



# A new Jackknifing ridge estimator for logistic regression model

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(Communicated by Madjid Eshaghi Gordji)

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## Abstract

In reducing the effects of collinearity, the ridge estimator (RE) has been consistently demonstrated to be an attractive shrinkage method. In application, when the response variable is binary data, the logistic regression model (LRM) is a well-known model. However, it is known that collinearity negatively affects the variance of maximum likelihood estimator of the LRM. To address this problem, a logistic ridge estimator was proposed by several authors. In this work, a Jackknifing logistic ridge estimator (NJLRE) is proposed and derived. The Monte Carlo simulation results recommend that the NJLRE estimator can bring significant improvement relative to other existing estimators. Furthermore, the real application results demonstrate that the NJLRE estimator outperforms both LRE and MLE in terms of predictive performance.

*Keywords:* Collinearity; Jackknife estimator; ridge estimator; logistic regression model; Monte Carlo simulation.

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## 1. Introduction

Binary classification using a logistic regression model has often been adopted in several real data applications, “such as cancer classification. Various studies have attempted to apply the logistic regression model as a base to build a classification model.

In the presence of collinearity, when estimating the regression coefficients for logistic regression model using the maximum likelihood method (MLE), the estimated coefficients are usually become

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*Received:* May 2021    *Accepted:* October 2021

unstable with a high variance, and therefore low statistical significance (Kibria, Månsson, & Shukur, 2015)[17]. The ridge estimator (Hoerl & Kennard, 1970)[10] has been consistently demonstrated to be an attractive and alternative to the MLE (Asar & Genç, 2015)[3].

In linear regression, the ridge estimator is defined as

$$\hat{\beta}_{Ridge} = (X^T X + kI)^{-1} X^T y, \tag{1.1}$$

where  $y$  is an  $n \times 1$  vector of observations of the response variable,  $X = (x_1, \dots, x_p)$  is an  $n \times p$  known design matrix of explanatory variables,  $\beta = (\beta_1, \dots, \beta_p)$  is a  $p \times 1$  vector of unknown regression coefficients,  $I$  is the identity matrix with dimension  $p \times p$ , and  $k \geq 0$  represents the ridge parameter (shrinkage parameter) (Algamal & Lee, 2015; Hoerl & Kennard, 1970)[1, 10].

### 2. Logistic ridge regression model

In case of binary classification problem, logistic regression (LR) is a statistical model that is used frequently. In classification, the response variable of the LR has two values either 1 for the positive class or 0 for the normal class. Assume that we have  $n$  observations and  $p$  explanatory variables. Let  $y_i \in \{0, 1\}$  be the response variable value for observation  $i$ ,  $i = 1, 2, \dots, n$  and  $z_i = (z_{i1}, z_{i2}, \dots, z_{in})^T$  be the  $i^{th}$  explanatory variable vector of the design matrix  $Z$ . Then, the response variable is related to explanatory variables by

$$\psi_i = p(y_i = 1|z_i) = \frac{\exp(z_i^T \beta)}{1 + \exp(z_i^T \beta)}, \quad i = 1, 2, \dots, n \tag{2.1}$$

where  $\beta = (\beta_0, \beta_1, \dots, \beta_p)^T$  is a  $(p + 1) \times 1$  vector of unknown explanatory variables coefficients. The log-likelihood function of the logit transformation of Eq. (1.1) is defined as

$$\ell(\beta) = \sum_{i=1}^n \{y_i \log(\psi_i) + (1 - y_i) \log(1 - \psi_i)\}. \tag{2.2}$$

The MLE is then obtained by computing the first derivative of the Eq. (2.2) and setting it equal to zero, as

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^n [y_i - \psi_i] z_i = 0. \tag{2.3}$$

Because Eq. (2.3) is nonlinear in  $\beta$ , the iteratively weighted least squares (IWLS) algorithm can be used to obtain the MLE of the LR parameters as

$$\hat{\beta}_{LR} = (Z^T \hat{W} Z)^{-1} Z^T \hat{W} \hat{v}, \tag{2.4}$$

where  $\hat{W} = \text{diag}(\hat{\psi}_i(1 - \hat{\psi}_i))$  and  $\hat{v}$  is a vector where  $i^{th}$  element. The covariance is

$$\text{cov}(\hat{\beta}_{LR}) = \left[ -E \left( \frac{\partial^2 \ell(\beta)}{\partial \beta_i \partial \beta_k} \right) \right]^{-1} = (Z^T \hat{W} Z)^{-1}. \tag{2.5}$$

