OLSAVS: A NEW ALGORITHM FOR MODEL SELECTION

by

Nicklaus T. Hicks

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Approved by:

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Hasthika Rupasinghe, Ph.D., Thesis Director

_____

Lasanthi Watagoda, Ph.D., Second Reader

_____

William J. Cook, Ph.D., Honors Director, Department of Mathematical Sciences

_____

Eric S. Marland, Ph.D., Chair, Department of Mathematical Sciences

Abstract

The shrinkage methods such as Lasso and Relaxed Lasso introduce some bias in order to reduce the variance of the regression coefficients in multiple linear regression models. One way to reduce bias after shrinkage of the coefficients would be to apply ordinary least squares to the subset of predictors selected by the shrinkage method used. We extensively studied this idea in this work and developed a new variable selection algorithm. We named this technique OLSAVS (**O**rdinary **L**east **S**quares **A**fter **V**ariable **S**election). We have implemented the OLSAVS algorithms in R. Simulations were used to illustrate that the new method is able to produce better predictions with less bias for various error distributions. We compare the OLSAVS method with a few widely used shrinkage methods in terms of their achieved test root mean square error and bias.

Acknowledgments

My deepest gratitude goes to the Appalachian State University mathematics department for providing me with the knowledge to accomplish a milestone such as this. I wish to extend my gratitude to my thesis director, Dr. Hasthika Rupasinghe, for his continuous support and guidance throughout this thesis. Without his help, this would not be possible. An additional sincere thanks to my second reader, Dr. Lasanthi Watagoda, for taking the time out of her schedule to analyze this paper. Furthermore, I wish to acknowledge my honors director, Dr. William J. Cook, for providing me with this opportunity to express my knowledge.

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Contents

1 Introduction

Suppose we have a response predictor Y_i and p distinct predictors, then our multiple linear regression model (MLR) takes the form of

$$Y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon \tag{1}$$

where X_j represents each predictor and β_j represents the corresponding relationship between the variable and response, with β_0 representing the intercept. MLR is an important tool for this study and helps lay a foundation for more complex models.

1.1 MLR model in matrix notation

MLR introduced in equation (1) can oftentimes become lengthy depending on the number of predictors. Therefore, using matrix notation, we can write the multiple linear regression model in the form of $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ according to [8]. Analyzing this form,

$$\boldsymbol{Y}_{n\times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \tag{2}$$

Where $\boldsymbol{Y}$ is a $n \times 1$ vector, and n is the sample size. The matrix $\boldsymbol{X}$ below,

$$\boldsymbol{X}_{n\times p} = \begin{bmatrix} 1 & X_{11} & X_{12} & \dots & X_{1,p-1} \\ 1 & X_{21} & X_{22} & \dots & X_{2,p-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{n,p-1} \end{bmatrix} \tag{3}$$

is a $n \times p$ matrix of predictors. Then, $\boldsymbol{\beta}$,

$$\boldsymbol{\beta}_{p\times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix} \tag{4}$$

is an unknown p x 1 vector of coefficients, and $\boldsymbol{\epsilon}$,

$$\boldsymbol{\epsilon}_{n\times 1} = \begin{bmatrix} \boldsymbol{\epsilon}_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} \tag{5}$$

is $n \times 1$ vector representing the random error in each predictor.

Note that $\boldsymbol{Y}$ and $\boldsymbol{\epsilon}$ are the same as for simple linear regression. The $\boldsymbol{\beta}$ vector contains additional regression parameters, and the $\boldsymbol{X}$ matrix contains a column of 1's as well as a column of n observations for each $p-1$ explanatory variable in the regression model. Additionally, the row subscript for each element in X_{ik} in the matrix, $\boldsymbol{X}$ represents the trial/case, and the column subscript identifies the $\boldsymbol{X}$ variables. See [1].

1.2 Estimation of Regression Coefficients

This section closely follows [4] and covers the theory for estimating simple linear and MLR regression model coefficients.

1.2.1 Estimating simple liner regression model coefficients

Consider the simple linear regression model where there is only one predictor variable and this function is linear, we can describe this model below,

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i \tag{6}$$

Where,

Y_i is the value we obtain of the response variable in the ith trial

β_0 and β_1 are parameters that are defined in section 1.2 through the least squares method

X_i is a known constant that represents the value of the predictor variable in the ith trial.

ϵ_i represents the random error in the mean with mean 0 and variance σ^2

Additionally we can expand equation (6) below,

$$\boldsymbol{Y}_{n\times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \tag{7}$$

Where $\boldsymbol{Y}$ is a n x 1 vector with n being the number of response variables. Next, we look at the matrix $\boldsymbol{X}$,

$$\boldsymbol{X}_{n\times 2} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \tag{8}$$

Following this we have vectors for $\boldsymbol{\beta}$ and $\boldsymbol{\epsilon}$ respectively,

$$\boldsymbol{\beta}_{2\times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \tag{9}$$

$$\boldsymbol{\epsilon}_{n\times 1} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} \tag{10}$$

In order to perform any kind of statistical testing, we must first understand and describe the regression coefficients. These coefficients are parameters in the regression model and are typically described as β_0 and β_1. The β_1 represents the slope of the regression line and β_0 represents the y-intercept in the line.

However, in many cases, the values for these two parameters are not known. Therefore, we must estimate these values. We will estimate these values through either observational data or experimental data.

In order to estimate values for β_0 and β_1, we will use the least squares method. By using observations in a data set (X_i, Y_i), we can build a formula that considers the deviation of Y_i from its expected value,

$$Y_i - (\beta_0 + \beta_1 X_i) \tag{11}$$

Now, we can build off equation (11) and consider the sum of n squared deviations. We will use Q to define this,

$$Q = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2 \tag{12}$$

In equation (12), we will estimate β_0 and β_1 with b_0 and b_1, which are values that help minimize Q for n sample observations.

The idea for least squares is to find the estimate values, b_0 and b_1, for the parameters that help minimize Q. We can find these estimates in two ways, through numerical search procedures or analytical procedures. By using the analytical procedure, we can show that b_0 and b_1 that minimize Q are given by the following,

$$\sum Y_i = nb_0 + b_1 \sum X_i \tag{13}$$

$$\sum X_i Y_i = b_0 \sum X_i + b_1 \sum X_i^2 \tag{14}$$

where these two equations are known as normal equations and b_0 and b_1 are known as the point estimators for β_0 and β_1. Now, we can solve equations (13) and (14) for b_0 and b_1,

$$b_1 = \frac{\sum(X_i - \bar{X})(Y_i - \bar{Y})}{\sum(X_i - \bar{X})^2} \tag{15}$$

$$b_0 = \frac{1}{n}(\sum Y_i - b_1 \sum X_i) = \bar{Y} - b_1\bar{X} \tag{16}$$

Here, $\bar{X}$ and $\bar{Y}$ are the means of the X_i and Y_i observations.

1.2.2 Estimating MLR model coefficients

Extending equation (12) using the MLR model in equation (1) we get;

$$Q = \sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_{i1} - \ldots - \beta_{p-1}X_{i,p-1})^2 \tag{17}$$

In this equation, the least squares estimators are $\beta_0, \beta_1, \ldots, \beta_{p-1}$, which help minimize Q. However, the least squares estimated regression coefficients $b_0, b_1, \ldots, b_{p-1}$, where $\boldsymbol{b}$,

$$\boldsymbol{b}_{p\times 1} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix} \tag{18}$$

where the least squares normal equations for the general linear regression model are,

$$\boldsymbol{X'Xb} = \boldsymbol{X'Y} \tag{19}$$

and the least squares estimators are,

$$\boldsymbol{b}_{p\times 1} = (\boldsymbol{X'X})^{-1}\boldsymbol{X'Y} \tag{20}$$

1.2.3 Fitted Values and Residuals

Let $\hat{\boldsymbol{Y}}$ be a vector of fitted values and the vector of residuals $e_i = Y_i - \hat{Y}_i$ be represented by $\boldsymbol{e}$:

$$\hat{\boldsymbol{Y}}_{n\times 1} = \begin{bmatrix} \hat{Y_1} \\ \hat{Y_2} \\ \vdots \\ \hat{Y_n} \end{bmatrix} \tag{21}$$

$$\boldsymbol{e}_{n\times 1} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} \tag{22}$$

Where the fitted values are represented by,

$$\hat{\boldsymbol{Y}}_{n\times 1} = \boldsymbol{X}\boldsymbol{b} \tag{23}$$

since,

$$\begin{bmatrix} \hat{Y_1} \\ \hat{Y_2} \\ \vdots \\ \hat{Y_n} \end{bmatrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} b_0 + b_1 X_1 \\ b_0 + b_1 X_2 \\ \vdots \\ b_0 + b_1 X_n \end{bmatrix} \tag{24}$$

and the residual terms by,

$$\boldsymbol{e}_{n\times 1} = \boldsymbol{Y} - \hat{\boldsymbol{Y}} = \boldsymbol{Y} - \boldsymbol{X}\boldsymbol{b} \tag{25}$$

The residual value represents the difference between the observed response value and the value predicted by the specific model being used. Now we can define the residual sum of squares (RSS) as follows,

$$RSS = {e_1}^2 + {e_2}^2 + \ldots + {e_n}^2 \tag{26}$$

or expanded as,

$$RSS = (y_1 - \hat{\beta}_0 + \hat{\beta}_1 X_1)^2 + (y_2 - \hat{\beta}_0 + \hat{\beta}_1 X_2)^2 + \ldots + (y_n - \hat{\beta}_0 + \hat{\beta}_1 X_n)^2 \tag{27}$$

where the least squares method mentioned previously helps determine β_0 and β_1 to minimize the RSS.

1.3 Variable selection

Variable selection is the search for a subset of predictor variables that can be deleted with little loss of information, and so the model with the remaining predictors is useful for prediction. The variable selection methods being looked at in this study are the following, Ridge regression, Lasso, Relaxed Lasso, and Elastic Net models.

1.3.1 Ridge regression

According to [3], similar to least squares, ridge regression finds the best coefficients to make the RSS small. Ridge Regression coefficient estimates $\hat{\beta}^R$, are values that minimize,

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p}\beta^2 = RSS + \lambda \sum_{j=1}^{p}\beta_j^2 \tag{28}$$

Where $\lambda \geq 0$ is a tuning parameter. The second term in the equation,

$$\lambda \sum_{j=1}^{p}\beta_j^2 \tag{29}$$

is known as the shrinkage penalty. This penalty value is small when $\beta_1, ..., \beta_p$ are close to zero, sending the β_j values to zero but never reaching zero. For this reason, ridge regression includes all predictors p in the model.

1.3.2 Lasso

Another method for estimating β is known as Lasso regression, which contains qualities similar to ridge regression models. Lasso improves on one specific that ridge does not. Lasso sets variables to zero, unlike ridge. See [7]. The Lasso coefficients,

$$\hat{\beta_\lambda}^L, \text{minimizes the quantity} \tag{30}$$

$$RSS + \lambda \sum_{j=1}^{p} |\beta_j| \tag{31}$$

Where RSS is given in equation (26).

