A Liu estimator in inverse Gaussian regression model with application in chemometrics

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Abstract

The presence of multicollinearity among the explanatory variables has undesirable effects on the maximum likelihood estimator (MLE). Liu estimator (LE) is a wide used estimator in overcoming this issue. The LE enjoys the advantage that its mean squared error (MSE) is less than MLE. The inverse Gaussian regression (IGR) model is a well-known model in application when the response variable positively skewed. The purpose of this paper is to derive the LE of the IGR under multicollinearity problem. In addition, the performance of this estimator is investigated under numerous methods for estimating the Liu parameter. Monte Carlo simulation results indicate that the suggested estimator performs better than the MLE estimator in terms of MSE. Furthermore, a real chemometrics dataset application is utilized and the results demonstrate the excellent performance of the suggested estimator when the multicollinearity is present in IGR model.

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

1. Introduction

In many applications of regression model, there exists a natural correlation among the explanatory variables. When the correlations are high, it causes unstable estimation of the regression parameters leading to difficulties in interpreting the estimates of the regression coefficients [Månsson and Shukur (2011)]. When the problem of multicollinearity exists, it is difficult to estimate the individual effects of each explanatory variable in the regression model. Moreover, the sampling variance of the regression coefficients will inflate affecting both inference and prediction. There are numerous methods that have been proposed to solve multicollinearity problem in the literature. In linear regression model, Hoerl and Kennard (1970) proposed a ridge estimator to deal with multicollinearity. This proposed estimator is biased, but it gives smaller mean squared error (MSE) than ordinary least squares (OLS) estimator. Nevertheless, ridge estimator has drawbacks that the estimated parameters are nonlinear functions of the ridge parameter and that the small ridge parameter chosen in the process may not be large enough to overcome multicollinearity [Asar and Genç (2015), Algamal (2018, (2018, (2018), Algamal and Alanaz (2018), Algamal and Asar (2018), Algamal (2018), Yahya Algamal (2018), Rashad and Algamal (2019), Shamany et al. (2019), Al-Taweel et al. (2020), Algamal (2020), Alkhateeb and Algamal (2020), Abdulazeez and Algamal (2021), Algamal and Abonazel (2021), Alobaidi et al. (2021), Lukman, Algamal, et al. (2021), Lukman, Dawoud, et al. (2021), Mohammed and Algamal (2021), Rashad et al. (2021)].

Liu (1993) proposed an estimator, which is called Liu estimator, combining the Stein estimator with the ridge estimator. Comparing with ridge estimator, the Liu estimator is a linear function of the shrinkage parameter, therefore it is easy to choose the shrinkage parameter than to choose ridge parameter.

The inverse Gaussian regression (IGR) has been widely used in industrial engineering, life testing, reliability, marketing, and social sciences [Folks and Davis (1981), Bhattacharyya and Fries (1982), Fries and Bhattacharyya (1986), Ducharme (2001), 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 (2011)]. When the response variable is extremely skewness, the IGR is preferable than gamma regression model [De Jong and Heller (2008)].

The purpose of this paper is to drive the Liu estimator for the inverse Gaussian regression model when the multicollinearity issue exists. Furthermore, several methods of estimating the Liu shrinkage parameter are explored and investigated. This paper is organized as follows. The model specification and estimation is given in Section 2. Section 3 contains the theoretical aspects of the Liu inverse Gaussian estimator. In Sections 4 and 5, the simulation and the real application results are presented. Finally, Section 6 covers the conclusion of this paper.

2. Model Specification and estimation

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

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

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

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

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

where $C(y,\tau)=-(1/2)\ln(2\pi y^3)-(1/2)\ln(\tau)$ 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 $\eta_i=\mathbf{x}_i^T\boldsymbol{\beta}$, where $\mathbf{x}_i$ is the ith row of $\mathbf{X}$ and $\boldsymbol{\beta}$ is a $(p+1)\times 1$ vector of unknown regression coefficients. Because η_i depends on $\boldsymbol{\beta}$ and the mean of the response variable is a function of η_i, then $E(y_i)=\mu_i=g^{-1}(\eta_i)=g^{-1}(\mathbf{x}_i^T\boldsymbol{\beta})$. Related to the IGR, the $\mu=1/\sqrt{\mathbf{x}_i^T\boldsymbol{\beta}}$. Another possible link function for the IGR is log link function, $\mu=\exp(\mathbf{x}_i^T\boldsymbol{\beta})$.

