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A new two-parameter estimator for the inverse Gaussian regression model with application in chemometrics

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The presence of multicollinearity among the explanatory variables has undesirable effects on the maximum likelihood estimator (MLE). The inverse Gaussian regression (IGR) model is a well-known model in application when the response variable positively skewed. To address the problem of multicollinearity, a two-parameter estimator is proposed (TPE). The TPE enjoys the advantage that its mean squared error (MSE) is less than MLE. The TPE is derived and the performance of this estimator is investigated under several conditions. Monte Carlo simulation results indicate that the proposed 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,two-parameter estimator,inverse Gaussian regression model, 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,

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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).

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 idea of the two-parameter estimator, which is a merging between the ridge estimator and Liu estimator, was proposed by Özkale and Kaciranlar (2007); Yang and Chang (2010).

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, 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 two-parameter estimator for the inverse Gaussian regression model when the multicollinearity issue exists. Furthermore, several methods of estimating the shrinkage parameter are explored and investigated. This paper is organized as follows. The model specification is given in Section 2. Section 3 contains the theoretical aspects of the proposed 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

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

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

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 $p \times 1$ vector of unknown regression coefficients. Because $\eta_i$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, $\mu = \exp(x_i^T\beta)$.

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

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

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 nonlinear 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 β^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 $B=(X^T\hat{W}X)$, $\hat{W}=\mathbf{diag}(\hat{\mu}_i^3)$, $\hat{m}$ 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

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

where λ_j is the eigenvalue of the B matrix and the dispersion parameter, τ, is estimated by Uusipaikka (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 The proposed estimator

The ridge estimator (RE) for the inverse Gaussian regression model can be defined as follows (Algamal, 2018):

$$\hat{\beta}_{RE} = (S+kI_P)^{-1}\ S\hat{\beta}_{IGR}, \qquad k>0 \tag{10}$$

where $S = X^T\hat{W}X$and $I_p$is the $p\times p$identity matrix. The Liu estimator can be defined for the IGR model as

$$\hat{\beta}_{LE} = (S+I_p)^{-1}\ (S+dI_p)\ \hat{\beta}_{IGR}, \tag{11}$$

where $0<d<1$.

Inspired by the work of Asar and Genç (2018); Kandemir Çetinkaya and Kaçıranlar (2019); Özkale and Kaciranlar (2007); Yang and Chang (2010), the proposed two-parameter estimator of the inverse Gaussian regression model (TPE) is defined as:

$$\hat{\beta}_{TPE} = (S+kI_p)^{-1}(S+kdI_p)\,\hat{\beta}_{IGR} \tag{12}$$

The MMSE and the MSE being the trace of MMSE of the proposed estimators are derived so that $MSE(\beta_{TPE}) < MSE(\beta_{MLE})$. The MMSE and MSE of an estimator $\tilde{\beta}$ are, respectively, define by

$$\begin{aligned}MMSE\left(\tilde{\beta}\right) &= E\left[\left(\tilde{\beta}-\beta\right)\left(\tilde{\beta}-\beta\right)^T\right]\\ &= var\left(\tilde{\beta}\right)+bias\left(\tilde{\beta}\right)\ bias\left(\tilde{\beta}\right)^T\ ,\end{aligned} \tag{13}$$

$$MSE\left(\tilde{\beta}\right) = tr\left(MMSE\left(\tilde{\beta}\right)\right) = E\left[\left(\tilde{\beta}-\beta\right)^T\left(\tilde{\beta}-\beta\right)\right] \tag{14}$$

where tr is the trace operator, $var\left(\tilde{\beta}\right)$is the variance covariance matrix of the estimator, and $bias\left(\tilde{\beta}\right)$ is the bias of the estimator $\tilde{\beta}$ such that $bias\left(\tilde{\beta}\right)= E\left(\tilde{\beta}\right)-\beta$. If $\tilde{\beta}_1$ and

$\tilde{\beta}_2$ are two estimators of the coefficient vector, then $\tilde{\beta}_2$ is superior to $\tilde{\beta}_1$ if and only if $MMSE\left(\tilde{\beta}_1\right) - MMSE\left(\tilde{\beta}_2\right) \geq 0$.