The mean squared error (MSE) of Eq. (2.4) can be obtained as

$$\begin{aligned} \text{MSE}(\hat{\beta}_{LR}) &= E(\hat{\beta}_{LR} - \beta)^T (\hat{\beta}_{LR} - \beta) \\ &= \text{tr}[(Z^T \hat{W} Z)^{-1}] \\ &= \sum_{j=1}^p \frac{1}{\lambda_j}, \end{aligned} \tag{2.6}$$

where  $\lambda_j$  is the eigenvalue of the  $Z^T \hat{W} Z$  matrix.

The LRE (Le Cessie & Van Houwelingen, 1992; Lee & Silvapulle, 1988; Schaefer, Roi, & Wolfe, 1984)[18, 19] as

$$\begin{aligned} \hat{\beta}_{LRE} &= (Z^T \hat{W} Z + kI)^{-1} Z^T \hat{W} Z \hat{\beta}_{LR} \\ &= (Z^T \hat{W} Z + kI)^{-1} Z^T \hat{W} \hat{v}, \end{aligned} \tag{2.7}$$

where  $k \geq 0$ (Kibria et al., 2015; Rashad & Algamal, 2019)[17, 24].

$$\text{MSE}(\hat{\beta}_{LRE}) = \sum_{j=1}^p \frac{\lambda_j}{(\lambda_j + k)^2} + k^2 \sum_{j=1}^p \frac{\alpha_j}{(\lambda_j + k)^2}, \tag{2.8}$$

where  $\alpha_j$  is defined as the  $j^{th}$  element of  $\gamma \hat{\beta}_{LR}$  and  $\gamma$  is the eigenvector of the  $Z^T \hat{W} Z$  matrix.

### 3. The proposed estimator

Let  $D = (d_1, d_2, \dots, d_p)$  and  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_p)$ , respectively, be the matrices of eigenvectors and eigenvalues of the  $Z^T \hat{W} Z$  matrix, such that  $M^T Z^T \hat{W} Z D = S^T \hat{W} S = \Lambda$ , where  $S = XD$ . Consequently, the logistic regression estimator of Eq. (2.4),  $\hat{\beta}_{LR}$ , can be written as

$$\begin{aligned} \hat{\gamma}_{LR} &= \Lambda^{-1} S^T \hat{W} \hat{v} \\ \hat{\beta}_{LR} &= D \hat{\gamma}_{LR}. \end{aligned} \tag{3.1}$$

Accordingly, the logistic ridge estimator,  $\hat{\beta}_{LRE}$ , is rewritten as

$$\begin{aligned} \hat{\gamma}_{LRE} &= (\Lambda + K)^{-1} S^T \hat{W} \hat{v} \\ &= (I - K B^{-1}) \hat{\gamma}_{LR}, \end{aligned} \tag{3.2}$$

where  $B = \Lambda + K$  and  $K = \text{diag}(k_1, k_2, \dots, k_p)$ ;  $k_i \geq 0, i = 1, 2, \dots, p$ . Equation (3.2) represents the generalized ridge logistic regression estimator (Batah, Ramanathan, & Gore, 2008; Khurana, Chaubey, & Chandra, 2014; Özkale, 2008)[8, 15, 23].

In GRE, the Jackknifing approach was used (Khurana et al., 2014; Nyquist, 1988; Singh, Chaubey, & Dwivedi, 1986)[15, 22, 27]. Batah et al. (2008)[8] proposed a modified Jackknifed ridge estimator in LRM. Related to Poisson regression model, Türkan and Özel (2015) proposed a modified Jackknifed Poisson ridge estimator depending on the study of Singh et al. (1986).

