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RESEARCH ARTICLE

Fiducial confidence limits and prediction limits for a gamma distribution: Censored and uncensored cases

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The problems of finding confidence limits for the mean and an upper percentile, and upper prediction limits for the mean of a future sample from a gamma distribution are considered. Simple methods based on cube root transformation and fiducial approach are proposed for constructing confidence limits and prediction limits when samples are uncensored or censored. Monte Carlo simulation studies indicate that the methods are accurate for estimating the mean and percentile and for predicting the mean of a future sample as long as the percentage of nondetects is not too large. Algorithms for computing confidence limits and prediction limits are provided. Necessary R programs for calculating confidence limits and prediction limits are also provided as a supplementary file. The methods are illustrated using some real uncesnored/censored environmental data sets.

KEYWORDS
coverage probability, detection limits, fiducial approach, fiducial quantity, maximum likelihood estimates, normal-based methods, tolerance limits

1 | INTRODUCTION

Environmental data and pollution data are often right-skewed, and skewed distributions such as the lognormal and gamma are routinely used to model such data. In particular, lognormal distribution is often used to model the pollution data from a workplace, while the gamma model is commonly used to model environmental data. Gibbons and Coleman (2001, pp. 34–47) noted that the use of a gamma distribution is more appropriate than a normal distribution when variability and concentration are related, as in the case of many environmental constituents. In environmental monitoring, upper tolerance limits of a gamma distribution are often constructed based on a background sample (groundwater or air pollution data) and used to determine whether a potential source of contamination (e.g., landfill by a waste management facility or hazardous material storage facility) has adversely impacted the environment (Bhaumik & Gibbons 2006). For other applications in environmental data analysis, see the books by Gibbons and Coleman (2001) and Gibbons, Bhaumik, and Aryal (2009).

Most of the methods available in the literature are for uncensored samples. Even for uncensored samples, the natural maximum likelihood estimates (MLEs) are not in closed-form, and the MLEs can be obtained only numerically. Recently, Krishnamoorthy and Luis (2014) and Krishnamoorthy, Lee and Wang (2015) have proposed likelihood-based approaches for testing the equality of shape parameters, equality of scale parameters, equality of means, and homogeneity of several gamma distributions. For estimating the mean, Krishnamoorthy and Luis (2014) have proposed a parametric bootstrap (PB) approach, and Fraser, Reid and Wong (1997) have proposed a Modified Likelihood Ratio Test (MLRT) that can be inverted to find a CI for the mean. The likelihood methods are accurate even for small samples, but they either require repeated calculations of the MLEs based on simulated samples or numerically complex. Furthermore, a numerical search method is required to find a CI based on the likelihood ratio tests proposed in Fraser *et al.* (1997) and Krishnamoorthy and Luis (2014). For other methods and applications, see Bhaumik and Gibbons (2006), Krishnamoorthy, Mathew and Mukherjee (2008) and Bhaumik, Kapur and Gibbons (2009), and the references therein.

In environmental sampling, concentration levels are often found to be below the detection limit (DL), thus resulting in nondetect values and causing the data to be Type I left-censored. Samples with multiple DLs arise when the measurements are obtained using different devices, each with its own limitation of detecting contaminant levels, or samples are analyzed by different laboratories. A nondetect indicates that the concentration present in the sample is somewhere below the DL. Even though nondetects provide some important information about the analyte concentrations, nondetects make statistical analyses more complicated because of the unknown quantitative values. As noted by Daniel (2015), there is rarely a single optimal mechanism for analyzing data with nondetects. Early recommendations were often to replace the nondetects with *DL*/2, but such substitution methods often lead to inaccurate results. In his editorial note, Ogden (2010) has noted that “the substitution method is so flawed compared to other methods that journals should reject papers that use it.” Inference on a gamma distribution based on samples with nondetects has received only limited attention. Wilks (1990) has derived necessary equations to find the MLEs for a gamma distribution based on a sample with a single DL. Bolstad (1998) has described expectation–maximization (EM) method to compute the MLEs based on sample with single DL. Wilks' results along with the Fisher information matrix can be used to find large sample approximate CIs for the parameters and for the mean. This approach as well as EM algorithm, however, involve repeated calculation of incomplete gamma integrals, which makes the methods to be numerically complex.

The approximate solutions that we propose in this article are obtained by applying the fiducial approach to cube root transformed samples. As the cube root transformed samples are approximately normally distributed, fiducial distributions for the gamma parameters can be obtained from those of normal parameters. The idea of fiducial probability and fiducial inference was introduced by Fisher (1930, 1935). Zabell (1992) has noted some criticisms concerning the interpretation of fiducial distribution. However, Efron (1998) has concluded in section 8 of his paper that “maybe Fishers biggest blunder will become a big hit in the 21st century!” Fiducial approach is a useful tool to find solutions to many complex problems with satisfactory frequentist properties. In fact, fiducial inference in many situations are now well accepted. For example, Clopper and Pearson (1934) fiducial limits for a binomial proportion and Garwoods (1936) fiducial limits for a Poisson mean are now commonly referred to as the exact (in the frequentist sense) confidence intervals. Furthermore, the exact conditional CI for the ratio of two Poisson means by Chapman (1952), and the exact CI for the correlation coefficient of a bivariate normal distribution (see Anderson, 1984, section 4.2) are also fiducial intervals. For other situations where fiducial inference led to exact CIs, see Dawid and Stone (1982).

In the sequel, we first consider the uncensored case and provide approximate solutions to the problems of (a) constructing confidence limits (CLs) for the parameters and the mean of a gamma distribution, (b) upper confidence limit (UCL) for an upper percentile, and (c) for constructing prediction limits for the mean of a future sample based on a background sample. The uncensored case is considered mainly to illustrate the fiducial approach so that a reader can comprehend the idea of the fiducial inference and to demonstrate the simplicity and accuracy of the approach. The solutions to the uncensored case are extended to the case of samples with multiple DLs. For such censored case, we address the following problems: (a) construction of confidence intervals for the mean and parameters, (b) upper confidence limits (UCLs) for an upper percentile, (c) upper prediction limits (UPLs) for the mean of a future sample, and (d) UPLs that include at least l of a sample of m observations from each of r locations.

We briefly review the relevant literature and practical applications for each of the problems noted in the preceding paragraph. A 95% UCL for the mean is used to demonstrate compliance with the Remediation Standard Regulation. As the gamma distribution is often used to model environmental data, it is of interest to find a UCL for the gamma mean. Another important problem in environmental monitoring is the comparison of the mean of a small number of on-site measurements with a larger collection of background measurements. Using these back ground data collected from locations that are unaffected by the ecological hazard of concern, a prediction limit for the mean of a future sample is constructed. The potentially impacted on-site data are then compared with the statistical prediction limit directly. If the mean of the on-site data is less than the UPL, then one can conclude that the on-site data are consistent with background data (Bhaumik & Gibbons 2004). For the uncensored case, assuming lognormality, Bhaumik and Gibbons (2004) have provided a few methods of finding UPL for the mean of a future sample. The UPL for l of m futures samples at each of r locations is required for simultaneous determinations of an analyte of concern in multiple locations. In the event of an initial exceedance of the UPL, a few more samples are collected to confirm evidence of an impact on the environment (see chapter 4 of Gibbons *et al.*, 2009). For the uncensored case, Bhaumik and Gibbons (2006) and Krishnamoorthy *et al.* (2008) have provided approximate methods to find such a UPL.

The rest of the article is organized as follows. In Section 2, we develop approximate fiducial quantities for the parameters of a gamma distribution based on the fiducial quantities of normal parameters. In Section 3, we consider the uncensored case and propose approximate CLs for the mean and parameters, UCL for an upper percentile, and an approximate UPL for the mean of a future sample. The results for the uncensored case are extended to the censored case in Section 4. Furthermore, an approximate fiducial prediction limit that includes at least l of m future observations from each of r locations is also provided in Section 4. To judge the accuracy of the proposed methods, coverage probabilities of the proposed confidence limits and prediction limits are estimated using Monte Carlo simulation. All the methods are illustrated using some real data. Some concluding remarks are given in Section 5.

