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Improved LARS Algorithm for Adaptive LASSO in the Linear Regression Model

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Abstract

The adaptive LASSO method has been employed for reliable variable selection as an alternative to LASSO in linear regression models. This paper introduces an adjusted LARS algorithm that integrates adaptive LASSO with several biased estimators, including the Almost Unbiased Ridge Estimator (AURE), Liu Estimator (LE), Almost Unbiased Liu Estimator (AULE), Principal Component Regression Estimator (PCRE), r-k class estimator, and r-d class estimator. The effectiveness of the proposed algorithm is evaluated through Monte Carlo simulation and empirical examples.

Keywords: Adaptive LASSO; LARS; biased estimators; monte carlo simulation.

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1 Introduction

Let us consider a linear regression model

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}. \tag{1.1}$$

Here, $\boldsymbol{y}$ represents the $n \times 1$ vector of observations on the dependent variable, $\boldsymbol{X}$ is the $n \times p$ matrix of observations on the non-stochastic predictor variables, $\boldsymbol{\beta}$ stands for a $p \times 1$ vector of unknown coefficients, and $\boldsymbol{\varepsilon}$ denotes the $n \times 1$ vector of random error terms. These errors are assumed to be independent and identically normally distributed with mean zero and common variance σ^2.

It is well-established that the Ordinary Least Squares Estimator (OLSE) as the Best Linear Unbiased Estimator (BLUE) for estimating the unknown parameter vector in model (1.1), defined as:

$$\begin{aligned} \hat{\boldsymbol{\beta}}_{\text{OLSE}} &= \arg\min_{\boldsymbol{\beta}} \left\{ (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) \right\} \\ &= (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}. \end{aligned} \tag{1.2}$$

Nevertheless, the OLSE demonstrates instability and yields parameter estimates with high variance in the presence of multicollinearity within $\boldsymbol{X}$. To mitigate this multicollinearity issue, many researchers resort to biased estimators.

As per Kayanan and Wijekoon [1], the generalized representation of biased estimators including Ridge Estimator (RE), Almost Unbiased RidgeEstimator (AURE), Liu Estimator (LE), Almost Unbiased Liu Estimator (AULE), Principal Component Regression Estimator (PCRE), r-k class estimator and r-d class estimator can be expressed as:

$$\hat{\boldsymbol{\beta}}_G = \boldsymbol{G}\hat{\boldsymbol{\beta}}_{\text{OLSE}} \tag{1.3}$$

where

$$\hat{\boldsymbol{\beta}}_G = \begin{cases} \hat{\boldsymbol{\beta}}_{\text{RE}} & \text{if } \boldsymbol{G} = (\boldsymbol{X}'\boldsymbol{X} + k\boldsymbol{I})^{-1}\boldsymbol{X}'\boldsymbol{X} \\ \hat{\boldsymbol{\beta}}_{\text{AURE}} & \text{if } \boldsymbol{G} = \left(\boldsymbol{I} - k^2(\boldsymbol{X}'\boldsymbol{X} + k\boldsymbol{I})^{-2}\right) \\ \hat{\boldsymbol{\beta}}_{\text{LE}} & \text{if } \boldsymbol{G} = (\boldsymbol{X}'\boldsymbol{X} + \boldsymbol{I})^{-1}(\boldsymbol{X}'\boldsymbol{X} + d\boldsymbol{I}) \\ \hat{\boldsymbol{\beta}}_{\text{AULE}} & \text{if } \boldsymbol{G} = \left(\boldsymbol{I} - (1-d)^2(\boldsymbol{X}'\boldsymbol{X} + \boldsymbol{I})^{-2}\right) \\ \hat{\boldsymbol{\beta}}_{\text{PCRE}} & \text{if } \boldsymbol{G} = \boldsymbol{T}_h\boldsymbol{T}_h' \\ \hat{\boldsymbol{\beta}}_{\text{rk}} & \text{if } \boldsymbol{G} = \boldsymbol{T}_h\boldsymbol{T}_h'(\boldsymbol{X}'\boldsymbol{X} + k\boldsymbol{I})^{-1}\boldsymbol{X}'\boldsymbol{X} \\ \hat{\boldsymbol{\beta}}_{\text{rd}} & \text{if } \boldsymbol{G} = \boldsymbol{T}_h\boldsymbol{T}_h'(\boldsymbol{X}'\boldsymbol{X} + \boldsymbol{I})^{-1}(\boldsymbol{X}'\boldsymbol{X} + d\boldsymbol{I}) \end{cases}$$