1.3.3 Relaxed Lasso

Relaxed Lasso, according to [5] controls model selection and shrinkage estimation by two separate parameters λ and ϕ. The Relaxed Lasso estimator is defined for $\lambda \in [0, \infty)$ and $\phi \in (0, 1]$ as

$$\hat{\boldsymbol{\beta}}^{\lambda,\phi} = \underset{\beta}{\operatorname{argmin}}\, n^{-1} \sum_{i=1}^{n} (\boldsymbol{Y}_i - \boldsymbol{X}_i^T \{\boldsymbol{\beta} \cdot \mathbf{1}_{\mathcal{M}_\lambda}\})^2 + \phi\lambda|\boldsymbol{\beta}|_1 \tag{32}$$

Where $\mathcal{M}_\lambda$ is the indicator function on the set of variables $\mathcal{M} \subseteq \{1, ..., p\}$ so that for all $k \in \{1, \ldots, p\}$

$$\boldsymbol{\beta} \cdot \mathbf{1}_{\mathcal{M}_\lambda} = \begin{cases} 0 & k \notin \mathcal{M}_\lambda \\ \boldsymbol{\beta}_k & k \in \mathcal{M}_\lambda \end{cases}$$

Relaxed Lasso is a generalization from Lasso. Unlike Lasso, the Relaxed Lasso takes into account two regularization parameters. This method produces not only Lasso solutions but also a least-squares solution that controls the regularization applied to the selected variables.

1.3.4 Elastic Net

As explained in [10], given data ($\boldsymbol{y}$,$\boldsymbol{X}$) and penalty parameters (λ_1,λ_2) and some augmented data ($\boldsymbol{y}^*$, $\boldsymbol{X}^*$) the naïve Elastic Net model takes the following form,

$$\hat{\boldsymbol{\beta}}^* = \underset{\boldsymbol{\beta}^*}{\operatorname{argmin}} |\boldsymbol{y}^* - \boldsymbol{X}^*\boldsymbol{\beta}^*|^2 + \frac{\lambda_1}{\sqrt{(1+\lambda_2)}}|\boldsymbol{\beta}|_1 \tag{33}$$

This form of the Elastic Net solves a Lasso-type problem, where the corrected Elastic Net estimates $\hat{\boldsymbol{\beta}}$ are defined as,

$$\hat{\boldsymbol{\beta}}(\text{elastic net}) = \sqrt{(1+\lambda_2}\hat{\boldsymbol{\beta}}^* \tag{34}$$

and $\hat{\boldsymbol{\beta}}$(naïve elastic net) $= 1/\sqrt{1+\lambda_2}\ \hat{\boldsymbol{\beta}}^*$ then,

$$\hat{\boldsymbol{\beta}}(\text{elastic net}) = (1+\lambda_2)\hat{\boldsymbol{\beta}}(\text{naïve elastic net}). \tag{35}$$

This then shows that our Elastic Net model takes form from a rescaled naïve Elastic Net. Additionally, the scaling factor $(1+\lambda_2)$ comes from a decomposition of the Ridge operator. However, this is outside the scope of this paper but does give insight into how the Elastic Net model includes Ridge regression as well.

Lastly, Elastic Net (Enet) regression is another method of variable selection. This model takes into account two regularization parameters. These two parameters come for the Lasso and Ridge models. Therefore, Elastic Net does produce variables equal to zero. In many cases, Elastic Net is better to use than Lasso or Ridge, because in this scenario you do not have to choose between the two.

2 Method

2.1 Assessing Model Accuracy

In statistical learning, it is key to determine the model's accuracy with some value and decide which method works better. This metric is called the Mean Squared Error (MSE), and we will use this measure to represent the extent to which the predicted response value is close to the true response value for a

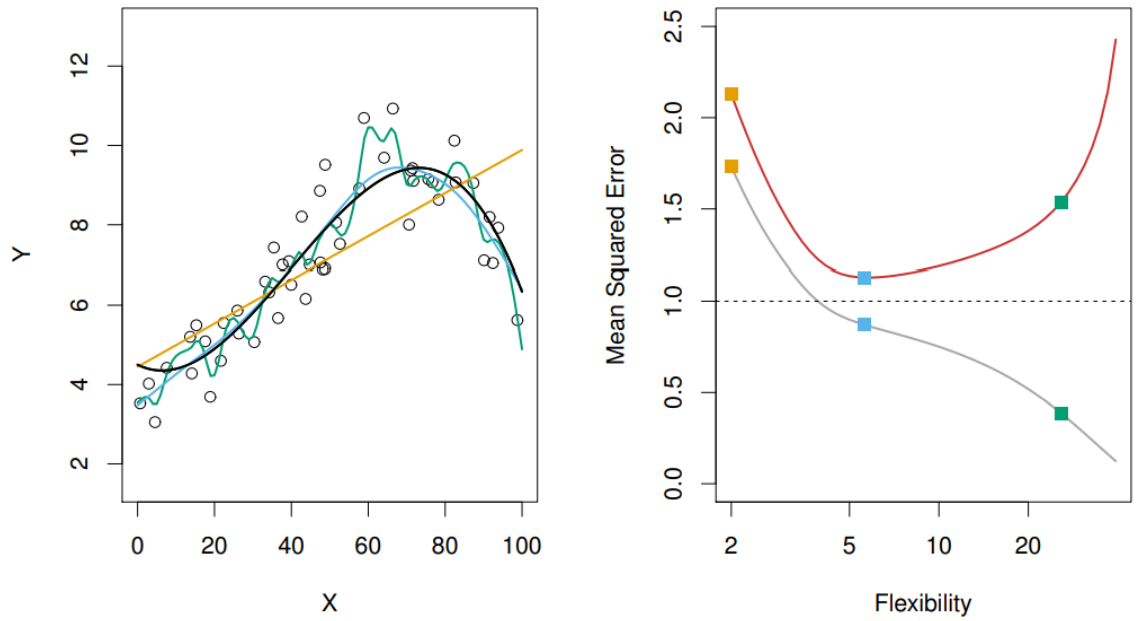


Figure 1: Left: Data simulated from f, shown in black. We estimate f with the following: the linear regression line (orange curve), and two smoothing spline fits (blue and green curves). Right: Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed line). Squares represent the training and test MSEs for the three fits shown on the left.

given observation. The MSE is given by the formula,

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2 \tag{36}$$

Where $\hat{f}(x_i)$ is the prediction that $\hat{f}$ gives for the ith observation. This value will be small if the predicted values are close to the true values. See [1].

Although we would like this value to be small for training data, the key value will come from the test MSE as shown below in figure 1,

Here we see a data set fitted with three different models. Based on the first judgment it appears the green cubic spline fits the data best. However, on the right, we can see how the training and test MSE values compare. Notice that the green square represents the respective cubic line in the left image. Here we can see that although this line has a very low training MSE, the test MSE is noticeably high. This specific scenario is known as over-fitting and happens when we a model fits the data too closely. In this particular case, it is actually the blue line that fits the model the best, and we can look at our test MSE to help prove this.

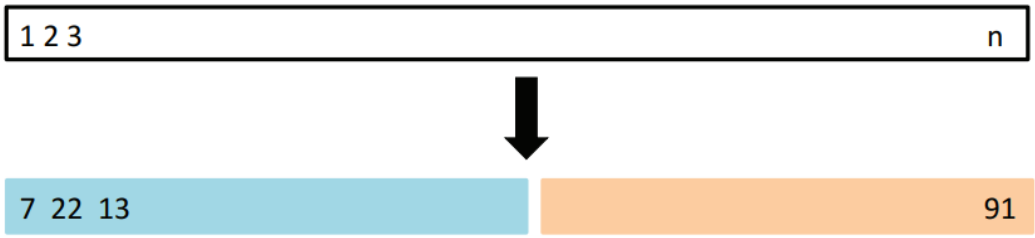


Figure 2: A display of the validation set approach provided in [1]. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.

2.2 Cross Validation

Thus far, we have learned how to predict model accuracy, and what variable helps us determine this measure. Both the training MSE and test MSE are useful pieces of information, but we determined that the test MSE would be the most beneficial in determining model accuracy. However, in many cases, we are unable to perform a test MSE calculation on a designated test set. Instead, we use methods to help gather an estimate for this error rate by using the training data. In particular, we will hold out a subset of the training observations from the fitting process, and then apply the statistical method to those held-out observations. We will focus on two main forms of cross-validations, "Leave One Out Cross Validation (LOOCV)" and "k-Fold Cross-Validation".

2.2.1 The Validation Set Approach

When looking for a test error associated with fitting a statistical learning method on a specific set of observations, the validation approach is a simple strategy for this. This approach involves randomly dividing the observations into two sets, a training set and a validation set (hold-out set). We can see how this split is performed in figure 2.

We fit the model on the training set and then use the fitted model to predict the observations in the validation set. The MSE produced from the estimated validation set provides an estimate for the test error rate.

We can also see how the validation set works graphically. By using a data set in R, we can show

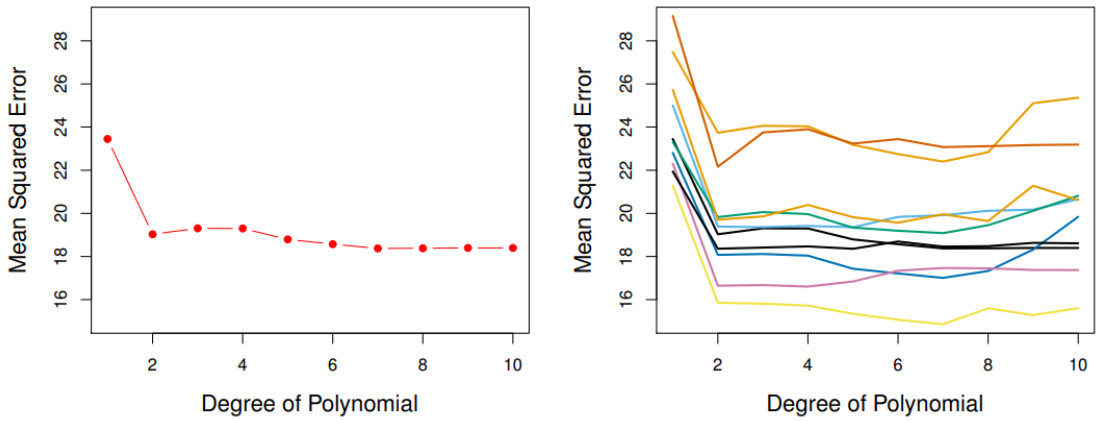


Figure 3: The validation set approach was used on a data set to estimate the test error for a response variable using polynomial functions of an explanatory variable. Left: Validation error estimates for a single split into training and validation data sets. Right: The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This shows the variability in the test MSE. See [1]

how the validation set error rates result from fitting various regression models on the training set. Then, evaluate their performance on the validation set, using MSE as a measure of test set error. In figure 3, on the left, we can see that the validation set error is noticeably smaller for a quadratic fit than a linear fit. However, increasing the fit to the cubic term results in a larger MSE. This showing that adding a higher polynomial term does not result in a better fit. Likewise, the figure on the right shows the same dataset performing ten random splits of the observations into training and test sets. Still, in every split, we can see the drastic drop in test set error from a linear fit to a quadratic fit. Furthermore, showing that higher polynomial fits do not benefit the model much.

Although this approach is beneficial in many ways, there are a couple of drawbacks. These include high variability and over-fitting. Since the method is looking to perform the best on the data set, it may try to include too many variables and overestimate. See [1] for more details.