The 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

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

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

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

Unfortunately, the first derivative cannot be solved analytically because Eq. (4) is nonlinear in $\boldsymbol{\beta}$. 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

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

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

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

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

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

and the MSE equals

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

where λ_j is the eigenvalue of the $\mathbf{B}$ matrix and the dispersion parameter, τ, is estimated by [Uusipaikka (2009)]

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

3. Inverse Gaussian Liu estimator

The maximum likelihood estimator (MLE) often yields unstable estimation results in the multicollinearity situation [Asar and Genç (2015)]. This is because the MSE (Eq. (8)) becomes inflated when the eigenvalues of the highly correlated explanatory be small [Mackinnon and

Puterman (1989), Segerstedt (1992), Liu and Piantadosi (2016)]. To settle on the problem, ridge estimator (RE) is proposed [Hoerl and Kennard (1970)] by imposing a positive amount to the diagonal of $\mathbf{X}^T\mathbf{X}$ in case of linear regression model. However, RE has drawbacks that the estimated parameters are nonlinear functions of the ridge parameter and that the small ridge parameter chosen in the process may not be large enough to overcome multicollinearity (Asar & Genç, 2015).

K. Liu (1993) proposed an estimator, which is called Liu estimator, combining the Stein estimator with the ridge estimator. Comparing with ridge estimator, the Liu estimator is a linear function of the shrinkage parameter, therefore it is easy to choose the shrinkage parameter than to choose ridge parameter.

Consequently, the Liu estimator in IGR, the inverse Gaussian Liu estimator (IGLE), is defined as

$$\hat{\boldsymbol{\beta}}_{IGLE} = (\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+\mathbf{I})^{-1}(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}+d\,\mathbf{I})\hat{\boldsymbol{\beta}}_{IGR} \tag{10}$$

where d is a shrinkage parameter, $0<d<1$. For $d=1$, $\hat{\boldsymbol{\beta}}_{IGLE}=\hat{\boldsymbol{\beta}}_{IGR}$ and for $0<d<1$, $\left\|\hat{\boldsymbol{\beta}}_{IGLE}\right\| < \left\|\hat{\boldsymbol{\beta}}_{IGR}\right\|$.

3.1. The MSE properties

The Liu estimator is a shrinkage estimator and it is assumed to perform better than the MLE estimator in the presence of multicollinearity [Månsson (2013)]. The matrix mean squared error (MMSE) of $\hat{\boldsymbol{\beta}}_{IGLE}$ is defined as follows:

$$\begin{aligned}\text{MMSE}(\hat{\boldsymbol{\beta}}_{IGLE}) &= E(\hat{\boldsymbol{\beta}}_{IGLE}-\boldsymbol{\beta})(\hat{\boldsymbol{\beta}}_{IGLE}-\boldsymbol{\beta})^T \\ &= Var(\hat{\boldsymbol{\beta}}_{IGLE}) + \left[bias(\hat{\boldsymbol{\beta}}_{IGLE})\right]\left[bias(\hat{\boldsymbol{\beta}}_{IGLE})\right]^T,\end{aligned} \tag{11}$$

where

$$Var(\hat{\boldsymbol{\beta}}_{IGLE}) = \tau\, \mathbf{V}_d\, \mathbf{B}^{-1} \mathbf{V}_d^T \,, \tag{12}$$

and

$$bias(\hat{\boldsymbol{\beta}}_{IGLE}) = \left[\mathbf{V}_d - \mathbf{I}\right] \boldsymbol{\beta}, \tag{13}$$

where $\mathbf{B} = \mathbf{X}^T \hat{\mathbf{W}} \mathbf{X}$ and $\mathbf{V}_d = (\mathbf{B}+\mathbf{I})^{-1}(\mathbf{B}+d\,\mathbf{I})$. The MSE of the estimator $\hat{\boldsymbol{\beta}}_{IGLE}$ can be defined as

$$\begin{aligned} \mathrm{MSE}(\hat{\boldsymbol{\beta}}_{IGRE}) &= tr\left[\tau\, \mathbf{V}_d \mathbf{B}^{-1} \mathbf{V}_d^T\right] + \left[\mathbf{V}_d - \mathbf{I}\right] \boldsymbol{\beta}\boldsymbol{\beta}^T \left[\mathbf{V}_d - \mathbf{I}\right]^T \\ &= \tau \sum_{j=1}^{p} \frac{(\lambda_j + d)^2}{\lambda_j (\lambda_j + 1)^2} + (d-1)^2 \sum_{j=1}^{p} \frac{\alpha_j^2}{(\lambda_j + 1)^2} \,, \end{aligned} \tag{14}$$

where α_j is defined as the j[th] element of $\gamma \hat{\boldsymbol{\beta}}_{IGR}$ and γ is the eigenvector of the $\mathbf{X}^T \hat{\mathbf{W}} \mathbf{X}$.

