Comparison of the scale parameter estimators for Maxwell distribution using different prior distributions

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Abstract

The Maxwell distribution plays an important role in physics, chemistry and other allied sciences. In this paper used the maximum likelihood estimation and Bayesian using different priors information for estimating the scale parameter of Maxwell distribution of life time are presented. Monte – Carlo simulation is used to compare of these estimators with respect to the Mean Square Error (MSE) ,and the results of comparison showed that for all the varying sample size, the estimators of Bayes method when the prior distribution is inverted gamma is smaller MSE compared to others, and in all cases for both methods the MSE decrease as sample size increases.

Key words : Maxwell distribution , Bayes method, Prior distributions

Introduction

The Maxwell distribution is usually thought of as the distribution for molecular speeds, and it can also refer to the distribution for velocities, momenta, and magnitude of the momenta of the molecules, each of which will have a different probability distribution function.

Maxwell distribution[5] (2008), and Maxwell– Boltzmann[4] (2008) are giving a summary of this applications. In (2005) Bekker and Roux[1], studied empirical Bayes estimation for Maxwell distribution, and we have assumed that complete sample information is available, Sanku Dey[6] (2011) studies on Bayes estimators of the parameter of a Maxwell distribution and obtain associated based on conjugate prior under scale invariant symmetric and a symmetric loss functions.

The object of the present paper is to obtain on maximum likelihood and Bayes estimators of the parameter θ using two prior distributions. And a simulation study has been performed in the last section of this paper to compare between these estimators according to the measure of statistics Mean Square Error (MSE).

Model Description[4],[5]

The Maxwell (or Maxwell – Boltzmann) distribution gives the distribution of speeds of molecules in thermal equilibrium as given by statistical mechanics.

Defining $\theta = \frac{2KT}{m}$, where K is the Maxwell constant, T is temperature, m is the mass of a molecule. The probability density function and the cumulative distribution function of Maxwell distribution over the rang $x \in [0, \infty)$ are given by:

$$f(X\,;\theta) = \frac{4}{\sqrt{\pi}}\ \frac{1}{\theta^{\frac{3}{2}}}\ X^2\ e^{-\frac{X^2}{\theta}}\ ;\ \theta > 0 \qquad \dots\ (1)$$

$$F(X\,;\theta) = \frac{1}{\Gamma\left(\frac{3}{2}\right)}\ \Gamma\left(\frac{X^2}{\theta}, \frac{3}{2}\right) \qquad \dots\ (2)$$

where $\Gamma(x, a) = \int_0^x e^{-w}\, W^{a-1}\, dw,$ is the incomplete gamma function.

It can also be expressed as follows:–

$$F(X\,;\theta) = 2erf\left(\frac{x}{\sqrt{\theta}}\right) - \frac{2}{\sqrt{\pi}}\ \frac{x}{\theta}\ e^{-\frac{X^2}{\theta}}$$

Where $erf(x) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-w2}\, dw$, is the error function.

Properties of Maxwell distribution[5]

1– The nth row moment is :

$$\mu_n' = \frac{2}{\sqrt{\pi}}\ \Gamma\left(\frac{n+3}{2}\right)\ \theta^{\frac{n}{2}}; n > -3$$

So that :

If n=1 , then $\mu_1' = 2\sqrt{\frac{\theta}{\pi}}$

If n=2 , then $\mu_2' = 3\frac{\theta}{2}\ ;\ etc.$

2- Mean = $2\sqrt{\frac{\theta}{\pi}}$

3- Variance = $\frac{\theta}{2\pi}\ (3\pi - 8)$

4- Mode = $\sqrt{\theta}$

5- Median = $\frac{1}{3}$(Mode + 2 Mean)

$= \frac{1}{3}\sqrt{\frac{\theta}{\pi}}\ \left(\sqrt{\pi} + 4\right)$

= 1.0856 $\sqrt{\theta}$

6– R(t)= P$(x > t) = \int_t^{\infty} \frac{4}{\sqrt{\pi}}\ \frac{1}{\theta^{\frac{3}{2}}}\ x^2\ e^{-\frac{x^2}{\theta}}\ dx$

$= \frac{4}{\sqrt{\pi}}\ \frac{1}{\theta^{\frac{3}{2}}}\ J(t, 2, \theta)\ ; t > 0$

