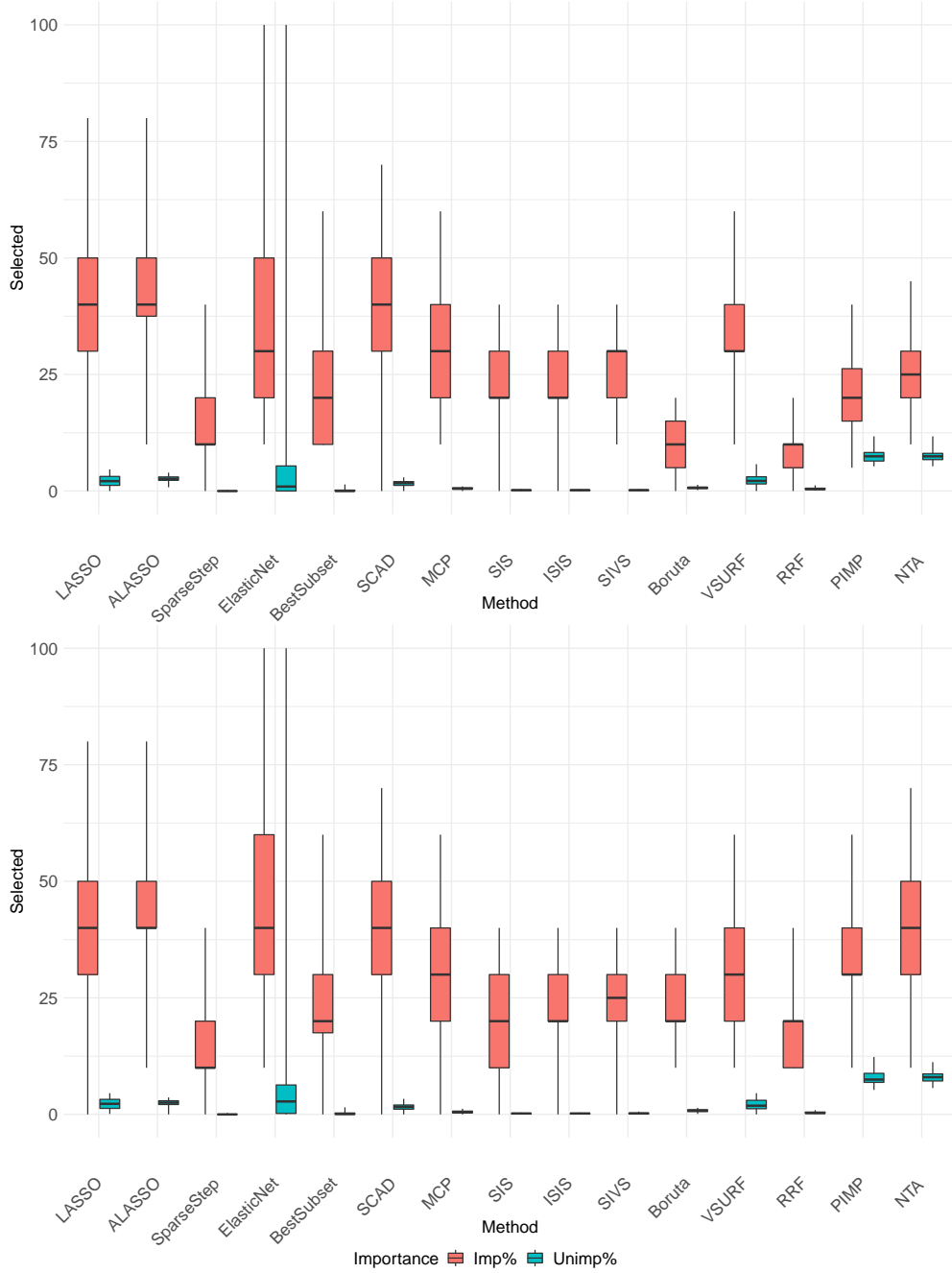
There are some common patterns that emerge in the four typologies. Across all scenarios, SparseStep is observed to be the most parsimonious method. We see that the MSE values decrease significantly for the screening based methods from low to moderate to high dimensional setups i.e. performance of these methods in estimating the regression coefficient is better when the number of variables is higher. Concave penalty based methods record higher accuracy in the correlated case than in the uncorrelated one. In contrast, SparseStep, ElasticNet, Best Subset and VSURF depict little improvement in accuracy in the correlated case than the independent setting.

Let us now explore the high-dimensional results in detail. In our simulation framework, there are ten important variables out of thousand, and Table 3 demonstrates that only MCP and Boruta tend to select near to correct number of variables. Meanwhile, LASSO, ALASSO, ElasticNet, SCAD, VSURF, PIMP and NTA pick more number of variables in general, whereas SparseStep, Best Subset and RRF choose only a few in all iterations. Screening-based methods generally are more conservative in this aspect. Another interesting finding is that the difference in accuracy measures between the uncorrelated and the correlated situation is less prominent in case of high-dimensional data than in low or moderate-dimensional data. In fact, tree-based methods such as Boruta and RRF enjoy more than 5% increase in accuracy when the covariates are correlated.

To examine the selection patterns in more detail, we next present the boxplots of the Imp% and Unimp% metrics for all methods, in Figure 1. It is evident that in case of the correlated

structure in high dimensional setup, the tree-based methods such as Boruta, RRF, PIMP and NTA, in addition to ElasticNet, perform significantly well compared to the independent case in selecting the important variables as well as to record good prediction accuracy. Consequently, in these cases, one can rely on the aforementioned methods more than the rest.

Figure 1: Boxplots of the percentage of important and unimportant variables selected by each method across various iterations in the high-dimensional setup ($n = 100, m = 1000$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.

