

14.5 ESTIMATORS FOR PARAMETERS OF DROP-SIZE DISTRIBUTION FUNCTIONS: SAMPLING FROM GAMMA DISTRIBUTIONS

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Abstract

This work represents a continuation in the investigation of techniques to estimate the parameters for rain-drop-size-distribution (DSD) functions. Although moment estimators are often used to estimate these parameters, our previous work (Smith and Kliche, 2005; Smith *et al.*, 2005) showed that the method of moments produces biased results that can lead to misleading extrapolations, and that the resulting functions often do not represent correctly the drop populations. These findings triggered our interest in searching for more robust parameter-fitting techniques. In the present paper we describe some findings of our investigation using Maximum Likelihood (ML) estimators as an alternative to the moment method. The ML method is asymptotically unbiased and seeks to find the parameter values of the assumed gamma size distribution function by maximizing the likelihood function. Monte Carlo simulation of raindrop sampling with various sample sizes was considered in this investigation. In cases where the data encompassed the full range of raindrop sizes, the ML method gave better estimates for the parameters of the gamma DSD function than the moment method. We also investigated the case of poor instrument response at small raindrop sizes by removing the drops smaller than a given threshold from all samples. The MLE parameter values are quite sensitive to missing observations of small drops, and the method of moments often gave superior results in estimating the parameters for the gamma function in these situations.

1. INTRODUCTION

Determining the correct drop-size-distribution (DSD) function for raindrop samples is an important issue for radar meteorologists, cloud physicists and cloud modelers. The radar meteorologists are interested in finding the mathematical relationships between radar echoes and the experimental records of rainfall rate. The DSD is of concern for cloud physicists in studies of precipitation physics. Cloud modelers are interested in having a mathematical function that describes the drop size distribution for the purpose of simulating the lifetime of clouds and for a better representation of the cloud microphysics.

The traditional approach with experimental DSD data is the use of moment methods to estimate the parameters for the DSD functions. However, it is well known that such methods are biased; Smith and Kliche (2005) gave examples of this bias for the case of sampling from an exponential raindrop size distribution, and examples for the gamma

DSD are described in Smith *et al.* (2005). The fact that the estimated or “fitted” parameters obtained using the moment method tend to differ significantly from the true values of the parameters of the underlying raindrop population, especially for small sample sizes, represents a serious problem. The biased values can lead to wrong conclusions about the features of the DSD being sampled.

The present work shows some preliminary results of our search for more robust parameter-fitting techniques. To test various techniques and their ability to estimate the parameters of a DSD, we decided to start with a known gamma DSD from which we took numerous random samples. We used computer-simulated gamma populations (with DSD shape parameter $\mu = 2$) and applied a Monte Carlo procedure to repetitively sample rain-drops from any given population. The moment method and the maximum likelihood (ML) method were then used to estimate the parameters of the known DSD. The analysis using the method of moments is described in detail in Smith and Kliche (2005) and Smith *et al.* (2005). The ML method is described in detail in the appendix of the present paper.

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2. SIMULATION OF RAINDROP SAMPLING

To test the effectiveness of the moment method and ML method in recovering the parameters of the known gamma DSD function, we designed a computer-simulated raindrop population. For simplicity, we started with the gamma DSD expressed in terms of N_T , the total drop concentration, μ , the distribution shape parameter, and D_m , the mass-weighted mean drop diameter. Thus the DSD form is

$$n(D; \mu, D_m) = N_T \frac{(\mu + 4)^{\mu+1}}{\Gamma(\mu + 1)} \frac{D^\mu}{D_m^{\mu+1}} \exp[-(\mu + 4)D/D_m] \quad (1)$$

Here D is the drop diameter and D_m is related to the usual gamma size (scale) parameter λ by $D_m = (\mu + 4) / \lambda$.