2 | APPROXIMATE FIDUCIAL QUANTITIES FOR GAMMA PARAMETERS

We shall now develop approximate fiducial quantities (FQs) based on cube root transformed samples, which are approximately normally distributed. Another transformation, due to Hawkins and Wixley (1986), is that the distribution of fourth-root-transformed gamma random variable can also be approximated by a normal distribution. Krishnamoorthy *et al.* (2008) have compared the cube root and the fourth root approximations, and recommended that the cube root approximation due to Wilson and Hilferty (1931) is preferred overall. So we shall consider developing FQs on the basis of cube root transformed samples. Let $Y_1, \ldots, Y_n$ be a sample from a gamma(a, b) distribution with shape parameter a and the scale parameter b. Let $X_i = Y_i^{\frac{1}{3}}$, $i = 1, \ldots, n$. On the basis of the Wilson and Hilferty (1931) approximation, X_i's are approximately normally distributed with mean μ and variance σ^2 given by

$$\mu = (ba)^{\frac{1}{3}}\left(1 - \frac{1}{9a}\right) \quad \text{and} \qquad \sigma^2 = \frac{b^{2/3}}{9a^{1/3}}. \tag{1}$$

The above relations between (μ, σ^2) and (a, b) are not needed to find tolerance intervals or to find confidence limits for a survival probability. For example, let $\overline{X}$ and S denote the mean and standard deviation of a cube root transformed sample of size n from a gamma distribution. Then

$$\left(\overline{X} + \frac{1}{\sqrt{n}} t_{n-1;1-\alpha}(z_p\sqrt{n})S\right)^3 \tag{2}$$

is a $100(1-\alpha)\%$ upper confidence limit (UCL) for the $100p$ percentile of the sampled gamma population. In the above expression, z_p is the $100p$ percentile of the standard normal distribution, and $t_{m;q}(\delta)$ denotes the $100q$ percentile of the noncentral t distribution with the degrees of freedom (df) m and noncentrality parameter δ. Similarly, notice that the survival probability of a component at time t is $P(X > t) = P(X^{1/3} > t^{1/3})$. Because $X^{1/3}$ is approximately normally distributed, normal-based method can be used to find a lower confidence bound for the survival probability; for more details, see Krishnamoorthy *et al.* (2008). However, to find confidence intervals for the mean ab, such approach is not useful because $E(X^{1/3}) \neq [E(X)]^{1/3}$, where E denotes the expectation. To find CIs for a parameter or for the mean, we shall use the following approach that requires the expressions in Equation 1.

Define

$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \quad \text{and} \quad S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X})^2.$$

To obtain fiducial quantities for μ and σ^2, consider the stochastic representations

$$\overline{X} \stackrel{d}{=} \mu + Z\frac{\sigma}{\sqrt{n}} \quad \text{and} \quad S^2 \stackrel{d}{=} \sigma^2 \frac{\chi^2_{n-1}}{n-1},$$

where Z is the standard normal random variable, χ^2_m denotes the chi-square random variable with degrees of freedom (df) m and the notation "$\stackrel{d}{=}$" means "distributed as." Furthermore, Z and χ^2_{n-1} are independent random variables. Let $(\bar{x}, s)$ be an observed value of $(\overline{X}, S)$. Solving the above equations for μ and σ^2, and replacing $(\overline{X}, S)$ with $(\bar{x}, s)$, we obtain the FQs for the parameters as

$$G_\mu = \bar{x} + \frac{Z\sqrt{n-1}}{\sqrt{\chi^2_{n-1}}}\frac{s}{\sqrt{n}} \quad \text{and} \quad G_{\sigma^2} = \frac{(n-1)s^2}{\chi^2_{n-1}}. \tag{3}$$

Notice that in the above FQs, $\bar{x}$ and s are fixed, and Z and χ^2_{n-1} are random variables whose distributions do not depend on any parameters. A FQ for a real-valued function, say, $h(\mu,\sigma^2)$ can be obtained by simple substitution as $h\left(G_\mu, G_{\sigma^2}\right)$.

FQs for a and b can be obtained by first expressing a and b in terms of (μ, σ^2) and then substituting FQs for μ and σ^2. Solving the set of equations in Equation 1 for a and b, we see that

$$\begin{aligned} a &= \frac{1}{9}\left\{\left(1 + .5\frac{\mu^2}{\sigma^2}\right) + \left[\left(1 + .5\frac{\mu^2}{\sigma^2}\right)^2 - 1\right]^{\frac{1}{2}}\right\} \quad \text{and} \\ b &= 27a^{\frac{1}{2}}\left(\sigma^2\right)^{\frac{3}{2}}. \end{aligned} \tag{4}$$

Replacing the parameters (μ, σ^2) by (G_μ, G_{σ^2}), we obtain the FQs for a and b as

$$\begin{aligned} G_a &= \frac{1}{9}\left\{\left(1 + .5\frac{G_\mu^2}{G_{\sigma^2}}\right) + \left[\left(1 + .5\frac{G_\mu^2}{G_{\sigma^2}}\right)^2 - 1\right]^{\frac{1}{2}}\right\} \quad \text{and} \\ G_b &= 27(G_a)^{\frac{1}{2}}(G_\sigma)^3, \end{aligned} \tag{5}$$

where $G_{\mu^2} = (G_\mu)^2$ and $G_\sigma = \sqrt{G_{\sigma^2}}$. For calculation purpose, we note that

$$\frac{G_\mu^2}{G_{\sigma^2}} = \left(\bar{x}\sqrt{\frac{\chi^2_{n-1}}{(n-1)s^2}} + \frac{Z}{\sqrt{n}}\right)^2. \tag{6}$$

3 | CONFIDENCE LIMITS AND PREDICTION LIMITS: UNCENSORED CASE

3.1 | Confidence limits for the mean and parameters

Noting that the mean of a gamma(a, b) distribution is given by $M = ab$, a FQ for the mean can be obtained as $G_M = G_a G_b$. Alternatively, we can express the FQ for the mean as follows.

Let $M = ab$ so that we can write Equation 1 as

$$\mu = M^{\frac{1}{3}}\left(1 - \frac{b}{M}\right) \quad \text{and} \quad \sigma^2 = \frac{b}{9M^{\frac{1}{3}}}.$$

Solving the above equations for M, we find $M = \left(\mu/2 + \sqrt{\mu^2/4 + \sigma^2}\right)^3$. Thus, a FQ for the gamma mean is obtained as

$$G_M = \left(\frac{G_\mu}{2} + \sqrt{\left(\frac{G_\mu}{2}\right)^2 + G_{\sigma^2}}\right)^3, \tag{7}$$

where G_μ and G_{σ^2} are defined in Equation 3. For a given $(\bar{x}, s)$, the distribution of G_M does not depend on any unknown parameters, and so its percentiles can be estimated using Monte Carlo simulation. In fact, a 95% CI for the mean can be obtained using the following R codes:

```
nr <- 100000

u <- rchisq(nr, n-1)/(n-1); z = rnorm(nr)

Gu <- xbar + z*s/sqrt(n)/sqrt(u); Gsigsq <- s^2/u

Gm <-  (.5*Gu+sqrt(.25*Gu^2+Gsigsq))^3

ci <- quantile(Gm, c(.025,.975))
```

In the above, (xbar, s) denotes the (mean, standard deviation) based on a cube-root-transformed sample of size n.

The CIs for the mean M and other parameters can be obtained using the following algorithm, which can be coded in any programming language.