2.2.2 Leave One Out Cross Validation (LOOCV)

Similar to our previous validation approach, Leave One Out Cross Validation (LOOCV), attempts to fix some of the issues mentioned for the validation set approach. In this approach, we will still split the data into training and test sets. However, instead of making the two sets comparable in size, we will now remove one observation and allow it to be the validation set with the remaining sets making up the

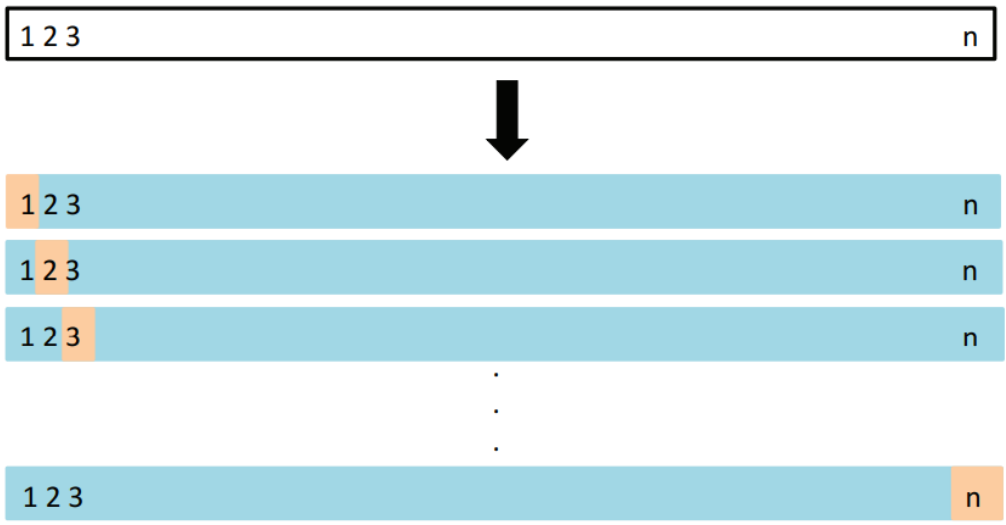


Figure 4: A display of LOOCV provided in [1]. A set of n data points is repeatedly split into a training set (blue) containing all but one observation,and a validation set that contains only that observation (beige). The test error is then estimated by averaging the MSE's, n times. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth

training set. Figure 4 gives a nice visualization of how this split is performed,

Unlike the previous validation approach and using a single estimate for the test MSE, the LOOCV estimate for the test MSE is the average of the n test error estimates shown in the formula,

$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} MSE_i \tag{37}$$

According to [1], LOOCV, also has a couple of advantages over the validation set approach. First, this method is less-bias since LOOCV uses $n-1$ training observation sets which nearly cover the entire data set. Secondly, LOOCV tends to not overestimate the test error rate as much as the validation set approach.

2.2.3 k-Fold Cross-Validation

The last validation approach we have is *k-fold* $\boldsymbol{CV}$. This approach is still similar to the other by forming training and validation sets, but now these sets are split into k groups, or folds of the same size. The first fold will be treated as the validation set, where the remaining k-1 folds fit with our method. Figure 5 shows an example of a 5-fold cross-validation,

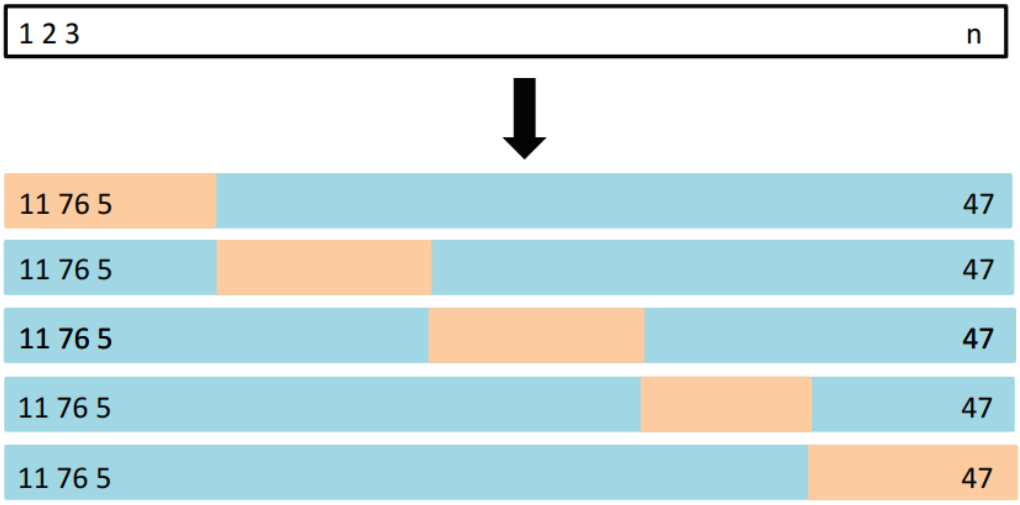


Figure 5: A display of 5-fold CV provided in [1]. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.

To test the accuracy for the k-1 approach, we compute the MSE for each held-out observation. Since we have k folds, this operation will be produced k times. The k-1 fold estimate is computed by averaging these values,

$$\boldsymbol{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k} MSE_i \tag{38}$$

Typically, we will only use $k = 5$ folds or $k = 10$ folds. This is due to the time it takes to compute each of these estimates. We can see how k fold validation compares to simulated data through the figure 6.

Here we can see how both methods compare to the test MSE. Including one case where both underestimate the true MSE. Although this underestimate is shown, it is beneficial to see, because in some cases locating the minimal point for the estimated curve is used to compare with other methods to determine which is best.

2.3 Bias of a model

The bias for a statistical machine learning model can be described as systematic error that occurs in the model when the model draws incorrect assumptions of the data in the modeling process according

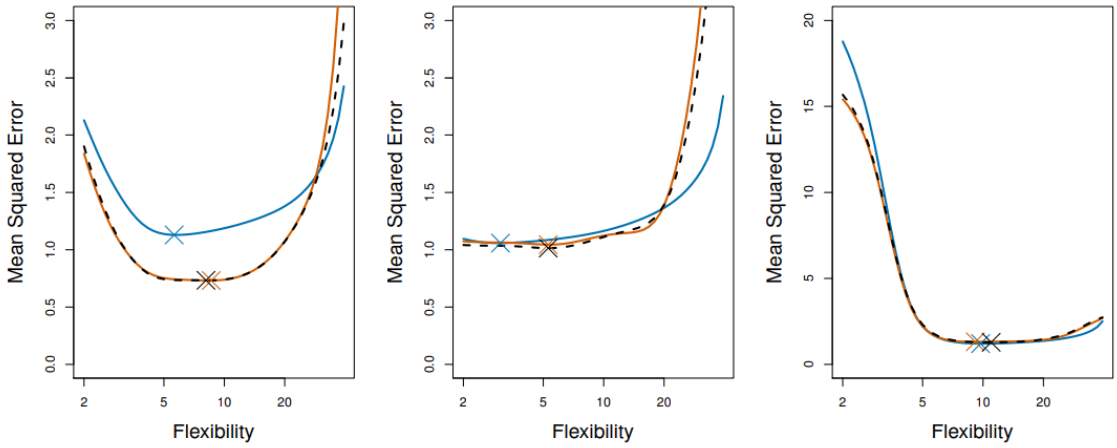


Figure 6: True and estimated test MSE for simulated data sets provided in [1]. The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the 10-fold CV estimate is shown in orange. The crosses indicate the minimum of each of the MSE curves.

to [9]. Bias is often referred to as the error that is introduced by approximating a real-life scenario. Additionally, bias in a model can also describe how closely our model follows our training data. Higher bias resembles a low-fitting model, low bias resembles a close-fitting model.

2.4 Variance of a model

Variance in a model is best described as a value in which the model changes when introduced to different values in the training set. Running the model on different training sets will result in different values for the variance, however, this value should not change too much between sets. Variance tends to correlate directly to complexity in a model. A model with high variability relates to a more complex model, whereas a less complex model tends to have low variability. See [1]

2.5 Bias-Variance Trade off

Referring back to the test MSE mentioned in 2.1, we can form an equation using the bias and variance to measure the expected test MSE. This equation is shown below,

$$E(y_0 - \hat{f}(x_0))^2 = Var(\hat{f}(x_0)) + [Bias(\hat{f}(x_0))]^2 + Var(\epsilon) \tag{39}$$

Where $E(y_0 - \hat{f}(x_0))^2$ defines the expected test MSE at X_0. Equation (39) shows that in order to

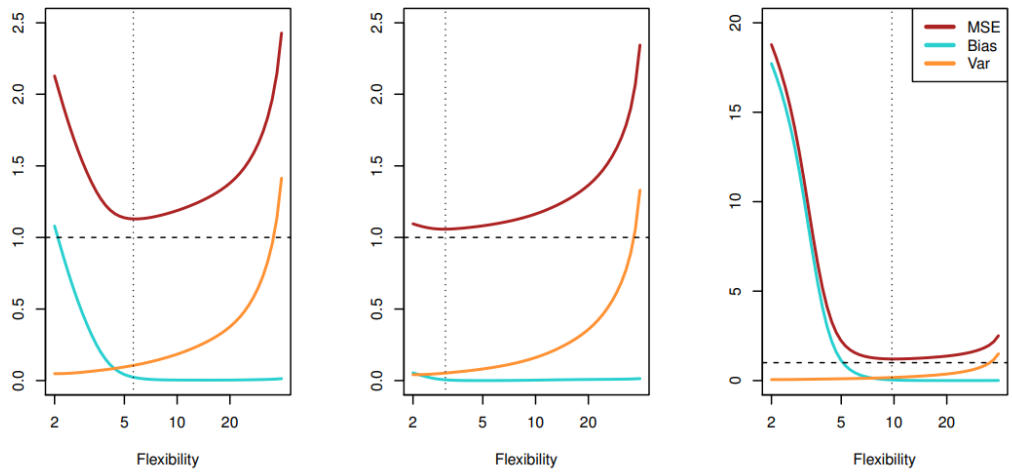


Figure 7: Squared bias (blue curve), variance (orange curve), Var(ϵ) (dashed line), and test MSE (red curve) for the three given data sets. The vertical dotted line shows the flexibility level that results in the smallest test MSE.

make the test MSE small, two things are required. The model requires both low variance and low bias in order to obtain a low MSE.

When computing machine learning models, to determine the best model, Bias and Variance are typically two points that are examined. The goal is to get low bias and variance to create the best model for the data. However, one contradicts the other, and this is known as the bias-variance trade-off. When we get a model that has high variability, that model has low bias. In the same manner, a model with low variability has high bias. Determining a point where the model performs well for both bias and variability is one of the main goals for all learning models. The graphs in figure 7 help us understand this trade-off better.

Notice, in each of the three graphs, there is a distinct point where the test MSE is the smallest. At this point, there is a corresponding variance and bias level for each graph, giving us some sort of indication of what type of model is being performed.

2.6 A new method for model selection: OLSAVS

The shrinkage methods such as Lasso and Relaxed Lasso introduce some bias in order to reduce the variance of the regression coefficients. As briefly mentioned in [2], one way to reduce bias after shrinkage of the coefficients would be to apply ordinary least squares to the subset of predictors se-

lected by the shrinkage method used. In this work, we extensively study this idea to develop a new variable selection algorithm. We name this technique Ordinary Least Squares After Variable Selection (OLSAVS). We have implemented OLSAVS method in R. The set of functions can be found at `https://hasthika.github.io/olsvspack.txt`. The algorithm of the OLSAVS method is as follows:

Algorithm: Ordinary Least Squares After Variable Selection (OLSAVS)

Repeat: following steps with a different shrinkage method

1) Apply the first shrinkage method to $(Y_i, \boldsymbol{x}_i)$ for $i = 1, ..., n$.