Where $J\ (t, k, \theta) = \int_t^{\infty} e^{-\frac{w^2}{\theta}}\ w^k\ dw$, is the Jacobian function

7- $h(t) = \frac{f(t)}{R(t)} = \frac{t^2\ e^{-\frac{t^2}{\theta}}}{J\ (t,2,\theta)}$

Estimation of Parameter

In this section we can used two methods to estimation parameter θ

Maximum likelihood estimation[2]

We introduce the concept of maximum likelihood estimation with Maxwell distribution. Let n items have an independent and identically distributed, then the *likelihood of the sample from Maxwell distribution with parameter* θ *is given by*:

$$L\,(x_i\ ;\theta) = \pi_{i=1}^{n} f(x_i\ ;\ \theta) = \left(\frac{4}{\sqrt{\pi}}\right)^{n} \frac{1}{\theta^{\frac{3n}{2}}}\ (\pi_{i=1}^{n}\ x_i^2\ )\ e^{-\ \frac{\sum_{i=1}^{n} x_i^2}{\theta}} \quad \dots (3)$$

From which we calculate the log−likelihood function:

$$\text{In } L(x_i;\ \theta) = nIn\left(\frac{4}{\sqrt{\pi}}\right) + In\ 1 - \frac{3n}{2}\ In\theta + 2\sum_{i=1}^{n} In\ x_i - \frac{\sum_{i=1}^{n} x_i^2}{\theta} \quad \dots (4)$$

Now, differentiating partially equation(4) with respect to θ:

$$\frac{\partial\ In\ L(x_i\ ;\theta)}{\partial\ \theta} = \frac{-3n}{2\ \theta} + \frac{\sum_{i=1}^{n} x_i^2}{\theta^2} \quad \dots (5)$$

The MLE of θ is the solution of the likelihood equation(5)equal to zero, then the maximum likelihood estimator of θ is:

$$\hat{\theta} = \frac{2}{3n} \sum_{i=1}^{n} x_i^2 \quad \dots (6)$$

Bayes Estimation[6]

Let x_1 , x_2 ,…, x_n be a random sample of size n with probability density function given in equation (1) and likelihood function given in equation(3).

We consider the Bays estimation of the parameter θ under different prior distributions which is mentioned below, here we consider two types of priors:

(a) when the prior distribution of θ can be taken as general uniform distribution with pdf:

$$g_1(\theta) = \frac{(a-1)(\alpha\beta)^{a-1}}{\beta^{a-1} - \alpha^{a-1}} \cdot \frac{1}{\theta^{a}} \quad ; 0 < \alpha \le \theta \le \beta < \infty, a > 0 \quad \dots (7)$$

Then the posterior distribution of θ given the data (x_1,…,x_n) is

$$h(x_1, \dots, x_n\ ;\ \theta) = \frac{\pi_{i=1}^{n} f(x_i\ ;\theta)\ g(\theta)}{\int_0^{\infty} \pi_{i=1}^{n} f(x_i\ ;\theta)\ g(\theta)\ d\theta} \quad \dots (8)$$

substituting the equation(3) and the equation(7)in equation(8) ,we get:

$$h(x_1, \dots, x_n\ ;\ \theta) = \frac{e^{-\frac{\sum_{i=1}^{n} x_i^2}{\theta}}\ \frac{1}{\theta^{\frac{3n}{2}+a}}}{\frac{\Gamma\left(\frac{3n}{2}+a-1\right)}{\left(\sum_{i=1}^{n} x_i^2\right)^{\frac{3n}{2}+a-1}}}$$

by using squared error loss function $\ell(\hat{\theta} - \theta) = (\hat{\theta} - \theta)^2$, the risk function is:

$$R(\hat{\theta} - \theta) = E[\ell(\hat{\theta} - \theta)\,]$$

$$= \int_0^{\infty} \ell\,(\hat{\theta} - \theta) h(x_1, \dots, x_n\ ;\ \theta) d\theta$$

$$= \hat{\theta}^2 - 2\,\hat{\theta} \int_0^{\infty} \theta \,.\, \frac{e^{-\frac{\sum_{i=1}^{n} x_i^2}{\theta}} \frac{1}{\theta^{\frac{3n}{2}+a}}}{\frac{\Gamma\left(\frac{3n}{2}+a-1\right)}{-\left(\sum_{i=1}^{n} x_i^2\right)^{\frac{3n}{2}+a-1}}} \; d\theta + k(\theta)$$

