A new shrinkage estimator in Inverse Gaussian Regression model

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Abstract
The ridge estimator has been consistently demonstrated to be an attractive shrinkage method to reduce the effects of multicollinearity. The inverse Gaussian regression model (INGRM) is a well-known model in application when the response variable is a skewed data. However, it is known that the variance of maximum likelihood estimator (MLE) of the INGRM coefficients can negatively affected in the presence of multicollinearity. In this paper, a new shrinkage estimator is proposed to overcome the multicollinearity problem in the INGRM. Our Monte Carlo simulation and real data application results suggest that the proposed estimator is better than the MLE estimator and ridge estimator, in terms of MSE.

Keywords: Multicollinearity; ridge estimator; inverse Gaussian regression model; Monte Carlo simulation.

1. Introduction

The inverse Gaussian regression model (IGRM) has been widely used in industrial engineering, life testing, reliability, marketing, and social sciences [1-7]. “Specifically, IGRM is used when the response variable under the study is positively skewed [8-10]. When the response variable is extremely skewness, the IGRM is preferable than gamma regression model [11]. In dealing with the IGRM, it is assumed that there is no correlation among the explanatory variables [12-32]. In practice, however, this assumption often not holds, which leads to the problem of multicollinearity. In the presence of multicollinearity, when estimating the regression coefficients for IGRM using the maximum likelihood (ML) method, the estimated coefficients are usually become unstable with a high variance, and therefore low statistical significance [33]. Numerous remedial methods have been proposed to overcome the problem of multicollinearity [34-58]. The ridge regression method [59] has been consistently demonstrated to be an attractive and alternative to the ML estimation method.

Ridge regression is a biased method that shrinks all regression coefficients toward zero to reduce the large variance [60]. This done by adding a positive amount to the diagonal of $\mathbf{X}^T\mathbf{X}$. As a result, the ridge estimator is biased but it guaranties a smaller mean squared error than the ML estimator.

In linear regression, the ridge estimator is defined as

$$\hat{\boldsymbol{\beta}}_{Ridge} = (\mathbf{X}^T \mathbf{X} + k\,\mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}, \tag{1}$$

where $\mathbf{y}$ is an $n \times 1$ vector of observations of the response variable, $\mathbf{X} = (\mathbf{x}_1, ..., \mathbf{x}_p)$ is an $n \times p$ known design matrix of explanatory variables, $\boldsymbol{\beta} = (\beta_1, ..., \beta_p)$ is a $p \times 1$ vector of unknown regression coefficients, $\mathbf{I}$ is the identity matrix with dimension $p \times p$, and $k \geq 0$ represents the ridge parameter (shrinkage parameter). The ridge parameter, k, controls the shrinkage of $\boldsymbol{\beta}$ toward zero. The OLS estimator can be considered as a special estimator from Eq. (1) with $k = 0$. For larger value of k, the $\hat{\boldsymbol{\beta}}_{Ridge}$ estimator yields greater shrinkage approaching zero [59, 61].

2. The proposed estimator

To improve ridge estimator in dealing with multicollinearity in inverse Gaussian ridge regression model, a new shrinkage estimator of ridge estimator is proposed by extending the works of Lukman, et al. [62], Lukman, et al. [63], Lukman, et al. [64]. The proposed estimator (INGMRE) is defined as:

$$\hat{\boldsymbol{\beta}}_{INGMRE} = (\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X} + k\,(1+d)\mathbf{I})^{-1} \mathbf{X}^T \hat{\mathbf{W}} \mathbf{X} \hat{\boldsymbol{\beta}}_{INGRM} = \mathbf{C} \hat{\boldsymbol{\beta}}_{INGRM}\,, \tag{2}$$

where $\mathbf{C} = (\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X} + k\,(1+d)\mathbf{I})^{-1} \mathbf{X}^T \hat{\mathbf{W}} \mathbf{X}$, $k > 0$, and $0 < d < 1$. The MSE of Eq. (2) can be obtained as

$$MSE\left[\hat{\boldsymbol{\beta}}_{INGMRE}\right] = \mathbf{C}(\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X})^{-1} \mathbf{C}^T + (\mathbf{C} - \mathbf{I})\boldsymbol{\beta}\boldsymbol{\beta}^T (\mathbf{C} - \mathbf{I})^T, \tag{3}$$

where the bias and variance of $\hat{\boldsymbol{\beta}}_{INGMRE}$ is defined as, respectively,

$$\text{bias}\left[\hat{\boldsymbol{\beta}}_{INGMRE}\right] = (\mathbf{C} - \mathbf{I})\boldsymbol{\beta} \tag{4}$$

$$\text{var}\left[\hat{\boldsymbol{\beta}}_{INGMRE}\right] = \mathbf{C}(\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X})^{-1} \mathbf{C}^T \tag{5}$$

