

A Study of Understand the Weighted Maxwell-Boltzmann Distribution

Meenakshi^{1*}, Dr. Sudesh Kumar²

¹ Research Scholar, Sunrise University, Alwar, Rajasthan

² Professor, Sunrise University, Alwar, Rajasthan

Abstract - The Maxwell Distribution is often used in physics, especially statistical mechanics, to describe the speed of a particle in an idealized gas. James Clerk Maxwell, a Scottish physicist, suggested this distribution in 1859. In 1871, a German scientist named Ludwig Boltzmann built on Maxwell's work to explain how energy is distributed among molecules. The speed of a particle travelling through three-dimensional space may be seen as a collection of independent and normally distributed random variables, each with a mean and variance equal to one-third of the rate parameter, which is the focus of the majority of the study. Derivation of weighted Maxwell-Boltzmann distribution, weighted distribution, Maximum likelihood estimation, Structural properties, Estimation of parameters, Maximum likelihood estimation

Keyword - Maxwell, distributed

-----X-----

INTRODUCTION

To characterize the speed of a particle in an idealized gas, the Maxwell Distribution (MD) is frequently used in physics, particularly statistical mechanics. In addition, this distribution may be used to explain the distribution of values. of $\sqrt{e_1 + e_2 + e_3}$ where e_1, e_2 and e_3 are the measurement errors in position coordinates of a particle in a 3-dimensional space. In 1859, Scottish physicist James Clerk Maxwell proposed this distribution. Ludwig Boltzmann, a German physicist, expanded Maxwell's finding in 1871 to describe the distribution of energy among molecules. One way to think about the speed of a particle travelling across three-dimensional space is to think of it as a set of independent and normally distributed random variables, each having a mean and variance equal to one-third of the rate parameter. However, if a particle travels in a two-dimensional space rather than a three-dimensional one, the Rayleigh distribution better describes its speed. A particle's kinetic energy (E), which is inversely proportional to its velocity, may be determined using MD. ($v = x$) by the formula $E = \frac{1}{2}mx^2$, provided the distribution of speed is known. The p.d.f. of MD is given by

$$f(x) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi x^2 \exp\left(-\frac{mx^2}{2kT}\right) \quad (2.1)$$

where m denotes the mass of particle, k the Boltzmann's constant and T thermodynamic temperature.

Re-parameterizing equation (2.1) by $m = kT = \theta$, we have the resulting p.d.f. as given in (2.2).

$$f(x; \theta) = \sqrt{\frac{2}{\pi}} \theta^{3/2} x^2 \exp\left(-\frac{\theta x^2}{2}\right), x \geq 0, \theta > 0 \quad (2.2)$$

MD has several uses in both physics and chemistry. Pressure and diffusion are only two of the many basic phenomena of gases that may be explained using MD. The distribution of velocities, energies, and magnitudes of molecular momenta is commonly referred to as this. When it came to researching randomness in physical and chemical sciences, MD was key. An investigation of its statistical qualities may be done in a variety of different ways in Statistics

Derivation of weighted Maxwell-Boltzmann distribution

Consider the weight functions $w(x) = x^\omega$, where $\omega > 0$ the weight parameter is. Therefore,

$$E[w(x)] = \frac{2^{\frac{\omega}{2}+1} \Gamma((\omega+3)/2)}{\sqrt{\pi \theta^\omega}} \quad (2.3)$$

Now, using the definition of weighted distribution given by (1.53), we get the p.d.f. of weighted

Maxwell-Boltzmann distribution (WMD) and is given by (2.4).

$$f_W(x; \theta, \omega) = \frac{\theta^{(\omega+3)/2} x^{\omega+2} \exp(-\theta x^2/2)}{2^{(\omega+1)/2} \Gamma((\omega+3)/2)}, x > 0, \theta > 0, \omega > 0 \quad (2.4)$$

We use $X \sim WMD(\theta, \omega)$ as the notation for denoting a random variable X following WMD with rate θ and weight parameter ω in the rest of chapter. C.d.f., reliability function and hazard rate of WMD are respectively given by (2.5), (2.6) and (2.7).