This form can be treated as the product of the mean number concentration N_T and the gamma probability density function (PDF) of drop size. The unknown parameters in this case are N_T , μ and D_m . For our simulations, we used a new dimensionless variable $y = D/D_m$ which allows us to create simulations which are independent of the specific value of D_m . So, (1) becomes

$$n(y) = N_T \frac{(\mu + 4)^{\mu+1}}{\Gamma(\mu + 1)} y^\mu \exp[-(\mu + 4)y] \quad (2)$$

For the gamma distribution with $\mu = 2$, our simulations started from selecting values of N_T , which we designated to be the mean number of drops in a sample. This assumption is similar to considering a sampling instrument with a sample volume of 1 m^3 , and it also applies for a sample volume of $\alpha \text{ m}^3$ and a mean drop concentration of N_T / α , because it leads to the same mean sample size. Once N_T is selected, we draw from a Poisson distribution with mean value N_T to determine the actual number of drops in a given sample. For each value in the Poisson array, we then extract corresponding values of y from the gamma PDF and establish the sizes of the drops in each sample (in this case y representing the normalized values).

For the simulations the drop sizes are classified in intervals of $\Delta y = 0.02$, starting from $y = 0$ and truncating the gamma PDF at $y = 3.0$. This size channeling method is a common procedure for the drop measuring instruments. The goal is to use

about 1,000,000 drops in the simulations; therefore for $N_T = 10$, a total of 100,000 samples are selected, for $N_T = 50$, the total number of samples is 20,000, and for $N_T = 500$, 2,000 samples are selected.

3. THE BIAS IN MOMENT ESTIMATORS

The general form for the moments of a gamma DSD can be written as

$$M_i = N_T (\mu + 1)(\mu + 2) \dots (\mu + i) \left[\frac{D_m}{(\mu + 4)} \right]^i \quad (3)$$

In these simulations the sample moments are expressed as $M_{iS} = m_i D_m^i$ where the m_i represent the normalized sample moments. This format has the advantage of allowing dimensionless expressions for the parameter estimates of the DSD, where the actual drop size is not included. For this study we usually only considered the case of estimators based on M_2 , M_3 , and M_4 . In this new format, the estimated parameters $\hat{\mu}$, $\hat{\lambda}$, \hat{N}_T , and \hat{D}_m for the gamma DSD are calculated using the following moment expressions:

$$\hat{\mu} = \frac{3m_4 m_2 - 4m_3^2}{m_3^2 - m_4 m_2} \quad (4)$$

$$\frac{\hat{\lambda}}{\lambda} = \frac{(\hat{\mu} + 4)m_3}{(\mu + 4)m_4} \quad (5)$$

$$\hat{N}_T = \left(\frac{m_2^2}{m_4} \right) \frac{\alpha}{(2 - 3\alpha)(1 - 2\alpha)} \quad (6)$$

with
$$\alpha = \frac{m_3^2}{m_4 m_2},$$

and
$$\frac{\hat{D}_m}{D_m} = \frac{m_4}{m_3}. \quad (7)$$

For each sample we calculated the gamma DSD parameters using the moment methods. Figure 1 (taken from Smith *et al.*, 2005) shows the variation of the median value of gamma DSD shape parameter $\hat{\mu}$ with mean sample size N_T . The figure demonstrates that the gamma functions "fitted" this way tend to have overestimated shape parameters. Three sets of sample moments were

used for this illustration; the first set is based on moments M_2, M_3, M_4 , as suggested in Smith (2003), and leads to (4) above. The second set is based on moments M_3, M_4, M_6 , as used by Ulbrich (1983), Kozu and Nakamura (1991), and Tokay and Short (1996), and the third one is based on moments M_2, M_4, M_6 , as suggested by Ulbrich and Atlas (1998). In this simulation the underlying DSD population is a gamma distribution with shape parameter $\mu = 2$; the horizontal dashed line represents the population value. Figure 1 shows that the “fitted” parameters determined by the moment methods are biased, and this bias increases with the order of the moments used in the “fitting” process. Consequently, we use only the M_2, M_3, M_4 set in the work below. As the sample size increases, the bias decreases, which suggests that for samples having hundreds or thousands of drops, the moment estimators’ bias can be small or negligible.