Kayanan and Wijekoon [1] illustrated that the r-k class estimator and r-d class estimator yield superior performance compared to other estimators within a particular range of regularization parameter values in the presence of multicollinearity among predictor variables. Nonetheless, biased estimators can introduce significant bias when the number of predictor variables is large, which may result in the inclusion of irrelevant predictors in the final model. To mitigate this problem, Tibshirani [2] introduced the Least Absolute Shrinkage and Selection Operator (LASSO) as

$$\hat{\boldsymbol{\beta}}_{\text{LASSO}} = \arg\min_{\boldsymbol{\beta}} \left\{ (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) \right\} \text{ subject to } \sum_{j=1}^{p} |\beta_j| \leq t, \tag{1.4}$$

where $t \geq 0$ is a turning parameter. The LASSO solutions has been obtained by the Least Angle Regression (LARS) algorithm.

Zou and Hastie [3] observed that LASSO does not surpass the Ridge Estimator in scenarios where high multicollinearity is present among predictors, and its performance becomes unstable when the number of predictors exceeds the number of

observations. To address this issue, Zou and Hastie [3] proposed the Elastic Net (ENet) estimator, which integrates LASSO and Ridge Estimator as

$$\hat{\boldsymbol{\beta}}_{\text{ENet}} = \arg\min_{\boldsymbol{\beta}} \left\{ (\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta}) + k\sum_{j=1}^{p}\beta_j^2 \right\} \text{ subject to } \sum_{j=1}^{p}|\beta_j| \le t. \tag{1.5}$$

The LARS-EN algorithm, an adaptation of the LARS-LASSO algorithm, has been employed to derive solutions for the Elastic Net (ENet) estimator.

Further, Zou and Hastie [3] noted that LASSO does not care about variable importance when a group of variables among which the pairwise correlations are very high.

To handle this problem, Zou [4] proposed adaptive LASSO by giving different weights to regression coefficients in L1 penalty of LASSO. By taking weight vector $\hat{\boldsymbol{w}} = |\hat{\boldsymbol{\beta}}_{\text{OLSE}}|^{-\alpha}$ for any $\alpha > 0$, the adaptive LASSO is defined as

$$\hat{\boldsymbol{\beta}}_{\text{adpLASSO}} = \arg\min_{\boldsymbol{\beta}} \left\{ (\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta}) \right\} \text{ subject to } \sum_{j=1}^{p}|w_j\beta_j| \le t. \tag{1.6}$$

In addition to that Zou and Zhang [4] proposed adaptive Enet estimator by combining adaptive LASSO and RE, and it is defined as

$$\hat{\boldsymbol{\beta}}_{\text{adpENet}} = \arg\min_{\boldsymbol{\beta}} \left\{ (\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta}) + k\sum_{j=1}^{p}\beta_j^2 \right\} \text{ subject to } \sum_{j=1}^{p}|w_j\beta_j| \le t, \tag{1.7}$$

where where $\hat{\boldsymbol{w}} = |\hat{\boldsymbol{\beta}}_{Enet}|^{-\alpha}$.

Kayanan and Wijekoon [5] introduced the generalized LARS (GLARS) algorithm, which integrates LASSO with various biased estimators, including the Ridge Estimator (RE), Almost Unbiased Ridge Estimator (AURE), Liu Estimator (LE), Almost Unbiased Liu Estimator (AULE), Principal Component Regression Estimator (PCRE), r-k class estimator, and r-d class estimator. They demonstrated that the combination of LASSO and the r-d class estimator performs effectively in high-dimensional linear regression models, particularly when there is significant multicollinearity among the predictor variables [6, 7, 8, 9, 10, 11].