In this paper, the new estimator (NLRE) is derived by following the study of Batah et al. (2008). Let the Jackknife estimator (JE), in logistic regression, is defined as

$$\hat{\gamma}_{JE} = (I - K^2 B^{-2}) \hat{\gamma}_{LR}, \tag{3.3}$$

and the modified Jackknife estimator (MJE) of Batah et al. (2008)[8], in logistic regression model, is defined as

$$\hat{\gamma}_{MJE} = (I - K B^{-1})(I - K^2 B^{-2}) \hat{\gamma}_{LR}. \tag{3.4}$$

The new estimator can be defined by multiplying it with the amount  $[(I - K^3 B^{-3}) / (I - K^2 B^{-2})]$ . The new estimator is defined as

$$\hat{\gamma}_{NLRE} = (I - K B^{-1})(I - K^2 B^{-2}) \frac{(I - K^3 B^{-3})}{(I - K^2 B^{-2})} \hat{\gamma}_{LR}, \tag{3.5}$$

and

$$\hat{\beta}_{NLRE} = D^T \hat{\gamma}_{NLRE}. \tag{3.6}$$

3.1. the properties of the new estimator

The MSE of the new estimator can be obtained as

$$MSE(\hat{\gamma}_{NLRE}) = var(\hat{\gamma}_{NLRE}) + [bias(\hat{\gamma}_{NLRE})]^2 \tag{3.7}$$

According to Eq. (3.7), the bias and variance of  $\hat{\gamma}_{NLRE}$  can be obtained as, respectively,

$$\begin{aligned} bias(\hat{\gamma}_{NLRE}) &= E[\hat{\gamma}_{NLRE}] - \gamma \\ &= (I - KB^{-1})(I - K^3B^{-3})E[\hat{\gamma}_{LR}] - \gamma \\ &= -K [(KB^{-1})^{-1} - (KB^{-1})^{-1}(I - KB^{-1}) + K^2B^{-2}(I - KB^{-1})] B^{-1}\gamma, \end{aligned} \tag{3.8}$$

$$\begin{aligned} var(\hat{\gamma}_{NLRE}) &= (I - KB^{-1})(I - K^3B^{-3})var(\hat{\gamma}_{LR})(I - K^3B^{-3})^T(I - KB^{-1})^T \\ &= (I - KB^{-1})(I - K^3B^{-3})\Lambda^{-1}(I - K^3B^{-3})^T(I - KB^{-1})^T. \end{aligned} \tag{3.9}$$

Then,

$$\begin{aligned} MSE(\hat{\gamma}_{NLRE}) &= (I - KB^{-1})(I - K^3B^{-3})\Lambda^{-1}(I - K^3B^{-3})^T(I - KB^{-1})^T + \\ &\quad [-K [(KB^{-1})^{-1} - (KB^{-1})^{-1}(I - KB^{-1}) + K^2B^{-2}(I - KB^{-1})] B^{-1}\gamma] \\ &\quad [-K [(KB^{-1})^{-1} - (KB^{-1})^{-1}(I - KB^{-1}) + K^2B^{-2}(I - KB^{-1})] B^{-1}\gamma]^T \\ &= \Phi\Lambda^{-1}\Phi^T + K\Psi B^{-1}\gamma\gamma^T B^{-1}\Psi^T K, \end{aligned} \tag{3.10}$$

where  $\Phi = (I - K^3B^{-3})^T(I - KB^{-1})$  and  $\Psi = [I + KB^{-1} - KB^{-3}K]$ .

3.2. Selection of parameter  $k$

The efficiency of ridge estimator strongly depends on appropriately choosing the  $k$  parameter (Kibria et al., 2015)[17].

1. Hoerl and Kennard (1970) (HK), which is defined as

$$k_j(HK) = \frac{1}{\hat{\alpha}_{\max}^2}, \quad j = 1, 2, \dots, p, \tag{3.11}$$

2. Kibria et al. (2015) (KMS1), which is defined as

$$k_j(KMS1) = \text{Median} \left\{ \left[ \sqrt{\frac{1}{\hat{\alpha}_j^2}} \right]^2 \right\}, \quad j = 1, 2, \dots, p, \tag{3.12}$$

3. Kibria et al. (2015) (KMS2), which is defined as

$$k_j(KMS2) = \text{Median} \left\{ \frac{\lambda_{\max}}{(n - p) + \lambda_{\max}\hat{\alpha}_j^2} \right\} \tag{3.13}$$