Let $\frac{\partial R\,(\hat{\theta}-\theta)}{\partial \hat{\theta}} = 0\,, then$

$$\hat{\theta} = \int_0^{\infty} \frac{e^{-\frac{\sum_{i=1}^{n} x_i^2}{\theta}} \frac{1}{\theta^{\frac{3n}{2}+a-1}}}{\frac{\Gamma\left(\frac{3n}{2}+a-1\right)}{-\left(\sum_{i=1}^{n} x_i^2\right)^{\frac{3n}{2}+a-1}}} \; d\theta$$

Let $y = \frac{\left(\sum_{i=1}^{n} x_i^2\right)}{\theta}$

Then after substitution we find that :

$$\hat{\theta} = \frac{-\left(\sum_{i=1}^{n} x_i^2\right)^{\frac{3n}{2}+a-1}}{\Gamma\left(\frac{3n}{2}+a-1\right)} \int_0^{\infty} e^{-y} \frac{y^{\frac{3n}{2}+a-1}}{\left(\sum_{i=1}^{n} x_i^2\right)^{\frac{3n}{2}+a-1}} \frac{-\left(\sum_{i=1}^{n} x_i^2\right)}{y^2} \, dy$$

Hence , the Bayes estimator of θ is :

$$\hat{\theta}_1 = \frac{\left(\sum_{i=1}^{n} x_i^2\right)}{\left(\frac{3n}{2}+a-2\right)} \qquad \ldots (9)$$

(b) when the prior distribution of θ can be taken as inverted gamma with pdf:

$$g_2(\theta) = \frac{\alpha^{\beta}}{\Gamma(\beta)} \; \frac{1}{\theta^{\beta+1}} \; e^{-\frac{\alpha}{\theta}} \;\; ; \; \alpha, \beta, \theta > 0 \qquad \ldots (10)$$

Then the posterior distribution of θ given the data (x_1, …,x_n) is:

$$h(x_1, \ldots, x_n \,;\, \theta) = \frac{e^{-\frac{1}{\theta}\left(\sum_{i=1}^{n} x_i^2+\alpha\right)} \frac{1}{\theta^{\frac{3n}{2}+\beta+1}}}{\frac{\Gamma\left(\frac{3n}{2}+\beta\right)}{-\left(\sum_{i=1}^{n} x_i^2+\alpha\right)^{\frac{3n}{2}+\beta}}}$$

The risk function is:

$$R\left(\hat{\theta}-\theta\right) = E\left[\ell\left(\hat{\theta}-\theta\right)\right]$$

$$= \hat{\theta}^2 - 2\hat{\theta} \int_0^{\infty} \theta \,.\, \frac{e^{-\frac{1}{\theta}\left(\sum_{i=1}^{n} x_i^2+\alpha\right)} \frac{1}{\theta^{\frac{3n}{2}+B+1}}}{\frac{\Gamma\left(\frac{3n}{2}+\beta\right)}{-\left(\sum_{i=1}^{n} x_i^2+\alpha\right)^{\frac{3n}{2}+\beta}}}$$

Let $\frac{\partial R\,(\hat{\theta}-\theta)}{\partial \hat{\theta}} = 0$, and Let $y = \frac{\left(\sum_{i=1}^{n} x_i^2\right)}{\theta}$

Then after few steps we get:

$$\hat{\theta} = \frac{-\left(\sum_{i=1}^{n} x_i^2+\alpha\right)^{\frac{3n}{2}+\beta}}{\Gamma\left(\frac{3n}{2}+\beta\right)} \int_0^{\infty} e^{-y} \frac{y^{\frac{3n}{2}+\beta}}{\left(\sum_{i=1}^{n} x_i^2+\alpha\right)^{\frac{3n}{2}+\beta}} \frac{-\left(\sum_{i=1}^{n} x_{i+\alpha}^2\right)}{y^2} \, dy$$

Hence , the Bayes estimator of θ is :

$$\hat{\theta}_2 = \frac{\left(\sum_{i=1}^{n} x_i^2+\alpha\right)}{\left(\frac{3n}{2}+\beta-1\right)} \qquad \ldots (11)$$

Simulation Results

In this section. Monte – Carlo simulation study is performed to compare the methods of estimation by using mean square Error(MSE) where:

$$(\text{MSE})(\theta) = \frac{\sum_{i=1}^{R}(\hat{\theta}_i - \theta_i)^2}{R}$$

The number of replication was used R=1000, and we have chosen n=20,50,100 to represent small moderate and large sample size, with θ=3.0 , 4.5 , α=1.5 , 3.3 and β=2.0 , a=1 , 5

In each row of Tables(1,2) we have three values of estimators that is the Bayes estimator when prior distribution is general uniform distribution and Bayes estimator when prior distribution is inverted gamma and maximum likelihood estimator. The best method is the method that gives the smallest value of (MSE).