In this article, we propose an enhanced version of the GLARS algorithm that combines adaptive LASSO with various biased estimators, including the Almost Unbiased Ridge Estimator (AURE), Liu Estimator (LE), Almost Unbiased Liu Estimator (AULE), Principal Component Regression Estimator (PCRE), r-k class estimator, and r-d class estimator. Additionally, we compare the predictive performance of the proposed algorithm with existing adaptive LASSO and adaptive Elastic Net (ENet) algorithms through a Monte Carlo simulation study and an empirical example.

The article is structured as follows: Section 2 introduces the proposed adaptive GLARS algorithm, Section 3 assesses the performance of the algorithm, and Section 4 provides the conclusion.

2 Adaptive GLARS Algorithm for LASSO

Based on the methodology outlined by Kayanan and Wijekoon [5], we propose the adaptive GLARS algorithm as follows:

Algorithm 1 Adaptive GLARS

1: Standardize the predictor variables $\boldsymbol{X}$ to have a mean of zero and a standard deviation of one, and the response variable $\boldsymbol{y}$ to have a mean of zero.

2: Define $\hat{\boldsymbol{w}} = |\hat{\boldsymbol{\beta}}_G|^{-\alpha}$ for $\alpha > 0$, where $\hat{\boldsymbol{\beta}}_G$ is the general form of the biased estimators defined in equation (1.3), and $\boldsymbol{X} = \dfrac{\boldsymbol{X}}{\hat{\boldsymbol{w}}}$.

3: Initialize the estimated value of $\boldsymbol{\beta}$ as $\hat{\boldsymbol{\beta}} = 0$, and set the residual $\boldsymbol{r}_0 = \boldsymbol{y}$.

4: Identify the predictor variable most correlated with $\boldsymbol{r}_0$ by:

- Calculate $X_{j1} = \max_j |\text{Cor}(X_j, \boldsymbol{r}_0|$ for $j = 1, 2, ..., p$.
- Increase the estimate of $\hat{\beta}_{j1}$ from 0 until another predictor X_{j2} has a high correlation with the current residual as X_{j1} does.
- Proceed in the equiangular direction between X_{j1} and X_{j2}.
- Similarly, each subsequent variable X_{ji} earns its way into the active set, and proceed in the equiangular direction between all selected predictors
- Update coefficient estimates using the formula:

$$\hat{\boldsymbol{\beta}}_{ji} = \hat{\boldsymbol{\beta}}_{j(i-1)} + \rho_i \boldsymbol{u}_i, \tag{2.1}$$

  where α_i is a value between 0 and 1 representing the distance the estimate moves before another variable enters the model, and $\boldsymbol{u}_i$ is the equiangular vector.
- Calculate the direction $\boldsymbol{u}_i$ using:

$$\boldsymbol{u}_i = \boldsymbol{G}_E (\boldsymbol{E}_i' \boldsymbol{X}' \boldsymbol{X} \boldsymbol{E}_i)^{-1} \boldsymbol{E}_i' \boldsymbol{X}' \boldsymbol{r}_{i-1}, \tag{2.2}$$

  where **Ei** is the matrix with columns $(e_{j1}, e_{j2}, ..., e_{ji})$, e_j is the j-th standard unit vector in $\mathbb{R}^p$ with the indices of selected variables, and $\boldsymbol{G}_E$ depends on the specific estimator which can be substituted by respective expressions for any of estimators of our interest as listed in Table 2.
- Update ρ_i as:

$$\rho_i = \min \left\{ \rho_{ji}^+, \rho_{ji}^-, \rho_{ji}^* \right\} \in [0, 1] \tag{2.3}$$

  where

$$\rho_{ji}^{\pm} = \frac{\text{Cor}(\boldsymbol{r}_{i-1}, X_{ji}) \pm \text{Cor}(\boldsymbol{r}_{i-1}, X_j)}{\text{Cor}(\boldsymbol{r}_{i-1}, X_{ji}) \pm \text{Cor}(\boldsymbol{X}\boldsymbol{u}_i, X_j)} \text{for any } j \text{ such that } \hat{\boldsymbol{\beta}}_{j(i-1)} = 0, \tag{2.4}$$

  and

$$\rho_{ji}^* = -\frac{\hat{\boldsymbol{\beta}}_{j(i-1)}}{\boldsymbol{u}_i} \text{ for any } j \text{ such that } \hat{\boldsymbol{\beta}}_{j(i-1)} \neq 0. \tag{2.5}$$