2) Obtain the k non-zero predictors selected by the shrinkage method in 1)

3) Apply Ordinary Least Squares on the subset of k predictors obtained in 2)

Stop

4) Select a single best model using cross-validated prediction error, C_p , (AIC), BIC, or adjusted R^2

3 Simulation

3.1 Simulation setup

We used `R` to generate $(Y_i, \boldsymbol{x}_i)$ for $i = 1, ..., n$. The regression parameters $\boldsymbol{\beta}$ were set to (1, 1, ..., 1, 0, ..., 0) with $k + 1$ ones, $p - k - 1$ zeroes where p is the total number of predictors, and k is the number of non-trivial predictors. Then for a given regression method, the regression coefficients, $\hat{\boldsymbol{\beta}}$ were obtained using the proposed method. This process was repeated 5000 times (runs). For each run, the difference between the regression parameters $\boldsymbol{\beta}$ and the regression coefficients, $\hat{\boldsymbol{\beta}}$ were obtained using the Minkowski distance. The average difference (Diff) was calculated by averaging all 5000 runs. The root MSE was also obtained using a test of observations for each run that was averaged of the 5000 runs (TRMSE). We used $p = n/5, n/2$, or $n - 1$ as the total number of predictors and $k = 1, 19$, or $p - 1$ as the number of non-trivial predictors in the model. As per the easiness of coding we used the relation $cor(x_i, x_j) = \rho = (2\psi + (p - 3)\psi^2)/(1 + (p - 2)\psi^2)$, for $i \neq j$, where, x_i, x_j are non-trivial predictors. As ψ increases the correlation between preceptors, ρ grows. We used $\psi = 0, 0.3$ or 0.9. We considered five error distributions with zero mean.

1. The first distribution we used is the $N(0,1)$ which is commonly used in simulation studies.

2. As the second error distribution, we considered t_3, one of the heavy-tailed distributions.

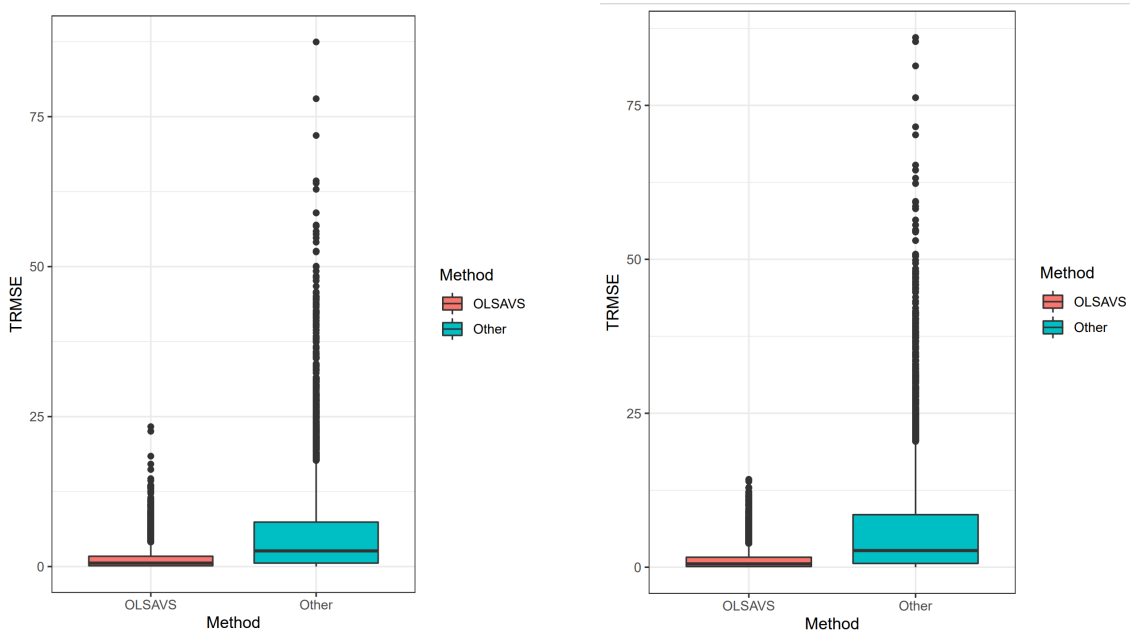
3. We also considered not very commonly used in simulations but found in many real-life situations, a non-symmetric error distribution $EXP(1) - 1$.

4. We also used $uniform(-1,1)$, and

5. $0.9N(0,1) + 0.1N(0,100)$.

The simulation study was conducted in R. See [6].

3.2 Simulation results



(a) Table 1, Plot 1 ($n = 100$)

(b) Table 1, Plot 2 ($n = 200$)

Figure 8: Box plots for table 1 showing simulation results for OLSAVS vs. Lasso regression with error type 1.

For figure 8, we assembled box plots to compare the TRMSE results in table 1. For each of the simulations tables, we will assemble two plots with $n = 100$ or $n = 200$ to compare the results. Here in figure 8, we see that in either sample size, OLSAVS has a smaller median TRMSE and lower variation in the results. However, it appears for this simulation, for Lasso with a normal error, that when the sample size increases, so do the variation in the plot.

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	Lasso
100	20	1	0	1.0478	1.021	0.01657	0.1449
100	20	1	0.3	1.0417	1.0199	0.1124	0.1549
100	20	1	0.9	1.0083	1.0057	0.6455	0.6635
100	20	19	0	1.1112	1.1107	0.0037	0.0122
100	20	19	0.3	1.1112	1.1377	0.0055	0.0158
100	20	19	0.9	1.1543	2.3451	1.5667	7.5674
100	50	1	0	1.0916	1.0369	0.0268	0.181
100	50	1	0.3	1.0708	1.0303	0.1654	0.2028
100	50	1	0.9	1.0142	1.0059	0.9511	0.5929
100	50	49	0	1.3973	1.4014	0.0043	0.0149
100	50	49	0.3	1.5522	4.353	0.0163	0.0557
100	50	49	0.9	2.1118	9.4775	8.8016	43.9716
200	40	1	0	1.0386	1.0175	0.0225	0.1208
200	40	1	0.3	1.0316	1.0157	0.1044	0.1327
200	40	1	0.9	1.0108	1.005	0.7825	0.4165
200	40	39	0	1.117	1.119	0.002	0.0095
200	40	39	0.3	1.117	2.5606	0.0028	0.0369
200	40	39	0.9	1.6985	6.8533	5.8545	32.8388
200	100	1	0	1.0691	1.0261	0.0354	0.1454
200	100	1	0.3	1.0605	1.0251	0.1392	0.1653
200	100	1	0.9	1.0184	1.0045	0.9712	0.0855
200	100	99	0	1.4495	1.4561	0.0034	0.0132
200	100	99	0.3	3.166	11.4553	0.1379	0.488
200	100	99	0.9	3.7274	27.9646	17.4699	93.9076

Table 1: TRMSE and difference values for Lasso for $e_i \sim N(0, 1)$

For table 1 we ran simulations to compare the OLSAVS method to Lasso regression. However, in this particular simulation, we compared OLSAVS to a Lasso regression with a normal distribution error type that has a mean of 0 and a variance of 1. Here, and for the remaining simulations, we will compare the methods for $n = 100, 200$.

In table 1 the first trend we can begin to see occurs in the TRMSE for the simulations. In the beginning, Lasso outperforms the method being proposed, and this occurs for the first trial where the non-trivial predictors (k) are low. However, as this value increases for both the predictors and the correlation among these predictors respectively, the OLSAVS method will eventually overtake the Lasso regression for the TRMSE value. This trend will continue throughout table 1, but as the sample size and non-trivial predictors increase, the distance between the OLSAVS and Lasso values gets noticeably larger. In comparing the two, the OLSAVS stays consistent throughout for the TRMSE, where Lasso has a lot of variability for this value.

Although the OLSAVS out-performed Lasso for certain cases, we need to analyze the table for the difference (Diff) values computed using Minkowski distance. There is not any noticeable trend unlike the TRMSE, but we can see that for small non-trivial predictors and high correlation values, the Lasso regression either comes close or betters OLSAVS in the difference value here. Other than this certain case, the new method significantly bettered the Lasso in table 1.

Figure 9 shows two simulation plots pulled from table 2. Looking at two cases, each varying in sample size, we see that our method does edge out Lasso regression with the error type being from a t-distribution. However, unlike 8 the variation in the plot now decreases as expected when the error type increases.

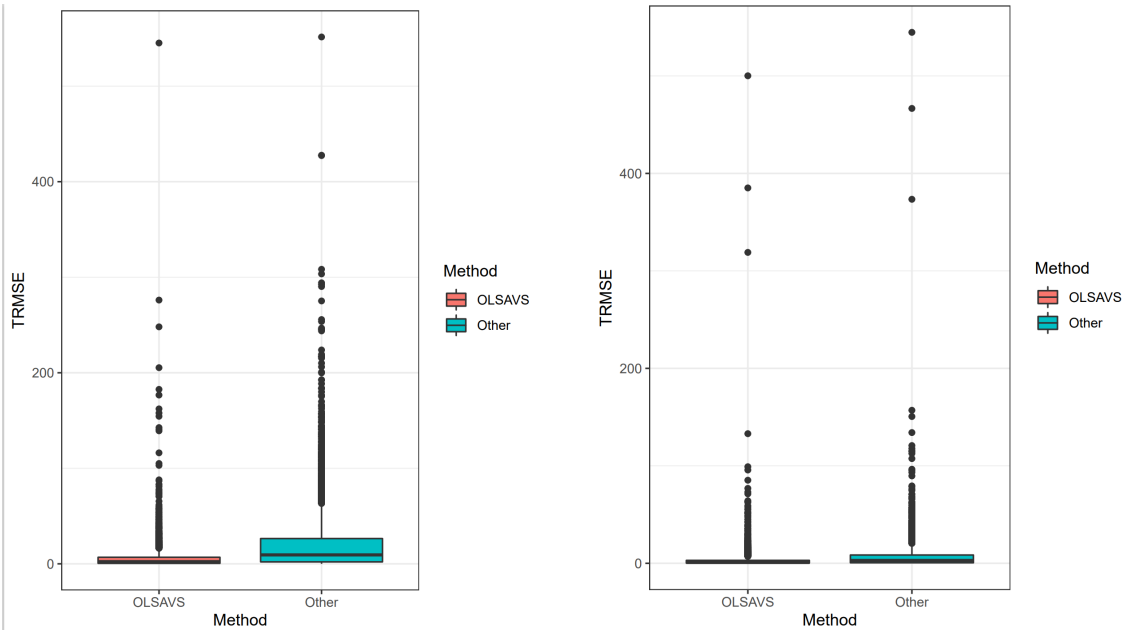
Table 2 is a similar simulation approach to the previous table 1, however the error type in table 2 changes for the Lasso regression. The error type for table 2 will be a t-distribution with zero mean.

Analyzing the TRMSE for table 2, a trend begins to form as the number of non-trivial predictors increases. The Lasso regression will outperform OLSAVS every time that the non-trivial predictor $k = 1$. However, once we go from one extreme to another in our simulations, the TRMSE favors our method once the non-trivial predictors are equal to $p - 1$. Additionally, as the correlation between the non-trivial predictors increases, we can see a large distance increase between the two methods.

For the difference in table 2, it is hard to establish any consistent trends throughout. However, it is notable that when $n = 100$, $p = 50$, and $k = 1, 49$ the Lasso slightly does better than the new method.