4. Simulation study

4.1. Simulation design

The response variable of  $n$  observations is generated from logistic regression model by Eq. (1.1) with  $\sum_{j=1}^p \beta_j^2 = 1$  and  $\beta_1 = \beta_2 = \dots = \beta_p$  (Kibria, 2003; Månsson & Shukur, 2011)[16, 20]. In addition, the explanatory variables  $z_i^T = (z_{i1}, z_{i2}, \dots, z_{in})$  have been generated from the following formula

$$z_{ij} = (1 - \rho^2)^{1/2}w_{ij} + \rho w_{i,p+1}, \quad i = 1, 2, \dots, n, \quad j = 1, 2, \dots, p, \tag{4.1}$$

where  $\rho$  is the correlation between the explanatory variables and  $w_{ij}$ 's are independent standard normal pseudo-random numbers.  $n=30, 100$  and  $150$ . In addition,  $p = 4$  and  $p = 8$ . Further, because we are interested in the effect of multicollinearity,  $\rho = \{0.90, 0.95, 0.99\}$ . For a combination of these different values of  $n, p$ , and  $\rho$  the generated data is repeated 1000 times and the averaged mean squared errors (MSE) is calculated as

$$\text{MSE}(\hat{\beta}) = \frac{1}{1000} \sum_{i=1}^{1000} (\hat{\beta} - \beta)^T (\hat{\beta} - \beta), \quad (4.2)$$

where  $\hat{\beta}$  is the estimated coefficients for the used estimator.

#### 4.2. Simulation results

The estimated MSE of Eq. (4.2) for MLE, LRE, and NLRE, for all the different selection methods of  $k$  and the combination of  $n, p$ , and  $\rho$ , are respectively summarized in Tables 1 and 2. Several observations can be made.

First, in terms of  $\rho$  values, there is increasing in the MSE values when the  $\rho$  increases regardless the value of  $n, p$ . However, NLRE performs better than LRE and MLE for all the different selection methods of  $k$ . For instance, in Table 1, when  $p = 4, n = 100$ , and  $\rho = 0.95$ , the MSE of NRLR was about 51.64%, 35.81%, and 20.81% lower than that of LRE for KH, KMS1 and KMS2, respectively. In addition, the MSE of NLRE was about 94.73% lower than that of MLE.

Second, regarding  $p$ , it is easily seen that there is increasing in the MSE values when the  $p$  increasing from four variables to eight variables. Although this increasing can affected the quality of an estimator, NLRE is achieved the lowest MSE comparing with MLE and LRE, for different  $n, \rho$  and different selection methods of  $k$ .

Third, with respect to the value of  $n$ , The MSE values decreases when  $n$  increases, regardless the value of  $\rho, p$ , and the value of  $k$ . However, NLRE still consistently outperforms LRE and MLE by providing the lowest MSE.

Finally, for the different selection methods of  $k$ , the performance of all methods suggesting that the NLRE estimator is better than the other used two estimators. The KMS1 efficiently provides less MSE comparing with the KMS1 and KH for both NLRE and LRE estimators. Besides, KH is more efficient for providing less MSE than KMS2 or both NRLE and RLE estimators.

To summary, all the considered values of  $n, \rho, p$ , and the value of  $k$ , NLRE is superior to LRE, clearly indicating that the new proposed estimator is more efficient".

Table 1: MSE values when  $p = 4$ 

		MLE	KH		KMS1		KMS2	
			LRE	NLRE	LRE	NLRE	LRE	NLRE
$\rho$								
$n = 30$	0.90	5.707	1.746	1.593	1.386	1.285	2.131	2.031
	0.95	6.335	1.977	1.826	1.835	1.734	2.292	2.189
	0.99	6.733	2.627	2.475	2.367	2.266	2.636	2.535
$n = 100$	0.90	4.078	1.379	1.226	1.297	1.196	1.672	1.571
	0.95	5.153	1.651	1.498	1.406	1.305	1.768	1.667
	0.99	5.345	1.968	1.815	2.296	2.195	1.981	1.881
$n = 150$	0.90	3.921	1.181	1.028	1.268	1.167	1.529	1.428
	0.95	4.131	1.305	1.152	1.295	1.194	1.545	1.444
	0.99	4.886	2.331	2.178	2.071	1.971	1.663	1.562