3. Superiority of the proposed estimator in terms of MSE

With availability of different estimators for a parameter in the regression model, it is of interest to compare their performances in terms of MSE. For two given estimators $\hat{\boldsymbol{\beta}}_A$ and $\hat{\boldsymbol{\beta}}_B$ of $\boldsymbol{\beta}$, the estimator $\hat{\boldsymbol{\beta}}_B$ is said to be superior to $\hat{\boldsymbol{\beta}}_A$ under the MSE criterion if and only if $\Delta = \text{MSE}(\hat{\boldsymbol{\beta}}_A) - \text{MSE}(\hat{\boldsymbol{\beta}}_B) \geq 0$.

Lemma 1: [65] Let $\mathbf{D}$ is a $p \times p$ positive definite matrix, $\mathbf{b}$ is a $p \times 1$ vector, and ϑ is a positive constant. Then $\vartheta \mathbf{D} - \mathbf{b}\mathbf{b}^T$ is a nonnegative definite if and only if $\mathbf{b}^T \mathbf{D}^{-1} \mathbf{b} \leq \vartheta$ is hold.

3.1. Comparison between $\hat{\boldsymbol{\beta}}_{INGMRE}$ and $\hat{\boldsymbol{\beta}}_{INGRM}$

The proposed estimator $\hat{\boldsymbol{\beta}}_{INGMRE}$ is better than $\hat{\boldsymbol{\beta}}_{INGRM}$ if and only if (iff),

$$\boldsymbol{\beta}^T(\mathbf{C}-\mathbf{I})^T\left[(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}-\mathbf{C}(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{C}^T)\right]^{-1}(\mathbf{C}-\mathbf{I})^T\boldsymbol{\beta}<1 \tag{6}$$

The difference between Eq. (6) and Eq. (3) is defined as

$$\Delta=((\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}-\mathbf{C}(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{C}^T))-(\mathbf{C}-\mathbf{I})\boldsymbol{\beta}\boldsymbol{\beta}^T(\mathbf{C}-\mathbf{I})^T \tag{7}$$

Since $(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k(1+d))^2-(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^T>0$, then $(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}-\mathbf{C}(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{C}^T)$ is positive definite. By lemma 1, the proof is complete.

3.2. Comparison between $\hat{\boldsymbol{\beta}}_{INGMRE}$ and $\hat{\boldsymbol{\beta}}_{Ridge}$

The proposed estimator $\hat{\boldsymbol{\beta}}_{INGMRE}$ is better than $\hat{\boldsymbol{\beta}}_{Ridge}$ if and only if (iff),

$$\boldsymbol{\beta}^T(\mathbf{C}-\mathbf{I})^T\left[\mathbf{H}+k^2(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\boldsymbol{\beta}\boldsymbol{\beta}^T\left((\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\right)^T\right]^{-1}(\mathbf{C}-\mathbf{I})\boldsymbol{\beta}\le 1 \tag{8}$$

where

$$\mathbf{H}=(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}\left((\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\right)^T-\mathbf{C}(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X})^{-1}\mathbf{C}^T \tag{9}$$

The difference between Eq. (8) and Eq. (6) is defined as

$$\Delta=\mathbf{H}+k^2(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\boldsymbol{\beta}\boldsymbol{\beta}^T\left((\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\right)^T-(\mathbf{C}-\mathbf{I})\boldsymbol{\beta}\boldsymbol{\beta}^T(\mathbf{C}-\mathbf{I})^T \tag{10}$$

Because $\mathbf{H}+k^2(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\boldsymbol{\beta}\boldsymbol{\beta}^T\left((\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+k\mathbf{I})^{-1}\right)^T$ is positive, $\Delta>0$ iff Eq. (10) is satisfied.

4. Simulation study

In this section, a Monte Carlo simulation experiment is used to examine the performance of used estimators with different degrees of multicollinearity.