$$F_W(x; \theta, \omega) = 1 - \frac{\Gamma((\omega+3)/2, \theta x^2/2)}{\Gamma((\omega+3)/2)} \quad (2.5)$$

$$R_W(x; \theta, \omega) = \frac{\Gamma((\omega+3)/2, \theta x^2/2)}{\Gamma((\omega+3)/2)} \quad (2.6)$$

$$h_W(x; \theta, \omega) = \frac{\theta^{(\omega+3)/2} x^{\omega+2} \exp(-\theta x^2/2)}{2^{(\omega+1)/2} \Gamma((\omega+3)/2, \theta x^2/2)} \quad (2.7)$$

Weighted Distribution

Weighted distribution may be traced back to the work of Fisher (1934), in which it is examined how ascertainment procedures might affect how recorded observations are distributed. Rao (1965) used it to represent statistical data when conventional distributions were determined to be inappropriate for the task. Rao then refined and formalized it in generic terms. Consequently, Fisher (1934) and Rao (1965) are credited with first pondering non-experimental, non-replicated, and non-random observation conditions before introducing the notion of weighted distribution. Observations are only recorded when they are encountered, and this may be shown best via encounter sampling. Conditions where observations are collected with probability proportional to some weight function w may be described more broadly (x). Every observation must be given an equal opportunity to be recorded if we are to get the true distribution of the seen data while researching real world random occurrences. If this does not occur, the recorded data will not have the original distribution. Rao (1965) came up with the idea of weighted distributions as a unifying technique for the issue of model design and statistical inference after researching comparable cases.

Maximum Likelihood Estimation

Let $0 \leq x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(n)} \leq \theta$ be an ordered sample of size n from WTPFD $(\alpha, \theta, \beta, \omega)$. As a result, the logarithmic likelihood function is equal to

$$\log[l(\alpha, \theta, \beta, \omega | \underline{x})] = \sum_{i=1}^n \log((\beta+1)\theta^\alpha - 2\beta x_i^\alpha) + (\alpha + \omega - 1) \sum_{i=1}^n \log x_i + n \log(\alpha + \omega) - n \log(2\alpha - \beta\omega + \omega) - n(2\alpha + \omega) \log \theta + n \log(2\alpha + \omega) \quad (3.28)$$

Differentiating (3.28) w.r.t. θ we get the following gradient:

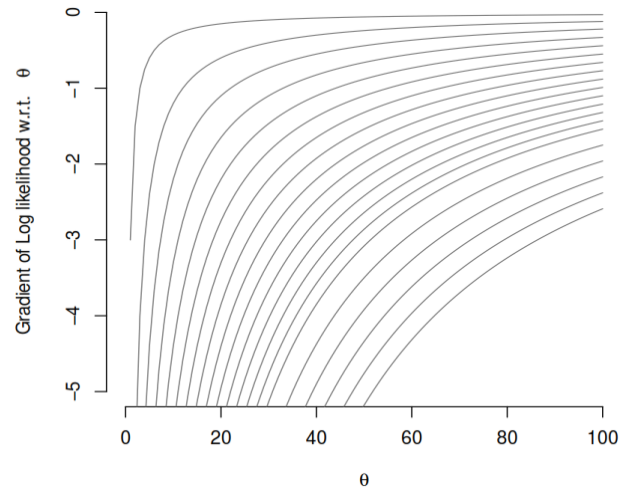


Figure 1: Gradient of log likelihood function w.r.t. θ at different values of α, β and ω .

$$\frac{\partial \log[l(\alpha, \theta, \beta, \omega | \underline{x})]}{\partial \theta} = \sum_{i=1}^n \frac{(\beta+1)\alpha}{(\beta+1)\theta^\alpha - 2\beta x_i^\alpha} - \frac{n(2\alpha + \omega)}{\theta} \quad (3.29)$$

From Figure 3.5, it is clear that the gradient given by (3.29) is negative for all possible values of θ , which implies that (3.28) is a decreasing function w.r.t. θ . Therefore, M.L.E. of θ under the restriction $x_{(n)} \leq \theta$ is given by $\hat{\theta}_{MLE} = x_{(n)}$, whereas, M.L.E.'s for the rest of three parameters ω, α and β are obtained by solving simultaneously the equation (3.30), (3.31) and (3.32). the following system of equations is obtained by equating the gradients of (3.28) w.r.t. ω, α and β to zero.