Table 2: MSE values when  $p = 8$ 

		MLE	KH		KMS1		KMS2	
			LRE	NLRE	LRE	NLRE	LRE	NLRE
$\rho$								
$n = 30$	0.90	6.211	2.249	2.096	1.889	1.788	2.634	2.533
	0.95	6.838	2.481	2.329	2.338	2.237	2.793	2.692
	0.99	7.236	3.132	2.978	2.871	2.769	3.139	3.038
$n = 100$	0.90	4.581	1.882	1.729	1.801	1.699	2.175	2.074
	0.95	5.656	2.154	2.001	1.909	1.808	2.271	2.172
	0.99	5.848	2.471	2.318	2.799	2.698	2.484	2.383
$n = 150$	0.90	4.424	1.684	1.531	1.771	1.671	2.032	1.931
	0.95	4.634	1.808	1.655	1.798	1.697	2.048	1.947
	0.99	5.389	2.834	2.681	2.574	2.473	2.166	2.065

## 5. Real data application

A dataset of 121 molecules of anti-hepatitis C virus activity of thiourea derivatives was used for constructing quantitative structure-activity relationship (QSAR) model. The molecules were divided into two categories by the threshold value of  $0.1 \mu\text{M}$ : actives ( $\text{EC}_{50} < 0.1 \mu\text{M}$ ) and inactive ( $\text{EC}_{50} \geq 0.1 \mu\text{M}$ ). First, the deviance test (Montgomery, Peck, & Vining, 2015) is used to check whether the LRM is fit well to this data or not. The result of the residual deviance test is equal to 8.027 with 120 degrees of freedom and the p-value is 0.837. Second, the relationships between the explanatory variables is listed in Table 3. Then, the eigenvalues of the matrix  $Z^T \hat{W} Z$  are obtained as 941.295, 201.332, 71.385, 36.588, 20.602, and 1.324. The determined condition number  $\text{CN} = \sqrt{\lambda_{\max}/\lambda_{\min}}$  of the data is 29.9026.663 indicating that the collinearity issue is existing.

The estimated LRM and MSE values for the MLE, LRE, and NLRE estimators are listed in Table 4. According to Table 4, it is clearly seen that the NLRE estimator shrinkages the value of the estimated coefficients efficiently. Additionally, in terms of the calculated standard errors, the LRE and NLRE show substantial decreasing comparing with MLE, regardless of the selection method of  $k$ . Furthermore, in terms of the selection method of  $k$ , NLRE shows the superiority results of both coefficient estimation and standard error using KMS1. In terms of MSE, the NLRE using KMS1 achieves the lowest MSE.

Table 3: The correlation matrix among the five explanatory variables.

	Mor02u	RDF015u	Mor25v	PJI3
CIC3	0.912	0.102	0.889	0.957
Mor02u		0.875	0.947	0.624
RDF015u			0.913	0.806
Mor25v				0.962

Table 4: The estimated coefficients and MSE values for the MLE, LRE, and NLRE estimators. The number in parenthesis is the standard error.

	KH			KMS1		KMS2	
	MLE	LRE	NLRE	LRE	NLRE	LRE	NLRE
$\hat{\beta}_1$	-3.041 (0.111)	-2.105 (0.103)	-1.516 (0.097)	-1.604 (0.088)	-1.415 (0.078)	-1.213 (0.077)	-0.844 (0.071)
$\hat{\beta}_2$	2.329 (0.123)	2.035 (0.113)	2.004 (0.101)	2.032 (0.111)	1.924 (0.102)	1.440 (0.089)	1.451 (0.084)
$\hat{\beta}_3$	1.561 (0.124)	1.107 (0.124)	1.016 (0.118)	0.986 (0.114)	0.911 (0.098)	0.546 (0.108)	0.393 (0.088)
$\hat{\beta}_4$	-3.168 (0.214)	-2.046 (0.204)	-1.934 (0.188)	-1.863 (0.124)	-1.521 (0.117)	1.604 (0.102)	1.019 (0.079)
$\hat{\beta}_5$	2.0431 (0.127)	1.017 (0.110)	1.008 (0.104)	1.014 (0.111)	0.984 (0.103)	0.919 (0.103)	0.636 (0.094)
MSE	4.102	3.557	2.397	1.981	1.761	1.242	0.977

## 6. Conclusion

In this work, a new estimator of LRM is proposed to overcome the collinearity problem in the logistic regression model. According to Monte Carlo simulation studies, the proposed estimator has better performance than MLE and LRE, in terms of MSE. The superiority of the proposed estimator of real data application based on the resulting MSE was consistent with Monte Carlo simulation results.

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