4.1. Simulation design

The response variable is drawn from inverse Gaussian distribution $y_i \sim IG(\mu_i,\tau)$ with sample sizes $n=100$ and 150, respectively, where $\tau\in\{0.5,1.5,3\}$. The explanatory variables $\mathbf{x}_i^T=(x_{i1},x_{i2},...,x_{in})$ have been generated from the following formula

$$x_{ij}=(1-\rho^2)^{1/2}w_{ij}+\rho w_{ip},\ i=1,2,...,n,\quad j=1,2,...,p, \tag{11}$$

where ρ represents the correlation between the explanatory variables and w_{ij}'s are independent pseudo-random numbers. Three values of the number of the explanatory variables: 4, 8, and 12, and three different values of ρ corresponding to 0.90, 0.95, and 0.99 are considered. Depending on the type of the link function, μ_i, the log link function is investigated. The log link function is defined as

$$\mu_i = \exp(\mathbf{x}_i^T \boldsymbol{\beta}), \quad i = 1, 2, ..., n. \tag{12}$$

Here, the vector $\boldsymbol{\beta}$ is chosen as the normalized eigenvector corresponding to the largest eigenvalue of the $\mathbf{X}^T \mathbf{W}\mathbf{X}$ matrix subject to $\boldsymbol{\beta}^T \boldsymbol{\beta} = 1$ [66]. In addition, the w_{ij} in Eq. (11) are generated from normal distribution (0,1).

The estimated average MSE is calculated as

$$\text{MSE}(\hat{\boldsymbol{\beta}}) = \frac{1}{R} \sum_{i=1}^{R} (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}), \tag{13}$$

where R equals 1000 corresponding to the number of replicates used in our simulation. All the calculations are computed by R program.

4.2. Simulation results

The average estimated MSE of Eq. (13) for all the combination of n, τ, p, and ρ, are respectively summarized in Tables 1 – 3. According to Tables 1 – 3, the proposed estimator, INMRE, gives low bias comparing with Ridge estimator. This finding indicates that the proposed estimator is significantly decreasing the bias. Meanwhile, INMRE estimator performs well not only in terms of bias, but also in terms of MSE. It is noted that INMRE ranks first with respect to MSE. In the second rank, Ridge estimator performs better than INGRM estimator. Additionally, INGRM estimator has the worst performance among Ridge and INMRE which is significantly impacted by the multicollinearity.

Furthermore, with respect to ρ, there is increasing in the bias and MSE values when the correlation degree increases regardless the value of n, τ and p. Regarding the number of explanatory variables, it is easily seen that there is a negative impact on both bias and MSE, where there are increasing in their values when the p increasing from three variables to ten variables. In Addition, in terms of the sample size n, the bias and the MSE values decrease when n increases, regardless the value of ρ, τ and p. Clearly, in terms of the dispersion parameter τ, both bias and MSE values are decreasing when τ increasing.

Table 1: Averaged MSE values for the log link function when $p = 4$

n	τ	ρ	INGRM	Ridge	INGMRE
100	0.5	0.90	11.5361	1.6041	**1.2721**
		0.95	14.7541	2.0181	**1.4111**
		0.99	17.6511	2.3631	**2.0041**
	1.5	0.90	10.5511	1.4831	**1.2581**

		0.95	13.4141	1.6681	**1.3451**
		0.99	17.1631	1.9861	**1.6321**
	3	0.9	7.1141	1.4041	**1.2221**
		0.95	11.2151	1.4321	**1.3251**
		0.99	14.6531	1.5841	**1.5331**
150	0.5	0.9	11.3191	1.3871	**1.0551**
		0.95	14.5371	1.8011	**1.1941**
		0.99	17.4341	2.1461	**1.7871**
	1.5	0.9	10.3651	1.2971	**1.0511**
		0.95	13.2281	1.4821	**1.1591**
		0.99	16.9771	1.8011	**1.4441**
	3	0.90	10.3431	1.2751	**1.0291**
		0.95	13.2061	1.4611	**1.1371**
		0.99	16.9551	1.7781	**1.4221**