Algorithm 1

1. For a given sample from a gamma distribution, compute the mean $\bar{x}$ and variance s^2 of the cube root transformed sample.
2. Generate a standard normal variate Z and a chi-square variate χ^2_{n-1}.
3. Compute G_μ and G_{σ^2} using Equation 3.
4. Calculate the FQs G_a and G_b using Equations 5 and 6, respectively, and G_M using Equation 7.
5. Repeat Steps 2–5 for a large number of times, say, 10,000
6. Let $G_{M;q}$ denote the $100q$ percentile of 10,000 G_M's generated in the preceding step. Then $(G_{M;\alpha}, G_{M;1-\alpha})$ is a 100 $(1 - 2\alpha)$% CI for the mean of the sampled gamma population, and $G_{M;1-\alpha}$ is a $100(1 - \alpha)$% UCL for the mean.

CIs for a and b can be obtained similarly. For example, if $G_{a;\alpha}$ denote the 100αth percentile of 10,000 G_a's generated using the above algorithm, then $(G_{a;\alpha}, G_{a;1-\alpha})$ is a 100 $(1 - 2\alpha)$% CI for the shape parameter a.

3.2 | Upper confidence limit for an upper percentile

Let $F(x|a, b) = P(X \leqslant x|a, b)$, where X is a gamma (a, b) random variable. Let $F^{-1}(p\,|a, b)$,$0 < p < 1$, denote the inverse function of $F(x|a, b)$. Then, a FQ for finding an UCL for $F^{-1}(p \mid a, b)$ is given by

$$F^{-1}(p|G_a, G_b). \tag{8}$$

For a given (mean, SD) based on a cube root transformed sample and p, we can generate $F^{-1}(p|G_a, G_b)$ for a large number of times, and $100(1 - \alpha)$ percentile of such simulated values is a $100(1 - \alpha)$% UCL for the $100p$th percentile of the sampled gamma(a, b) distribution.

Noting that an approximate $100p$ percentile of a gamma (a, b) distribution is $(\mu + z_p\sigma)^3$, alternatively, an approximate FQ for finding a UCL for an upper percentile can be expressed as

$$\begin{aligned}\left(G_\mu + z_p G_\sigma\right)^3 &= \left(\bar{x} + \frac{Z + z_p\sqrt{n}}{\sqrt{\chi^2_{n-1}/(n-1)}}\frac{s}{\sqrt{n}}\right)^3 \\ &= \left(\bar{x} + \frac{1}{\sqrt{n}}t_{n-1}(z_p\sqrt{n})s\right)^3,\end{aligned} \tag{9}$$

where $Z \sim N(0, 1)$ independently of χ^2_{n-1} and $\frac{Z+z_p\sqrt{n}}{\sqrt{\chi^2_{n-1}/(n-1)}} = t_{n-1}(z_p\sqrt{n})$ denotes the noncentral t random variable with df $= n - 1$ and the noncentrality parameter $z_p\sqrt{n}$. Thus, this alternative approach produces the closed-form UCL in Equation 2, which is the same as the one given in Krishnamoorthy *et al.* (2008).

Between the two UCLs described above, the one in Equation 2 is simple to compute, and our preliminary simulation studies (not reported here) indicated that both UCLs are comparable with respect to coverage probabilities and precision. The UCL based on Equation 8 involves repeated calculation of gamma percentiles; as a result, it is time consuming. The UCL based on the noncentral t percentile is simple to compute and is very satisfactory for applications (Krishnamoorthy *et al.*, 2008).

3.3 | Upper confidence limit for the mean of a future sample

A fiducial UPL for the mean of a future sample can be estimated using the fiducial quantities G_a and G_b on the basis of a background sample. Specifically, let $Z_1, \ldots, Z_N$ be independent standard normal random variables, and let $\chi^2_{1,n-1}, \ldots \chi^2_{N,n-1}$ be independent chi-square random variables with df $= n - 1$. Define

$$G_{i,\mu} = \bar{x} + \frac{Z_i\sqrt{n-1}}{\sqrt{\chi^2_{i,n-1}}}\frac{s}{\sqrt{n}}, \text{ and } G_{i,\sigma^2} = \frac{(n-1)s^2}{\chi^2_{i,n-1}}, i = 1, \ldots, N,$$

where $(\bar{x}, s^2)$ is the (mean, variance) based on a cube root transformed background sample of size n. Define $G_{i,a}$ and $G_{i,b}$ using Equation 5 with (G_μ, G_{σ^2}) replaced by $(G_{i,\mu}, G_{i,\sigma^2})$, $i = 1, \ldots, N$. The joint fiducial distribution of the mean of a future sample of size m and the background sample can be obtained empirically by simulating means from gamma $(G_{i,a}, G_{i,b})$, $i = 1, \ldots, N$. Noting that the mean of a sample of m observations from a gamma distribution also follows a gamma distribution with the shape parameter multiplied by m and the scale parameter divided by m, we can find the joint fiducial distribution by simulating

$$\overline{Y}_i \sim \text{gamma}\left(mG_{i,a}, G_{i,b}/m\right), \quad i = 1, \ldots, N.$$

The $100(1-\alpha)$ percentile of the $\overline{Y}_i$'s is an approximate UPL for the mean of a future sample from the gamma population from which the background sample was collected.

For a given $(\bar{x}, s^2)$, the distribution of $\overline{Y}_i$'s does not depend on any parameters, and so its percentiles can be estimated using Monte Carlo simulation as shown in the following algorithm.

Algorithm 2

1. For a given sample from a gamma(a, b) distribution, compute the mean $\bar{x}$ and variance s^2 of the cube root transformed sample.
2. Generate a chisquare variate χ^2_{n-1} and a standard normal variate Z.
3. Compute the FQs G_μ and G^2_σ using Equation 3.
4. Compute the FQs G_a and G_b using Equations 5 and 6.
5. Generate the mean $\overline{Y}$ from gamma(mG_a,G_b/m) distribution.
6. Repeat Steps 2–5 for a large number of times, say, 10,000
7. The $100(1-\alpha)$ percentile of these 10,000 $\overline{Y}$'s is a 100 $(1-\alpha)$% UPL for the mean of a future sample of size m.

Remark 1. If the sizes of the background sample and future sample are the same, then a closed-form approximate prediction limit for the mean of a future sample can be obtained as follows. Let $\overline{Y}$ denote the mean of a random sample $Y_1, \ldots, Y_n$ from a gamma distribution, and let S denote the standard deviation of $Y_1^{1/3}, \ldots, Y_n^{1/3}$. Then $\overline{Y} \sim$ gamma $(na, b/n)$, and $\overline{Y}^{1/3} \sim N(\mu_n, \sigma_n^2)$, approximately, where $\mu_n = (ab)^{1/3}$ $[1 - 9/(an)]$ and $\sigma_n^2 = \sigma^2/n$, with σ^2 defined in Equation 1. Let $\overline{Y}_F$ denote the mean of a future sample of size m. Let $\mu_d = b^{1/3}(1/m - 1/n)/(9a^{2/3})$. Then, it is easy to see that $\overline{Y}^{1/3} - \overline{Y}_F^{1/3} \sim N(\mu_d, \sigma^2(1/n + 1/m))$ approximately and independently of $(n-1)S^2/\sigma^2 \sim \chi^2_{n-1}$. Therefore, if $n = m$, then $\mu_d = 0$ and $\left(\overline{Y}^{\frac{1}{3}} - \overline{Y}_F^{\frac{1}{3}}\right) / \left[S\sqrt{\frac{1}{n} + \frac{1}{m}}\right] \sim t_{n-1}$, approximately, where t_{n-1} denotes the Student's t distribution with df $= n - 1$. On the basis of this distributional result, we obtain

$$\left(\overline{Y}^{\frac{1}{3}} \pm t_{n-1;1-\alpha/2} S\sqrt{\frac{1}{n} + \frac{1}{m}}\right)^3 \tag{10}$$

as an approximate $100(1-\alpha)$% prediction interval for $\overline{Y}_F$. Our simulation studies (not reported here) indicate that the above approximate prediction interval is very satisfactory in terms of coverage probabilities as long as $n \geqslant 3$ and the shape parameter $a \geqslant .5$. Furthermore, preliminary simulation studies indicated that the above prediction interval can be used in application if $m/n \leqslant 3$, which maybe the case in most applications; see Examples 1 and 2.