As a last piece in this section, we investigate the time complexity of the fifteen methods under different setups. Since the computational challenges are not dependent on the correlation structures

of the regressors, we calculate the average time for all the methods, taking the correlated and the independent case together, for different choices of n, m, p. These values are displayed in Figure 2, and one can notice that the time consumption increases as the number of features increases. The time for all penalty-based methods except ElasticNet is very low. Because of selecting more variables most of the times, the computational burden is greater for ElasticNet. Among screening-based methods, SIVS takes a significant amount of time compared to the others. We also note that VSURF is the most expensive approach among the tree-based methods, while PIMP and NTA also take a significant amount of time. RRF is the fastest tree-based method and its complexity does not change substantially across different settings.

Figure 2: Average computation time for the fifteen methods corresponding to the different setups in the simulation study.

4   An application to a real dataset

In this section, we consider a high dimensional classification dataset that uses the gene expression data of prostate cancer patients. It is originally from the study of Singh et al. [2002], is freely available in the R package sda (Ahdesmaki et al. [2021]), and has been widely studied by many researchers (see e.g. Efron [2009], Genuer et al. [2010]). The dataset contains relevant information of 6033 genes for 102 subjects – 52 prostate cancer patients and 50 healthy men. It falls within the regime of the LRM, as the response variable can be taken as whether a subject is a cancer patient or not, and the objective is to identify which genes are responsible for prostate cancer.

We analyze and compare the performances of all of the variable selection methods discussed and explored in the previous sections for this dataset. To begin with, using the complete data, we investigate the number of selected variables, running time and the accuracy in fitting the data for the fifteen methods. These results are detailed in Table 4. Note that, because the true set of important variables are unknown, we can only present the selected number of variables, brier score

for the fitted probability distributions and the time taken by each method. To further understand how well the models fit the data, we calculate and report the area under the curve (AUC) as well.

Table 4: Comparison of the fifteen methods in the real data ($n = 102, m = 6033$).

Method	Selected	AUC	Brier	Time
LASSO	75	1	0.000	0.019
ALASSO	44	1	0.000	0.118
SparseStep	1	0.764	0.185	0.450
ElasticNet	875	1	0.000	1.058
Best Subset	19	1	0.005	0.161
SCAD	50	1	0.018	0.102
MCP	15	0.999	0.057	0.066
SIS	5	0.935	0.092	0.006
ISIS	5	0.956	0.077	0.120
SIVS	5	0.945	0.088	4.731
Boruta	195	1	0.002	4.209
VSURF	13	1	0.002	379.289
RRF	6	1	0.002	0.291
PIMP	550	1	0.003	11.113
NTA	1325	1	0.004	4.907

Among the norm-based penalty methods, we notice that except for the SparseStep method, all other techniques register great accuracy in classifying the patients correctly. However, the number of variables selected varies substantially among all the methods. While LASSO and ALASSO select a moderately high number of variables, ElasticNet, potentially due to the properties of ridge regularization, selects as many as 875 variables and renders an immensely complex model. On the contrary, SparseStep selects only one gene, and it is still found to have the AUC value of 0.764. The Best Subset method, in the sense of parsimony and accuracy, tends to be the most appropriate approach as it selects 19 variables and records an AUC value of 1 and a fitted brier score of 0.005.

Among the concave penalty-based methods, MCP is more parsimonious compared to SCAD, and both have near to one AUC score. We also find that all screening-based methods select only five genes and record good AUC and brier scores, reflecting their usefulness in high dimensional data. Meanwhile, all the tree-based methods are found to fit the data very well. So far as the feature selection goes, except for RRF and VSURF, other three techniques pick many genes to be important. They take considerable time to run as well. VSURF in particular is exceedingly time-consuming, which is inline with the discussion of time complexity in Section 3.3. Overall, we can infer that RRF is the most effective model as it selects only six genes to classify the patients' category and incurs the least computational time of all the tree-based methods.

Next, to further demonstrate the effectiveness of these methods, we focus on the consistency in variable selection and estimation, as well as prediction performance. Here, we randomly select 80% of the dataset as a training set and the remaining 20% as a test set. This process is repeated for many iterations and the results are recorded. Due to the excessive computational burden, PIMP and VSURF are not considered here. For the other thirteen methods, in an attempt to evaluate how consistently a method determines the set of important variables across different iterations, we define a measure of similarity following the Sokal-Michener index (Valsecchia and Todeschinia [2020]). Let us use $\hat{\beta}_{ik}$ to denote the estimated value of the ith coefficient in the kth iteration. Then the Sokal-Michener similarity index, for the kth and the lth iteration corresponding to a method, is

computed as

$$\text{SM}_{kl} = \frac{\#\left\{1 \leqslant i \leqslant m : \left(\hat{\beta}_{ik} \neq 0 \text{ and } \hat{\beta}_{il} \neq 0\right) \text{ or } \left(\hat{\beta}_{ik} = 0 \text{ and } \hat{\beta}_{il} = 0\right)\right\}}{m}. \tag{4.1}$$

Using the above, if r is the total number of iterations, then the global similarity index for a method is given as

$$\text{SM} = \frac{1}{\binom{r}{2}} \sum_{k=1}^{r-1} \sum_{l=k+1}^{r} \text{SM}_{kl}. \tag{4.2}$$

Furthermore, to estimate how consistently a method estimates the coefficients of the variables across different iterations, we define the following consistency index (CI)

$$\text{CI} = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{(r-1)} \sum_{j=1}^{r} \left(\hat{\beta}_{ij} - \frac{1}{r} \sum_{j=1}^{r} \hat{\beta}_{ij}\right)^2. \tag{4.3}$$

The above measure signifies the average variation in the estimated coefficients across all iterations. Observe that the consistency index is not defined for tree-based methods as coefficient values are not estimated in those cases. Hence it is calculated for the other ten methods. A lower value of this index is desired to obtain consistency in estimating the coefficients of the variables.