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	Lasso
100	20	1	0	1.3677	1.3362	0.0260	0.1882
100	20	1	0.3	1.3551	1.3317	0.1497	0.2031
100	20	1	0.9	1.3178	1.3169	0.6539	0.7482
100	20	19	0	1.4441	1.4442	0.0047	0.0130
100	20	19	0.3	1.4441	1.4590	0.0061	0.0142
100	20	19	0.9	1.4487	2.4245	1.8395	7.2843
100	50	1	0.3	1.3704	1.3311	0.2075	0.2549
100	50	1	0.9	1.3060	1.3015	0.9523	0.6991
100	50	49	0	1.8360	1.8418	0.0076	0.0076
100	50	49	0.3	1.9877	4.4636	0.0245	0.0245
100	50	49	0.9	2.2778	9.6242	8.8102	43.9438
200	40	1	0	1.3453	1.3165	0.0351	0.1550
200	40	1	0.3	1.3324	1.3163	0.1351	0.1707
200	40	1	0.9	1.3075	1.3033	0.8243	0.5671
200	40	39	0	1.4351	1.4355	0.0036	0.0107
200	40	39	0.3	1.4351	2.5826	0.0048	0.0376
200	40	39	0.9	1.8981	6.7108	5.7510	32.8242
200	100	1	0	1.3837	1.3189	0.0460	0.1847
200	100	1	0.3	1.3559	1.3153	0.1774	0.2115
200	100	1	0.9	1.3096	1.2998	1.1920	0.2210
200	100	99	0	1.8397	1.8487	0.0058	0.0147
200	100	99	0.3	3.3891	11.4710	0.1501	0.4976
200	100	99	0.9	3.8424	27.4098	17.2990	93.9071

Table 2: TRMSE and difference values for Lasso for $e_i \sim t_3$



(a) Table 1, Plot 1 ($n = 100$)

(b) Table 1, Plot 2 ($n = 200$)

Figure 9: Box plots for table 2 showing simulation results for OLSAVS vs. Lasso regression with error type 2.

Overall, the new method outperforms Lasso by a large majority.

Figure 10 shows boxplots gathered from two simulations in table 3. In the two plots shown, we see yet again that OLSAVS edges out the Lasso and has a much shorter variation in the box plot. Lasso with an exponential error does compete in the $n = 100$ plot but then has a much larger gap when the sample size is increased.

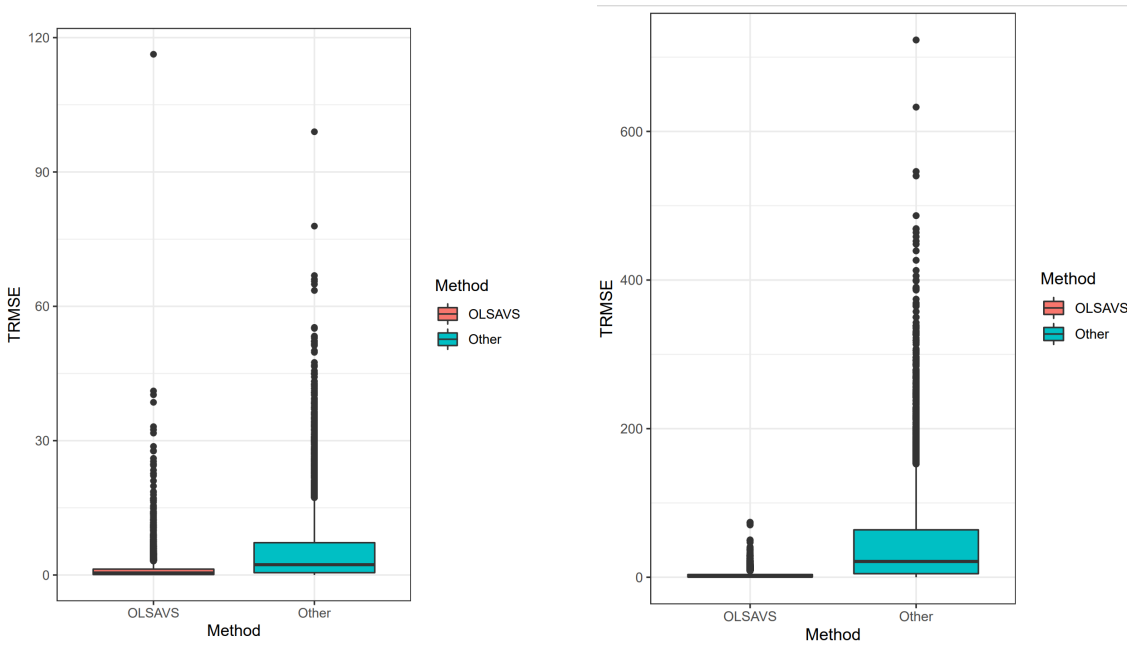
In table 3 we will compare our method to Lasso again, but this time we will compare to the Lasso regression with the error types being from the exponential distribution. Again, with a mean of zero, will analyze the TRMSE and Diff for both methods.

Upon analyzing the TRMSE for both methods, we can see a very similar trend occurring. Much like our simulations from table 2, as the non-trivial predictors are increased to $p - 1$ we can see our method produces a lower TRMSE than Lasso. Additionally, the same gap occurs when the correlation is increased for the $p - 1$ predictors as well.

The differences in table 3 appear to have no consistent trends. OLSAVS seems to dominate for the majority of the difference values. Still, much like the previous simulations, there is this interesting difference that occurs when the correlation between predictors is equal to 0.9 and $k = 1$. At this particular point, Lasso does better than our method, but only at this point.

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	Lasso
100	20	1	0	1.0589	1.0366	0.0208	0.1416
100	20	1	0.3	1.0287	1.0099	0.1123	0.1533
100	20	1	0.9	0.9913	0.9900	0.6264	0.6519
100	20	19	0	1.1055	1.1063	0.0033	0.0118
100	20	19	0.3	1.1055	1.1583	0.0046	0.0148
100	20	19	0.9	1.1335	2.3835	1.5415	7.5833
100	50	1	0	1.0948	1.0456	0.0232	0.1804
100	50	1	0.3	1.0767	1.0414	0.1689	0.2039
100	50	1	0.9	1.0263	1.0188	0.9343	0.5814
100	50	49	0	1.4078	1.4105	0.0045	0.0147
100	50	49	0.3	1.5744	4.3752	0.0153	0.0520
100	50	49	0.9	2.1137	9.5345	8.8138	44.0251
200	40	1	0	1.0298	1.0071	0.0202	0.1201
200	40	1	0.3	1.0202	1.0037	0.1063	0.1331
200	40	1	0.9	0.9969	0.9925	0.7664	0.4067
200	40	39	0	1.1034	1.1048	0.0026	0.0097
200	40	39	0.3	1.1034	2.4771	0.0035	0.0380
200	40	39	0.9	1.7076	6.7040	5.8761	32.8648
200	100	1	0	1.0522	1.0122	0.0371	0.0371
200	100	1	0.3	1.0356	1.0101	0.1402	0.1657
200	100	1	0.9	1.0067	0.9953	0.9636	0.0896
200	100	99	0	1.4138	1.4192	0.0037	0.0131
200	100	99	0.3	3.1658	11.2754	0.1451	0.4836
200	100	99	0.9	3.6705	27.4919	17.5606	93.9063

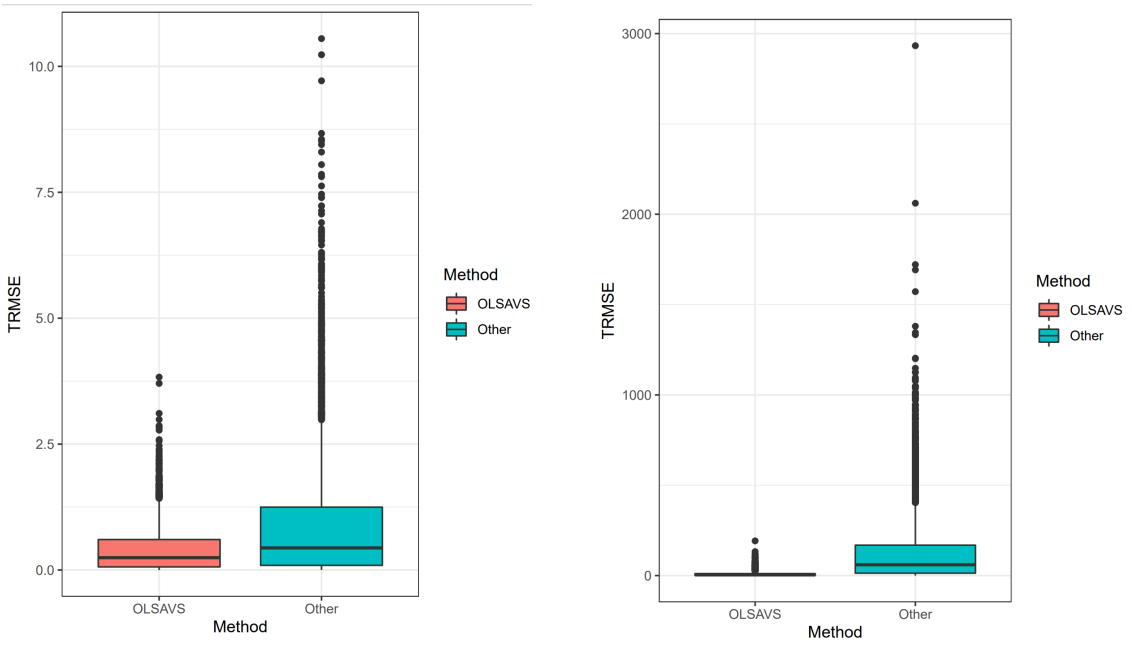
Table 3: TRMSE and difference values for Lasso for $e_i \sim EXP(1) - 1$



(a) Table 1, Plot 1 ($n = 100$)

(b) Table 1, Plot 2 ($n = 200$)

Figure 10: Box plots for table 3 showing simulation results for OLSAVS vs. Lasso regression with error type 3.



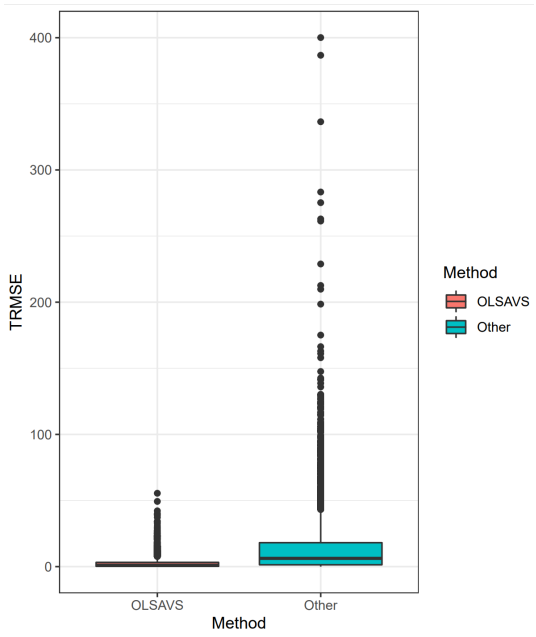
(a) Table 1, Plot 1 ($n = 100$)

(b) Table 1, Plot 2 ($n = 200$)

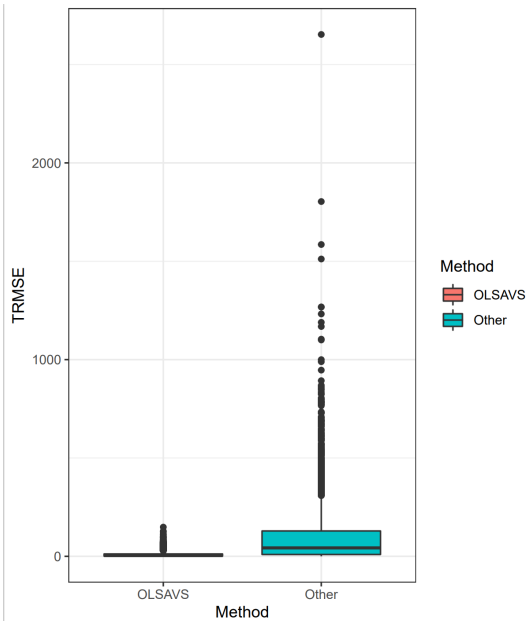
Figure 11: Box plots for table 4 showing simulation results for OLSAVS vs. Lasso regression with error type 4.

