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Restricted ridge estimator in the Inverse Gaussian regression model

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The Inverse Gaussian regression (IGR) model is a well-known model in application when the response variable positively skewed. Its parameters are usually estimated using maximum likelihood (ML) method. However, the ML method is very sensitive to multicollinearity. Ridge estimator was proposed in Inverse Gaussian regression model. A restricted ridge estimator is proposed. Simulation and real data example results demonstrate that the proposed estimator is outperformed ML and Inverse Gaussian ridge estimator.

keywords: multicollinearity, ridge regression, restricted estimator, shrinkage, Monte Carlo simulation.

1 Introduction

The Inverse Gaussian regression (IGR) has been widely used in industrial engineering, life testing, reliability, marketing, and social sciences (Bhattacharyya and Fries, 1982; Ducharme, 2001; Folks and Davis, 1981; Fries and Bhattacharyya, 1986; Heinzl and Mittlböck, 2002; Lemeshko et al., 2010; Malehi et al., 2015). Specifically, IGR model is used when the response variable under the study is positively skewed (Babu and Chaubey, 1996; Chaubey, 2002; Wu and Li, 2012). When the response variable is extremely skewness, the IGR is preferable than gamma regression model (De Jong et al., 2008). In dealing with the IGR, it is assumed that there is no correlation among the explanatory variables. In practice, however, this assumption often not holds, which leads to the problem of multicollinearity. In the presence of multicollinearity, when estimating the

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regression coefficients for IGR using the maximum likelihood (ML) method, the estimated coefficients are usually become unstable with a high variance, and therefore low statistical significance with incorrect signs (Alheety and Kibria, 2014; Batah et al., 2009; Jou et al., 2014). Numerous remedial methods have been proposed to overcome the problem of multicollinearity. The ridge regression method (Hoerl and Kennard, 1970). has been consistently demonstrated to be an attractive and alternative to the ML estimation method. Ridge regression is a shrinkage method that shrinks all regression coefficients toward zero to reduce the large variance (Asar and Genç, 2016). The ridge regression performance greatly relies on the choice of shrinkage parameter. Consequently, choosing a suitable value of the shrinkage parameter is an important part of ridge regression model fitting (Söküt Açar and Özkale, 2016). Several methods, which they are based on the original ridge regression of (Hoerl and Kennard, 1970), are available for estimating the ridge shrinkage parameter in the literature (Alkhamisi et al., 2006; Yasin et al., 2013; Hamed et al., 2013; Hefnawy and Farag, 2014; Khalaf and Shukur, 2005; Kibria, 2003; Muniz and Kibria, 2009; Algamal, 2018b,a; Mohammed and Algamal, 2021; Algamal et al., 2018; Qasim and Algamal, 2020; Algamal and Lee, 2017a; Algamal, 2017; Algamal et al., 2016b, 2017b; Algamal, 2012; Rashad and Algamal, 2019; Algamal et al., 2017a, 2016a; Algamal and Asar, 2020; Qasim et al., 2018; Algamal and Alanaz, 2018; Yahya Algamal, 2019; Shamany et al., 2019; Lukman et al., 2021a,b; Noeel and Algamal, 2021).

2 Inverse Gaussian ridge regression model

The Inverse Gaussian distribution is a continuous distribution with two positive parameters: location parameter ,μ, and scale parameter, τ, denoted as $IG(\mu, \tau)$. Its probability density function is defined as

$$f(y, \mu, \tau) = \frac{1}{\sqrt{2\pi y^3 \tau}} \exp\left[-\frac{1}{2y}\left(\frac{y-\mu}{\mu\sqrt{\tau}}\right)^2\right], \quad y > 0. \tag{1}$$

The mean and variance of this distribution are, respectively, $E(y) = \mu$ and $var(y) = \tau \mu^3$.