In order to obtain the MMSE and MSE of the estimators, we use the spectral decomposition of the matrix S such that $S = \varphi \wedge \varphi'$, where φ is the matrix whose columns are the eigenvectors of S and $\wedge$ is a diagonal matrix containing the eigenvalues of S such that $\wedge = diag(\lambda_1, \lambda_2, ..., \lambda_{p+1})$. To obtain the MMSE and MSE of TPE, we firstly compute the variance and bias of the estimator, respectively, as follows:

$$var(\hat{\beta}_{TPE}) = \tau \left[\varphi \wedge_k^{-1} \wedge_{kd} \wedge^{-1} \wedge_{kd} \wedge_k^{-1} \varphi^T\right] \tag{15}$$

$$bias(\hat{\beta}_{TPE}) = k(d-1)\varphi \wedge_k^{-1} \alpha \tag{16}$$

where $\alpha = \varphi^T \beta,\ \wedge_k = diag(\lambda_1 + k, \lambda_2 + k, ..., \lambda_{p+1} + k)$, and
$\wedge_{kd} = diag(\lambda_1 + kd, \lambda_2 + kd, ..., \lambda_{p+1} + kd)$. Thus, the MMSE and MSE of TPE are computed by

$$MMSE(\hat{\beta}_{TPE}) = \tau \left[\varphi \wedge_k^{-1} \wedge_{kd} \wedge^{-1} \wedge_{kd} \wedge_k^{-1} \varphi^T\right] + bb^T \tag{17}$$

$$MSE(\hat{\beta}_{TPE}) = \sum_{j=1}^{p+1} \left(\tau \frac{(\lambda_j + kd)^2}{\lambda_j(\lambda_j + k)^2} + \frac{k^2(d-1)^2\alpha_j^2}{(\lambda_j + k)^2}\right) \tag{18}$$

where $\alpha_j$is the jth element of α.
Theorem 1

Let $k > 0$,$0 < d < 1$ and $b = bias(\underset{TPE}{\overset{\wedge}{\beta}})$Then $MMSE(\hat{\beta}_{IGR}) - MMSE(\hat{\beta}_{TPE}) > 0$ if $b'\left[\Lambda^{-1} - \Lambda_k^{-1}\Lambda_{kd}\Lambda_k^{-1}\right]^{-1} b < 1$
Proof
The difference between MMSE function of MLE and TPE is obtained by

$$\begin{aligned} MMSE(\hat{\beta}_{IGR}) - MMSE(\hat{\beta}_{TPE}) &= \tau Q(\Lambda^{-1} - \Lambda_k^{-1}\Lambda_{kd}\Lambda_k^{-1}\Lambda_{kd}\Lambda_k^{-1})Q' - bb' \\ &= \tau Q diag\left\{\tfrac{1}{\lambda_j} - \tfrac{(\lambda_j+kd)^2}{\lambda_j(\lambda_j+k)^2}\right\}_{j+1}^{p+1} - bb \end{aligned} \tag{19}$$

The matrix $\Lambda_k^{-1}\Lambda_{kd}\Lambda_k^{-1}\Lambda_{kd}\Lambda_k^{-1}$ is p.d. if $(\lambda_j + k)^2 - (\lambda_j + kd) > 0$ which is equivalent to$[(\lambda_j + k) - (\lambda_j + kd)]\left[(\lambda_j + k) + (\lambda_j + kd)\right] > 0$ simplifying the last inequality, one gets $k(\textbf{??})(2\lambda_j - k(1 + d)) > 0$. Thus if $0 < d < 1$, then the proof is done by Theorem 1.

There is no definite rule of estimating the shrinkage parameter k which is a positive constant and d which is between zero and one. To estimate the parameters, we start by taking derivative of Eq. (18) with respect to$k$and equating the resulting function to zero and solving for the parameter k, we obtain the following individual parameter

$$k_j = \frac{\tau\lambda_j}{\lambda_j \overset{\wedge}{\alpha_j^2}(1-d) - d} \tag{20}$$

Since each individual parameter should be positive, we obtain the following upper bound for the parameter d so that $k_j > 0$:

$$d < \min \left(\frac{\tau \lambda_j \hat{\alpha}_j^2}{1 + \lambda_j \hat{\alpha}_j^2} \right)_{j=1}^{p+1} \tag{21}$$