Table 5: Comparison of similarity and consistency in variable selection, estimation, prediction and computational complexity for all the methods (except VSURF and PIMP) across randomly generated train-test splits of the real data.

Method	Selected	Similarity	Consistency (in 10^{-4})	Time	Brier
LASSO	51.15 ± 6.59	0.989	3.917	0.047	0.155
ALASSO	41.90 ± 4.02	0.992	8.045	0.234	0.152
SparseStep	1.00 ± 0.65	0.999	3.219	0.246	0.244
ElasticNet	630.95 ± 306.18	0.892	1.902	1.602	0.069
BestSubset	18.30 ± 1.45	0.996	2.498	0.161	0.153
SCAD	38.80 ± 4.73	0.992	0.079	0.058	0.153
MCP	11.55 ± 2.31	0.997	0.190	0.052	0.203
SIS	4.00 ± 0.32	0.999	8.257	0.008	0.236
ISIS	4.10 ± 0.45	0.999	27.647	0.141	0.261
SIVS	4.25 ± 0.55	0.999	2.696	2.923	0.246
Boruta	161.55 ± 6.89	0.986		2.338	0.028
RRF	5.25 ± 1.16	0.999		0.147	0.064
NTA	1121.60 ± 26.87	0.810		1.642	0.042

Table 5 demonstrates that the behavior of all methods except Boruta, in terms of the number of variables selected, are pretty similar to the simulation study conducted for the high-dimensional data. SparseStep is identified to be the sparsest method. It typically selects only one gene in this real application. Best Subset and MCP choose moderate number of variables with less variability. LASSO, ALASSO, and SCAD on average select moderate number of variables; whereas ElasticNet and NTA select a very high number of covariates. It is however interesting that despite selecting more than 1000 variables on an average, NTA is very consistent, i.e. there is minimal variation in the number of the selected genes by this method. Contrary to that, ElasticNet shows high

variability in variable selection, although the estimated coefficients do not differ much. Finally, akin to the simulation study, screening-based methods tend to select only a handful of variables. It clearly depicts their tightness in picking only an appropriate and small set of variables in such a high dimensional data.

The above observations are reaffirmed from the similarity index column of Table 5. Methods with a high number of selected variables are generally not uniform in selecting the same set of genes across the iterations, while the screening-based methods are most homogeneous in selecting the important covariates. A conflicting point is noted from the consistency index which indicates that the estimated coefficients in screening-based typology are not homogeneous and that the concave penalty-based methods are the most dependable in this front. In fact, ISIS appears to be the most inconsistent method among all the non-tree-based methods in estimating the coefficients of the variables.

Among the procedures of the last type, the behaviors are found to be drastically different. RRF selects quite a low number of features but has higher variability in selecting the variables than the screening-based methods. It is one of the fastest algorithms as well. In comparison, Boruta and NTA select many features in general and are more time-consuming methods.

As a final piece of this section, we compare the prediction performance of the thirteen methods. The last column of Table 5 displays the average Brier scores across different iterations. We find that the screening-based methods are in general the least effective in predicting the true classes. In contrast, the tree-based methods and the ElasticNet are the best to classify the category of a patient in the out-of-sample data. Their Brier scores are, in truth, about four times better than the screening-based methods and more than two times better than other penalty-based methods. ElasticNet, possibly due to the selection of a bigger set of relevant genes, registers higher prediction accuracy than other penalty or screening-based methods. We note that Boruta selects a moderate number of genes to classify the category and record the best brier score among all the methods. RRF selects very few genes compared to Boruta, but the latter's brier score is more than two times better than RRF.

From the above results, we make a conjecture that in a medical study, it is important to recognise all the essential genes which are potentially correlated with an illness. Therefore, in an application like this, Boruta can be the most appropriate method, as it selects moderate number of variables and registers the highest prediction accuracy. RRF is one of the most parsimonious methods with a low brier score. Amongst the penalty or screening based methods, only ElasticNet can be an effective method, and it usually chooses an exhaustive set of features that would provide good predictive performance.

5   Conclusion

In this study, we have considered four types of classical variable selection methods in the regression model for the binary data, and assessed their efficacy in six different simulation setups related to low, moderate and high dimensional cases of correlated and uncorrelated covariates. The accuracy of the methods deviate from one setting to another. For instance, in the low dimensional data where the number of observations is much higher than the number of predictors, penalty-based methods such as LASSO, Best Subset and MCP are appropriate to use. In these cases, screening-based methods should be avoided as they provide misleading regression coefficients. In a moderate dimensional setting where the number of predictors is comparable to the number of observations, Best Subset and MCP still continue to perform well. LASSO and SCAD can also be used in these cases as they are fast and accurate in out-of-sample predictions, albeit the former tends to select

slightly greater number of covariates than the truth.

The results for the high-dimensional setting is more intriguing. We notice that the screening-based methods lean towards selecting very less number of variables. Thus, if the purpose is to choose a sparse yet good model, then these methods can be very useful. They provide acceptable prediction accuracy as well. Otherwise, concave penalty-based methods like SCAD and MCP can be good choices as they select appropriate number of total and important variables and record the lowest Brier scores in high dimensional setup. Based on the real application, we can also ascertain that Boruta is an excellent choice in gene expression studies as it selects the appropriate number of important variables and registers the best accuracy. On a related note, practitioners are often interested in detecting an exhaustive list of covariates which may be correlated with the binary response variable in such research problems. ElasticNet or NTA, which tend to select a higher number of variables, can be more fitting algorithms for such requirements. Since LASSO can only select up to $\min\{n, m\}$ number of variables, it is not recommended in these problems, despite its predictive accuracy being at par with other penalty-based methods. We also note that SIVS, VSURF and PIMP take a lot of time to function, and thus they should be avoided while working with very high dimensional data.