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	Lasso
100	20	1	0	0.6087	0.5952	0.0112	0.0843
100	20	1	0.3	0.6024	0.5945	0.0662	0.0900
100	20	1	0.9	0.5905	0.5879	0.5773	0.4067
100	20	19	0	0.6360	0.6369	0.0023	0.0103
100	20	19	0.3	0.6360	0.9626	0.0031	0.0308
100	20	19	0.9	0.7599	2.3075	1.3762	7.8005
100	50	1	0	0.6265	0.5999	0.0177	0.1043
100	50	1	0.3	0.6169	0.5955	0.0943	0.1160
100	50	1	0.9	0.5917	0.5826	0.7318	0.2120
100	50	49	0	0.8221	0.8299	0.0028	0.0127
100	50	49	0.3	1.0467	4.3592	0.0121	0.0573
100	50	49	0.9	1.9089	9.4600	9.0251	44.0993
200	40	1	0	0.6078	0.5907	0.0127	0.0697
200	40	1	0.3	0.6016	0.5904	0.0604	0.0760
200	40	1	0.9	0.5886	0.5836	0.4935	0.1028
200	40	39	0	0.6506	0.6506	0.0013	0.0088
200	40	39	0.3	0.6506	2.5639	0.0018	0.0388
200	40	39	0.9	1.4729	6.8174	5.9630	33.0055
200	100	1	0	0.6130	0.5903	0.0123	0.0831
200	100	1	0.3	0.5967	0.5967	0.0898	0.0973
200	100	1	0.9	0.5902	0.5830	0.5646	0.0216
200	100	99	0	0.8125	0.8243	0.0021	0.0119
200	100	99	0.3	2.9615	11.3001	0.1460	0.4744
200	100	99	0.9	3.5458	27.3187	17.4181	93.9087

Table 4: TRMSE and difference values for Lasso for $e_i \sim uniform(-1, 1)$



(a) Table 1, Plot 1 ($n = 100$)



(b) Table 1, Plot 2 ($n = 200$)

Figure 12: Box plots for table 5 showing simulation results for OLSAVS vs. Relaxed Lasso regression with error type 1.

For table 4 in our Lasso simulations, we look at a Lasso regression with a uniform distribution error type. Here in figure 11, the variation for each method is large, however, OLSAVS still has the smaller average TRMSE. Once the sample size increases, both the variation and the average TRMSE shrinks for each method, but the OLSAVS still maintains the advantage in each.

The last table we will analyze for Lasso regression is table 4. This table keeps the same ideas, but again our distribution for the errors is changed. We will look at a uniform distribution this time with zero mean.

Once again for our TRMSE simulations, the same trend appears between the OLSAVS and Lasso estimates as before. However, this time we get an output where the two functions are equal for observation 16. Compared to the other simulations, this Lasso regression stands out since the other simulations for this observation were larger than the OLSAVS value.

The difference for the simulations remains mostly the same as for our previous simulations for Lasso with an exponential distribution. Here our method outperforms Lasso again, with the same occurrence of only one certain scenario when the correlation between predictors is equal to 0.9 and $k = 1$.

Figure 12 shows our first boxplots for the Relaxed Lasso simulations with error type 1. Here in

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	R Lasso
100	20	1	0	1.05004	1.03955	0.01180	0.04069
100	20	1	0.3	1.04307	1.03993	0.11183	0.11699
100	20	1	0.9	1.00809	1.00586	0.63942	0.67805
100	20	19	0	1.11518	1.11527	0.00315	0.00298
100	20	19	0.3	1.11518	1.12323	0.00384	0.00384
100	20	19	0.9	1.14518	1.44021	1.54564	7.55956
100	50	1	0	1.10563	1.08454	0.02597	0.05857
100	50	1	0.3	1.09096	1.08971	0.16601	0.16668
100	50	1	0.9	1.03093	1.02483	0.95682	0.60006
100	50	49	0	1.42151	1.42127	0.00415	0.00446
100	50	49	0.3	1.57851	3.89696	0.01567	0.01567
100	50	49	0.9	2.12296	4.80282	8.87674	45.66343
200	40	1	0	1.03855	1.03304	0.02126	0.02466
200	40	1	0.3	1.03295	1.03285	0.10517	0.10524
200	40	1	0.9	1.01005	1.00655	0.78436	0.42916
200	40	39	0	1.12531	1.12531	0.00267	0.00267
200	40	39	0.3	1.12531	1.80026	0.00386	0.12240
200	40	39	0.9	1.70105	3.57716	5.88467	33.41152
200	100	1	0	1.06191	1.05162	0.02599	0.03373
200	100	1	0.3	1.04883	1.04896	0.13610	0.13720
200	100	1	0.9	1.01643	1.00291	0.96788	0.96788
200	100	99	0	1.40641	1.40518	1.40518	0.00281
200	100	99	0.3	3.15561	10.08956	0.14074	0.92836
200	100	99	0.9	3.71833	9.86930	17.35998	97.95932

Table 5: TRMSE and difference values for Relaxed Lasso for $e_i \sim N(0, 1)$

these plots, we can see immediately that OLSAVS has the lower average TRMSE and variation. If the sample size is increased, the same comparison results hold, while making the variation for OLSAVS even smaller.

Table 5 introduces simulations using the Relaxed Lasso method. In this method comparison, we will keep the same variables and simulation values while only changing the method in which we're applying. For the Relaxed Lasso simulations, we also will look at the same error types as the Lasso regression.

For table 5, we compare our method with a Relaxed Lasso regression with a normal distribution error type. Again, our mean will remain zero and we compare the simulations results for TRMSE and the average difference. Much like our results for Lasso regression, we see that Relaxed Lasso appears to have the advantage when $k = 1$. However, once k is increased to $p - 1$ predictors, OLSAVS begins to have the smaller TRMSE. Still, Relaxed Lasso is more competitive than Lasso for a normal distribution error.

The differences for table 5 do not have much of a trend occurring. However, our method does perform better than Relaxed Lasso for the majority of the simulations. Yet again, Relaxed Lasso does compete well with the error type coming from a normal distribution. Our method does get beat in various errors in the table, but no trends seem to appear in these spots.

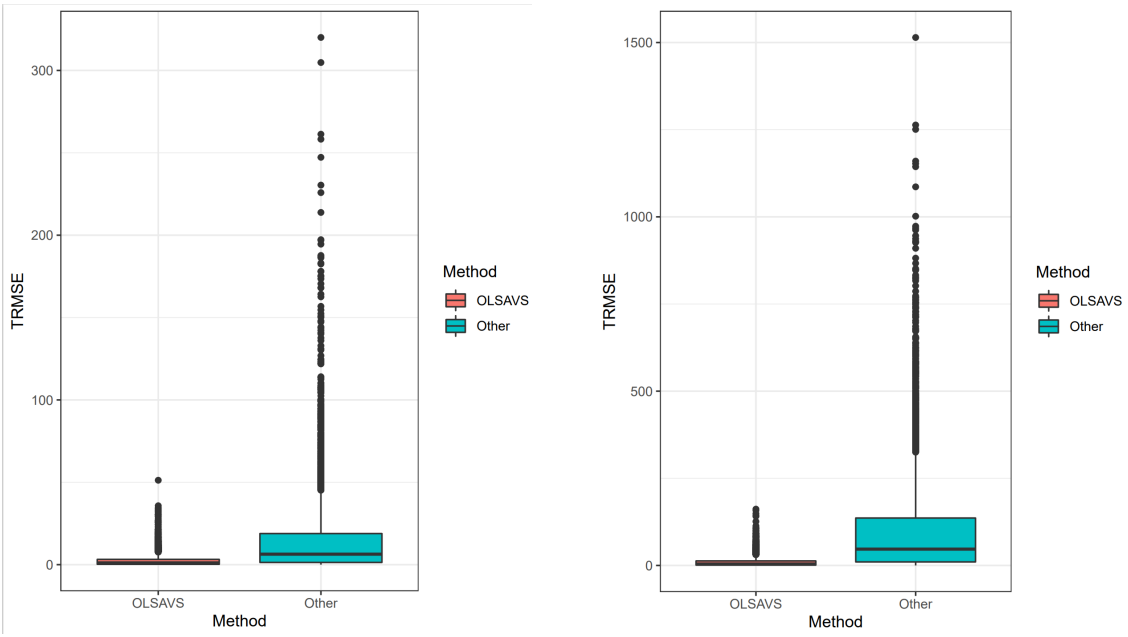
Figure 13 shows simulation results between OLSAVS and Relaxed Lasso with error type 2. Figure 13 follows closely to the results from figure 12, but here both methods in figure 13 seem to contain larger variation for error type 2. However, OLSAVS still maintains the lower quantities for the TRMSE.

By looking at the results in table 6, we are going to get almost the exact same trend for TRMSE values as our values in table 5. Again, we see that Relaxed Lasso has the advantage in the TRMSE when $k = 1$. However, once k is increased to $p - 1$ predictors, OLSAVS has the smaller test error value.

Lastly, our differences in table 6 show our method performing well once again for the bias values. We can see that our method does compete with relxaed Lasso with error type 2, but judging on the majority of simulations, our method wins outright. Additionally, we can see OLSAVS also provides more consistent differences overall.

				TRMSE		Diff	
n	p	k	ψ	OLSAVS	Lasso	OLSAVS	R Lasso
100	20	1	0	1.36487	1.34437	0.02908	0.08346
100	20	1	0.3	1.34847	1.34209	1.34209	0.15530
100	20	1	0.9	1.30332	1.30211	0.62132	0.74412
100	20	19	0	1.44316	1.44326	0.00553	0.00605
100	20	19	0.3	1.44316	1.44720	0.00764	0.03972
100	20	19	0.9	1.43871	1.65548	1.83681	7.26831
100	50	1	0	1.44446	1.40636	0.03604	0.10807
100	50	1	0.3	1.41096	1.40477	0.20648	0.21225
100	50	1	0.9	1.34176	1.33864	0.95980	0.71164
100	50	49	0	1.85165	1.85164	0.00554	0.00698
100	50	49	0.3	2.00740	4.14320	4.14320	4.14320
100	50	49	0.9	2.31574	4.91246	8.71224	45.59930
200	40	1	0	1.33118	1.31585	0.03086	0.05388
200	40	1	0.3	1.31769	1.31472	0.13591	0.13865
200	40	1	0.9	1.29278	1.28860	0.84014	0.58889
200	40	39	0	1.44431	1.44436	0.00272	0.00272
200	40	39	0.3	1.44431	2.02409	0.00388	0.13289
200	40	39	0.9	1.91426	3.72937	5.77462	33.17816
200	100	1	0	1.35272	1.32707	0.04958	0.07102
200	100	1	0.3	1.33008	1.32910	0.18092	0.18116
200	100	1	0.9	1.28972	1.27810	1.19952	0.21588
200	100	99	0	1.80251	1.80167	0.00513	0.00464
200	100	99	0.3	3.31817	10.32727	0.14145	0.92488
200	100	99	0.9	3.76114	9.86319	17.36192	97.95763

Table 6: TRMSE and difference values for Relaxed Lasso for $e_i \sim EXP(1) - 1$



(a) Table 1, Plot 1 ($n = 100$)

(b) Table 1, Plot 2 ($n = 200$)

Figure 13: Box plots for table 6 showing simulation results for OLSAVS vs. Relaxed Lasso regression with error type 2.