Therefore, we propose to estimate the parameter d by

$$d + \frac{1}{2} \min \left(\frac{\tau \lambda_j \hat{\alpha}_j^2}{1 + \lambda_j \hat{\alpha}_j^2} \right)_{j=1}^{p+1} \tag{22}$$

As in Kibria (2003), the following method was proposed to estimate the k value as

$$k = median \quad \left(\frac{\tau \lambda_j}{\lambda_j \hat{\alpha}_j^2 (1-d) - d} \right)_{j=1}^{p+1} \tag{23}$$

4 Simulation study

In this section, a Monte Carlo simulation experiment is used to examine the performance of TPE in the IGR model with different degrees of multicollinearity for both the canonical link function and the log link function. 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 $\tau \in \{0.5, 3.5\}$. The explanatory variables $x_i^T = (x_{i1}, x_{i2}, ..., x_{in})$ have been generated from the following formula

$$x_{ij} = (1 - \rho^2)^{1l2} w_{ij} + \rho w_{ip}, \quad i = 1, 2, ..., n, \quad j = 1, 2, ..., p, \tag{24}$$

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: 3 and 10, 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. The canonical link function is defined as

$$\mu_i = \frac{1}{\sqrt{x_i^T \beta}}, \quad i = 1, 2, ..., n, \tag{25}$$

To grantee that $x_i^T \beta$ 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. (24) are generated from uniform distribution. In addition, the log link function is defined as

$$\mu_i = \exp(x_i^T \beta), \quad i = 1, 2, ..., n. \tag{26}$$

Here, the vector β is chosen as the normalized eigenvector corresponding to the largest eigenvalue of the X^TWX matrix subject to $\beta^T\beta = 1$ (Kibria, 2003). In addition, the w_{ij}in Eq. (24) are generated from normal distribution $[0, 1]$.

The estimated average MSE is calculated as

$$MSE(\hat{\beta}) = \frac{1}{R}\sum_{i=1}^{R}(\hat{\beta} - \beta)^T(\hat{\beta} - \beta), \qquad (27)$$

where R equals 1000 corresponding to the number of replicates used in our simulation. All the calculations are computed by R program. The average estimated MSE of Eq. (27) and bias for all the combination of n, τ, p, and ρ, are respectively summarized in Tables 1 and 2. The best value of the averaged bias and MSE is highlighted in bold. As Table 1 shows, the proposed method, TPE, gives low bias comparing with RE. This finding indicates that the proposed estimator is significantly decreasing the bias. Meanwhile, TPE estimator performs well not only in terms of bias, but also in terms of MSE (Table 2). It is noted from Table 2 that TPE ranks first with respect to MSE. In the second rank, RE estimator performs better than IGR estimator. Additionally, IGR estimator has the worst performance among RE and TPE 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 $\rho, \tau$and p. Clearly, in terms of the dispersion parameter τ, both bias and MSE values are decreasing when τ increasing.

Table 1: Averaged bias values for RE and TPE estimators

			$\tau = 0.5$		$\tau = 3.5$	
n	p	ρ	RE	TPE	RE	TPE
100	3	0.90	0.9652	0.8512	0.8449	0.7309
		0.95	0.9956	0.8816	0.8753	0.7613
		0.99	1.0072	0.8932	0.8869	0.7729
	10	0.90	1.0853	0.9713	0.9651	0.8522
		0.95	1.1157	1.0017	0.9954	0.8814
		0.99	1.1273	1.0133	1.0071	0.8934
150	3	0.90	0.7234	0.6094	0.6031	0.4891
		0.95	0.7538	0.6398	0.6335	0.5195
		0.99	0.7654	0.6514	0.6451	0.5311
	10	0.90	0.8435	0.7295	0.7232	0.6092
		0.95	0.8739	0.7599	0.7536	0.6396
		0.99	0.8855	0.7715	0.7652	0.6512