- If $\rho_i = \rho_{ji}^*$, update $\boldsymbol{E}_i$ by removing the column e_j from $\boldsymbol{E}_{i-1}$. Calculate the new residual $\boldsymbol{r}_i$ as:

$$\boldsymbol{r}_i = \boldsymbol{r}_{i-1} - \rho_i \boldsymbol{X} \boldsymbol{u}_i, \tag{2.6}$$

  and move to the next step where j_{i+1} is the value of j such that $\rho_i = \rho_{ji}^+$ or $\rho_i = \rho_{ji}^-$ or ρ_{ji}^*.
- End this step when $\rho_i = 1$.

5: Output $\hat{\boldsymbol{\beta}}_{adp} = \dfrac{\hat{\boldsymbol{\beta}}}{\hat{\boldsymbol{w}}}$.

In Table 1, $\boldsymbol{I}p_E$ denotes the $p_E \times p_E$ identity matrix, where p_E represents the number of selected variables at each iterative step, and $\boldsymbol{T}_{h_E} = (t_1, t_2, ..., t_{h_E})$ comprises the first h_E columns of the standardized eigenvectors of $\boldsymbol{E}_i' \boldsymbol{X}' \boldsymbol{X} \boldsymbol{E}_i$.

The adaptive GLARS algorithm iteratively updates the combined estimates of adaptive LASSO and other estimators. The algorithm requires $O(m^3 + pm^2)$ operations, with m representing the number of steps. However, this study does not consider computational efficiency. The evaluation of prediction performance is based on the Root Mean Square Error (RMSE) criterion, as detailed in Section 3. The adaptive GLARS method enables the integration of adaptive LASSO with any of the estimators listed in Table 1.

Table. 1. G_E of the estimators for GLARS

Estimators	G_E
OLSE	E_i
RE	$E_i(E_i'(X'X+kI)E_i)^{-1}(E_i'X'XE_i)$
AURE	$E_i(I_{p_E}-k^2(E_i'(X'X+kI)E_i)^{-2})$
LE	$E_i(E_i'(X'X+I)E_i)^{-1}(E_i'(X'X+dI)E_i)$
AULE	$E_i(I_{p_E}-(1-d)^2(E_i'(X'X+I)E_i)^{-2})$
PCRE	$T_{h_E}T_{h_E}'E_i$
r-k class	$T_{h_E}T_{h_E}'E_i(E_i'(X'X+kI)E_i)^{-1}(E_i'X'XE_i)$
r-d class	$T_{h_E}T_{h_E}'E_i(E_i'(X'X+I)E_i)^{-1}(E_i'(X'X+dI)E_i)$

It is worth noting that when G_E corresponds to the expressions of OLSE and RE, adaptive GLARS provides solutions akin to adaptive LASSO and adaptive ENet, respectively. For ease of reference, we denote adaptive GLARS as adpLARS-LASSO, adpLARS-EN, adpLARS-AURE, adpLARS-LE, adpLARS-AULE, adpLARS-PCRE, adpLARS-rk, and adpLARS-rd when G_E corresponds to the expressions of OLSE, RE, AURE, LE, AULE, PCRE, r-k class, and r-d class estimators, respectively.

We can use two-dimensional cross-validation to find the suitable value of α and shrinkage parameter k or d for adaptive GLARS.