Table 2: Averaged MSE values for the log link function when $p = 8$

n	τ	ρ	INGRM	Ridge	INGMRE
100	0.5	0.90	11.8271	1.8951	**1.5631**
		0.95	15.0451	2.3091	**1.7021**
		0.99	17.9421	2.6541	**2.2951**
	1.5	0.90	10.8421	1.7741	**1.5491**
		0.95	13.7051	1.9591	**1.6361**
		0.99	17.4541	2.2771	**1.9231**
	3	0.9	7.4051	1.6951	**1.5131**
		0.95	11.5061	1.7231	**1.6161**
		0.99	14.9441	1.8751	**1.8241**
150	0.5	0.9	11.6101	1.6781	**1.3461**
		0.95	14.8281	2.0921	**1.4851**

		0.99	17.7251	2.4371	**2.0781**
	1.5	0.9	10.6561	1.5881	**1.3421**
		0.95	13.5191	1.7731	**1.4501**
		0.99	17.2681	2.0921	**1.7351**
	3	0.90	10.6341	1.5661	**1.3201**
		0.95	13.4971	1.7521	**1.4281**
		0.99	17.2461	2.0691	**1.7131**

Table 3: Averaged MSE values for the log link function when $p = 12$

n	τ	ρ	INGRM	Ridge	INGMRE
100	0.5	0.90	11.9251	1.9931	**1.6611**
		0.95	15.1431	2.4071	**1.8001**
		0.99	18.0401	2.7521	**2.3931**
	1.5	0.90	10.9401	1.8721	**1.6471**
		0.95	13.8031	2.0571	**1.7341**
		0.99	17.5521	2.3751	**2.0211**
	3	0.9	7.5031	1.7931	**1.6111**
		0.95	11.6041	1.8211	**1.7141**
		0.99	15.0421	1.9731	**1.9221**
150	0.5	0.9	11.7081	1.7761	**1.4441**
		0.95	14.9261	2.1901	**1.5831**
		0.99	17.8231	2.5351	**2.1761**
	1.5	0.9	10.7541	1.6861	**1.4401**
		0.95	13.6171	1.8711	**1.5481**
		0.99	17.3661	2.1901	**1.8331**
	3	0.90	10.7321	1.6641	**1.4181**
		0.95	13.5951	1.8501	**1.5261**
		0.99	17.3441	2.1671	**1.8111**

5. Real data application

To demonstrate the usefulness of the IGLE in real application, we present here a chemistry dataset with $(n, p) = (65,15)$, where n represents the number of imidazo[4,5-b]pyridine derivatives, which are used as anticancer compounds. While p denotes the number of molecular descriptors, which are treated as explanatory variables [67]. The response of interest is the biological activities (IC_{50}). Quantitative structure-activity relationship (QSAR) study has become a great deal of importance in chemometrics. The principle of QSAR is to model several biological activities over a

collection of chemical compounds in terms of their structural properties [68]. Consequently, using of regression model is one of the most important tools for constructing the QSAR model.
First, to check whether the response variable belongs to the inverse Gaussian distribution, a Chi-square test is used. The result of the test equals to 5.2762 with p-value equals to 0.2601. It is indicated form this result that the inverse Gaussian distribution fits very well to this response variable. That is, the following model is set

$$\hat{y}_{IC_{50}} = \exp(\sum_{j=1}^{15} \mathbf{x}_j \hat{\beta}_j). \tag{14}$$

Second, to check whether there is a relationship among the explanatory variables or not, Figure 1 displays the correlation matrix among the 15 explanatory variables. It is obviously seen that there are correlations greater than 0.90 among MW, SpMaxA_D, and ATS8v ($r = 0.96$), between SpMax3_Bh(s) and ATS8v ($r = 0.92$), and between Mor21v with Mor21e ($r = 0.93$).
Third, to test the existence of multicollinearity after fitting the inverse Gaussian regression model using log link function and the estimated dispersion parameter is 0.00103, the eigenvalues of the matrix $\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X}$ are obtained as 1.884×10^9, 3.445×10^6, 2.163×10^5, 2.388×10^4, 1.290×10^3, 9.120×10^2, 4.431×10^2, 1.839×10^2, 1.056×10^2, 5525, 3231, 2631, 1654, 1008, and 1.115". The determined condition number $\text{CN} = \sqrt{\lambda_{\max} / \lambda_{\min}}$ of the data is 40383.035 indicating that the severe multicollinearity issue is exist.