3.2. Comparison of $\hat{\boldsymbol{\beta}}_{IGLE}$ with $\hat{\boldsymbol{\beta}}_{IGR}$

For two given estimators $\hat{\boldsymbol{\beta}}_1$ and $\hat{\boldsymbol{\beta}}_2$ of $\boldsymbol{\beta}$, the estimator $\hat{\boldsymbol{\beta}}_2$ is said to be superior to $\hat{\boldsymbol{\beta}}_1$ under the MMSE criterion if and only if $\mathrm{MMSE}(\hat{\boldsymbol{\beta}}_1) - \mathrm{MMSE}(\hat{\boldsymbol{\beta}}_2) \geq 0$.

Lemma 1: [Rao and Toutenburg (1995)] Let $\mathbf{A}_1$ and $\mathbf{A}_2$ are $n \times n$ matrices such that $\mathbf{A}_1 > 0$ and $\mathbf{A}_2 \geq 0$, then $\mathbf{A}_1 + \mathbf{A}_2 > 0$.

Lemma 2: [Rao et al. (2008)] Let $\mathbf{A}_1$ and $\mathbf{A}_2$ are $n \times n$ matrices such that $\mathbf{A}_1 > 0$ and $\mathbf{A}_2 \geq 0$, then $\mathbf{A}_1 > \mathbf{A}_2$ if and only if $\lambda_{\max}(\mathbf{A}_2 \mathbf{A}_1^{-1}) < 1$.

Theorem 1: $\mathrm{MMSE}(\hat{\boldsymbol{\beta}}_{IGR}) - \mathrm{MMSE}(\hat{\boldsymbol{\beta}}_{IGLE}) > 0$ if and only if

$$\lambda_{\max}\left(\left[\left[\tau\, \mathbf{V}_d \mathbf{B}^{-1} \mathbf{V}_d^T\right] + \left[\mathbf{V}_d - \mathbf{I}\right] \boldsymbol{\beta}\boldsymbol{\beta}^T \left[\mathbf{V}_d - \mathbf{I}\right]^T\right]\left[\tau \mathbf{B}^{-1}\right]^{-1}\right) < 1.$$

Proof From Eqs. (8), (12), and (13), the matrix difference is

$$\begin{aligned}\Delta &= \mathrm{MMSE}(\hat{\boldsymbol{\beta}}_{IGR}) - \mathrm{MMSE}(\hat{\boldsymbol{\beta}}_{IGLE}) \\ &= \tau\mathbf{B}^{-1} - \left\{\left[\tau\,\mathbf{V}_d\mathbf{B}^{-1}\mathbf{V}_d^T\right] + \left[\mathbf{V}_d - \mathbf{I}\right]\boldsymbol{\beta}\boldsymbol{\beta}^T\left[\mathbf{V}_d - \mathbf{I}\right]^T\right\} \\ &= \mathbf{Q}_1 - \mathbf{Q}_2,\end{aligned}$$

where $\mathbf{Q}_1 = \tau\mathbf{B}^{-1}$ and $\mathbf{Q}_2 = \left[\tau\,\mathbf{V}_d\mathbf{B}^{-1}\mathbf{V}_d^T\right] + \left[\mathbf{V}_d - \mathbf{I}\right]\boldsymbol{\beta}\boldsymbol{\beta}^T\left[\mathbf{V}_d - \mathbf{I}\right]^T$. It is obvious that $\mathbf{B}^{-1}$ and $\mathbf{V}_d\mathbf{B}^{-1}\mathbf{V}_d^T$ are positive definite matrices. Further, $\left[\mathbf{V}_d - \mathbf{I}\right]\boldsymbol{\beta}\boldsymbol{\beta}^T\left[\mathbf{V}_d - \mathbf{I}\right]^T$ is a non-negative definite matrix. By Lemma 1, it is clear that $\mathbf{Q}_2$ is a positive definite matrix. Moreover, by Lemma 2, $\lambda_{\max}(\mathbf{Q}_2\mathbf{Q}_1^{-1}) < 1$ the $\mathbf{Q}_1 - \mathbf{Q}_2$ is a positive definite matrix, where $\lambda_{\max}(\mathbf{Q}_2\mathbf{Q}_1^{-1})$ is the largest eigenvalue of $\mathbf{Q}_2\mathbf{Q}_1^{-1}$. Consequently, the proof is completed.