Inverse Gaussian regression model is considered a member of the generalized linear models (GLM) family, extending the ideas of linear regression to the situation where the response variable is following the Inverse Gaussian distribution. Following the GLM methodology, Eq. (1) can re-write in terms of exponential family function as

$$f(y, \mu, \tau) = \frac{1}{\tau}\left\{-\frac{y}{2\mu^2} + \frac{1}{\mu}\right\} + \left\{-\frac{1}{2}\ln(2\pi y^3) - \frac{1}{2}\ln(\tau)\right\}, \tag{2}$$

where $C(y, \tau) = -\frac{1}{2}\ln(2\pi y^3) - (1/2)\ln(\tau)$ and $\frac{y\theta - a(\theta)}{\phi} = \frac{1}{\tau}\left\{-\frac{y}{2\mu^2} + \frac{1}{\mu}\right\}$. Here, τ represents the dispersion parameter and $1/\mu^2$ represents the canonical link function. In GLM, a monotonic and differentiable link function connects the mean of the response variable with the linear predictor $\eta_i = x_i^T \beta$, where x_i is the ith row of X and β is a

$(p + 1) \times 1$ vector of unknown regression coefficients. Because η_i depends on β and the mean of the response variable is a function of η_i, then $E(y_i) = \mu_i = g^{-1}(\eta_i) = g^{-1}(x_i^T \beta)$. Related to the IGR, the $\mu = 1/\sqrt{x_i^T \beta}$. Another possible link function for the IGR is log link function, $\mu = \exp(x_i^T \beta)$. he model estimation of the IGR is based on the maximum likelihood method (ML). The log likelihood function of the IGR under the canonical link function is defined as

$$\ell(\beta) = \sum_{i=1}^{n} \left\{ \frac{1}{\tau} \left[\frac{y_i x_i^T \beta}{2} - \sqrt{x_i^T \beta} \right] - \frac{1}{2\tau y_i} - \frac{\ln \tau}{2} - \ln(2\pi y_i^3) \right\}. \tag{3}$$

The ML estimator is then obtained by computing the first derivative of the Eq.(3) and setting it equal to zero, as

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^{n} \frac{1}{2\tau} \left[y_i - \frac{1}{\sqrt{x_i^T \beta}} \right] x_i = 0. \tag{4}$$

Unfortunately, the first derivative cannot be solved analytically because Eq.(4) is non-linear in β. The iteratively weighted least squares (IWLS) algorithm or Fisher-scoring algorithm can be used to obtain the ML estimators of the IGR parameters. In each iteration, the parameters are updated by

$$\beta^{(r+1)} = \beta^{(r)} + I^{-1}(\beta^{(r)})S(\beta^{(r)}), \tag{5}$$

where $S(\beta^{(r)})$ and $I^{-1}(\beta^{(r)})$ are $S(\beta) = \partial \ell(\beta)/\partial \beta$ and $I^{-1}(\beta) = \left(-E \left(\partial^2 \ell(\beta)/\partial \beta \partial \beta^T \right) \right)^{-1}$ evaluated at $\beta^{(r)}$), respectively. The final step of the estimated coefficients is defined as

$$\hat{\beta}_{IGR} = B^{-1} X^T \hat{W} \hat{m}, \tag{6}$$

where $B = (X^T \hat{W} X)$, $\hat{W} = \text{diag}(\hat{\mu}_i^3)$, $\hat{m}$ is a vector where ith element equals to $\hat{m}_i = (1/\hat{\mu}_i^2) + ((y_i - \hat{\mu}_i)/\hat{\mu}_i^3)$, and $\hat{\mu} = 1/\sqrt{x_i^T \hat{\beta}}$. The covariance matrix of $\hat{\beta}_{IGR}$ equals

$$cov(\hat{\beta}_{IGR}) = \left[-E \left(\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} \right) \right]^{-1} = \tau B^{-1}, \tag{7}$$

and the MSE equals

$$\begin{aligned} \text{MSE}(\hat{\beta}_{IGR}) &= E(\hat{\beta}_{IGR} - \hat{\beta})^T (\hat{\beta}_{IGR} - \hat{\beta}) \\ &= \tau \, tr[B^{-1}] \\ &= \tau \sum_{j=1}^{p} \frac{1}{\lambda_j}, \end{aligned} \tag{8}$$

where λ_j is the eigenvalue of the B matrix and the dispersion parameter, τ, is estimated by (Uusipaikka, 2008).

$$\hat{\tau} = \frac{1}{(n-p)} \sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{\hat{\mu}_i^3}. \tag{9}$$