$$\sum_{i=1}^n \frac{(4\beta x_i^\alpha - (\beta+1)x_{(n)}^\alpha)(\log x_{(n)} - \log x_i)}{(\beta+1)x_{(n)}^\alpha - 2\beta x_i^\alpha} - \frac{2n}{2\alpha - \omega + \omega\beta} + \frac{n(4\alpha + 3\omega)}{(\alpha + \omega)(2\alpha + \omega)} = 0 \quad (3.30)$$

$$\sum_{i=1}^n \frac{2\beta(2\alpha + \omega)x_i^\alpha - (\beta+1)x_{(n)}^\alpha(\alpha + \omega)}{(\beta+1)x_{(n)}^\alpha - 2\beta x_i^\alpha} = 0 \quad (3.31)$$

$$\sum_{i=1}^n \frac{x_{(n)}^\alpha(\alpha + \omega) - (2\alpha - \omega)x_i^\alpha}{(\beta+1)x_{(n)}^\alpha - 2\beta x_i^\alpha} = 0 \quad (3.32)$$

The above system of equations is non-linear. Therefore, to obtain the estimates in closed form is very tedious. Thus, R programming is used to find the required estimates of parameters after the fitting of WTPFD to some considered data sets.

Structural Properties

Here, the structural characteristics of WMD have been described. m.g.f. and characteristic function expressions for r th instant about origin and mean are provided. Also included are expressions for r th

moment about variance and coefficient of variation.

Theorem 2.1. The r^{th} moment about origin of a random variable $X \sim WMD(\theta, \omega)$ is given by

$$\mu_r' = \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma((\omega+3)/2)}, r = 1, 2, 3, \dots \quad (2.8)$$

Proof. By the definition of r^{th} moment about origin we have

$$\begin{aligned} \mu_r' &= E[x^r] \\ \mu_r' &= \int_0^\infty x^r f_W(x; \theta, \omega) dx \\ \mu_r' &= \int_0^\infty x^r \frac{\theta^{(\omega+3)/2} x^{\omega+2}}{2^{(\omega+1)/2} \Gamma((\omega+3)/2)} \exp(-\theta x^2/2) dx \\ \mu_r' &= \frac{\theta^{(\omega+3)/2}}{2^{(\omega+1)/2} \Gamma((\omega+3)/2)} \int_0^\infty \theta^{\omega+r+2} \exp(-\theta x^2/2) dx \\ \mu_r' &= \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma((\omega+3)/2)}, r = 1, 2, 3, \dots \end{aligned}$$

Theorem 2.2. Square of sample coefficient of variation is asymptotically unbiased estimator of the square of population coefficient of variation, i.e., $\lim_{n \rightarrow \infty} E\left[\frac{S_n^2}{\bar{X}_n^2}\right] = \left(\frac{\sigma}{\mu}\right)^2$, where $\bar{X}_n$ and S_n^2 are respectively the mean and variance of a sample.

Proof. Let $X_1, X_2, \dots, X_n$, be a random sample of size n with $\bar{X}_n$ and variance S_n^2 drawn from $WMD(\theta, \omega)$. Therefore,

$$E[\bar{X}_n] = \mu \text{ \& \; } var[\bar{X}_n] = \sigma^2/n \quad (2.17)$$

$$\text{Also, } E[\bar{X}_n^2] = var[\bar{X}_n] + [E(\bar{X}_n)]^2 \quad (2.18)$$

Using (2.17), (2.13) and (2.9) in (2.18), we get

$$E[\bar{X}_n^2] = \frac{2[\Gamma(w_3)\Gamma(w_5) - (1-n)\{\Gamma(w_4)\}^2]}{n\theta[\Gamma(w_3)]^2} \quad (2.19)$$

$$\text{Also, } E[S_n^2] = \sigma^2 = \frac{2[\Gamma(w_3)\Gamma(w_5) - \{\Gamma(w_4)\}^2]}{\theta[\Gamma(w_3)]^2} \quad (2.20)$$

$$\text{Now, } E[S_n^2] = E\left[\frac{S_n^2}{\bar{X}_n^2} \bar{X}_n^2\right] = E\left[\frac{S_n^2}{\bar{X}_n^2}\right] E[\bar{X}_n^2]$$

$$\text{Therefore, } E\left[\frac{S_n^2}{\bar{X}_n^2}\right] = \frac{E[S_n^2]}{E[\bar{X}_n^2]}$$