3.4 | Simulation studies: uncensored case

The CIs and UPLs based on the fiducial approach are quite simple to compute as they do not involve calculation of the MLEs of a and b. So, it is desired to evaluate their validity in terms of coverage probabilities. The CIs for the mean and the scale parameter are equivariant under a scale transformation of the data. Furthermore, the CI for the shape parameter is invariant under a scale transformation. Therefore, without loss of generality, we can take the scale parameter b to be unity in our simulation studies. We estimated the coverage probabilities of the approximate fiducial CIs for the mean for values a ranging from .5 to 5 and sample sizes ranging from 5 to 25. The coverage probabilities were estimated using 10,000 runs for generating a gamma sample of size n, and for each generated sample, Algorithm 1 was used with 10,000 runs to obtain a CI. The percentage of 10,000 CIs that include the true assumed mean is an estimate of the coverage probability.

Coverage probabilities for CIs for the mean, shape parameter, and the scale parameter are reported in Table 1. For the

TABLE 1 Coverage probabilities of 95% CIs for the mean, shape parameter and scale parameter

	Mean					Shape parameter					Scale parameter				
	n					n					n				
a	5	10	15	20	25	5	10	15	20	25	5	10	15	20	25
0.50	.926	.930	.929	.930	.943	.964	.965	.966	.966	.964	.954	.950	.956	.943	.946
1.00	.952	.944	.946	.947	.951	.960	.961	.965	.964	.962	.953	.954	.958	.960	.954
1.50	.956	.946	.948	.951	.954	.954	.960	.953	.955	.962	.952	.955	.951	.958	.950
2.00	.951	.955	.953	.951	.952	.953	.964	.960	.955	.952	.952	.954	.949	.953	.952
3.00	.954	.956	.956	.950	.947	.954	.950	.960	.951	.949	.950	.954	.957	.960	.950
4.00	.950	.953	.953	.962	.948	.956	.956	.951	.955	.950	.951	.948	.952	.954	.956
5.00	.951	.951	.946	.948	.953	.949	.957	.950	.945	.952	.948	.954	.950	.948	.953

TABLE 2 Powers of the MLRT* and the (Fiducial) test

$M_0 = 3$	n			$M_0 = 5$	n		
M	10	15	20	M	10	15	20
3.0	.050(.049)	.051(.048)	.051(.049)	5.0	.050(.049)	.050(.053)	.050(.047)
2.7	.119(.120)	.147(.140)	.174(.168)	4.7	.101(.093)	.120(.118)	.139(.130)
2.4	.236(.232)	.325(.322)	.408(.399)	4.4	.182(.169)	.242(.241)	.297(.292)
2.1	.402(.401)	.565(.560)	.696(.676)	4.1	.296(.280)	.409(.413)	.514(.512)
1.8	.585(.580)	.784(.787)	.894(.898)	3.8	.435(.415)	.603(.599)	.730(.727)
1.6	.702(.702)	.882(.889)	.959(.954)	3.6	.534(.511)	.719(.718)	.839(.829)
$M_0 = 3$	n			$M_0 = 5$	n		
M	30	35	40	M	30	35	40
3.0	.050(.048)	.050(.050)	.049(.049)	5.0	.049(.054)	.050(.051)	.050(.052)
2.7	.224(.218)	.246(.245)	.272(.277)	4.7	.171(.173)	.188(.183)	.202(.206)
2.4	.560(.555)	.623(.607)	.675(.672)	4.4	.401(.407)	.452(.449)	.494(.505)
2.1	.858(.860)	.907(.899)	.939(.936)	4.1	.677(.688)	.741(.744)	.793(.799)
1.8	.978(.981)	.991(.989)	.996(.996)	3.8	.884(.890)	.926(.922)	.952(.959)
1.6	.997(.995)	.999(.999)	1(1)	3.6	.955(.954)	.975(.974)	.988(.987)

Note. * The modified likelihood ratio test by Fraser *et al.* (1997). MLRT = Modified Likelihood Ratio Test.

H_0:$M = M_0$vs.H_a:$M < M_0$; $M = ab$; $b = 1$

mean, the estimated coverage probabilities being close to the nominal level .95, indicating that the fiducial CIs are quite satisfactory even for a sample of size five. The results for estimating the shape parameter a are similar except that the CIs could be slightly conservative for small values of a. In general, we observe from Table 1 that the CIs for the mean and the shape parameter are not very accurate when the shape parameter is 0.5. This is because the cube root transformation is not accurate for very small values of the shape parameter a; see Krishnamoorthy *et al.* (2008). CIs for b, however, seem to be accurate for all values of the shape parameters considered in the study. Overall, the CIs based on the fiducial approach are reasonably accurate for $a \geqslant .5$.

The likelihood-based methods by Fraser *et al.* (1997) and by Krishnamoorthy and Luis (2014) are very similar, so we compare the fiducial method with the MLRT by Fraser *et al.* (1997). For comparison, we estimated the powers of the MLRT and the test based on the fiducial CI determined by Equation 7. The powers are estimated for testing H_0:$M = M_0$ versus H_a:$M < M_0$ at the level of .05. The Monte Carlo estimates of powers are reported in Table 2 for sample sizes ranging from 10 to 40. Notice that the power at $M = M_0$ is the Type I error rate. We observe from Table 2 that both tests control Type I error rates around the nominal level .05 and are comparable in terms of Type I error rates and powers. This comparison shows that the CIs based on these two tests should be similar. As noted earlier, an advantage of the fiducial approach over the MLRT is that the fiducial method is simple and easy to find CIs for the mean.

In Table 3, we present estimated coverage probabilities of the 95% UPLs for the mean of a future sample of size m based on a background sample of size n. All estimated coverage probabilities are very close to the nominal level .95 for some small to moderate values of (n, m). Even for $a = .5$,

TABLE 3 Coverage probabilities of 95% UPLs for the mean of a sample

	(Background sample size, future sample size) = (n, m)							
a	(5,5)	(5,7)	(10,2)	(10,5)	(10,15)	(16,3)	(20,7)	(20,12)
0.50	.943	.944	.941	.940	.930	.943	. 944	.934
1.00	.947	.951	.948	.950	.953	.951	.950	.940
1.50	.951	.950	.951	.946	.952	.954	.954	.942
2.00	.945	.950	.949	.950	.950	.952	.951	.952
3.00	.949	.955	.956	.944	.950	.947	.951	.952
4.00	.952	.952	.953	.957	.953	.948	.948	.959
5.00	.951	.949	.949	.953	.951	.953	.949	.945

the coverage probabilities are close to .95. Overall, we see that the fiducial UPL for the mean of a future sample is quite satisfactory in terms of coverage probability.

3.5 | Examples: uncensored case

Example 1. In this example, we use the measurements in Gibbons (1994, p. 261), that represent alkalinity concentrations in groundwater obtained from a “greenfield” site (i.e., the site of a waste disposal landfill before disposal of waste) and are reproduced here in Table 4.