We want to conclude this paper with a succinct account of some future scopes of our work. Throughout the simulation study in this article, the number of important variables is taken to be substantially smaller than the number of observations, which may not be the case in some real-life applications. For example, in the application in Section 4, typically the tree-based methods are performing better and they are found to select more than 100 variables. Moreover, in such instances, covariates are likely to be correlated and can have grouping effects. Therefore, though the considered penalty-based approaches fail to provide good results in these situations, one may take resort to group LASSO type of estimators which are not evaluated in this work. To that end, it would be a valuable exercise to extend the review and simulations to include methods that incorporate the inherent group structures in the regressor set.

It is also worth mention that we work with continuous predictors in this paper, and discrete or categorical variables can be added as covariates, although that is not expected to affect the findings significantly. Furthermore, because of computational constraints, we have not incorporated ultra high-dimensional cases in this paper and it would be interesting to see if the performances of the methods alter much in those cases. Naturally, there is a sizeable scope of extending the simulations to more experimental frameworks.

Regarding the review and comparison of methods, we reiterate that our focus has been restricted on the frequentist approaches in the four typologies. Therefore, Bayesian variable selection procedures such as horseshoe shrinkage priors are not included in this work. Few other recent advances in machine learning (e.g. genetic algorithms and its variants) are also not included here. A prospective direction to our work would be to cover all such possible techniques and use appropriate measures to compare their virtues across various settings. Last but not the least, we earlier pointed out that there are several methods (CASE, FA-CAR, RSO etc.) the theory of which have been developed for the linear models, but the implementation in generalised linear models are yet to be explored. A future endeavor to improve the existing research on that note would be extremely valuable for both statisticians and practitioners.

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Appendix

A Additional tables and figures

Table A1: Performance metrics of the fifteen methods in the low dimensional simulation setting ($n = 100, m = 10, p = 3$).

Method	Selected	Imp%	Unimp%	MSE	MAE	Accuracy	Precision	Recall	Time	Brier
Independent case										
LASSO	6.430	96.000	50.714	0.763	0.408	83.300	0.832	0.853	0.004	0.112
ALASSO	3.910	89.667	17.429	0.485	0.307	83.900	0.838	0.857	0.004	0.110
SparseStep	2.540	77.333	3.143	0.649	0.324	84.000	0.849	0.839	0.006	0.113
ElasticNet	6.330	87.333	53.000	3.208	0.885	82.300	0.836	0.826	0.217	0.166
Best Subset	3.670	85.333	15.857	0.473	0.336	84.150	0.846	0.846	0.004	0.111
SCAD	3.470	86.333	12.571	8.289	0.480	84.350	0.852	0.850	0.004	0.111
MCP	3.090	84.667	7.857	0.514	0.317	84.650	0.854	0.852	0.004	0.109
SIS	2.710	77.667	5.429	8.556	0.540	83.600	0.852	0.827	0.001	0.113
ISIS	2.710	77.667	5.429	8.556	0.540	83.600	0.852	0.827	0.003	0.113
SIVS	3.076	90.217	9.162	0.974	0.466	84.565	0.855	0.850	2.389	0.108
Boruta	2.857	78.388	7.221			81.703	0.821	0.815	0.061	0.132
VSURF	2.959	79.252	8.309			81.276	0.811	0.824	0.330	0.131
RRF	3.327	76.871	14.577			80.969	0.815	0.815	0.001	0.133
PIMP	2.439	73.577	3.310			80.549	0.805	0.804	0.052	0.139
NTA	3.432	79.649	14.887			80.368	0.809	0.801	0.006	0.133
Correlated case										
LASSO	5.910	89.667	46.000	0.549	0.408	82.600	0.817	0.822	0.002	0.118
ALASSO	3.750	83.333	17.857	0.442	0.324	83.750	0.829	0.836	0.003	0.115
SparseStep	2.350	69.667	3.714	1.757	0.386	83.050	0.826	0.830	0.007	0.122
ElasticNet	6.950	87.333	61.857	19.651	1.225	81.650	0.821	0.801	0.110	0.158
Best Subset	3.510	80.000	15.857	0.543	0.360	83.100	0.823	0.832	0.005	0.119
SCAD	3.200	79.333	11.714	0.672	0.366	82.450	0.824	0.820	0.004	0.121
MCP	2.780	77.000	6.714	0.657	0.349	82.800	0.826	0.826	0.004	0.118
SIS	2.450	70.333	4.857	24.431	1.006	82.050	0.828	0.813	0.001	0.130
ISIS	2.450	70.333	4.857	24.431	1.006	82.050	0.828	0.813	0.002	0.130
SIVS	2.954	86.743	11.364	1.002	0.472	83.750	0.832	0.837	1.074	0.113
Boruta	3.905	76.596	22.796			78.404	0.782	0.770	0.075	0.149
VSURF	3.333	76.042	15.625			79.062	0.800	0.777	0.143	0.148
RRF	3.837	76.768	19.336			78.939	0.792	0.782	0.001	0.146
PIMP	2.884	71.648	10.181			78.621	0.795	0.747	0.053	0.153
NTA	4.789	79.649	34.286			78.579	0.791	0.773	0.006	0.147

Table A2: Performance metrics of the fifteen methods in the moderate dimensional simulation setting ($n = 100, m = 100, p = 5$).