3.3. Estimating d

To find the optimal value of d, the first derivative of Eq. (14) with respect to d is defined as

$$\frac{d\,\mathrm{MSE}(\hat{\boldsymbol{\beta}}_{IGLE})}{dd} = 2\hat{\tau}\sum_{j=1}^{p}\frac{\lambda_j + d}{\lambda_j(\lambda_j+1)^2} + 2(d-1)\sum_{j=1}^{p}\frac{\alpha_j^2}{(\lambda_j+1)^2}. \tag{15}$$

By setting the resulting $d\,\mathrm{MSE}(\hat{\boldsymbol{\beta}}_{IGLE})/dd$ to zero and solving for d, the optimal value is obtained as [Månsson (2013)]

$$d_{optimal} = \frac{\tau(\alpha^2-1)}{(1/\lambda)+\alpha^2}. \tag{16}$$

According to Eq. (16), when $\alpha_j^2 < 1$ the $d_{optimal}$ becomes negative and becomes positive when $\alpha_j^2 > 1$. To guarantee that $d_{optimal}$ be between 0 and 1, the following methods have been proposed to estimate the $d_{optimal}$ [Mansson et al. (2012), Månsson (2013)]:

$d_1 = \max\left(0, \frac{\hat{\tau}(\hat{\alpha}_{\max}^2 - 1)}{(1/\hat{\lambda}_{\max}) + \hat{\alpha}_{\max}^2}\right)$, $d_2 = \max\left(0, median\left(\frac{\hat{\tau}(\hat{\alpha}_j^2 - 1)}{(1/\hat{\lambda}_j) + \hat{\alpha}_j^2}\right)\right)$,

$d_3 = \max\left(0, \frac{\hat{\tau}}{p}\sum_{j=1}^{p}\frac{(\hat{\alpha}_j^2 - 1)}{(1/\hat{\lambda}_j) + \hat{\alpha}_j^2}\right)$, $d_4 = \max\left(0, \max\left(\frac{\hat{\tau}(\hat{\alpha}_j^2 - 1)}{(1/\hat{\lambda}_j) + \hat{\alpha}_j^2}\right)\right)$, and

$d_5 = \max\left(0, \min\left(\frac{\hat{\tau}(\hat{\alpha}_j^2 - 1)}{(1/\hat{\lambda}_j) + \hat{\alpha}_j^2}\right)\right)$, where $\hat{\alpha}$ is defined as the j$^{\text{th}}$ element of $\gamma\hat{\boldsymbol{\beta}}_{IGR}$ and γ is the eigenvector of the $\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}$ matrix, $\hat{\alpha}_{\max}$ is the maximum value of $\hat{\alpha}$.

4. Simulation study

In this section, a Monte Carlo simulation experiment is used to examine the performance of IGLE with different degrees of multicollinearity for both the canonical link function and the log link function.

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

$$x_{ij} = (1-\rho^2)^{1/2} w_{ij} + \rho w_{ip}, \quad i = 1, 2, ..., n, \quad j = 1, 2, ..., p, \tag{17}$$

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 three type of the link function, μ_i , the canonical and log link functions are investigated.

4.1.1 Canonical link function

The canonical link function is defined as

$$\mu_i = \frac{1}{\sqrt{\mathbf{x}_i^T \boldsymbol{\beta}}}, \quad i = 1, 2, ..., n, \tag{18}$$

To grantee that $\mathbf{x}_i^T \boldsymbol{\beta}$ values are positive, the regression parameters are assumed to be equal to 1 because the results can be generalized to any value for the parameters [Hefnawy and Farag (2013)]. Additionally, the w_{ij} in Eq. (17) are generated from uniform distribution (0,1).

4.1.2 Log link function

The log link function is defined as

$$\mu_i = \exp(\mathbf{x}_i^T \boldsymbol{\beta}), \quad i = 1, 2, ..., n. \tag{19}$$

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 $\boldsymbol{\beta}^T \boldsymbol{\beta} = 1$ [Kibria (2003)]. In addition, the w_{ij} in Eq. (17) are generated from normal distribution (0,1).

The estimated average MSE is calculated as

$$\text{MSE}(\hat{\boldsymbol{\beta}}_{\text{IGLE}}) = \frac{1}{R} \sum_{i=1}^{R} (\hat{\boldsymbol{\beta}}_{\text{IGLE}} - \boldsymbol{\beta})^T (\hat{\boldsymbol{\beta}}_{\text{IGLE}} - \boldsymbol{\beta}), \tag{20}$$

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. (20) for all the different selection methods of d and the combination of n, τ, p, and ρ, are respectively summarized in Tables 1 – 6. Several observations can be obtained as follows:

1- Generally, the MSE of IGLE is smaller than that of MLE.