The mean and standard deviation of the cube root transformed concentrations are $\bar{x} = 3.8274$ and $s = 0.4298$. Using Algorithm 1 with 100,000 runs, we found 90% CI for the shape parameter as (5.40, 13.46), 90% CI for the scale parameter as (4.29, 10.99), and 95% UCL for the mean concentration as 65.12. Using the software StatCalc* by Krishnamoorthy (2015), which uses the parametric bootstrap method, we found the 90% CI for the shape parameter as (5.42, 13.43), 90% CI for the scale parameter as

*visit www.ucs.louisiana.edu/∼kxk4695/ for free download

TABLE 4 Alkalinity concentrations in groundwater

58	**82**	**42**	**28**	**118**	**96**	**49**	**54**	**42**	**51**	**66**	**89**	**40**	**51**
54	55	59	42	39	40	60	63	59	70	32	52	79	

Note. UPLs = upper prediction limits.

TABLE 5 Vinyl concentrations in groundwater

5.1	**2.4**	**.4**	**.5**	**2.5**	**.1**	**6.8**	**1.2**	**.5**	**.6**	**5.3**	**2.3**
1.8	1.2	1.3	1.1	.9	3.2	1.0	.9	.4	.6	8.0	.4
2.7	.2	2.0	.2	.5	.8	2.0	2.9	.1	4.0		

(4.30, 10.98), and 95% UCL for the mean as 65.04. The 95% UCL for the 90th percentile of alkalinity concentration distribution is calculated as $\left(\bar{x} + \frac{1}{\sqrt{n}} t_{n-1;.95}(z_{.9}\sqrt{n})s\right)^3 = (3.8274 + 1.8114 \times .4298)^3 = 97.71$. We also estimated the 95% UPLs using Algorithm 2 for the means of future samples of sizes 5, 10, and 15 as 75.6, 71.4, and 69.6, respectively. That is, using alkalinity concentrations in Table 4 as background data, we predict the mean of a future sample of size 5 is no more than 75.6 with confidence 95%. Other UPLs can be interpreted similarly. The 95% UPLs based on the approximate formula in Equation 10 for the means of future samples of sizes 5, 10, and 15 are 75.7, 71.2, and 69.4, respectively. Notice that these UPLs are practically the same as those based on Algorithm 2.

Example 2. We shall now use the vinyl chloride data to illustrate our methods for uncensored samples. The data given in Table 1 of Bhaumik and Gibbons (2006) are reproduced here in Table 5. These vinyl chloride concentrations were collected from clean upgradient monitoring wells. A quantile-quantile plot of Bhaumik and Gibbons showed an excellent fit of these data to a gamma distribution.

The mean of the cube root transformed data in Table 5 is $\bar{x} = 1.10223$ and the standard deviation is $s = 0.39992$. Using Algorithm 1 with 100,000 simulation runs, we calculated the 90% CI for the mean vinyl concentration as (1.44, 2.53). For this data, the third-order likelihood method by Fraser *et al.* (1997) yielded (1.45, 2.56); see Krishnamoorthy and Luis (2014). To compute a 95% UCL for the 90th percentile of the distribution of vinyl concentrations, we found the 90th percentile of the standard normal distribution as $z_{.9} = 1.2816$ and noncentral t critical value as $t_{33;.95}(1.2816 \times \sqrt{34}) = 10.1478$. Thus, the desired UCL for the 90th percentile is $\left(1.10223 + \frac{1}{\sqrt{34}} t_{33;.95}(z_{.9}\sqrt{34}) \times .39992\right)^3 = (1.10223 + 1.7403 \times .39992)^3 = 5.81$. That is, 90% of the vinyl chloride concentrations are no more than 5.81 with confidence 95%.

The 95% UPLs for the means of future samples of sizes 5, 10, and 15 are 3.66, 3.20, and 3.02, respectively. For example, the mean of a future sample of size 15 will be no more than 3.02 with confidence 95%. These UPLs were obtained using Algorithm 2 with 100,000 runs. The 95% UPLs based on the approximate formula in Equation 10 for the means of future samples of sizes 5, 10, and 15 are 3.78, 3.23, and 3.01, respectively. We once again see that these UPLs are practically the same as those based on Algorithm 2.

4 | CONFIDENCE LIMITS AND PREDICTION LIMITS: CENSORED CASE

We shall now extend the fiducial approach for the uncensored case to the censored case. Recall that for the uncensored case, the FQs are a function of the mean and standard deviation based on cube root transformed samples. We shall develop similar FQs as functions of the MLEs based on cube root transformed censored sample. In particular, we will use the MLEs of μ and σ^2 (the parameters defined in Equation 1) based on cube root transformed uncensored observations and cube root transformed DLs. In the following section, we describe some approximate distributional results of the MLEs and provide the FQs for the normal mean and standard deviation. These FQs for the normal mean and standard deviation are used to obtain approximate FQs for the shape and scale parameters of a gamma distribution.

4.1 | Maximum likelihood estimates and fiducial quantities

Consider a simple random sample of n observations subject to k detection limits, say, $DL_1, \ldots, DL_k$, from a normal distribution with mean μ and variance σ^2. Let us assume without loss of generality that $DL_1 < DL_2 < \ldots < DL_k$, and all the measurements are expressed in the same measurement unit. Let m_i denotes the number of nondetects that are below DL_i, and let $m = \sum_{i=1}^{k} m_i$, Let us denote the detected observations by $x_1, \ldots, x_{n-m}$. Define

$$\bar{x}_d = \frac{1}{n-m}\sum_{i=1}^{n-m} x_i \quad \text{and} \quad s_d^2 = \frac{1}{n-m}\sum_{i=1}^{n-m}(x_i - \bar{x}_d)^2. \tag{11}$$

The log-likelihood function for the censored case, after omitting a constant term, can be written as

$$l(\mu, \sigma) = \sum_{i=1}^{k} m_i \ln\ \Phi(z_i^*) - (n-m)\ln\sigma - \frac{(n-m)\left(s_d^2 + (\bar{x}_d - \mu)^2\right)}{2\sigma^2}, \tag{12}$$

where $z_i^* = \frac{DL_i - \mu}{\sigma}$, $i = 1, \ldots, k$. The MLE $(\hat{\mu}, \hat{\sigma})$ of (μ, σ) is obtained by maximizing the above log-likelihood function. For more details on obtaining the MLEs numerically, see Krishnamoorthy and Xu (2011) and Krishnamoorthy, Mathew and Xu (2014).

To develop FQs, we first describe the distributional results given in Krishnamoorthy and Xu (2011). Let $\widehat{\mu}^*$ and $\widehat{\sigma}^*$ denote the MLEs based on a sample from a $N(0,1)$ distribution with DLs $DL_i^* = (DL_i - \mu)/\sigma$, $i = 1, \ldots, k$. Then $\frac{\widehat{\mu}-\mu}{\sigma} \sim \widehat{\mu}^*$ and $\frac{\widehat{\sigma}}{\sigma} \sim \widehat{\sigma}^*$. Approximate distributions can be obtained by replacing DL_i^* with $\widehat{DL}_i^* = (DL_i - \widehat{\mu})/\widehat{\sigma}$, $i = 1, \ldots, k$, where $\widehat{\mu}$ and $\widehat{\sigma}$ are the MLEs. Because the MLEs are consistent estimators, the approximations should be very satisfactory for large samples. However, Krishnamoorthy and Xu's (2011) simulation studies indicated that the CIs based on such approximations are very satisfactory even for small samples. On the basis of the approximate distributional results, we have the following approximate stochastic representations:

$$\mu \overset{d}{=} \mu + \widehat{\mu}^*\sigma \text{ and } \widehat{\sigma} \overset{d}{=} \sigma\widehat{\sigma}^*, \text{ approximately,}$$

where $\widehat{\mu}^*$ and $\widehat{\sigma}^*$ denote the MLEs based on a sample from a $N(0,1)$ distribution with DLs $\widehat{DL}_i^* = (DL_i - \widehat{\mu})/\widehat{\sigma}$, $i = 1, \ldots, k$. Let $(\widehat{\mu}_0, \widehat{\sigma}_0)$ be an observed value of $(\widehat{\mu}, \widehat{\sigma})$. Solving the above equations for μ and σ, and then replacing $(\widehat{\mu}, \widehat{\sigma})$ with $(\widehat{\mu}_0, \widehat{\sigma}_0)$, we obtain the FQs for μ and σ as

$$Q_\mu = \widehat{\mu}_0 - \frac{\widehat{\mu}^*}{\widehat{\sigma}^*}\widehat{\sigma}_0 \quad \text{and} \quad Q_\sigma = \frac{\widehat{\sigma}_0}{\widehat{\sigma}^*}. \tag{13}$$