Method	Selected	Imp%	Unimp%	MSE	MAE	Accuracy	Precision	Recall	Time	Brier
Independent case										
LASSO	20.550	83.000	17.263	0.211	0.112	82.90	0.852	0.821	0.003	0.127
ALASSO	13.820	76.000	10.547	0.142	0.096	81.90	0.840	0.812	0.004	0.127
SparseStep	2.430	46.600	0.105	0.168	0.072	80.70	0.836	0.788	0.068	0.134
ElasticNet	20.730	71.600	18.053	0.357	0.170	78.20	0.816	0.780	0.163	0.183
Best Subset	4.570	59.600	1.674	0.158	0.080	80.80	0.836	0.799	0.051	0.131
SCAD	10.350	79.000	6.737	0.574	0.094	82.90	0.851	0.828	0.013	0.121
MCP	5.910	70.200	2.526	0.158	0.079	82.50	0.846	0.822	0.011	0.123
SIS	3.320	48.400	0.947	0.171	0.081	80.00	0.836	0.785	0.001	0.140
ISIS	3.860	61.000	0.853	0.166	0.075	82.20	0.847	0.818	0.003	0.127
SIVS	4.210	60.800	1.232	0.242	0.095	82.90	0.853	0.826	5.000	0.126
Boruta	5.505	55.152	2.892			74.95	0.734	0.746	0.138	0.166
VSURF	7.140	56.800	4.526			75.90	0.779	0.766	0.659	0.172
RRF	3.657	46.061	1.425			76.57	0.752	0.766	0.004	0.160
PIMP	7.530	52.600	5.158			75.55	0.748	0.747	0.189	0.167
NTA	12.360	62.600	9.716			74.60	0.729	0.752	0.032	0.176
Correlated case										
LASSO	16.790	74.800	13.737	0.222	0.108	81.65	0.814	0.820	0.002	0.133
ALASSO	12.720	70.000	9.705	0.148	0.096	81.75	0.818	0.814	0.003	0.131
SparseStep	2.450	45.600	0.179	0.151	0.071	82.75	0.831	0.832	0.023	0.129
ElasticNet	17.630	66.000	15.084	0.429	0.184	78.55	0.795	0.791	0.122	0.195
Best Subset	4.100	56.600	1.337	0.172	0.083	82.80	0.819	0.843	0.018	0.128
SCAD	8.830	69.600	5.632	0.150	0.079	83.20	0.831	0.847	0.010	0.119
MCP	5.250	64.000	2.158	0.144	0.075	83.65	0.838	0.847	0.008	0.116
SIS	2.600	40.800	0.590	0.178	0.083	79.20	0.796	0.799	0.001	0.146
ISIS	3.720	54.600	1.042	3.453	0.110	81.85	0.816	0.829	0.002	0.136
SIVS	3.940	58.200	1.084	0.239	0.094	82.60	0.821	0.831	3.823	0.124
Boruta	6.870	50.800	4.558			74.20	0.745	0.748	0.166	0.175
VSURF	6.430	52.600	4.000			76.25	0.771	0.761	0.526	0.162
RRF	3.959	41.224	1.998			72.96	0.728	0.732	0.004	0.180
PIMP	8.700	49.600	6.547			75.10	0.754	0.752	0.188	0.173
NTA	14.510	59.000	12.168			74.20	0.738	0.741	0.064	0.180

Table A3: Performence metrics of the fifteen methods in the high dimensional simulation setting $(n = 100, m = 1000, p = 10)$.

					Independent case					
Method	Selected	Imp%	Unimp%	MSE	MAE	Accuracy	Precision	Recall	Time	Brier
LASSO	25.610	41.200	2.170	0.073	0.025	73.40	0.733	0.749	0.003	0.179
ALASSO	30.200	43.000	2.616	0.061	0.027	72.70	0.731	0.737	0.013	0.195
SparseStep	1.640	15.100	0.013	0.064	0.021	70.90	0.715	0.732	0.032	0.192
ElasticNet	56.440	36.400	5.333	0.078	0.029	69.90	0.729	0.698	0.236	0.224
Best Subset	4.410	23.700	0.206	0.068	0.022	72.10	0.734	0.737	0.031	0.182
SCAD	19.790	39.600	1.599	0.065	0.023	75.10	0.766	0.766	0.015	0.168
MCP	8.590	33.200	0.532	0.067	0.022	74.80	0.756	0.759	0.012	0.167
SIS	3.800	20.500	0.177	0.063	0.022	71.00	0.713	0.718	0.001	0.205
ISIS	4.000	23.300	0.169	0.301	0.024	71.80	0.722	0.726	0.009	0.217
SIVS	4.160	25.900	0.159	0.070	0.022	74.60	0.758	0.752	6.281	0.185
Boruta	8.900	10.500	0.694			60.45	0.615	0.608	0.201	0.243
VSURF	26.470	32.200	2.348			65.20	0.662	0.650	3.696	0.219
RRF	6.500	8.750	0.484			62.00	0.624	0.639	0.029	0.241
PIMP	77.820	21.600	7.500			59.90	0.599	0.618	1.331	0.236
NTA	78.840	26.100	7.512			61.10	0.627	0.626	0.284	0.234
					Correlated case					
Method	Selected	Imp%	Unimp%	MSE	MAE	Accuracy	Precision	Recall	Time	Brier
LASSO	26.330	40.800	2.247	0.070	0.025	75.300	0.750	0.750	0.003	0.177
ALASSO	29.500	43.400	2.541	0.058	0.026	73.550	0.736	0.717	0.013	0.194
SparseStep	1.660	14.700	0.019	0.062	0.021	71.350	0.725	0.715	0.032	0.192
ElasticNet	80.190	43.400	7.662	0.073	0.030	69.450	0.700	0.717	0.236	0.231
Best Subset	5.100	24.800	0.265	0.067	0.023	72.250	0.722	0.720	0.031	0.187
SCAD	19.100	38.300	1.542	0.062	0.023	75.000	0.746	0.760	0.014	0.173
MCP	7.990	30.500	0.499	0.065	0.023	74.650	0.750	0.751	0.012	0.173
SIS	3.590	20.000	0.161	0.061	0.022	72.950	0.729	0.722	0.001	0.194
ISIS	4.000	24.300	0.159	0.052	0.020	73.700	0.733	0.737	0.008	0.197
SIVS	4.260	24.800	0.180	0.068	0.023	74.300	0.736	0.756	5.977	0.185
Boruta	10.240	22.800	0.804			67.400	0.689	0.657	0.217	0.212
VSURF	24.220	31.500	2.128			66.550	0.658	0.682	3.730	0.216
RRF	5.190	18.300	0.339			68.750	0.690	0.679	0.029	0.210
PIMP	81.040	34.800	7.835			64.850	0.691	0.609	1.326	0.225
NTA	82.590	39.800	7.941			63.750	0.688	0.611	0.287	0.226