Using (2.19) and (2.20), we obtain

$$E\left[\frac{S_n^2}{\bar{X}_n^2}\right] = \frac{\Gamma(w_3)\Gamma(w_5) - \{\Gamma(w_4)\}^2}{\frac{1}{n}\Gamma(w_3)\Gamma(w_5) - \left(\frac{1}{n} - 1\right)\{\Gamma(w_4)\}^2}$$

Applying $\lim_{n \rightarrow \infty}$ on both sides, we get

$$\lim_{n \rightarrow \infty} E\left[\frac{S_n^2}{\bar{X}_n^2}\right] = \frac{\Gamma(w_3)\Gamma(w_5) - \{\Gamma(w_4)\}^2}{\{\Gamma(w_4)\}^2}$$

$$\lim_{n \rightarrow \infty} E\left[\frac{S_n^2}{\bar{X}_n^2}\right] = \left[\frac{\sqrt{\Gamma(w_3)\Gamma(w_5) - \{\Gamma(w_4)\}^2}}{\Gamma(w_4)}\right]^2 = (cv)^2$$

Theorem 2.3. The m.g.f. and characteristic function of $X \sim WMD(\theta, \omega)$ are respectively given by (2.21) and (2.22).

$$M_X(t) = \sum_{r=0}^{\infty} \frac{t^r}{r!} \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma(w_3)}, t \in \mathbb{R} \quad (2.21)$$

$$\Phi_X(t) = \sum_{r=0}^{\infty} \frac{(it)^r}{r!} \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma(w_3)} \quad (2.22)$$

Proof. From the definition of m.g.f. we have

$$M_X(t) = E[e^{tX}]$$

$$M_X(t) = \int_0^\infty e^{tx} f_W(x; \theta, \omega) dx$$

$$M_X(t) = \int_0^\infty e^{tx} \frac{\theta^{(\omega+3)/2} x^{\omega+2} \exp(-\theta x^2/2)}{2^{(\omega+1)/2} \Gamma((\omega+3)/2)} dx$$

$$M_X(t) = \sum_{r=0}^{\infty} \frac{t^r}{r!} \frac{\theta^{(\omega+3)/2} \int_0^\infty x^{\omega+r+2} \exp(-\theta x^2/2) dx}{2^{(\omega+1)/2} \Gamma((\omega+3)/2)}$$

$$M_X(t) = \sum_{r=0}^{\infty} \frac{t^r}{r!} \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma(w_3)}$$

Also, we know that $\Phi_X(t) = M_X(it)$. Therefore

$$\Phi_X(t) = \sum_{r=0}^{\infty} \frac{(it)^r}{r!} \left(\frac{2}{\theta}\right)^{r/2} \frac{\Gamma((\omega+r+3)/2)}{\Gamma(w_3)}$$

Estimation of Parameters

Maximal likelihood estimation and the technique of moments are used to estimate WMD parameters in

this section. Fisher information matrix is also obtained and is used to obtain the 100(1- α)% asymptotic confidence interval of M.L.E.'s.

1. Maximum likelihood estimation

Let $x_1, x_2, \dots, x_n$ be a random sample of size n from $WMD(\theta, \omega)$. Therefore, its likelihood function is given by (2.31).

$$l(\Theta|x) = \frac{\theta^{n(\omega+3)/2} \prod_{i=1}^n x_i^{\omega+2}}{2^{n(\omega+1)/2} \Gamma((\omega+3)/2)^n} \exp\left(-\frac{\theta}{2} \sum_{i=1}^n x_i^2\right), \text{ where } \Theta = (\theta, \omega) \quad (2.31)$$