To find the FQs for the gamma parameters a and b based on a censored sample, we simply apply the results for the normal case to the cube root transformed samples and cube root transformed DLs. Specifically, we use the MLEs $(\widehat{\mu}_0, \widehat{\sigma}_0)$ based on the cube root transformed samples with detection limits $DL_i^{\frac{1}{3}}$, and $\widehat{DL}_i^* = (DL_i^{\frac{1}{3}} - \widehat{\mu}_0)/\widehat{\sigma}_0$, $i = 1, \ldots, k$. The FQs for a and b can be obtained from Equation 4 as

$$Q_a = \frac{1}{9}\left\{\left(1 + .5\frac{Q_\mu^2}{Q_{\sigma^2}}\right) + \left[\left(1 + .5\frac{Q_\mu^2}{Q_{\sigma^2}}\right)^2 - 1\right]^{\frac{1}{2}}\right\} \quad \text{and}$$
$$Q_b = 27(Q_a)^{\frac{1}{2}}(Q_\sigma)^3. \tag{14}$$

4.2 | Confidence limits for the mean

Following Equation 7, the FQ for the gamma mean is obtained as

$$Q_M = \left(\frac{Q_\mu}{2} + \sqrt{\left(\frac{Q_\mu}{2}\right)^2 + Q_\sigma^2}\right)^3. \tag{15}$$

For a given $(\widehat{\mu}_0, \widehat{\sigma}_0)$ and the detection limits, the distribution of Q_M does not depend on any parameters, and so its percentiles can be estimated by Monte Carlo simulation. Appropriate percentiles of Q_M form a CI for the mean, and they can be estimated using the following algorithm.

Algorithm 3

1. For a given sample of size n with DLs $DL_1, \ldots, DL_k$, calculate the MLEs $\widehat{\mu}_0$ and $\widehat{\sigma}_0$ based on the cube root transformed sample and cube root transformed DLs. Set $\widehat{DL}_i^* = (DL_i^{\frac{1}{3}} - \widehat{\mu}_0)/\widehat{\sigma}_0$, $i = 1, \ldots, k$.
2. Generate a sample of size n from $N(0,1)$ with detection limits $\widehat{DL}_1^*, \ldots, \widehat{DL}_k^*$.
3. Calculate the MLEs $\widehat{\mu}^*$ and $\widehat{\sigma}^*$.
4. Calculate Q_μ and Q_σ using Equation 13.
5. Calculate Q_M using Equation 15.
6. Repeat Steps 2–5 for a large number of times, say, 10,000
7. The $100(1-\alpha)$ percentile of these 10,000 Q_M's is a $100(1-\alpha)\%$ UCL for the mean.

As noted earlier, computational details on MLEs and generating samples with multiple detection limits can be found in Krishnamoorthy and Xu (2011) and Krishnamoorthy *et al.* (2014). Algorithm 3 is also implemented in R and available at the journal's website and also can be downloaded from the first author's webpage http://www.ucs.louisiana.edu/~kxk4695/.

4.3 | Confidence limits for an upper percentile

Recall that the $100p$ percentile of a normal distribution with mean μ and the variance σ^2 is $\xi_p = \mu + z_p\sigma$, where z_p is the $100p$ percentile of the standard normal distribution. A FQ for ξ_p can be found by replacing the parameters by their FQs and is given by

$$Q_{\xi_p} = Q_\mu + z_p Q_\sigma = \widehat{\mu}_0 + \frac{z_p - \widehat{\mu}^*}{\widehat{\sigma}^*}\widehat{\sigma}_0, \tag{16}$$

where $\widehat{\mu}^*$ and $\widehat{\sigma}^*$ are the MLEs based on a sample of size n with detection limits $DL_i = (DL_i - \widehat{\mu})/\widehat{\sigma}$, $i = 1, \ldots, k$. Thus, for a given sample, the distribution of Q_{ξ_p} does not depend on any unknown parameters, and the percentiles Q_{ξ_p} can be estimated using Monte Carlo simulation.

The above approach can be applied to a gamma distribution after taking cube-root transformation of samples, and a UCL for a percentile can be obtained as the third power of the $100(1-\alpha)$ percentile of Q_{ξ_p}. Computational details are shown in the following algorithm.

Algorithm 4

1. For a given sample of size n with DLs $DL_1, \ldots, DL_k$, calculate the MLEs $\widehat{\mu}_0$ and $\widehat{\sigma}_0$ based on the cube root transformed sample and cube root transformed DLs. Set $\widehat{DL}_i^* = (DL_i^{\frac{1}{3}} - \widehat{\mu}_0)/\widehat{\sigma}_0$, $i = 1, \ldots, k$.
2. Generate a sample of size n from $N(0,1)$ with detection limits $\widehat{DL}_1^*, \ldots, \widehat{DL}_k^*$.
3. Calculate the MLEs $\widehat{\mu}^*$ and $\widehat{\sigma}^*$.
4. Set $Q_p^* = \frac{z_p - \widehat{\mu}^*}{\widehat{\sigma}^*}$.

5. Repeat steps 2 – 4 for a large number of times, say, 10,000.
6. Find the $100(1-\alpha)$ percentile of these 10,000 Q_p^*'s, and denote it by $Q_{p;1-\alpha}^*$.

Then

$$\left(\hat{\mu}_0 + Q_{p;1-\alpha}^*\hat{\sigma}_0\right)^3 \tag{17}$$

is an approximate $100(1-\alpha)\%$ UCL for the $100p$ percentile of the sampled gamma population.

4.4 | Prediction limits for the mean of a future sample

A prediction limit for the mean of a future sample of size m based on a background sample of size n can be estimated along the lines for the uncensored case in Section 3.3. Specifically, let $(\hat{\mu}_0, \hat{\sigma}_0)$ be an observed value of the MLE $(\hat{\mu}, \hat{\sigma})$ based on a cube root transformed censored sample from a gamma(a, b) distribution. Define

$$Q_{i,\mu} = \hat{\mu}_0 - \frac{\hat{\mu}_i^*}{\hat{\sigma}_i^*}\hat{\sigma}_0, \quad \text{and} \quad Q_{i,\sigma} = \frac{\hat{\sigma}_0}{\hat{\sigma}_i^*}, \quad i = 1, \dots, N,$$

where $(\hat{\mu}_i^*, \hat{\sigma}_i^*)$ is the MLE based on the ith censored sample generated from $N(0,1)$ distribution with detection limits $\widehat{DL}_j^* = (DL_j^{\frac{1}{3}} - \hat{\mu}_0)/\hat{\sigma}_0$, $j = 1, \dots, k$. Define $Q_{i,a}$ and $Q_{i,b}$ using Equation 14 with (Q_μ, Q_{σ^2}) replaced by $(Q_{i,\mu}, Q_{i,\sigma^2})$, $i =, \dots, N$. The joint fiducial distribution of the mean of a future sample of size m and the background sample can be obtained empirically by simulating means from the gamma$(Q_{i,a}, Q_{i,b})$ distribution, $i = 1, \dots, N$. Specifically, we can study the empirical joint fiducial distribution by simulating $\overline{Y}_i \sim$ gamma $\left(mQ_{i,a}, Q_{i,b}/m\right)$, $i = 1, \dots, N$. The $100(1-\alpha)$ percentile of the $\overline{Y}_i$'s is an approximate UPL for the mean of a future sample from the gamma population from which the background sample was collected. For a given $(\hat{\mu}_0, \hat{\sigma}_0)$, the distribution of $\overline{Y}_i$'s does not depend on any parameters, and so its percentiles can be estimated using Monte Carlo simulation as shown in the following algorithm.