3 Performance of the Adaptive GLARS Algorithms

Proposed algorithms are compared using the RMSE criterion, which is the expected prediction error of the algorithms, and is defined as

$$RMSE(\hat{\boldsymbol{\beta}}) = \sqrt{\frac{1}{n}(\boldsymbol{y}_{new}-\boldsymbol{X}_{new}\hat{\boldsymbol{\beta}})'(\boldsymbol{y}_{new}-\boldsymbol{X}_{new}\hat{\boldsymbol{\beta}})} \tag{3.1}$$

Here, $(\boldsymbol{y}_{\text{new}},\boldsymbol{X}_{\text{new}})$ represents the new data set not utilized in estimating the parameters, and $\hat{\boldsymbol{\beta}}$ signifies the estimated value of $\boldsymbol{\beta}$ obtained through the corresponding algorithm. A comparison is conducted using both a Monte Carlo simulation study and empirical examples.

3.1 Simulation study

As outlined by McDonald and Galarneau [12], initially, the predictor variables are generated utilizing the following mathematical expression:

$$x_{i,j} = \sqrt{(1-\rho^2)}z_{i,j}+\rho z_{i,m+1} \qquad ;i=1,2,...,n.\ \ j=1,2,...,m. \tag{3.2}$$

In this context, $z_{i,j}$ represents an independent standard normal pseudo-random number, and ρ denotes the theoretical correlation between any pair of explanatory variables.

In this investigation, we employed a linear regression model comprising 100 observations and 20 predictors. The dependent variable is generated utilizing the subsequent equation:

$$y_i = \beta_1 x_{i,1}+\beta_2 x_{i,2}+...+\beta_5 x_{i,20}+\varepsilon_i \qquad ;i=1,2,...,100. \tag{3.3}$$

where ε_i is a normal pseudo random number with mean zero and common variance σ^2. We choose $\boldsymbol{\beta}=(\beta_1,\beta_2,...,\beta_{20})$ as

the normalized eigenvector corresponding to the largest eigenvalue of $\boldsymbol{X}'\boldsymbol{X}$ for which $\boldsymbol{\beta}'\boldsymbol{\beta} = 1$. To explore the impacts of varying degrees of multicollinearity on the estimators, we select $\rho = (0.5, 0.7, 0.9)$, representing weak, moderate, and high multicollinearity, respectively. For our analysis, we simulate 50 datasets, each comprising 50 observations, to fit the model, and another 50 observations are used to calculate the Root Mean Square Error (RMSE).

The Cross-validated RMSE values of the adaptive GLARS algorithms are depicted in Figs. 1 through 3, while the median cross-validated RMSE values of the algorithms are presented in Tables 2 through 4.

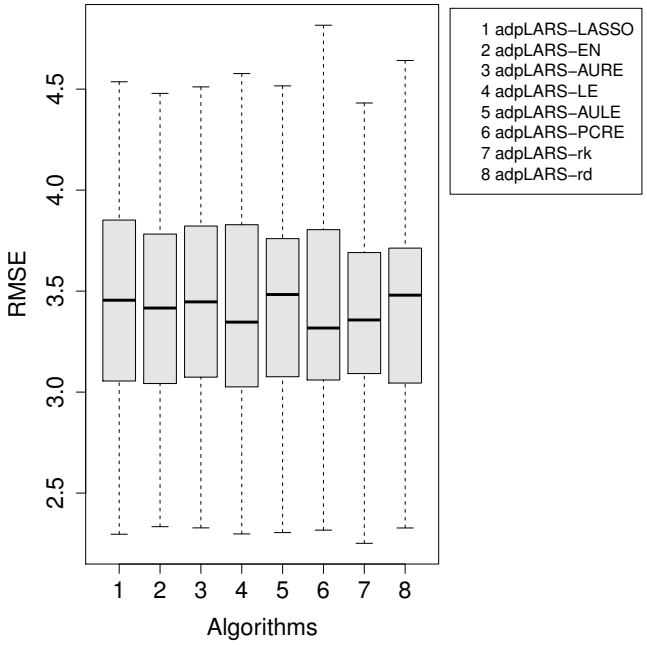

Fig. 1. Cross-validated RMSE values of the adaptive GLARS algorithms under the condition where $\rho = 0.5$