In the presence of multicollinearity, the matrix $X^T \hat{W} X$ becomes ill-conditioned leading to high variance and instability of the ML estimator of the IGR. As a remedy, the ridge estimator (IGRR)

$$\hat{\beta}_{IGRR} = (X^T \hat{W} X + kI)^{-1} X^T \hat{W} X \hat{\beta}_{ML}$$
$$= (X^T \hat{W} X + kI)^{-1} X^T \hat{W} \hat{v}, \tag{10}$$

where $k \geq 0$. The ML estimator can be considered as a special estimator from Eq. (10) with $h = 0$. Regardless of h value, the MSE of the $\hat{\beta}_{IGRR}$ is smaller than that of $\hat{\beta}_{ML}$ because the MSE of $\hat{\beta}_{IGRR}$ is equal to

$$\text{MSE}(\hat{\beta}_{PRE}) = \tau \sum_{j=1}^{p} \frac{\lambda_j}{(\lambda_j + k)^2} + \sum_{j=1}^{p} \frac{\alpha_j}{(\lambda_j + k)^2}, \tag{11}$$

where α_j is defined as the jth element of $\gamma \hat{\beta}_{ML}$ and γ is the eigenvector of the $X^T \hat{W} X$ matrix. Comparing with the MSE of Eq.(10), MSE($\hat{\beta}_{PRE}$) is always small for $k > 0$.

3 The proposed estimator

In addition to the sample information, there are some exact or restrictions for the unknown parameter of the model exist which may help to reduce the multicollinearity problem. Therefore, suppose that we have some prior information about β in the form of independent linear restrictions as:

$$H\beta = h, \tag{12}$$

where H denotes a $q \times (p + 1)$ $(q \leq p + 1)$ known matrix and h shows a $q \ x \ I$ vector of pre-specified know constants. Considering such a restriction, Duffy and Santner (1989a). defined the restricted maximum likelihood estimator (RMLE) with the following from:

$$\hat{\beta}_{RMLE} = \hat{\beta}_{MLE} - (X^T \hat{W} X)^{-1} H^T (H(X^T \hat{W} X)^{-1} H^T)^{-1} (H\hat{\beta}_{MLE} - h) \tag{13}$$

Based on the Eq. (10) and Eq. (7), we propose a restricted Inverse Gaussian ridge estimator (RIGRE) which is given as follows:

$$\hat{\beta}_{RIGRE} = (X^T \hat{W} X + kI)^{-1} X^T \hat{W} \hat{v} - (X^T \hat{W} X + kI)^{-1} H^T \left[H(X^T \hat{W} X + kI)^{-1} H^T \right]^{-1}$$
$$\left[H(X^T \hat{W} X + kI)^{-1} X^T \hat{W} \hat{v} - h \right] \tag{14}$$

It is easy to see that when the biasing parameter, $k = 0$, Eq. (14) becomes the RMLE in Eq. (13). The restricted ridge estimator was studied by several authors, such as (Alheety and Kibria, 2014; Asar et al., 2017; Duffy and Santner, 1989b; Kurtoğlu and Özkale, 2019; Nagarajah et al., 2015; Najarian et al., 2013). The MSE of $\hat{\beta}_{RIGRE}$ is defined as

$$\text{MSE}(\hat{\beta}_{RPRE}) = \tau \sum_{j=1}^{p} \frac{(\lambda_j(\lambda_j + k - h_{jj})^2}{(\lambda_j + k)^4} + k \left[\sum_{j=1}^{p} \frac{\alpha_j(\lambda_j + k - h_{jj})}{(\lambda_j + 1)^2} \right]^2, \tag{15}$$

4 Simulation results

In this section, a Monte Carlo simulation experiment is used to examine the performance of the new estimator with different degrees of multicollinearity. The response variable is drawn from Inverse Gaussian distribution $y_i \sim IG(\mu_i, \tau)$ with sample sizes $n = 50, 100$ and 150, respectively, where $\tau \in \{0.5, 1.5, 3\}$. The explanatory variables $x_i^T = (x_{i1}, x_{i2}, ..., x_{in})$ have been generated from the following formula

$$x_{ij} = (1 - \rho^2)^{1/2} w_{ij} + \rho w_{ip}, \ \ i = 1, 2, ..., n, \ \ \ j = 1, 2, ..., p, \tag{16}$$

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, and 7, 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 functions is investigated.