Table 2: Averaged MSE values for IGR, RE, and TPE estimators

			$\tau = 0.5$			$\tau = 3.5$		
n	p	ρ	IGR	RE	TPE	IGR	RE	TPE
100	3	0.90	4.894	4.653	4.2	4.785	4.55	4.097
		0.95	4.938	4.703	4.25	4.834	4.599	4.146
		0.99	5.204	4.969	4.516	5.101	4.866	4.413
	10	0.90	5.008	4.773	4.32	4.905	4.67	4.217
		0.95	5.058	4.823	4.37	4.954	4.719	4.265
		0.99	5.324	5.089	4.636	5.221	4.986	4.533
150	3	0.90	4.646	4.411	3.958	4.543	4.308	3.855
		0.95	4.696	4.461	4.008	4.593	4.357	3.904
		0.99	4.962	4.727	4.274	4.859	4.624	4.171
	10	0.90	4.772	4.531	4.078	4.663	4.428	3.975
		0.95	4.816	4.581	4.128	4.713	4.478	4.025
		0.99	5.082	4.847	4.394	4.979	4.744	4.291

5 Real Data Application

To demonstrate the usefulness of the TPE 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.

To check whether the response variable belongs to the inverse Gaussian distribution, Chi-square test is used. The result of the test equals to 11.0965 with p-value equals to 0.7752. It is indicated form this result that the inverse Gaussian distribution fits very well to this response variable. The estimated dispersion parameter is 0.0412.

Further, to test the existence of multicollinearity after fitting the inverse Gaussian regression model using log link function, the eigenvalues of the matrix $X^T\hat{W}X$ are obtained as 2.45×10^9,2.91×10^6, 2.53×10^5, 1.33×10^4, 2.13×10^3, 1.22×10^3,8.65×10^2, 5.62×10^2, 1.67×10^2, 5.88×10^1, 3.47×10^1, 2.63×10^1, 1.86×10^1, 9.71, and 2.57. The determined condition number $\mathbf{CN} = \sqrt{\lambda_{\max}/\lambda_{\min}}$ of the data is 30875.676 indicating that the severe multicollinearity issue is exist.

The estimated inverse Gaussian regression coefficients and MSE values for the RE and TPE estimators are listed in Table 3. According to Table 3, it is clearly seen that the TPE shrinkages the value of the estimated coefficients efficiently. Additionally, in terms of the MSE, there is an important reduction in favor of the TPE. Specifically, it can be seen that the MSE of the TPE estimator was about 36.45% and 15.82% lower than that of IGR and RE estimators, respectively.

Table 3: The estimated coefficients and MSE values for the three used estimators

	Estimators		
	IGR	RE	TPE
$\hat{\beta}_{\mathbf{1}}$	2.2514	1.9144	1.4021
$\hat{\beta}_{\mathbf{2}}$	1.1202	0.9981	0.7421
$\hat{\beta}_{\mathbf{3}}$	1.3366	1.1141	0.9841
$\hat{\beta}_{\mathbf{4}}$	0.1056	0.1088	0.1024
$\hat{\beta}_{\mathbf{5}}$	-3.9241	-3.4651	-2.3077
$\hat{\beta}_{\mathbf{6}}$	0.5156	0.5251	0.3054
$\hat{\beta}_{\mathbf{7}}$	-1.3581	-1.2584	-1.1661
$\hat{\beta}_{\mathbf{8}}$	5.1056	2.1056	1.1156
$\hat{\beta}_{\mathbf{9}}$	-1.1057	-1.7071	-1.0121
$\hat{\beta}_{\mathbf{10}}$	6.1056	5.1956	3.0256
$\hat{\beta}_{\mathbf{11}}$	-8.1171	-7.7183	-5.5172
$\hat{\beta}_{\mathbf{12}}$	6.3056	5.1006	4.2156
$\hat{\beta}_{\mathbf{13}}$	-3.1821	-2.7493	-1.0716
$\hat{\beta}_{\mathbf{14}}$	1.1156	1.1356	1.1006
$\hat{\beta}_{\mathbf{15}}$	3.6211	1.4475	1.1184
MSE	4.2247	3.5189	1.8875

6 Conclusions

In this paper, a new two-parameter estimator is proposed to overcome the multicollinearity problem in the inverse Gaussian regression model. According to Monte Carlo simulation studies, the proposed estimator has better performance than maximum likelihood estimator and ridge estimator, in terms of bias and MSE. Additionally, a real data application is also considered to illustrate benefits of using the new estimator in the context of inverse Gaussian regression model. 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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