4 Real data example

For this method, we will consider a Wisconsin nursing home data set provided by the Wisconsin Department of Health and Family Services. The goal of this data set is to utilize nursing home capacity. In the set we will look at the years of 2000 and 2001, with 362 and 355 facilities respectively. However, 10 observations were removed for containing missing values. Our data set contains 12 variables, with total patient years (TPY) being our response variable.

To determine how our methods perform, we will split our data into testing and training sets. In the sets, we will allocate 60% of the data to be in the training set and 40% to be in the testing set. We will compute the TRMSE from this data set and compare the values of the OLSAVS method to those of Lasso, Relaxed Lasso, and Elastic Net.

Below in table 7, we can see the results of using this real-world example. We can compare each of these side-by-side results and see that the OLSAVS method edges out each of these for this real-world example.

By analyzing table 7, it appears that OLSAVS does a nice job against the other common methods. If we look at each individual comparison, it turns out that OLSAVS has the lower test error for any method

Method	OLSAVS	ENET	OLSAVS	Lasso	OLSAVS	Relaxed Lasso
TRMSE	7.956877	8.071371	8.007678	8.044224	8.007678	8.013652

Table 7: TRMSE comparison for OLSAVS vs. common methods using real data

we choose. This showing that OLSAVS does have some practicality as it is able to perform in real-world scenarios.

5 R Package

In this section, we will briefly cover the R functions required to compute simulation results and plots shown in section 3. With each of these functions, our goal was to compare the OLSAVS with a few most common variable selection methods. Below, we will describe briefly what each of these functions do. To load this package: use `source("https://hasthika.github.io/olsvspack.txt")`

5.1 Function descriptions

`OLSAVS(x, y, method)`

Where x is a matrix of predictors, y is the response variable we are searching for, and the method determines what method we are applying OLSAVS with. Here the methods vary between Lasso, Ridge, Relaxed Lasso, and Elastic Net models. After a preferred method is selected, we will apply ordinary least squares to this model and gather a new model which will be the OLSAVS model.

`OLSAVSPredict(model, newx)`

This function will give us a vector of predictions ($\hat{y}$) for an OLSAVS model. 'OLSAVSPredict' will use the OLSAVS model and an argument newx, where newx is a matrix x values.

`olsafterlrsim(n, p, k, nruns, psi, type, alpha, pitype)`

This function was used to create Tables 1 through 6. This function requires the following arguments, n representing our sample size for the simulation, p, the number of predictors in the model, k as the number of non-trivial predictors in the model, nruns represents the number of simulations we run the model on, ψ as the correlation between non-trivial predictors, type defines the error distribution our model and rival model will use, and lastly, pitype represents which model we will compare our method

to. This could fall under Lasso, Ridge, Relaxed Lasso, or Elastic Net. This function results in four different outputs. Function outputs the TRMSE value for OLSAVS and the method selected, but also the difference between the estimated and the actual regssion coefficients computed by using the Minkowski distance.

```
olsafterlrsimplots(n, p, k, nruns, psi, type, alpha, pitype)
```

This function is very similar to olsafterlrsim(), however, this code now includes an output that produces plots. These plots produced show a side-by-side box plot of the TRMSE values for both methods defined in the code. The same variables are used here as in olsafterlrsim().

```
# Example

library(ISLR)

library(lars)

library(readr)

Wisc <- read_csv("WiscNursingHome (1).csv")

Wisc <- na.omit(Wisc)

set.seed(1008)


############ Splitting and preparing data ####################

train = sample(c(TRUE, FALSE), size = 0.6*nrow(Wisc), replace = TRUE)

test <- (!train)


xtrain <- model.matrix(TPY~., Wisc)[train,]

xtest <- model.matrix(TPY~., Wisc)[test,]


ytrain <- Wisc$TPY[train]

ytest <-  Wisc$TPY[test]
```

```
y <- ytrain

x <- xtrain


##################### Applying OLSAVS ############################

# Method - Lasso, RR, Enet or Relaxed Lasso (method = 1, method = 0,

# method = 0.5 or method = 2)

mod <- OLSAVS(x, y, method = 0.5) # Fitting the OLSAVS model

summary(mod)

# Predictions

# OLSAVSPredict: function for predictions for OLSAVS models

preds <- OLSAVSPredict(mod, xtest)

# Test root mean square error for OLSAVS

yhatTest <- preds$yhat

RMSE_test_OLSAVS <- sqrt(mean((ytest - yhatTest)^2))

RMSE_test_OLSAVS


###################### Lasso, Ridge, relax, enet ################

# Test root mean square error Lasso, Ridge, enet or relax (alpha = 1,

# 0 or 0.5 respectively. relax Lasso: see below)

# for relax Lasso: out <- cv.glmnet(x, y, relax = TRUE)

out <- cv.glmnet(x, y, relax = TRUE)

lam <- out$lambda.min

out_coef <- predict(out, s = lam, type = "coefficients")
```

```
yfhat <- predict(out, s = lam, newx = xtest)


RMSE_test_l <- sqrt(mean((ytest - yfhat)^2))

RMSE_test_l

########################## End Example ############################
```

6 Conclusions

The new method for variable selection, OLSAVS involves applying ordinary least squares to a subset of predictors selected from a specific variable selection method such as Lasso, relax Lasso, or Elastic Net. The proposed method is able to maintain the ability of consistency through the low variation applied from shrinkage methods, while also reducing bias by applying OLS to the predictors selected. We expected the OLSAVS to reduce the bias in the regression coefficients introduced by the shrinkage method and lead to the model being close-fitting while keeping the consistency of the reduced variance from the shrinkage method. Simulation results show that the OLSAVS method not only reduced the bias of the regression coefficient but also further reduced the variance of the estimates.

Furthermore, the OLSAVS method performs well in terms of predictions error as well. As discussed in section 3.2, the test root mean square errors when using OLSAVS for all error types studied are either significantly low or equal to the competing shrinkage method. It is interesting to notice that the prediction accuracy drastically decreases as the correlation between the predictors increases when using commonly used shrinkage methods. Prediction accuracy decreases further with number of non-trivial predictors. OLSAVS method outperformed the other shrinkage studied in both of above mentioned scenarios and produced much lower test root mean square error values. Lastly, when applied to the real world example of the Wisconsin nursing home data set, the method shows its usefulness by resulting in the lowest observed model accuracy values. Hence, this concludes that OLSAVS does have practically in variable selection techniques and is reliable for multiple error distributions.