2- Clearly, in terms of MSE, d_5 improved the performance of the inverse Gaussian Liu regression compared to MLE in all the cases. Furthermore, d_5 is the best estimation method for d among the others in all of the cases. On the other hand, d_1 and d_2 estimators attained poor results comparing with the other used estimators in all cases.

3- In terms of ρ values, there is increasing in the MSE values when the correlation degree increases regardless the value of n, τ and p.

4- Regarding the number of explanatory variables, it is easily seen that there is a negative impact on MSE, where there are increasing in their values when the p increasing.

5- With respect to the value of n, the MSE values decrease when n increases, regardless the value of ρ, τ and p.

6- For fixed n, p and degree of multicollinearity ρ, as the τ increases the MSE of all methods decreases.

7- All the selection methods of d are superior to the ML estimator in terms of MSE.

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

n	τ	ρ	MLE	d1	d2	d3	d4	**d5**
100	0.5	0.90	11.3231	7.6451	8.6501	1.3911	1.0591	**0.9429**
		0.95	14.5411	12.7411	13.0061	1.8051	1.1981	**1.1569**
		0.99	17.4381	13.2031	13.4411	2.1501	1.7911	**1.7019**
	1.5	0.90	10.3381	5.7821	5.1991	1.2701	1.0451	**0.9219**
		0.95	13.2011	8.5751	7.1691	1.4551	1.1321	**0.9969**
		0.99	16.9501	9.2051	8.5291	1.7731	1.4191	**1.3249**
	3	0.9	6.9011	4.5091	3.7291	1.1911	1.0091	**0.8909**
		0.95	11.0021	6.7721	5.4181	1.2191	1.1121	**0.9879**
		0.99	14.4401	7.8841	6.4681	1.3711	1.3201	**1.1909**
150	0.5	0.9	11.1061	7.4281	8.4331	1.1741	0.8421	**0.7259**
		0.95	14.3241	12.5241	12.7891	1.5881	0.9811	**0.9399**
		0.99	17.2211	12.9861	13.2241	1.9331	1.5741	**1.4849**
	1.5	0.9	10.1521	5.5961	5.0131	1.0841	0.8381	**0.7359**
		0.95	13.0151	8.3891	6.9811	1.2691	0.9461	**0.8109**
		0.99	16.7641	9.0191	8.3431	1.5881	1.2311	**1.1409**

	3	0.90	10.1301	5.5741	4.9911	1.0621	0.8161	**0.7139**
		0.95	12.9931	8.3711	6.9591	1.2481	0.9241	**0.7919**
		0.99	16.7421	8.9991	8.3211	1.5651	1.2091	**1.1169**

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

n	τ	ρ	MLE	d1	d2	d3	d4	**d5**
100	0.5	0.90	11.6801	8.0021	9.0071	1.7481	1.4161	**1.2999**
		0.95	14.8981	13.0981	13.3631	2.1621	1.5551	**1.5139**
		0.99	17.7951	13.5601	13.7981	2.5091	2.1481	**2.0609**
	1.5	0.90	10.6951	6.1391	5.5561	1.6491	1.4021	**1.3009**
		0.95	13.5581	8.9321	7.5241	1.8121	1.4891	**1.3539**
		0.99	17.3091	9.5621	8.8861	2.1301	1.7741	**1.6819**
	3	0.9	7.2581	4.8661	4.0861	1.5481	1.3661	**1.2459**
		0.95	11.3591	7.1291	5.7751	1.5761	1.4691	**1.3449**
		0.99	14.7991	8.2411	6.8241	1.7281	1.6771	**1.5479**
150	0.5	0.9	11.4631	7.7851	8.7901	1.5311	1.1991	**1.0829**
		0.95	14.6811	12.8811	13.1461	1.9451	1.3381	**1.2969**
		0.99	17.5781	13.3431	13.5811	2.2901	1.9311	**1.8419**
	1.5	0.9	10.5091	5.9531	5.3701	1.4411	1.1951	**1.0929**
		0.95	13.3721	8.7461	7.3381	1.6261	1.3031	**1.1679**
		0.99	17.1211	9.3761	8.7001	1.9441	1.5881	**1.5959**
	3	0.90	10.4871	5.9311	5.3481	1.4191	1.1731	**1.0709**
		0.95	13.3501	8.7241	7.3161	1.6041	1.2811	**1.1459**
		0.99	17.0991	9.3541	8.6781	1.9221	1.5661	**1.4739**