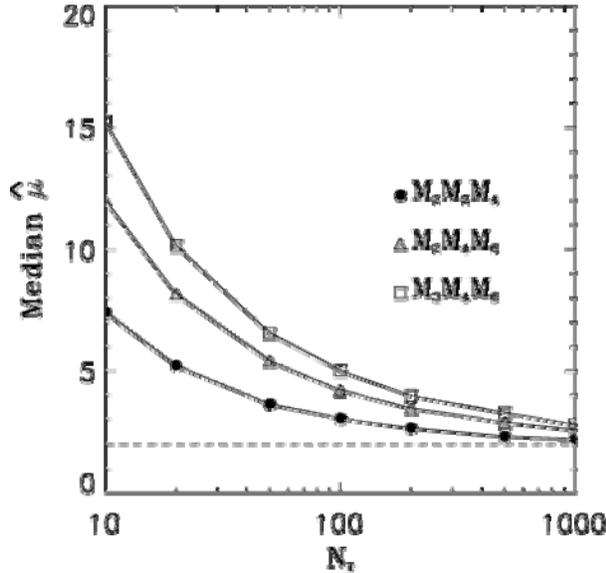


Figure 1: Variation of median value of gamma DSD shape parameter $\hat{\mu}$, as estimated from the indicated sets of three sample moments, with mean sample size N_T . Population DSD: gamma, $\mu = 2$ (horizontal dashed line indicates population value).

4. MAXIMUM LIKELIHOOD APPROACH

Although the moment method has the advantage of simplicity, its bias in estimating DSD parameters, which can lead to erroneous inferences, is of concern. The results of our simulations showed that the bias is strong with small sample sizes. Since the size of *in situ* drop samples is usually

limited, this bias is definitely a problem. Haddad *et al.* (1996, 1997) suggested the use of maximum likelihood methods as an alternative, since such methods should produce minimum-variance estimates. Choi and Wette (1969) showed that the ML methods are not without bias, but the advantage in using them is that the bias should be much smaller than the one produced by the method of moments.

The purpose of this work is to determine whether the ML method gives better estimates than the moment method. If we consider only the gamma PDF part of (1) then the two parameter gamma density function is given by

$$f(D) = \frac{(\mu + 4)^{\mu+1}}{\Gamma(\mu + 1)} \frac{D^\mu}{D_m^{\mu+1}} \exp[-(\mu + 4)D/D_m] \quad (8)$$

The maximum likelihood estimate of the shape parameter μ is obtained by solving the equation:

$$\ln(\hat{\mu}_{MLE} + 1) - \psi(\hat{\mu}_{MLE} + 1) = \ln \left[\frac{\bar{D}}{\left(\prod_{i=1}^n D_i \right)^{1/n}} \right] \quad (9)$$

where n is the number of drops in the sample, ψ the “psi” or “digamma” function defined by

$\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$, and \bar{D} is the arithmetic mean of variable D . By writing $D_i = y_i D_m$, (9) can be rewritten as

$$\ln(\hat{\mu}_{MLE} + 1) - \psi(\hat{\mu}_{MLE} + 1) = \ln \left[\frac{\bar{y}}{\left(\prod_{i=1}^n y_i \right)^{1/n}} \right] \quad (10)$$

where y_i is the corresponding dimensionless size value for each drop in the sample and \bar{y} is the arithmetic mean.

The expression (10) is solved by iteration, following the description in Bowman and Shenton (1988) and the steps described in the Appendix.

5. PRELIMINARY RESULTS

The shape parameter μ for each sample is estimated using both the moment method and the maximum likelihood method. Figure 2 illustrates the sampling distribution obtained for a mean

sample size of $N_T = 50$; the moment-method “fit” is based on the M_2 , M_3 , and M_4 moments. The vertical line represents the true value of the shape parameter ($\mu = 2$) for the underlying population. The mean value for the shape parameter as estimated using the moment method is found to be 3.80, while the mean ML estimate of the shape parameter is 2.18. The cumulative histograms for all 20,000 samples in the case of $N_T = 50$ show clearly that the bias resulting from the method of moments is much stronger than the bias observed using the ML method; the scatter of the moment estimates is also much greater.