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Appendices

A R Package

```
#############################################################
# To load this library: use source("https://hasthika.github.io/olsvspack.txt")
# Need library(ggplot2), library(leaps)
#############################################################

olsafterlrsim <- function(n = 10, p = 4, k = 2, nruns = 100, eps = 0.1,
                      shift = 9, psi = 0.0, type = 1, alpha = 0.05,
                      pitype = 1){
  # Needs library(glmnet).  Does Lasso, RR or Relaxed Lasso.
  ##slow        10 fold CV,
  # Simulates RMSE for lasso if pitype = 1, Ridge regression if
  pitype = 0, ralxed lasso for pitype = 2.
  # 1 <= k <= p-1, k is the number of nonnoise variables
  # Uses five iid error distributions:
  # type = 1 for N(0,1) errors, 2 for t5 errors, 3 for exp(1) - 1 errors
  # 4 for uniform(-1,1) errors, 5 for (1-eps) N(0,1) + eps N(0,(1+shift)^2)
  # errors.
  # constant = 1 so there are p = q+1 coefficients
  # need p > 1, beta = (1, 1, ..., 1, 0, ..., 0) with k+1 ones, p k-1  zeroes
  # Multiply x by A: for MVN data this results
```

```
# in a covariance matrix with eigenvector c(1, ..., 1)^T
# corresponding to the largest eigenvalue. As psi gets
# close to 1, the data clusters about the line in the
# direction of (1, ..., 1)^T. See Maronna and Zamar (2002).
# cor(X_i,X_j) = [2 psi +(q-2)psi^2]/[1 + (q-1)psi^2], i not = j
# when the correlation exists.
# set.seed(974) ##need p>2

e_lr <- rep(NA, nruns)
e_ols <- rep(NA, nruns)
RMSE_lr <- 0
RMSE_ols <- 0
ols_coef2 <- rep(0, p)
ols_coef_sum <- rep(0, p)
lr_coef_sum <-  rep(0, p)
ols_coef_avg <- rep(0, p)
lr_coef_avg <- rep(0, p)



q <- p-1
rho <- (2*psi + (q-2)*psi^2)/(1 + (q-1)*psi^2)
A <- matrix(psi,nrow=q,ncol=q)
diag(A) <- 1
b <- 0 * 1:q
```

```
b[1:k] <- 1 #b[1:0] acts like b[1:1] = b[1]
indx <- 1:n




for(i in 1:nruns) {
  x <- matrix(rnorm(n * q), nrow = n, ncol = q)
  x <- x %*% A
  xf <- rnorm(q) %*% A
  if(type == 1) {
    y <- 1 + x %*% b + rnorm(n)
    yf <- 1 + xf %*% b + rnorm(1)
  }
  if(type == 2) {
    y <- 1 + x %*% b + rt(n, df = 5)
    yf <- 1 + xf %*% b + rt(1, df = 5)
  }
  if(type == 3) {
    y <- 1 + x %*% b + rexp(n) - 1
    yf <- 1 + xf %*% b + rexp(1) - 1
  }
  if(type == 4) {
    y <- 1 + x %*% b + runif(n, min = -1, max = 1)
    yf <- 1 + xf %*% b + runif(1, min = -1, max = 1)
```

```
}
if(type == 5) {
  err <- rnorm(n, sd = 1 + rbinom(n, 1, eps) * shift)
  y <- 1 + x %*% b + err
  ef <- rnorm(1, sd = 1 + rbinom(1, 1, eps) * shift)
  yf <- 1 + xf %*% b + ef
} #make an MLR data set

# find the 10 fold CV lasso or Ridge regression model when
pitype == 1 || pitype == 0
if(pitype == 1 || pitype == 0){
out<-cv.glmnet(x, y, alpha = pitype)
lam <- out$lambda.min
out_coef <- predict(out,s = lam, type = "coefficients")
yfhat <- predict(out ,s = lam, newx = xf)
}

# find the 10 fold CV Relaxed lasso model when pitype == 2
if(pitype == 2){
rel_fit <- cv.glmnet(x, y, relax = TRUE)
lam <- rel_fit$lambda.min
out_coef <- predict(rel_fit, s = lam, type = "coefficients")
yfhat <- predict(rel_fit, s = lam, newx = xf)
```

```
}



# Filter out the non-zero coefficients
non_zero_indx <- which(out_coef[-1] != 0)
x_ols <- x[, non_zero_indx]

ols_mod <- lm(y~x_ols) # Apply OLS on the selected predictors
ols_coef <- ols_mod$coefficients

# For comparisons of coefficients
non_zero_coef_indx <- which(out_coef != 0)
ols_coef2[non_zero_coef_indx] <- ols_coef

xf_ols <- xf[, non_zero_indx]
xf_ols <- append(xf_ols, 1, after = 0) # modified xf so it
will work with ols
yfhat_ols <- xf_ols %*%  ols_coef

e_lr[i] <-  (yf - yfhat)^2
e_ols[i] <- (yf - yfhat_ols)^2



# Compare coefficients
```

```
  ols_coef_sum <- ols_coef2 + ols_coef_sum
  lr_coef_sum <-  out_coef + lr_coef_sum

}

# TRMSEs
RMSE_lr <- sqrt(sum(e_lr)/nruns)
RMSE_ols <- sqrt(sum(e_ols)/nruns)

# Coef avgs
ols_coef_avg <-ols_coef_sum/nruns
lr_coef_avg <- lr_coef_sum/nruns



# Minkowski distance
diff_ols <- (sum( (abs(append(b, 1, after = 0)
ols_coef_avg))^p ))^(1/p) # Sum of the absolute differences
between b and new ols coefficients estimates
diff_lr <- (sum( (abs(append(b, 1, after = 0) - lr_coef_avg))^p
))^(1/p) # Sum of the absolute differences between b and l or r
coefficients estimates

list(RMSE_ols = RMSE_ols, RMSE_lr = RMSE_lr, diff_ols=diff_ols,
diff_lr=diff_lr)
```

```
}

############################################################

olsafterlrsimplots <- function(n = 50, p = 4, k = 2, nruns = 100, eps = 0.1,
shift = 9, psi = 0.0, type = 1, alpha = 0.05,
pitype = 1){
  # Needs library(glmnet).  Does lasso, RR or Relaxed lasso
  simulations and produces a sid-by-side boxplot.
  ##slow        10 fold CV,
  # Simulates RMSE for lasso if pitype = 1, Ridge regression if
  pitype = 0, ralxed lasso for pitype = 2.
  # 1 <= k <= p-1, k is the number of nonnoise variables
  # Uses five iid error distributions:
  # type = 1 for N(0,1) errors, 2 for t3 errors, 3 for exp(1) - 1 errors
  # 4 for uniform(-1,1) errors, 5 for (1-eps) N(0,1) + eps N(0,(1+shift)^2)
  # errors.
  # constant = 1 so there are p = q+1 coefficients
  # need p > 1, beta = (1, 1, ..., 1, 0, ..., 0) with k+1 ones, p-k-1  zeroes
  # Multiply x by A: for MVN data this results
  # in a covariance matrix with eigenvector c(1, ..., 1)^T
  # corresponding to the largest eigenvalue. As psi gets
  # close to 1, the data clusters about the line in the
  # direction of (1, ..., 1)^T. See Maronna and Zamar (2002).
```

```
# cor(X_i,X_j) = [2 psi +(q-2)psi^2]/[1 + (q-1)psi^2], i not = j
# when the correlation exists.
# set.seed(974) ##need p>2

e_lr <- rep(NA, nruns)
e_ols <- rep(NA, nruns)
RMSE_lr <- 0
RMSE_ols <- 0
ols_coef2 <- rep(0, p)
ols_coef_sum <- rep(0, p)
lr_coef_sum <-  rep(0, p)
ols_coef_avg <- rep(0, p)
lr_coef_avg <- rep(0, p)



q <- p-1
rho <- (2*psi + (q-2)*psi^2)/(1 + (q-1)*psi^2)
A <- matrix(psi,nrow=q,ncol=q)
diag(A) <- 1
b <- 0 * 1:q
b[1:k] <- 1 #b[1:0] acts like b[1:1] = b[1]
indx <- 1:n
```

```
for(i in 1:nruns) {
  x <- matrix(rnorm(n * q), nrow = n, ncol = q)
  x <- x %*% A
  xf <- rnorm(q) %*% A
  if(type == 1) {
    y <- 1 + x %*% b + rnorm(n)
    yf <- 1 + xf %*% b + rnorm(1)
  }
  if(type == 2) {
    y <- 1 + x %*% b + rt(n, df = 3)
    yf <- 1 + xf %*% b + rt(1, df = 3)
  }
  if(type == 3) {
    y <- 1 + x %*% b + rexp(n) - 1
    yf <- 1 + xf %*% b + rexp(1) - 1
  }
  if(type == 4) {
    y <- 1 + x %*% b + runif(n, min = -1, max = 1)
    yf <- 1 + xf %*% b + runif(1, min = -1, max = 1)
  }
  if(type == 5) {
    err <- rnorm(n, sd = 1 + rbinom(n, 1, eps) * shift)
    y <- 1 + x %*% b + err
```

```
  ef <- rnorm(1, sd = 1 + rbinom(1, 1, eps) * shift)
  yf <- 1 + xf %*% b + ef
} #make an MLR data set

# find the 10 fold CV lasso or ridge regression model when
pitype == 1 || pitype == 0
if(pitype == 1 || pitype == 0){
  out<-cv.glmnet(x, y, alpha = pitype)
  lam <- out$lambda.min
  out_coef <- predict(out,s = lam, type = "coefficients")
  yfhat <- predict(out ,s = lam, newx = xf)
}

# find the 10 fold CV Relaxed lasso model when pitype == 2
if(pitype == 2){
  rel_fit <- cv.glmnet(x, y, relax = TRUE)
  lam <- out$lambda.min
  out_coef <- predict(rel_fit, s = lam, type = "coefficients")
  yfhat <- predict(rel_fit, s = lam, newx = xf)

}

# Filter out the non-zero coefficients
```

```
  non_zero_indx <- which(out_coef[-1] != 0)
  x_ols <- x[, non_zero_indx]

  ols_mod <- lm(y~x_ols) # Apply OLS on the selected predictors
  ols_coef <- ols_mod$coefficients

  # For comparisons of coefficients
  non_zero_coef_indx <- which(out_coef != 0)
  ols_coef2[non_zero_coef_indx] <- ols_coef

  xf_ols <- xf[, non_zero_indx]
  xf_ols <- append(xf_ols, 1, after = 0) # modified xf so it
  will work with ols
  yfhat_ols <- xf_ols %*%  ols_coef

  e_lr[i] <-  (yf - yfhat)^2
  e_ols[i] <- (yf - yfhat_ols)^2


  # Compare coefficients
  ols_coef_sum <- ols_coef2 + ols_coef_sum
  lr_coef_sum <-  out_coef + lr_coef_sum

}
```

```
# Plot TRMSEs
rmses <- data.frame(TRMSE = c(e_lr, e_ols), Method =
c(rep("Other", nruns), rep("OLSAVS", nruns)))

rmsePlot <- ggplot(data = rmses, aes(x= Method, y = TRMSE, fill
= Method)) + geom_boxplot() + theme_bw()

# TRMSEs
RMSE_lr <- sqrt(sum(e_lr)/nruns)
RMSE_ols <- sqrt(sum(e_ols)/nruns)

# Coef avgs
ols_coef_avg <-ols_coef_sum/nruns
lr_coef_avg <- lr_coef_sum/nruns

#nroot <- length(ols_coef_avg)

# Minkowski distance
diff_ols <- (sum( (abs(append(b, 1, after = 0) -
ols_coef_avg))^p ))^(1/p) # Sum of the absolute differences
between b and new ols coefficients estimates
diff_lr <- (sum( (abs(append(b, 1, after = 0) - lr_coef_avg))^p
))^(1/p) # Sum of the absolute differences between b and l or r
```

```
  coefficients estimates

  list(RMSE_ols = RMSE_ols, RMSE_lr = RMSE_lr, diff_ols=diff_ols,
  diff_lr=diff_lr, rmsePlot = rmsePlot)
}

OLSAVS <- function(x, y, method){
  # OLSAVS des the OLSAVS method
  # Needs library(glmnet).
  # need x as a model.matrix
  # y - matrix of predictors
  # y - response
  # Method - lasso, RR, Enet or Relaxed lasso (method = 1, method
  = 0, method = 0.5 or method = 2)
  # 10 fold CV

    # find the 10 fold CV lasso or ridge regression or enet model
    when method == 1 || method == 0 || method == 0.5
    if(method == 1 || method == 0 || method == 0.5){
      out<-cv.glmnet(x, y, alpha = method)
      lam <- out$lambda.min
      out_coef <- predict(out,s = lam, type = "coefficients")
```

```
  #yfhat <- predict(out ,s = lam, newx = xf)
}

# find the 10 fold CV Relaxed lasso model when method == 2
if(method == 2){
  rel_fit <- cv.glmnet(x, y, relax = TRUE)
  lam <- rel_fit$lambda.min
  out_coef <- predict(rel_fit, s = lam, type = "coefficients")
  #yfhat <- predict(rel_fit, s = lam, newx = xf)
}


# Filter out the non-zero coefficients
non_zero_indx <- which(out_coef[-1] != 0)
x_ols <- x[, non_zero_indx]

ols_mod <- lm(y~x_ols) # Apply OLS on the selected predictors
ols_coef <- ols_mod$coefficients

outPut <- list(ols_mod = ols_mod, ols_coef = ols_coef, out_coef = out_coef)
outPut$ols_mod

}
```

```
##########################################################



OLSAVSPredict <- function(model, newx){

  # Does predictions for OLSAVS


xtest <- newx

mod <- model


names(mod$coefficients) = gsub(pattern = "x_ols", replacement =

"", x = names(mod$coefficients))


xtest1 <- xtest[, names(mod$coefficients[-1])] # good

newxtest <- cbind(rep(1, nrow(xtest1)), xtest1) # Added a column

of ones to make xtest a design matrix

yhatTest <- newxtest %*% as.matrix(mod$coefficients)


pred <- list(yhat = yhatTest)

pred


}



##################### Example ###################################
```

```
library(ISLR)

library(lars)

data(Auto)


#set.seed(1111)


##################### Splitting and preparing data ##################


train = sample(c(TRUE, FALSE), size = 0.7*nrow(Auto), replace = TRUE)

test <- (!train)


xtrain <- model.matrix(mpg~., Auto)[train,]

xtest <- model.matrix(mpg~., Auto)[test,]


ytrain <- Auto$mpg[train]

ytest <-  Auto$mpg[test]


y <- ytrain

x <- xtrain


##################### Applying OLSAVS ##############################


#Method - lasso, RR, Enet or Relaxed lasso (method = 1, method =
```

```
0, method = 0.5 or method = 2)
mod <- OLSAVS(x, y, method = 0.5) # Fitting the OLSAVS model
mod
summary(mod)

# Predictions
preds <- OLSAVSPredict(mod, xtest) # OLSAVSPredict: separate
function for predictions

# Test root mean square error for OLSAVS
yhatTest <- preds$yhat
RMSE_test_OLSAVS <- sqrt(mean((ytest - yhatTest)^2))
RMSE_test_OLSAVS

######################## lasso, ridge, relax, enet ####################

# Test root mean square error lasso, ridge, enet or relax (alpha
= 1, 0, 0.5, relax: see below)
# for relax lasso: cv.glmnet(x, y, relax = TRUE)
out<-cv.glmnet(x, y, alpha = 0.5)
lam <- out$lambda.min
out_coef <- predict(out, s = lam, type = "coefficients")
yfhat <- predict(out, s = lam, newx = xtest)
```

```
RMSE_test_l <- sqrt(mean((ytest - yfhat)^2))

RMSE_test_l


########################## End Example ##############################
```