Table. 2. Median values of Cross-validated RMSE for the adaptive GLARS algorithms under the condition where $\rho = 0.5$

Algorithms	RMSE	(k, d)	α	t	Selected variables
adpLARS-LASSO	3.45489	–	1	6.6635	16
adpLARS-EN	3.41614	0.2	1	7.5795	17
adpLARS-AURE	3.44668	1.0	1	7.1685	17
adpLARS-LE	3.34648	0.3	1	7.1018	15
adpLARS-AULE	3.48312	0.2	1	8.0718	16
adpLARS-PCRE	**3.31719**	–	1	6.5019	16
adpLARS-rk	3.35712	0.2	1	6.0726	17
adpLARS-rd	3.47994	0.99	1	6.5019	16

Based on the insights gathered from Fig. 1 to Fig. 3 and Table 2 to Table 4, it is evident that the adpLARS-PCRE, adpLARS-rk, and adpLARS-rd algorithms consistently demonstrate superior performance in terms of RMSE criterion compared to other adaptive GLARS algorithms across varying degrees of multicollinearity, from weak to moderate and high levels, respectively.

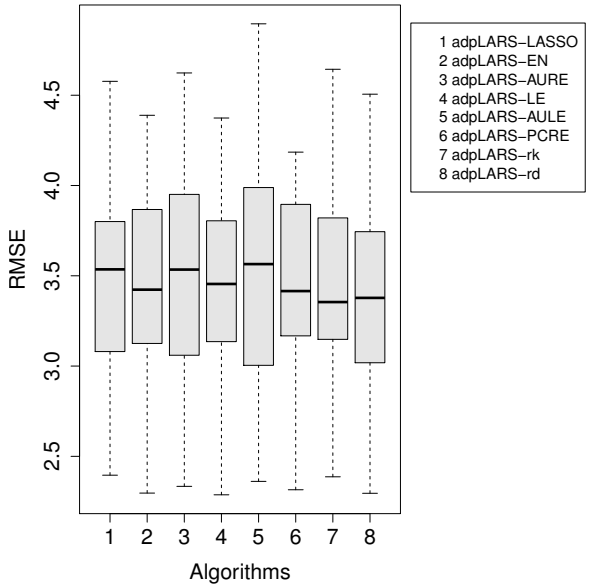

Fig. 2. Cross-validated RMSE values of the adaptive GLARS algorithms under the condition where $\rho = 0.7$

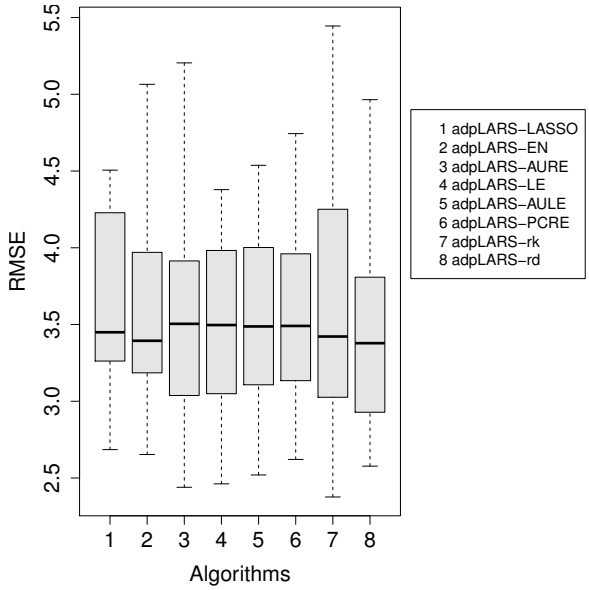

Fig. 3. Cross-validated RMSE values of the adaptive GLARS algorithms under the condition where $\rho = 0.9$

3.2 Real-world example

In our analysis, we utilized the Prostate Cancer Data [13], a well-established dataset explored by Tibshirani [2], Efron et al. [14] , and Zou and Hastie [3] to evaluate the efficacy of LASSO, LARS algorithm, and Enet.