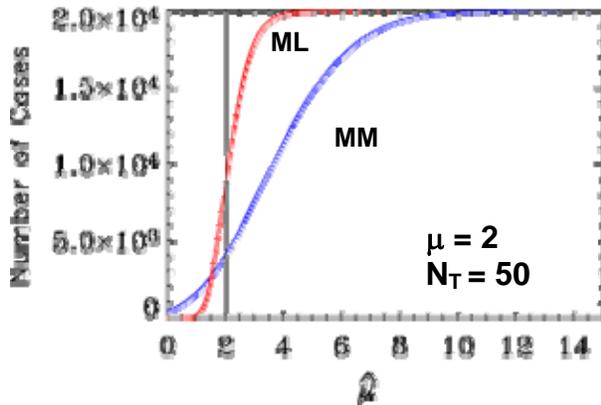


Figure 2: Sampling distributions of values of gamma DSD shape parameter $\hat{\mu}$, as estimated by method of moments (MM) and maximum likelihood (ML). Population DSD: gamma, $\mu = 2$ (vertical line indicates population value). Mean sample size: 50 drops.

Figure 3 shows that for the cases of $N_T = 10$, $N_T = 50$, and $N_T = 500$, the bias in the parameter estimates diminishes with increasing sample size, with both moment and ML estimators. However, ML estimates have much smaller bias than the moment estimates, and the latter become competitive only at large sample sizes.

A different picture emerges when small drops are not included in the sample. Sampling small drops can be a major instrumental problem, so this is a legitimate concern. We decided to investigate the effect of this problem in estimating the parameters of the DSD by withdrawing small drops from the simulated samples. For a start, we chose to eliminate from each generated sample the drops that have $y < 0.2$ (e.g. drops smaller than 0.2 mm with $D_m = 1$ mm or 0.6 mm with $D_m = 3$ mm). For the case of $\mu = 2$, 88% of the drops in the population

have $y \geq 0.2$, so that on average with $N_T = 50$ six of the drops will be removed from each sample by imposing this threshold. This has little effect on the moment estimates, but introduces a significant bias into the MLE results.

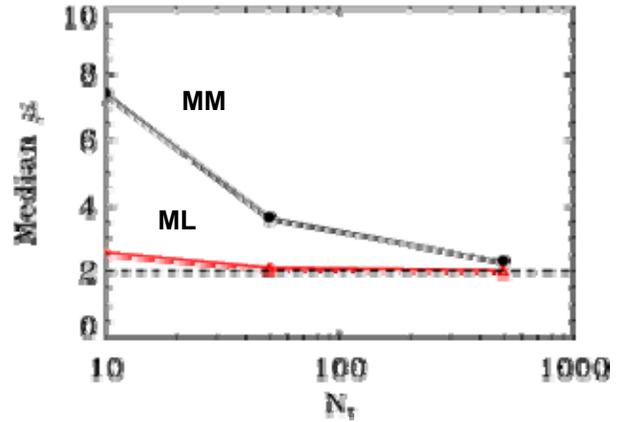


Figure 3: Variation of median value of gamma DSD shape parameter $\hat{\mu}$, as estimated by method of moments (MM) and maximum likelihood (ML), with mean sample size. Population DSD: gamma, $\mu = 2$ (horizontal dashed line indicates population value.)