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

n	τ	ρ	MLE	d1	d2	d3	d4	**d5**
100	0.5	0.90	11.8341	8.1561	9.1611	1.9021	1.5701	**1.4539**
		0.95	15.0521	13.2521	13.5191	2.3161	1.7091	**1.6679**
		0.99	17.9491	13.7141	13.9521	2.6611	2.3021	**2.2129**
	1.5	0.90	10.8491	6.2931	5.7101	1.7811	1.5561	**1.4329**
		0.95	13.7121	9.0861	7.6781	1.9661	1.6431	**1.5079**
		0.99	17.4611	9.7161	9.0401	2.2841	1.9281	**1.1359**
	3	0.9	7.4121	5.0201	4.2401	1.7021	1.5201	**1.3999**
		0.95	11.5131	7.2831	5.9291	1.7301	1.6231	**1.5009**
		0.99	14.9511	8.3951	6.9781	1.8821	1.8311	**1.6019**
150	0.5	0.9	11.6191	7.9391	8.9441	1.6851	1.3531	**1.2369**
		0.95	14.8351	13.0351	13.3001	2.0991	1.4921	**1.4509**
		0.99	17.7321	13.4991	13.7351	2.4441	2.0851	**1.9959**
	1.5	0.9	10.6631	6.1091	5.5241	1.5951	1.3491	**1.2469**
		0.95	13.5261	8.9001	7.4921	1.7801	1.4591	**1.3219**
		0.99	17.2751	9.5301	8.8541	2.0981	1.7421	**1.5499**

	3	0.90	10.6411	6.0851	5.5021	1.5731	1.3491	**1.2249**
		0.95	13.5041	8.8781	7.4701	1.7581	1.4351	**1.2999**
		0.99	17.2531	9.5081	8.8321	2.0761	1.7201	**1.5279**

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

n	τ	ρ	MLE	d1	d2	d3	d4	d5
100	0.5	0.90	11.8361	8.1581	9.1631	1.9041	1.5721	1.4559
		0.95	15.0541	13.2541	13.5191	2.3181	1.7111	1.6699
		0.99	17.9511	13.7161	13.9541	2.6631	2.3041	2.2149
	1.5	0.90	10.8511	6.2951	5.7121	1.7831	1.5581	1.4349
		0.95	13.7141	9.0881	7.6821	1.9681	1.6451	1.5099
		0.99	17.4631	9.7181	9.0421	2.2861	1.9321	1.7379
	3	0.9	7.4141	5.0221	4.2421	1.7041	1.5221	1.4039
		0.95	11.5151	7.2851	5.9311	1.7321	1.6251	1.5009
		0.99	14.9531	8.3971	6.9811	1.8841	1.8331	1.6039
150	0.5	0.9	11.6191	7.9411	8.9461	1.6871	1.3551	1.2389
		0.95	14.8371	13.0371	13.3021	2.1011	1.4941	1.4529
		0.99	17.7341	13.4991	13.7371	2.4461	2.0881	1.9979
	1.5	0.9	10.6651	6.1091	5.5261	1.5971	1.3511	1.2489
		0.95	13.5281	8.9021	7.4941	1.7821	1.4591	1.3239
		0.99	17.2771	9.5321	8.8561	2.1011	1.7441	1.6539
	3	0.90	10.6431	6.0871	5.5041	1.5751	1.3291	1.2269
		0.95	13.5061	8.8841	7.4721	1.7611	1.4381	1.3049
		0.99	17.2551	9.5121	8.8341	2.0781	1.7221	1.6299