The log link function is defined as

$$\mu_i = \exp(x_i^T \beta), \ \ \ i = 1, 2, ..., n. \tag{17}$$

Here, the vector β is chosen as the normalized eigenvector corresponding to the largest eigenvalue of the $X^T W X$ matrix subject to $\beta^T \beta = 1$ (Kibria, 2003). In addition, the w_{ij} in Eq. (16) are generated from normal distribution (0,1). The estimated average MSE is calculated as

$$\text{MSE}(\hat{\beta}) = \frac{1}{R} \sum_{i=1}^{R} (\hat{\beta} - \beta)^T (\hat{\beta} - \beta), \tag{18}$$

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

According to Asar et al. (2017), two restricted matrices are explained as

$$H_{p=4} = \begin{pmatrix} 1 & 0 & -3 & 2 \\ 1 & -2 & 1 & -1 \end{pmatrix} \text{ and } H_{p=7} = \begin{pmatrix} 1 & 0 & -3 & 1 & -1 & 2 & 1 \\ 1 & -2 & 1 & -1 & 0 & 1 & 1 \end{pmatrix} \text{ with } h = (0,0).$$ In addition, the method of determining the value of k is defined as $k = (1/\frac{2}{\max})$.

The estimated MSE of Eq. (15) for ML, IGRR, and our proposed estimator, RIGRE, for the combination of n, p, τ, and ρ, are respectively summarized in Tables 1, 2, and 3. Several observations can be made. First, in terms of ρ values, there is increasing in the MSE values when the correlation degree increases regardless the value of n, p, τ. However, RIGRE performs better than IGRR and ML. For instance, in Table 1, when $p = 4$, $n = 150$, and $\rho = 0.99$, the MSE of RIGRE was about 28.91% and 22.15% lower than that of ML and IGRR respectively.

Second, regarding the number of explanatory variables, it is easily seen that there is increasing in the MSE values when the p increasing from four variables to seven variables. Although this increasing can affected the quality of an estimator, RIGRE is achieved the lowest MSE comparing with ML and IGRR, for different n, ρ, τ.

Third, with respect to the value of n, The MSE values decreases when n increases, regardless the value of ρ, p, τ. However, RIGRE still consistently outperforms IGRR by providing the lowest MSE.

Fourth, in terms of the value of the τ and for a given values of ρ, p, n, RIGRE is always show smaller MSE comparing with the other methods.

To summary, all the considered values of n, ρ, p, τ, RIGRE is superior to IGRR, clearly indicating that the new proposed estimator is more efficient.

Table 1: Table 1: MSE values when $\tau = 0.5$

			ML	IGRR	RIGRE
		ρ			
$p = 4$	$n = 50$	0.9	5.0774	4.8304	3.9631
		0.95	5.7054	5.4584	4.5914
		0.99	6.1034	5.8564	4.9893
	$n = 100$	0.9	3.4484	3.2014	2.3344
		0.95	4.5234	4.2764	3.409
		0.99	4.7154	4.4684	3.6014
	$n = 150$	0.9	3.2914	3.0444	2.1771
		0.95	3.5014	3.2542	2.3874
		0.99	4.2564	4.009	3.1424
$p = 7$		0.9	5.1824	4.9354	4.0684
	$n = 50$	0.95	5.8014	5.5544	4.6874
		0.99	6.2164	5.9691	5.1024
		0.9	3.7174	3.4704	2.6034
	$n = 100$	0.95	4.8604	4.6134	3.7464
		0.99	5.1854	4.9384	4.0714
		0.9	3.6274	3.3804	2.5134
	$n = 150$	0.95	3.9024	3.6554	2.7884
		0.99	4.4604	4.2134	2.9464

Table 2: Table 2: MSE values when $\tau = 1.5$

			ML	IGRR	RIGRE
		ρ			
$p = 4$	$n = 50$	0.90	5.1011	4.8541	3.9873
		0.95	5.7291	5.4822	4.6151
		0.99	6.1271	5.8801	5.0131
	$n = 100$	0.90	3.4721	3.2251	2.3581
		0.95	4.5471	4.3001	3.4331
		0.99	4.7391	4.4922	3.6251
	$n = 150$	0.90	3.3151	3.0681	2.2011
		0.95	3.5251	3.2781	2.4111
		0.99	4.2801	4.0331	3.1661
$p = 7$	$n = 50$	0.90	5.2061	4.9592	4.0921
		0.95	5.8251	5.5781	4.7111
		0.99	6.2401	5.9931	5.1261
	$n = 100$	0.90	3.7411	3.4941	2.6271
		0.95	4.8841	4.6371	3.7701
		0.99	5.2091	4.9621	4.0951
	$n = 150$	0.90	3.6511	3.4041	2.5371
		0.95	3.9261	3.6791	2.8121
		0.99	4.4841	4.2371	3.3701