Figure 4 represents the cumulative histograms now obtained for the estimated gamma DSD shape parameter using the moment method and the ML method. The vertical line again represents the true value of the shape parameter for the underlying population; the mean value calculated using the moment method is 4.10, while the mean

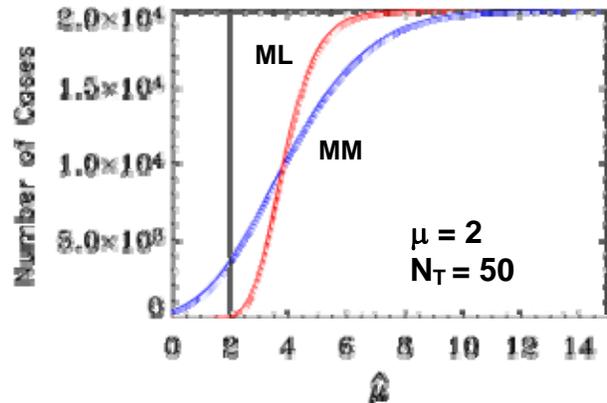


Figure 4: Same as Fig. 2, but with drops smaller than 0.2 D_m (i.e., $y < 0.2$) removed for each sample. The resulting effective mean sample size is about 44 drops.

value calculated with the ML method is now not much different, namely 3.96. Comparison of Figure 4 with Figure 2 clearly shows that the bias in estimating the shape parameter is stronger when a minimum-size threshold is applied to each sample, but the effect on the ML method is much greater.

The same minimum drop-size threshold was applied for various mean sample sizes, $N_T = 10$, $N_T = 50$, and $N_T = 500$. Figure 5 illustrates the trend of the median shape parameter with increasing sample size. The bias in the ML estimates of the shape parameter does decrease with the increase of the sample size, but only slightly. Thus the moment method, although it has much stronger bias at small sample sizes than the ML method, actually becomes superior as the sample size increases into hundreds of drops.

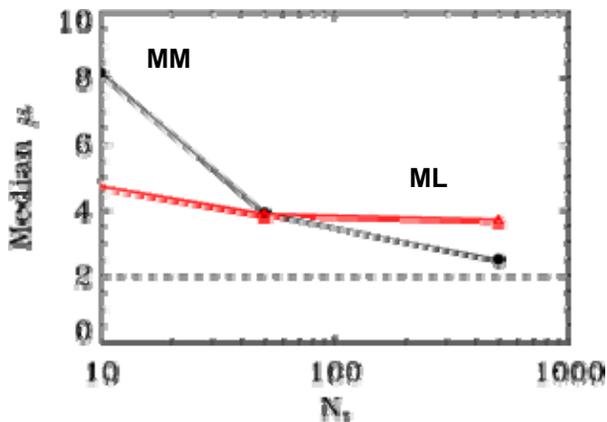


Figure 5: Same as Fig. 3, but with drops smaller than $0.2 D_m$ (i.e., $y < 0.2$) removed from each sample. The resulting effective sample size is about 12% smaller than the value indicated on the abscissa.

6. DISCUSSION AND CONCLUSIONS

Our results confirm the suggestions made in Haddad *et al.* (1996, 1997) that the maximum likelihood methods can produce minimum-variance estimates and demonstrate what statisticians describe as the ML method being asymptotically unbiased. Both techniques tested, the moment method and the ML method, have biases when estimating the gamma DSD parameters. The bias is significantly stronger with the moment method when the entire range of drop sizes is considered, i.e., small drops are included in the samples. Thus in the case of considering the full simulated sam-

ples, the ML method gives better estimates of the gamma parameters.

The computer-simulated gamma DSD populations had the advantage of including drops with all sizes in the interval $0 \leq D \leq 3.0 D_m$. However, in reality the available instruments respond poorly to small raindrop sizes. We explored the possible implication of such a problem by removing from the samples all drops having $D < 0.2 D_m$. Our computer simulation then shows that the ML method would have significant problems if applied to typical measured raindrop data; the bias in estimating the gamma parameters can equal, or even exceed, the bias encountered with the moment method for the same samples. The moment method bias decreases substantially with increased sample size, while that of the ML method diminishes only slightly. Thus in the case of samples on which a size threshold is imposed, the moment method can provide a better approximation of the gamma parameters than the ML method does when large samples are available.

The method of L-moments (Hosking, 1990; Hosking and Wallis, 1997) is currently being investigated for the parameter estimation problem described above. We hope to provide results of this procedure at the conference in July.