Table 5: Averaged MSE values for the log link function when $p = 8$

n	τ	ρ	MLE	d1	d2	d3	d4	**d5**
100	0.5	0.90	12.1931	8.5151	9.5201	2.2611	1.9291	**1.8129**
		0.95	15.4111	13.6111	13.8761	2.6751	2.0681	**2.0269**
		0.99	18.3081	14.0731	14.3111	3.0221	2.6611	**2.5739**
	1.5	0.90	11.2081	6.6521	6.0691	2.1621	1.9151	**1.8139**
		0.95	14.0711	9.4451	8.0381	2.3251	2.0021	**1.8669**
		0.99	17.8221	10.0751	9.3991	2.6431	2.2881	**2.1949**
	3	0.9	7.7711	5.3791	4.5991	2.0611	1.8791	**1.7609**
		0.95	11.8721	7.6421	6.2881	2.0891	1.9821	**1.8579**
		0.99	15.3121	8.7541	7.3391	2.2411	2.1901	**2.0609**
150	0.5	0.9	11.9761	8.2981	9.3031	2.0441	1.7121	**1.5959**
		0.95	15.1941	13.3941	13.6591	2.4581	1.8511	**1.8099**
		0.99	18.0911	13.8561	14.0941	2.8031	2.4441	**2.3549**
	1.5	0.9	11.0221	6.4661	5.8831	1.9541	1.7081	**1.6059**
		0.95	13.8851	9.2591	7.8511	2.1391	1.8161	**1.6809**
		0.99	17.6341	9.8891	9.2131	2.4571	2.1011	**2.0109**
	3	0.90	11.0001	6.4441	5.8611	1.9321	1.6861	**1.5839**
		0.95	13.8631	9.2391	7.8291	2.1191	1.7941	**1.6609**
		0.99	17.6121	9.8691	9.1911	2.4351	2.0791	**2.0169**

Table 6: Averaged MSE values for the log link function when $p = 12$

n	τ	ρ	MLE	d1	d2	d3	d4	**d5**
100	0.5	0.90	12.3491	8.6691	9.6741	2.4151	2.0831	**1.9669**
		0.95	15.5651	13.7651	14.0321	2.8291	2.2221	**2.1809**
		0.99	18.4621	14.2481	14.4651	3.1741	2.8151	**2.7259**
	1.5	0.90	11.3621	6.8061	6.2231	2.2941	2.0691	**1.9459**
		0.95	14.2251	9.5991	8.1911	2.4791	2.1561	**2.0209**
		0.99	17.9741	10.2291	9.5531	2.7981	2.4411	**2.6509**
	3	0.9	7.9251	5.5331	4.7531	2.2151	2.0331	**1.9129**
		0.95	12.0261	7.7961	6.4421	2.2431	2.1361	**2.0139**
		0.99	15.4641	8.9081	7.4911	2.3951	2.3441	**2.2149**
150	0.5	0.9	12.1321	8.4521	9.4591	2.1981	1.8661	**1.7499**
		0.95	15.3481	13.5481	13.8131	2.6121	2.0051	**1.9639**
		0.99	18.2451	14.0121	14.2481	2.9591	2.5981	**2.5109**
	1.5	0.9	11.1761	6.6221	6.0391	2.1081	1.8621	**1.7599**
		0.95	14.0391	9.4131	8.0051	2.2931	1.9721	**1.8349**
		0.99	17.7881	10.0431	9.3691	2.6111	2.2551	**2.1629**
	3	0.90	11.1541	6.5981	6.0151	2.0861	1.8621	**1.7379**
		0.95	14.0191	9.3911	7.9831	2.2711	1.9481	**1.8129**
		0.99	17.7661	10.0211	9.3451	2.5891	2.2331	**2.1409**

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 [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 (2017)]. Consequently, using of regression model is one of the most important tools for constructing the QSAR model. A description of the used explanatory variables is provided in Table 7. All the variables are numerical.

Table 7: Description of the used explanatory variables

Variable name's	description
MW	molecular weight
IC3	Information Content index (neighborhood symmetry of 3-order)
SpMaxA_D	normalized leading eigenvalue from topological distance matrix
ATS8v	Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume
MATS7v	Moran autocorrelation of lag 7 weighted by van der Waals volume
MATS2s	Moran autocorrelation of lag 2 weighted by I-state
GATS4p	Geary autocorrelation of lag 4 weighted by polarizability
SpMax8_Bh(p)	largest eigenvalue n. 8 of Burden matrix weighted by polarizability
SpMax3_Bh(s)	largest eigenvalue n. 3 of Burden matrix weighted by I-state
P_VSA_e_3	P_VSA-like on Sanderson electronegativity, bin 3
TDB08m	3D Topological distance based descriptors - lag 8 weighted by mass
RDF100m	Radial Distribution Function - 100 / weighted by mass
Mor21v	signal 21 / weighted by van der Waals volume
Mor21e	signal 21 / weighted by Sanderson electronegativity
HATS6v	leverage-weighted autocorrelation of lag 6 / weighted by van der Waals volume

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

$$\hat{y}_{IC_{50}} = \exp\left(\sum_{j=1}^{15} \mathbf{x}_j \hat{\beta}_j\right). \tag{21}$$

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 $\mathrm{CN} = \sqrt{\lambda_{\max} / \lambda_{\min}}$ of the data is 40383.035 indicating that the severe multicollinearity issue is exist.