Log likelihood function is given by

$$\begin{aligned} \log[l(\Theta|x)] &= \frac{n(\omega+3)}{2} \log \theta - \frac{n(\omega+1)}{2} \log 2 - n \log \Gamma((\omega+3)/2) \\ &+ (\omega+2) \sum_{i=1}^n \log x_i - \frac{\theta}{2} \sum_{i=1}^n x_i^2 \quad (2.32) \end{aligned}$$

Differentiating log likelihood function partially with respect to θ and ω we get the following two gradients:

$$\frac{\partial \log[l(\Theta|x)]}{\partial \theta} = \frac{n(\omega+3)}{2\theta} - \sum_{i=1}^n \frac{x_i^2}{2} \quad (2.33)$$

$$\frac{\partial \log[l(\Theta|x)]}{\partial \omega} = \frac{n}{2} \left[\log \theta - \log 2 - \Psi\left(\frac{\omega+3}{2}\right) + \frac{2}{n} \sum_{i=1}^n \log x_i \right] \quad (2.34)$$

On equating the derived gradients to zero and reducing them to simplified forms, we obtain following system of two equations:

$$\theta = \frac{n(\omega+3)}{\sum_{i=1}^n x_i^2} \quad (2.35)$$

$$\log \theta - \log 2 - \Psi\left(\frac{\omega+3}{2}\right) + \frac{2}{n} \sum_{i=1}^n \log x_i = 0 \quad (2.36)$$

Substituting (2.35) in (2.36), we get

$$\log\left(\frac{\omega+3}{2}\right) - \Psi\left(\frac{\omega+3}{2}\right) = \log \sum_{i=1}^n x_i^2 - \frac{2}{n} \sum_{i=1}^n \log x_i - \log n \quad (2.37)$$

It is impossible to obtain the M.L.E. of ω by solving (2.37) manually for ω . Therefore, an estimate of ω is computed numerically by using the following code written in Wolfram Mathematica programming language after supplying a guess value say $\omega = \omega_0$ and a data set say x .

```
FindRoot[Log[(\[\Omega]+3)/2]-PolyGamma[0,(\[\Omega]+3)/2]-log[Total[x^2]]
+(2Total[Log[x]]/Length[x]+log[Length[x]])==0,{\[\Omega],Subscript[\[\Omega],0]}]
```

After obtaining the numerical estimate $\hat{\omega}_{mle}$ of say $\hat{\omega}_{mle}$, it is substituted in (2.35) in order to have the corresponding estimate of θ which is given by

$$\hat{\theta}_{mle} = \frac{n(\hat{\omega}_{mle}+3)}{\sum_{i=1}^n x_i^2} \quad (2.38)$$

Now, on using (1.45) given in Section 1.2.10.2.1, we get Fisher information matrix associated with $WMD(\theta, \omega)$ and is given by

$$\begin{aligned} I(\Theta) &= -E \begin{bmatrix} \frac{\partial^2 \log l(\Theta|x)}{\partial \theta^2} & \frac{\partial^2 \log l(\Theta|x)}{\partial \theta \partial \omega} \\ \frac{\partial^2 \log l(\Theta|x)}{\partial \omega \partial \theta} & \frac{\partial^2 \log l(\Theta|x)}{\partial \omega^2} \end{bmatrix} \\ I(\Theta) &= - \begin{bmatrix} \frac{n(\omega+3)}{2\theta^2} & \frac{-n}{2\theta} \\ \frac{-n}{2\theta} & \frac{n}{4} \Psi'\left(\frac{\omega+3}{2}\right) \end{bmatrix} \quad (2.39) \end{aligned}$$

Where $\Psi(x) = \frac{\partial \log \Gamma(x)}{\partial x} = \frac{\Gamma'(x)}{\Gamma(x)}$ is known as digamma or Psi function. Thus, the asymptotic 100 (1- α)% confidence interval for Θ is given by

$$\Theta \in \left[\hat{\Theta}_{mle} \pm z_{\alpha/2} \sqrt{\text{diag}(I^{-1}(\hat{\Theta}_{mle}))} \right]$$