We report the results in the following tables:

Table(1): MSE estimated parameters of Maxwell distribution with α=1.5, β=2.0

size	θ	a	$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_{ML}$	MSE_1	MSE_2	MSE_{ML}
20	3.0	1	3.093	2.942	2.989	0.330	0.285	3.290
		5	2.718	2.942	2.989	0.328	0.285	3.290
	4.5	1	4.639	4.388	4.484	0.743	0.646	5.161
		5	4.077	4.388	4.484	0.738	0.646	5.161
50	3.0	1	3.034	2.974	2.994	0.118	0.112	3.108
		5	2.878	2.974	2.994	0.120	0.112	3.108
	4.5	1	4.551	4.451	4.490	0.266	0.252	4.747
		5	4.318	4.451	4.490	0.270	0.252	4.747
100	3.0	1	3.018	2.988	2.998	0.061	0.059	3.057
		5	2.939	2.988	2.998	0.064	0.059	3.057
	4.5	1	4.527	4.477	4.497	0.136	0.133	4.631
		5	4.409	4.477	4.497	0.137	0.133	4.631

Table(2): MSE estimated parameters of Maxwell distribution with α=3.3, β=2.0

size	θ	a	$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_{ML}$	MSE_1	MSE_2	MSE_{ML}
20	3.0	1	3.039	2.999	2.989	0.330	0.281	3.290
		5	2.718	2.999	2.989	0.328	0.281	3.290
	4.5	1	4.639	4.446	4.484	0.743	0.636	5.161
		5	4.077	4.446	4.484	0.738	0.636	5.161
50	3.0	1	3.034	2.998	2.994	0.118	0.111	3.108
		5	2.878	2.998	2.994	0.120	0.111	3.108
	4.5	1	4.551	4.745	4.490	0.266	0.250	4.747
		5	4.318	4.745	4.490	0.270	0.250	4.747
100	3.0	1	3.018	2.999	2.998	0.061	0.058	3.057
		5	2.939	2.999	2.998	0.064	0.058	3.057
	4.5	1	4.527	4.489	4.497	0.136	0.132	4.631
		5	4.409	4.489	4.497	0.137	0.132	4.631

Discussion

When we compared parametric estimators of Maxwell distribution by mean square Error (MSE) we find that the best estimator is Bayes when the prior is inverted gamma, followed Bayes when the prior is general uniform, and when the number of sample size increases the (MSE) decrease in all cases.

We find the values Bayes estimator of θ when the prior distribution is general uniform decrease as value of (a) increases, and when the value of α increases we find that the (MSE) of Bayes estimator when the prior is inverted gamma decrease, also same that to value of β.

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مقارنة مقدرات معلمة القياس لتوزيع ماكسويل

باستخدام توزيعات أولية مختلفة

نادية جعفر العبيدي

الجامعة المستنصرية/ كلية العلوم- قسم الرياضيات

المستخلص

لتوزيع ماكسويل دوراً مهماً في الفيزياء والكيمياء وعلوم أخرى . فقد تم في هذا البحث استخدام تقدير الإمكان الأعظم وتقدير بيز وباستخدام توزيعات أولية مختلفة لتقدير معلمة القياس لهدا التوزيع. فقد تم توظيف أسلوب المحاكاة وبطريقة مونت– كارلو للمقارنة بين هذه المقدرات باستخدام متوسط مربعات الخطأ وان نتائج هذه المقارنة ولحجوم العينة المختلفة وجدت إن مقدر بيز عندما التوزيع الأولي له هو معكوس كاما كان اقل متوسط مربعات الخطأ مقارنة بالمقدرات الأخرى كما وجدنا إلى إن في كل الحالات ولكلا الطريقتين إن متوسط مربعات الخطأ يقل عندما حجوم العينة تزداد