Algorithm 5

1. For a given sample of size n with DLs $DL_1, \dots, DL_k$, calculate the MLEs $\hat{\mu}_0$ and $\hat{\sigma}_0$ based on the cube root transformed sample and cube root transformed DLs. Set $\widehat{DL}_i^* = (DL_i^{\frac{1}{3}} - \hat{\mu}_0)/\hat{\sigma}_0$, $i = 1, \dots, k$.
2. Generate a sample of size n from $N(0,1)$ with detection limits $\widehat{DL}_1^*, \dots, \widehat{DL}_k^*$.
3. Calculate the MLEs $\hat{\mu}^*$ and $\hat{\sigma}^*$.
4. Calculate FQs (Q_μ, Q_σ) using Equation 13 and (Q_a, Q_b) using Equation 14.
5. Generate $\overline{Y}$ from gamma(mQ_a, Q_b/m).
6. Repeat steps 2 – 5 for a large number of times, say, 10,000.
7. The $100(1-\alpha)$ percentile of these 10,000 $\overline{Y}$'s is an approximate UPL for the mean of a future sample of size m.

4.5 | One-sided prediction limits for at least l of m observations from a gamma distribution at each of r locations

As noted earlier, this problem arises in ground water quality detection monitoring in the vicinity of hazardous waste management facilities and in process monitoring. Given a background sample of size n, the statistical problem is to construct an upper prediction limit so that at least l of m sample values are below the limit at each of r downgradient monitoring wells. A UPL satisfying these requirements can be estimated by applying the normal-based approach to cube root transformed samples. The following algorithm describes the method of finding such UPL.

Algorithm 6

1. For a given sample of size n with DLs $DL_1, \dots, DL_k$, calculate the MLEs $\hat{\mu}_0$ and $\hat{\sigma}_0$ based on the cube root transformed sample and cube root transformed DLs. Set $\widehat{DL}_i^* = (DL_i^{\frac{1}{3}} - \hat{\mu}_0)/\hat{\sigma}_0$, $i = 1, \dots, k$.
2. Generate a sample of size n from $N(0,1)$ with detection limits $\widehat{DL}_1^*, ..., \widehat{DL}_k^*$.
3. Calculate the MLEs $\hat{\mu}^*$ and $\hat{\sigma}^*$.
4. Calculate $Q_\mu = \hat{\mu}_0 - \frac{\hat{\mu}^*}{\hat{\sigma}^*}\hat{\sigma}_0$ and $Q_\sigma = \frac{\hat{\sigma}_0}{\hat{\sigma}^*}$.
5. Generate r samples, each of size m, from the normal distribution with mean Q_μ and standard deviation Q_σ. Find the lth order statistic for the ith sample, and denote it by $X_{(il)}$, $i = 1, \dots, r$.
6. Find $U_{r,m,l} = \max\{X_{(1l)}, \dots, X_{(rl)}\}$.
7. Repeat steps 2 – 6 for a large number of times, say, 10,000.
8. The $100(1-\alpha)$ percentile of these 10,000 $U_{r,m,l}$'s is an approximate UPL that includes at least l of m observations from each of r locations with confidence $1-\alpha$.

4.6 | Coverage studies: censored case

As the procedures that we proposed in the preceding sections are approximate, we need to appraise their accuracies in terms of coverage probabilities. We shall first estimate coverage probabilities of UCLs for the mean of a gamma distribution based on samples with multiple detection limits. As the proposed statistical procedures are scale equivariant, without loss of generality, we can take the scale parameter b to be unity in our coverage studies. To estimate the coverage probabilities of the UCL for the mean, we generated 2,500 samples, each of size n, from a gamma(a, 1) distribution. For each generated sample, we used Algorithm 3 with 5,000 runs to estimate the 95% UCL. The proportion of 2,500 UCLs that include the assumed mean is a Monte Carlo estimate of the coverage probability. The estimated coverage probabilities of 95% UCLs for the mean are reported in Table 6 for samples involving single detection limit and two detection limits. Simulation studies were conducted only for smaller values of a less than

TABLE 6 Coverage probabilities of 95% UCLs for the Mean based on samples with detection limits

	Single detection limit							
	n = 10				**n = 15**			
P_{DL_1}	**a = .5**	**a = 1**	**a = 2**	**a = 3**	**a = .5**	**a = 1**	**a = 2**	**a = 3**
.1	.944	.952	.947	.951	.940	.950	.953	.951
.2	.950	.951	.951	.951	.953	.952	.957	.945
.3	.952	.948	.955	.947	.954	.951	.945	.947
.5	.951	.949	.946	.946	.952	.944	.948	.950
.6	.946	.944	.951	.945	.950	.954	.953	.952
.7	—	—	—	—	.952	.946	.945	.948
	$n = 20$				$n = 25$			
P_{DL_1}	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
.1	.952	.950	.950	.943	.950	.950	.944	.950
.2	.951	.956	.950	.950	.951	.951	.950	.952
.3	.944	.945	.957	.946	.947	.953	.951	.946
.5	.947	.950	.954	.951	.952	.950	.953	.945
.6	.953	.952	.946	.951	.954	.953	.944	.950
.7	.944	.952	.951	.953	.951	.952	.950	.953
	Two detection limits							
	$n = 12$				$n = 16$			
(P_{DL_1}, P_{DL_2})	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
(.1,.2)	.951	.952	.948	.951	.947	.951	.953	.950
(.1,.3)	.946	.951	.952	.951	.948	.946	.951	.954
(.2,.2)	.951	.946	.950	.947	.950	.954	.949	.949
(.2,.3)	.945	.948	.948	.946	.947	.952	.954	.951
(.1,.5)	.947	.950	.954	.945	.946	.949	.947	.953
	$n = 20$				$n = 26$			
(P_{DL_1}, P_{DL_2})	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
(.1,.2)	.951	.951	.951	.953	.946	.950	.954	.951
(.1,.3)	.947	.951	.953	.950	.953	.951	.947	.951
(.2,.2)	.953	.944	.951	.949	.946	.951	.951	.954
(.2,.3)	.951	.952	.954	.952	.951	.947	.951	.946
(.1,.5)	.953	.946	.948	.946	.953	.954	.952	.946

Note. UCLs = upper prediction limits.

or equal to 3, because the cube root transformation is very satisfactory for moderate values of a, and so the results should be as good as those for the normal case. Furthermore, coverage probabilities were estimated assuming some values for proportion of concentrations below detection limit DL_i, and this proportion is denoted by P_{DL_i}. This is equivalent to setting detection limits as $100P_{DL_i}$ percentile of the gamma distribution. We observe in Table 6 that the estimated coverage probabilities for all cases are very close to the nominal level .95. In general, we see that the proposed interval estimation method for the mean of a gamma distribution works very satisfactorily for $n \geqslant 15$, and the percentage $(100 \times P_{DL_i})$ of nondetects is no more than 70. For sample size $n = 10$, the method works as long as the proportion of nondetects is around .6 or smaller. We like to note that for smaller n with high censoring, the number of detected values are often less than two with high probability, and the MLEs do not exist in such cases. For this reason, we were unable to estimate coverage probabilities when $n = 10$ and the proportion of nondetects is .7.