Since, $\Theta = (\theta, \omega)$ therefore we can write

$$\theta \in \left[\hat{\theta}_{mle} \pm z_{\alpha/2} \sqrt{I_{1,1}^{-1} \hat{\theta}_{mle}} \right] \text{ and } \omega \in \left[\hat{\omega}_{mle} \pm z_{\alpha/2} \sqrt{I_{2,2}^{-1} \hat{\omega}_{mle}} \right] \quad (2.40)$$

Therefore, 95% confidence interval for θ and ω is respectively given by

$$\theta \in \left[\hat{\theta}_{mle} \pm 1.96 \sqrt{I_{1,1}^{-1} \hat{\theta}_{mle}} \right] \text{ and } \omega \in \left[\hat{\omega}_{mle} \pm 1.96 \sqrt{I_{2,2}^{-1} \hat{\omega}_{mle}} \right] \quad (2.41)$$

where $z_{0.025} = 1.96$ and $I_{i,j}^{-1}$ represents the element belonging to i^{th} row and j^{th} column of inverse of Fisher information matrix.

CONCLUSION

A wide range of WMD-related characteristics have been investigated and explored in depth. The validity of WMD in statistical modelling is shown using three real-world data sets, including intensity, noise, wear, and a simulated one. By using inverse sampling, a simulated dataset is created. After fitting WMD to the input data, parameter moment estimates, maximum likelihood estimates, Fisher information matrices, and their inverses are calculated. When considering WMD, several statistical metrics such as the accuracies of weapons of mass destruction have been calculated. We already know that the distribution with the lowest AIC, BIC, and AICc is deemed to be the best fit. WMD is shown to have the lowest AIC, BIC, and AICc, followed by ABMD, LBMD,

and MD, correspondingly. It may therefore be stated that WMD is more flexible and the distribution of best fit for the given data sets in contrast to its specific circumstances..

weighted distributions". In: Journal of Nonparametric Statistics 12.6, pp. 861– 878.

REFERENCE

1. TasfaemEyob and Rama Shanker*(2019) "A Two-Parameter Weighted Rama Distribution with Properties and Application" Universal Journal of Mathematics and Applications, 2 (2) (2019) 48-58 Research paper Universal Journal of Mathematics and Applications Journal Homepage: www.dergipark.gov.tr/ujma ISSN 2619-9653 DOI: <http://dx.doi.org/10.32323/ujma.421980>
2. AamirSaghir, G. G. Hamedani (2017) "Weighted Distributions: A Brief Review, Perspective and Characterizations" International Journal of Statistics and Probability; Vol. 6, No. 3; May 2017 ISSN 1927-7032 E-ISSN 1927-7040 Published by Canadian Center of Science and Education
3. Mcdonald, L. L. (2010). "The Need For Teaching Weighted Distribution Theory: Illustrated With Applications In Environmental Statistics". In: Data And Context In Statistics Education Towards An Evidence-Based Society, ICOTS-8.
4. Aijaz Ahmad Dar, A. Ahmed and J. A. Reshi (2018) "Characterization and Estimation of Weighted Maxwell-Boltzmann Distribution" Appl. Math. Inf. Sci. 12, No. 1, 193-202 (2018) 193 Applied Mathematics & Information Sciences An International Journal <http://dx.doi.org/10.18576/amis/120119>
5. Alzaatreh, A., Lee, C., and Famoye, F. (2013). "A new method for generating families of continuous distributions". In: Metron 71.1, pp. 63–79.
6. Alzaatreh, A., Famoye, F., and Lee, C. (2012). "gamma-Pareto distribution and its applications". In: Journal of Modern Applied Statistical Methods 11.1, pp. 78–94.
7. Asgharzadeh, A. et al. (2016). "A new weighted Lindley distribution with application". In: Brazilian Journal of Probability and Statistics 30.1, pp. 1–27.
8. Balakrishnan, N. and Rao, C. R. (1998). Order statistics: applications. Vol. 17. Handbook of statistics. Elsevier. ISBN: 9780444829221.
9. Barmi, H. E. L. and Simonoff, J. S. (2000). "Transformation-based density estimation for

Corresponding Author

Meenakshi*

Research Scholar, Sunrise University, Alwar, Rajasthan