Figure A1: Boxplots of the percentage of important and unimportant variables selected by each method across various iterations in the low-dimensional setup ($n = 100, m = 10$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.
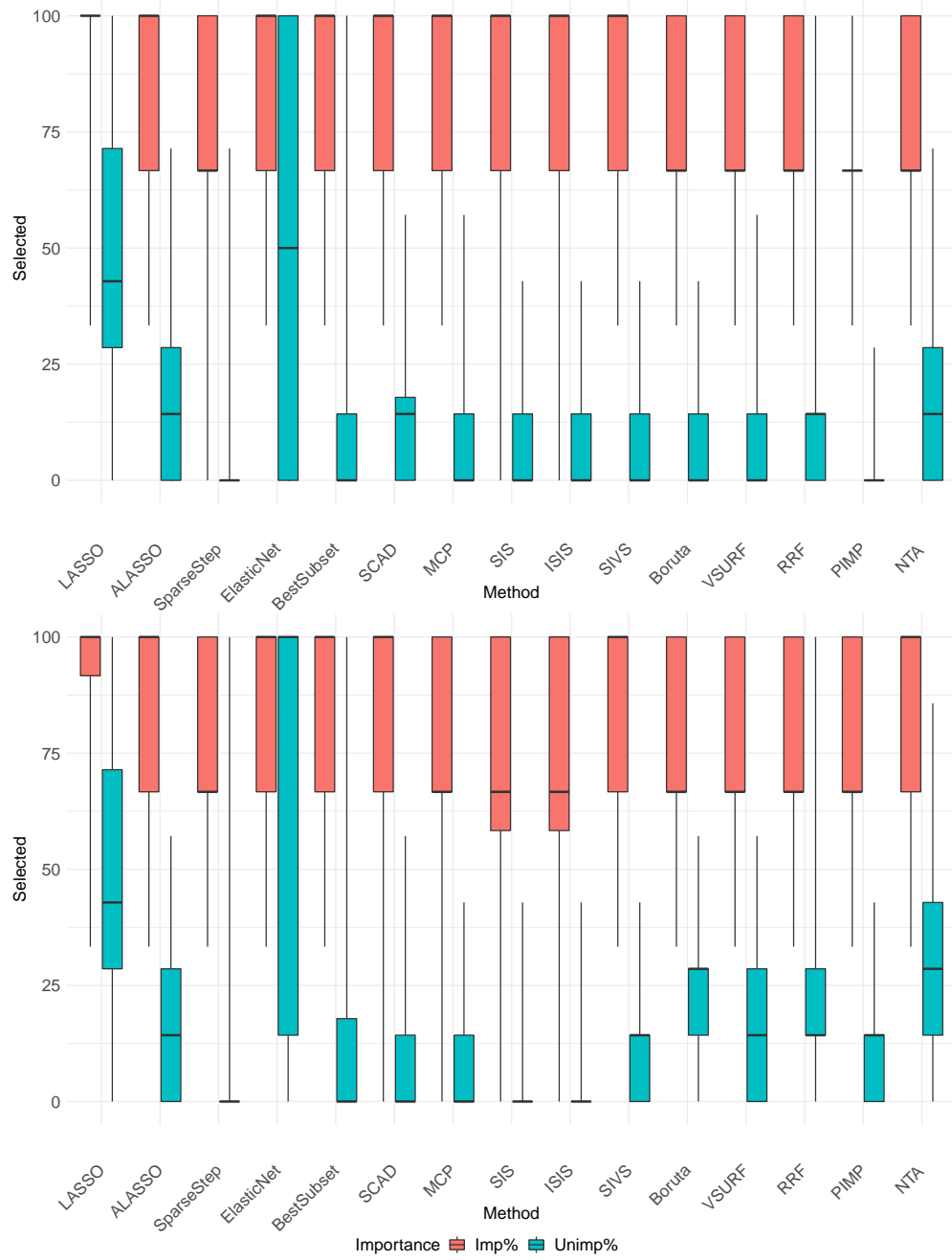
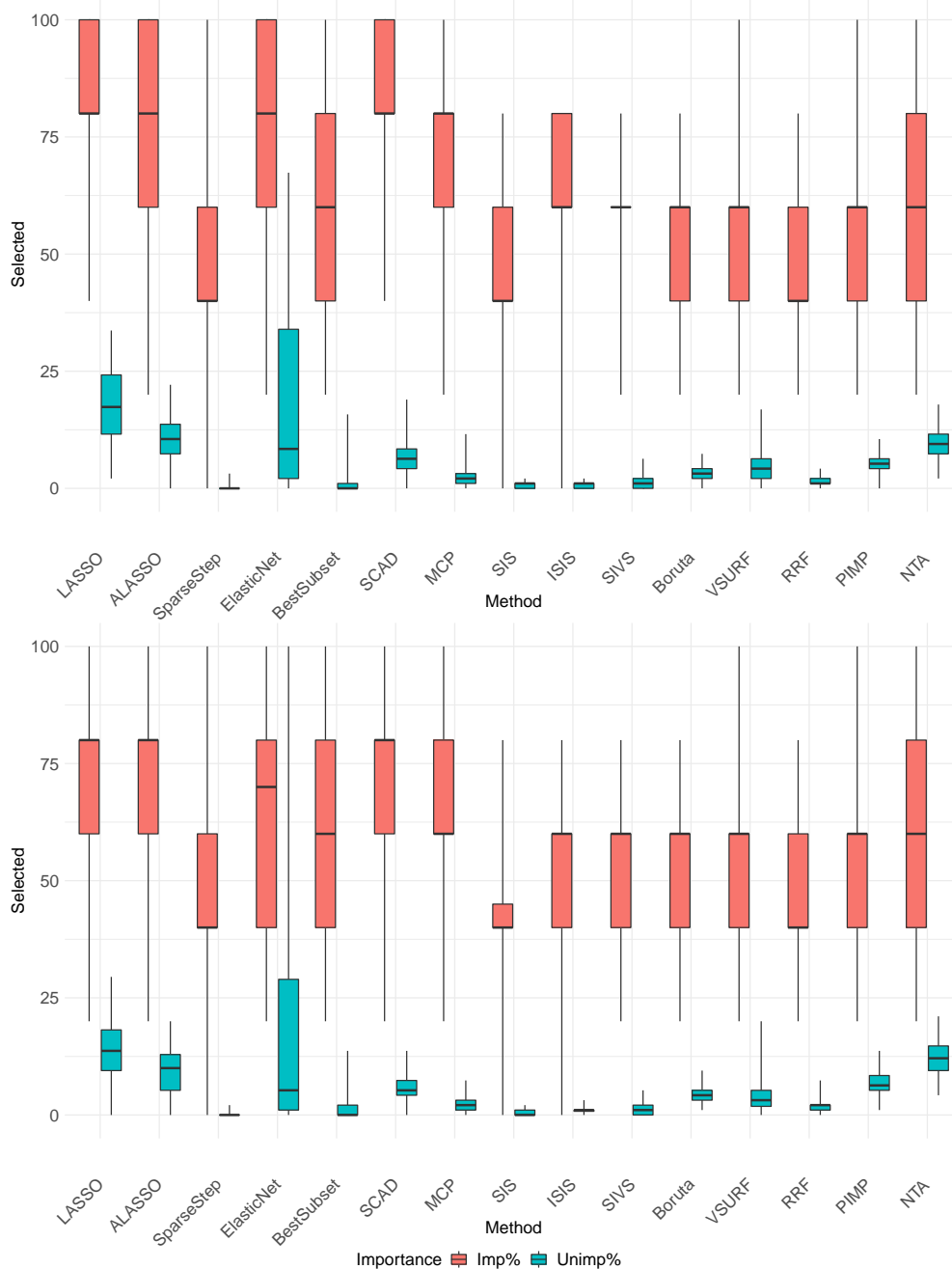Figure A2: Boxplots of the percentage of important and unimportant variables selected by each method across various iterations in the moderate-dimensional setup ($n = 100, m = 100$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.