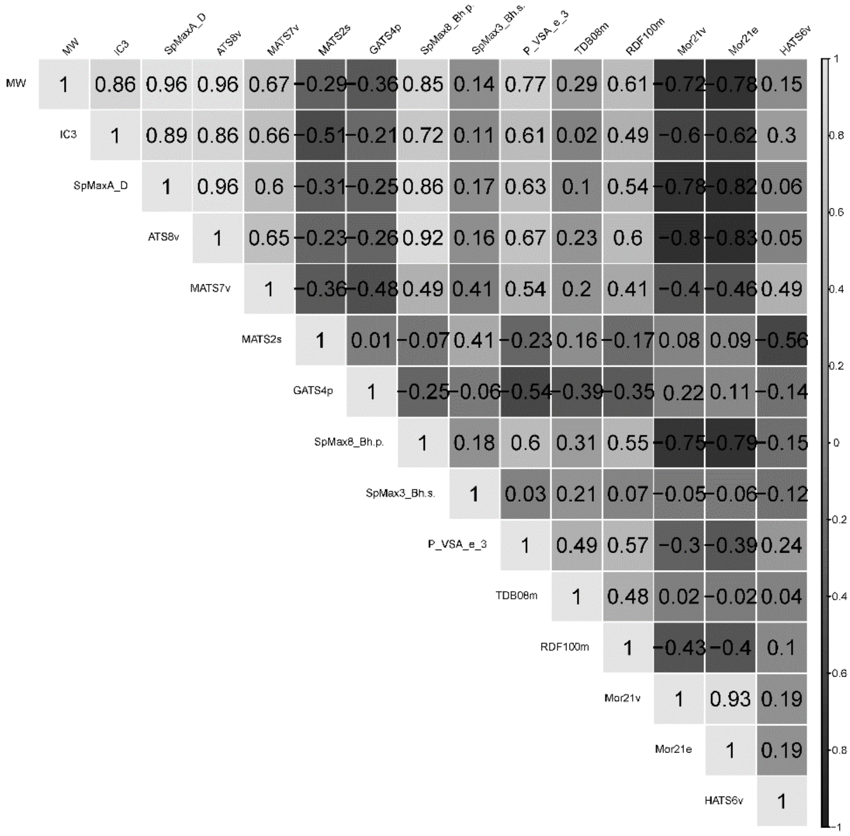

Figure 1. "Correlation matrix among the 15 explanatory variables of the real data.
The estimated inverse Gaussian regression coefficients and the estimated theoretical MSE values for the MLE, and the used estimators are listed in Table 4. According to Table 4, it is clearly seen

that the INGMRE shrinkages the value of the estimated coefficients efficiently. Additionally, in terms of the MSE, there is an important reduction in favor of the INGMRE. Specifically, it can be seen that the MSE of the INGMRE estimator was about 51.077% and 11.767% lower than that of INGRM and Ridge estimators, respectively.

Table 4: The estimated coefficients and MSE values of the used estimators"

	Methods		
$\hat{\beta}$	INGRM	Ridge	INGMRE
MW	1.002	0.835	0.734
IC3	1.237	1.07	0.969
SpMaxA_D	-1.102	-1.269	-0.902
ATS8v	-1.379	-1.546	-1.179
MATS7v	-1.219	-1.386	-1.019
MATS2s	-1.215	-1.382	-1.015
GATS4p	-1.237	-1.405	-1.037
SpMax8_Bh.p.	2.506	2.339	2.707
SpMax3_Bh.s.	2.069	1.902	2.269
P_VSA_e_3	2.001	1.833	2.2
TDB08m	-2.103	-2.27	-1.903
RDF100m	1.571	1.403	1.77
Mor21v	-2.434	-2.601	-2.235
Mor21e	-2.352	-2.519	-2.152
HATS6v	2.211	2.044	2.411
MSE	3.295	1.827	**1.612**

6. Conclusions

In this paper, “a new shrinkage estimator is proposed to overcome the multicollinearity problem in the inverse Gaussian regression model. According to Monte Carlo simulation studies, the INGMRE estimator has better performance than NIGRM and Ridge estimators, in terms of MSE. Additionally, a real data application is also considered to illustrate benefits of using INGMRE estimator. The superiority of the INGMRE estimator based on the resulting MSE was observed and it was shown that the results are consistent with Monte Carlo simulation results”. In conclusion, the use of the INGMRE estimator is recommended when multicollinearity is present in the inverse Gaussian regression model.

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