Table 3: Table 3: MSE values when $\tau = 3$

		ρ	ML	IGRR	RIGRE
$p = 4$	$n = 50$	0.90	5.299	5.052	4.185
		0.95	5.927	5.68	4.813
		0.99	6.325	6.078	5.211
	$n = 100$	0.90	3.67	3.423	2.556
		0.95	4.745	4.498	3.631
		0.99	4.937	4.69	3.823
	$n = 150$	0.90	3.513	3.266	2.399
		0.95	3.723	3.476	2.609
		0.99	4.478	4.231	3.364
$p = 7$	$n = 50$	0.90	5.404	5.157	4.29
		0.95	6.023	5.776	4.909
		0.99	6.438	6.191	5.324
	$n = 100$	0.90	3.939	3.692	2.825
		0.95	5.082	4.835	3.968
		0.99	5.407	5.16	4.293
	$n = 150$	0.90	3.849	3.602	2.735
		0.95	4.124	3.877	3.01
		0.99	4.682	4.435	3.568

5 Real 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 (Algamal et al., 2015). 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 (Algamal and

Lee, 2017b). 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

$$\hat{y}_{IC_{50}} = \exp(\sum_{j=1}^{15} x_j \hat{\beta}_j). \tag{19}$$

Second, to check whether there is a relationship among the explanatory variables or not. 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 $X^T \hat{W} X$ 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 CN $= \sqrt{\lambda_{\max}/\lambda_{\min}}$ of the data is 40383.035 indicating that the severe multicollinearity issue is exist.

The estimated IGR coefficients, standard errors which are computed by using bootstrap with 500 replications, and MSE values for the ML, IGRR and RIGRE estimators are listed in Table 4. According to Table 4, it is clearly seen that the RIGRE estimator shrinkages the value of the estimated coefficients efficiently. Additionally, in terms of the calculated standard errors, the RIGRE and IGRR show substantial decreasing comparing with ML.

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

	ML	IGRR	RIGRE
$\hat{\beta}_1$	-2.286	-1.8741	-1.259
	(0.147)	(0.007)	(0.127)
$\hat{\beta}_2$	0.441	0.510	0.031
	(0.151)	(0.001)	(0.132)
$\hat{\beta}_3$	0.575	0.416	0.224
	(0.175)	(0.008)	(0.103)
$\hat{\beta}_4$	-3.476	-2.034	-0.131
	(0.313)	(0.008)	(0.229)
$\hat{\beta}_5$	-2.432	-2.12	-1.007
	(0.160)	(0.004)	(0.132)
$\hat{\beta}_6$	5.121	0.004	0.173
	(0.387)	(0.003)	(0.225)
$\hat{\beta}_7$	6.211	2.308	2.418
	(0.317)	(0.003)	(0.225)
$\hat{\beta}_8$	3.206	2.66	1.974
	(0.388)	(0.003)	(0.225)
$\hat{\beta}_9$	-0.365	-0.225	-0.207
	(0.326)	(0.081)	(0.227)
$\hat{\beta}_{10}$	2.006	1.0687	0.887
	(0.225)	(0.103)	(0.230)
$\hat{\beta}_{11}$	-3.681	-2.067	-1.687
	(0.115)	(0.103)	(0.025)
$\hat{\beta}_{12}$	2.147	1.687	1.874
	(0.357)	(0.302)	(0.215)
$\hat{\beta}_{13}$	-0.664	-0.508	-0.484
	(0.314)	(0.266)	(0.230)
$\hat{\beta}_{14}$	0.121	0.114	0.103
	(0.387)	(0.003)	(0.225)
$\hat{\beta}_{15}$	5.661	4.528	3.607
	(0.311)	(0.153)	(0.025)
MSE	4.509	3.177	2.639

6 Conclusion

In this paper, a restricted ridge estimator of IGR was proposed. This proposed estimator allows us to handle multicollinearity. According to Monte Carlo simulation studies, the restricted estimator has better performance than maximum likelihood estimator and Inverse Gaussian ridge estimator, in terms of MSE. Additionally, a real data application is also considered to illustrate benefits of using the new estimator in the context of IGR. The superiority of the new estimator based on the resulting MSE was observed and it was shown that the results are consistent with Monte Carlo simulation results.

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