Figure A3: Boxplots of the prediction brier scores across various iterations in the low-dimensional setup ($n = 100, m = 10$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.
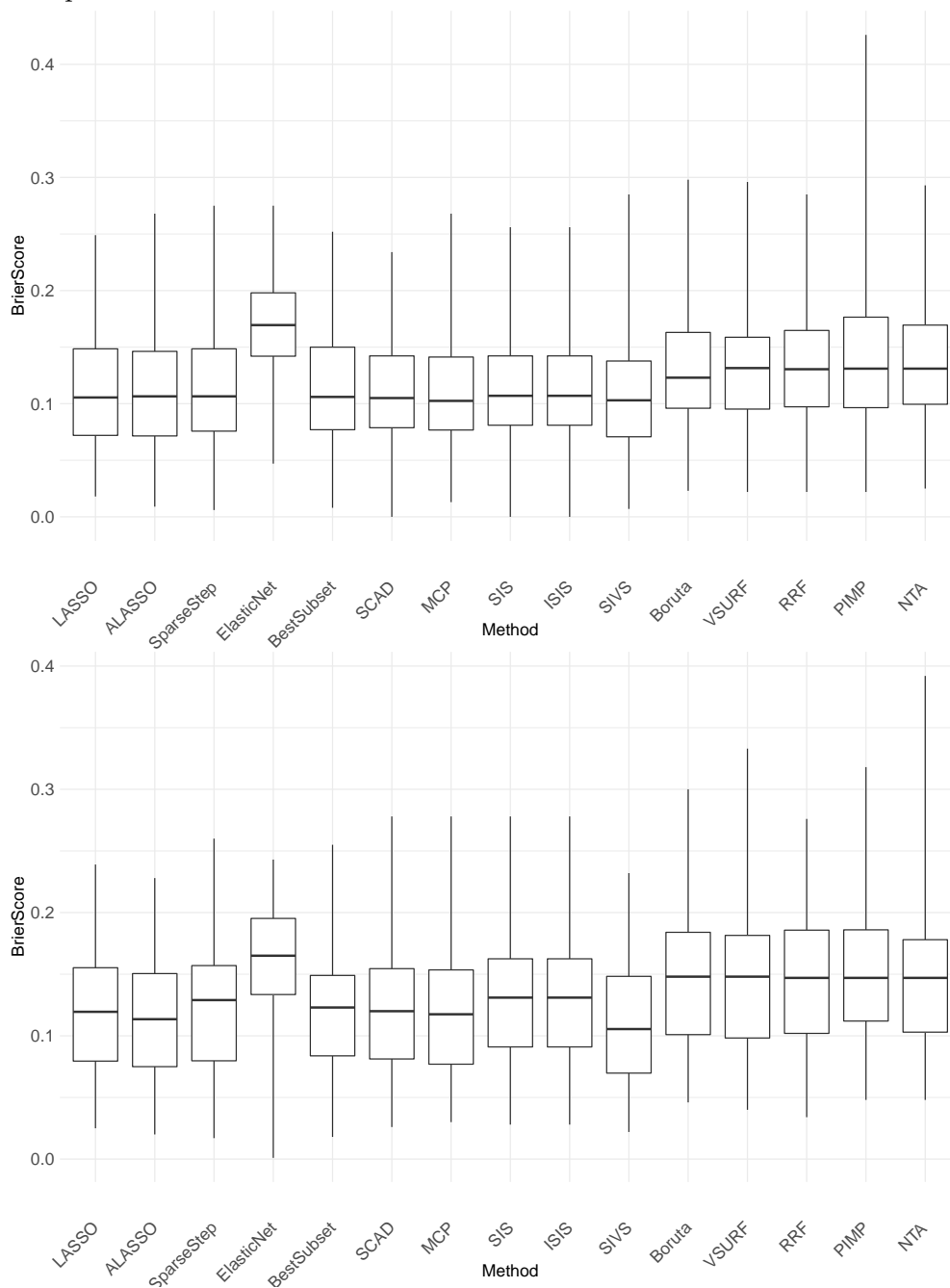
Figure A4: Boxplots of the prediction brier scores across various iterations in the moderate-dimensional setup ($n = 100, m = 100$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.
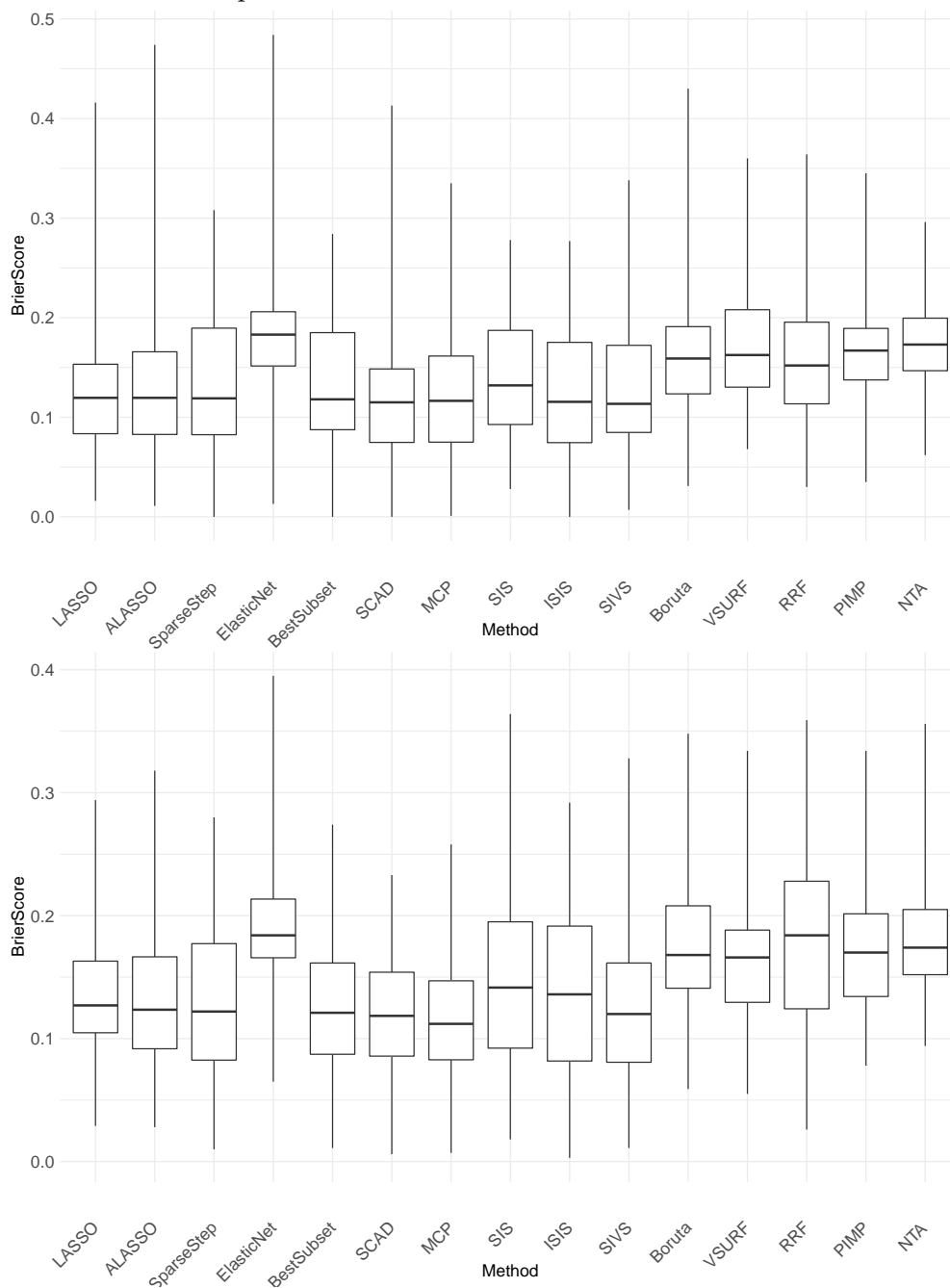
Figure A5: Boxplots of the prediction brier scores across various iterations in the high-dimensional setup ($n = 100, m = 1000$). Uncorrelated case is shown in the top panel and correlated case is shown in the bottom panel.