Table. 3. Median values of Cross-validated RMSE for the adaptive GLARS algorithms under the condition where $\rho = 0.7$

Algorithms	RMSE	(k, d)	α	t	Selected variables
adpLARS-LASSO	3.53553	–	1	8.7067	16
adpLARS-EN	3.42320	0.3	0.5	8.9330	17
adpLARS-AURE	3.53440	0.7	1	8.0610	17
adpLARS-LE	3.45469	0.1	0.5	9.1520	15
adpLARS-AULE	3.56472	0.1	1	8.0821	16
adpLARS-PCRE	3.41530	–	1	9.5873	16
adpLARS-rk	**3.35452**	0.1	1	8.9412	16
adpLARS-rd	3.37755	0.2	1	8.8207	16

Table. 4. Median values of Cross-validated RMSE for the adaptive GLARS algorithms under the condition where $\rho = 0.9$

Algorithms	RMSE	(k, d)	α	t	Selected variables
adpLARS-LASSO	3.44950	–	0.5	4.0460	15
adpLARS-EN	3.39404	1.0	1	8.2710	17
adpLARS-AURE	3.50448	0.9	1	10.045	17
adpLARS-LE	3.49651	0.1	0.5	10.005	15
adpLARS-AULE	3.48735	0.1	0.5	8.0684	16
adpLARS-PCRE	3.49078	–	0.5	10.682	17
adpLARS-rk	3.42176	0.3	1	10.433	16
adpLARS-rd	**3.37842**	0.99	0.5	7.0576	15

The Prostate Cancer Data comprises eight clinical metrics: log cancer volume (lcavol), log prostate weight (lweight), age, log of benign prostatic hyperplasia volume (lbph), seminal vesicle invasion (svi), log capsular penetration (lcp), Gleason score (gleason), and percentage Gleason score 4 or 5 (pgg45). The response variable is the log of prostate-specific antigen (lpsa), with a dataset size of 97 observations. Notably, the predictor variables exhibit Variance Inflation Factor (VIF) values of 3.09, 2.97, 2.47, 2.05, 1.95, 1.37, 1.36, and 1.32, indicating considerable multicollinearity, as evidenced by a high condition number of 243. This dataset is readily available within the "lasso2" R package. Our analysis involved fitting the model with 67 observations and computing the Root Mean Square Error (RMSE) using 30 observations.

Table. 5. Cross-validated RMSE values for the Prostate Cancer Data utilizing adaptive GLARS algorithm

Algorithms	RMSE	(k, d)	α	t	Selected variables
adpLARS-LASSO	0.77653	–	0.2	1.57112	7
adpLARS-EN	0.78716	0.3	1	0.80638	7
adpLARS-AURE	0.80638	1.0	0.9	0.80638	7
adpLARS-LE	0.80014	0.1	0.5	1.45884	7
adpLARS-AULE	0.79046	0.2	1	1.31322	6
adpLARS-PCRE	0.76890	–	0.9	1.44929	7
adpLARS-rk	0.77698	0.2	0.9	1.36273	7
adpLARS-rd	**0.76854**	0.7	0.9	1.44764	7

The cross-validated RMSE values obtained through the adaptive GLARS algorithms are summarized in Table 5. Upon examining Table 5, it becomes evident that the adpLARS-rd algorithm outperforms other algorithms when applied to the Prostate Cancer Data.

4 Conclusion

This study provides clear evidence of the effectiveness of the adpLARS-rk and adpLARS-rd algorithms in addressing high-dimensional linear regression challenges, particularly in the presence of numerous closely correlated independent variables. These improved algorithms emerge as reliable tools for tackling high dimensional regression models and offer promising avenues for future research and practical application in data-driven environments.

Disclaimer (Artificial Intelligence)

The author(s) hereby declare that generative AI technologies, such as Grammarly and ChatGPT, have been used to enhance the language of the manuscripts.

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Competing Interests

Authors have declared that no competing interests exist.

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