The estimated inverse Gaussian regression coefficients and the estimated theoretical MSE values for the MLE, and the used estimators are listed in Table 8. According to Table 8, it is clearly seen that the inverse Gaussian Liu estimators have MSE values less than the MSE of the MLE, in general. Moreover, the MSE of the d_5 estimator is the lowest among all estimators. Specifically, it can be seen that the MSE of d_5 estimator was about 44.24%, 38.56%, 33.68%, and 13.06% lower than that of d_1, d_2, d_3, and d_4 estimator, respectively. These findings come in agreement with the results of simulation.

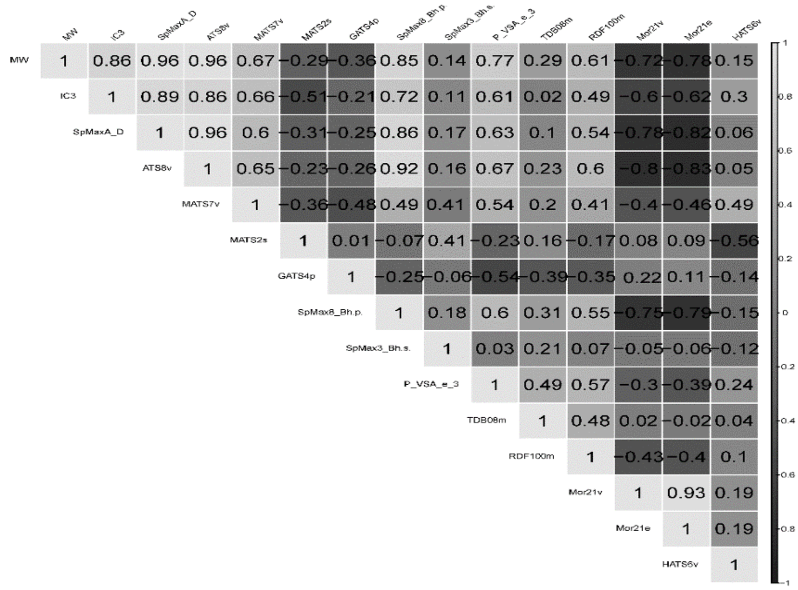

Figure 1. Correlation matrix among the 15 explanatory variables of the real data.

Table 8: The estimated coefficients and MSE values of the used estimators

	Methods					
$\hat{\beta}$	MLE	d1	d2	d3	d4	**d5**
MW	1.002	0.741	0.835	0.734	0.8	**0.617**
IC3	1.237	0.977	1.07	0.969	1.035	**0.852**
SpMaxA_D	-1.102	-1.363	-1.269	-0.902	-1.304	**-1.019**
ATS8v	-1.379	-1.64	-1.546	-1.179	-1.581	**-1.296**
MATS7v	-1.219	-1.48	-1.386	-1.019	-1.421	**-1.136**
MATS2s	-1.215	-1.476	-1.382	-1.015	-1.417	**-1.132**
GATS4p	-1.237	-1.498	-1.405	-1.037	-1.439	**-1.154**
SpMax8_Bh.p.	2.506	2.245	2.339	2.707	2.304	**2.589**
SpMax3_Bh.s.	2.069	1.808	1.902	2.269	1.867	**2.152**
P_VSA_e_3	2.001	1.739	1.833	2.2	1.798	**2.083**
TDB08m	-2.103	-2.365	-2.27	-1.903	-2.305	**-2.02**
RDF100m	1.571	1.309	1.403	1.77	1.368	**1.653**
Mor21v	-2.434	-2.695	-2.601	-2.235	-2.636	**-2.351**
Mor21e	-2.352	-2.613	-2.519	-2.152	-2.554	**-2.269**
HATS6v	2.211	1.95	2.044	2.411	2.009	**2.294**
MSE	3.295	2.041	1.855	1.716	1.309	**1.138**

6. Conclusions

In this paper, a Liu estimator was proposed in inverse Gaussian regression model. Further, numerous selection methods of the Liu parameter are explored and investigated. According to Monte Carlo simulation studies, the IGLE is always superior to the MLE in terms of MSE for all the used d estimation methods. Further, it has been seen that d_5 can bring significant improvement relative to others estimation methods of d , in terms of MSE in all the cases. In conclusion, based on the results of the simulation and real data application, the use of IGLE is recommended when multicollinearity is present in the inverse Gaussian regression model.

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