Acknowledgment: This material is based in part upon work supported by the National Science Foundation under Grant No. ATM-9907812.

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APPENDIX

Equations for Maximum Likelihood Estimates of Gamma DSD Parameters

This appendix shows how the expressions used to calculate the ML estimates of gamma DSD parameters are developed. The moment-method procedures as used in these simulations are described in detail in Smith *et al.* (2005). At this time we concentrate on showing the steps followed in the Maximum Likelihood method.

The general form of the gamma density function with the two parameters μ (shape) and λ (size) is given by

$$f(D; \mu, \lambda) = \frac{\lambda^{\mu+1}}{\Gamma(\mu+1)} D^\mu e^{-\lambda D}, D > 0 \quad (\text{A1})$$

The parameter λ is related to the mass-weighted mean diameter D_m by $\lambda = (\mu + 4)/D_m$, and equation (8) in the text gives the form of the gamma density function $f(D; \mu, D_m)$.

To implement the ML method mathematically, we note that the likelihood function is given by the product

$$L(D_i; \mu, D_m) = \prod_{i=1}^n f(D_i; \mu, D_m) \quad (\text{A2})$$

using the form in (8), where n is the number of drops in the sample.

The next step is to maximize the likelihood $L(D_i; \mu, D_m)$ over the parameters μ and D_m . However, it is equivalent to maximize the log of the likelihood instead. One may maximize the log of the likelihood function by differentiating with respect to parameter μ and parameter D_m . The resulting equations are given by

$$\ln(\hat{\mu}_{MLE} + 1) - \psi(\hat{\mu}_{MLE} + 1) = \ln \left[\frac{\bar{D}}{\left(\prod_{i=1}^n D_i \right)^{1/n}} \right] \quad (\text{A3})$$

and

$$\left(\hat{D}_m \right)_{MLE} = \frac{(\hat{\mu}_{MLE} + 4)}{(\hat{\mu}_{MLE} + 1)} \bar{D}$$

where ψ is the "psi" (or "digamma") function which is defined by $\psi(x) \equiv \frac{\Gamma'(x)}{\Gamma(x)}$. By writing $D_i = y_i D_m$, (A3) becomes equation (10) as shown in the text. The maximum likelihood estimate for the shape parameter is then obtained by solving (10).

Following Bowman and Shenton (1988) we may solve (10) by iteration using the recursion

$$\alpha_{(l+1)} = \alpha_l \frac{\ln(\alpha_l) - \psi(\alpha_l)}{\ln \left[\bar{y} / \left(\prod_{i=1}^n y_i \right)^{1/n} \right]} \quad (\text{A4})$$

with starting value $\alpha_1 = \frac{1 + \sqrt{1 + 4z/3}}{4z}$

where $z = \left[\bar{y} / \left(\prod_{i=1}^n y_i \right)^{1/n} \right]$

until the sequence converges to α . Then the maximum likelihood value for the shape parameter is given by $\hat{\mu}_{MLE} = \alpha - 1$. Bowman and Shenton (1988) indicated that this iterative procedure “is quite powerful and converges rapidly, on the evidence of computational results”.

To implement the iterative procedure it is necessary to evaluate the “psi” function. We use a method proposed by Moody (1967).

a. Apply the identity

$$\psi(x+1) = \frac{1}{x} + \psi(x) \quad \text{(A5)}$$

(repeatedly if necessary) to reduce the digamma calculation to computing $\psi(x+1)$ with x between 0 and 1.

b. Then use

$$\psi(x+1) \cong \frac{x}{x+1} - \gamma + \frac{x^7}{2} + \sum_{i=1}^6 c_i (x^i - x^7) \quad \text{(A6)}$$

where

i	c_i
1	+0.64493313
2	-0.20203181
3	+0.08209433
4	-0.03591665
5	+0.01485925
6	-0.00472050

and $\gamma = 0.57721566490153286061\dots$ is Euler's constant. This approximation is good to within 1.3×10^{-8} for $0 \leq x \leq 1$.