The coverage probabilities of 95% UCLs for the 90th percentile of a gamma distribution based on samples with multiple detection limits are presented in Table 7. These coverage probabilities were estimated along the lines for the mean in the preceding paragraph. We once again see that these coverage probabilities are very close to the nominal level .95, indicating that the approximate fiducial UCLs for the percentile are very accurate except for the case of single detection limit with proportion of nondetects is around .7 or more. The coverage probabilities being around .92, indicate that the fiducial UCLs could be anti-conservative when there is an intense censoring. Otherwise, the fiducial UCLs for an upper percentile are expected to be quite accurate.

Coverage probabilities of 95% UPLs for the mean of a future sample of size m based on a background sample of n are reported in Table 8 for some selected values of (n, m). Simulation studies were carried out for samples with single DL or with two DLs. We once again observe that the estimated coverage probabilities are very close to the nominal level .95.

TABLE 7 Coverage probabilities of 95% UCLs for the 90th percentile based on samples with detection limits

	Single detection limit							
	$n = 10$				$n = 15$			
P_{DL_1}	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
.1	.942	.952	.954	.952	.940	.950	.953	.951
.2	.954	.955	.953	.953	.953	.952	.957	.945
.3	.947	.952	.960	.963	.954	.951	.945	.947
.5	.945	.949	.946	.941	.952	.944	.948	.950
.6	.946	.949	.953	.950	.940	.934	.933	.934
.7	—	—	—	—	.922	.920	.925	.910
	$n = 20$				$n = 25$			
P_{DL_1}	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
.1	.952	.950	.950	.943	.950	.950	.944	.950
.2	.951	.956	.950	.950	.951	.951	.950	.952
.3	.944	.945	.957	.946	.947	.953	.951	.946
.5	.947	.950	.954	.951	.952	.950	.953	.945
.6	.953	.934	.934	.951	.932	.935	.934	.936
.7	.921	.919	.921	.917	.923	.918	.920	.924
	Two detection limits							
	$n = 12$				$n = 16$			
(P_{DL_1}, P_{DL_2})	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
(.1,.2)	.933	.950	.950	.950	.936	.950	.945	.952
(.1,.3)	.945	.947	.951	.946	.944	.945	.949	.952
(.2,.2)	.950	.949	.953	.951	.945	.954	.950	.945
(.2,.3)	.940	.944	.953	.953	.944	.946	.956	.948
(.1,.5)	.945	.950	.946	.949	.953	.953	.945	.945
	$n = 20$				$n = 26$			
(P_{DL_1}, P_{DL_2})	$a = .5$	$a = 1$	$a = 2$	$a = 3$	$a = .5$	$a = 1$	$a = 2$	$a = 3$
(.1,.2)	.931	.948	.945	.941	.933	.950	.951	.951
(.1,.3)	.942	.953	.951	.952	.951	.951	.947	.951
(.2,.2)	.942	.945	.951	.941	.947	.951	.951	.951
(.2,.3)	.949	.946	.954	.952	.951	.950	.951	.946
(.1,.5)	.934	.956	.953	.946	.951	.954	.952	.946

Note. P_{DL_i} = probability that a concentration is less than the detection limit DL_i; UPLs = upper prediction limits.

Even for the shape parameter $a = .5$, the coverage probabilities are close to the nominal level. Thus, the fiducial UPLs for the mean of a future sample are very satisfactory, and these UCLs can be safely used in applications.

Finally, we carried out some limited coverage studies on 95% UPLs that include at least l of m future observations from each of r locations. These coverage probabilities for $n = 12$ and some values of (r,m,l) are presented in Table 9. We observe in Table 9 that the coverage probabilities are very close to the nominal level .95 for all values of (r,m,l) considered. The coverage studies support that the fiducial approach for this type of prediction is accurate even for small shape parameter.

In general, the coverage probabilities are expected to be smaller than the nominal levels if the percentage of censored observations is high, say, 70% or more. In such situations, sample sizes should be at leat 20 for our methods to work satisfactorily. We also note that the normal approximation to cube-root-transformed samples is satisfactory provided the shape parameter $a \geqslant .5$. If a is less than 0.5, then the CIs are expected to be appreciably anti-conservative.

4.7 | Examples: censored case

Example 3. The data in Table 10 are concentrations of triphenyltin (TPT) measured in a sediment core given in Fent and Hunn (1991). Concentrations of TPT are in μg/kg dry weight. There are five nondetects that are below the detection limit 2. Gamma probability plot for the uncensored data in Figure 1 indicates that the data fit a gamma distribution well. The MLEs of μ and σ based on cube-root-transformed samples are 2.4401 and 1.6419, respectively. Using Algorithm 3 with 100,000 runs, we estimated 95% CI for the mean as (21.20, 72.98). That is, we can conclude with 94% confidence that the mean concentration is somewhere between 21.20 and 72.98. Similarly, we find 95% CI for the shape parameter as (.251, .757), and 95% CI for the scale parameter as (41.3, 215.9).

TABLE 8 Coverage probabilities of 95% UPLs for the mean of a future sample of size m based on a background sample of size n

	Single detection limit							
	(n = 12, m = 4)				**(n = 12, m = 8)**			
P_{DL_1}	**a = .5**	**a = 1**	**a = 2**	**a = 3**	**a = .5**	**a = 1**	**a = 2**	**a = 3**
.1	.932	.950	.948	.951	.940	.950	.951	.950
.2	.941	.953	.955	.951	.935	.952	.955	.944
.3	.943	.955	.956	.953	.939	.951	.940	.954
.5	.950	.949	.949	.952	.952	.944	.948	.952
.6	.940	.952	.944	.947	.945	.934	.948	.946
.7	—	—	—	—	.941	.940	.945	.940
	(n = 16, m = 4)				(n = 16, m = 10)			
P_{DL_1}	a = .5	a = 1	a = 2	a = 3	a = .5	a = 1	a = 2	a = 3
.1	.942	.950	.946	.953	.942	.946	.954	.950
.2	.941	.951	.956	.951	.941	.955	.951	.952
.3	.954	.947	.950	.955	.946	.951	.947	.946
.5	.947	.944	.950	.945	.950	.951	.951	.945
.6	.940	.947	.944	.946	.942	.945	.947	.936
.7	.944	.944	.941	.943	.941	.938	.943	.924
	Two detection limits							
	(n = 12, m = 4)				(n = 12, m = 6)			
(P_{DL_1}, P_{DL_2})	a = .5	a = 1	a = 2	a = 3	a = .5	a = 1	a = 2	a = 3
(.1,.2)	.933	.950	.951	.944	.939	.952	.945	.951
(.1,.3)	.945	.947	.945	.953	.944	.952	.950	.951
(.2,.2)	.950	.949	.943	.951	.945	.946	.944	.944
(.2,.3)	.940	.944	.954	.949	.944	.949	.956	.954
(.1,.5)	.945	.950	.956	.949	.943	.948	.953	.954
	(n = 16, m = 4)				(n = 16, m = 8)			
(P_{DL_1}, P_{DL_2})	a = .5	a = 1	a = 2	a = 3	a = .5	a = 1	a = 2	a = 3
(.1,.2)	.941	.950	.950	.950	.943	.953	.947	.945
(.1,.3)	.939	.951	.953	.946	.941	.947	.949	.948
(.2,.2)	.944	.955	.946	.946	.947	.946	.950	.951
(.2,.3)	.943	.949	.947	.953	.941	.951	.947	.955
(.1,.5)	.939	.952	.950	.954	.938	.944	.951	.953

P_{DL_i} = probability that a concentration is less than the detection limit DL_i.

Using Algorithm 4 with 100,000 runs, we found a 95% UCL for the 90th percentile of the distribution of concentration as 199.3. That is, 90% of concentration levels are no more than 199.3 with confidence .95.

Example 4. In order to illustrate the methods for samples with nondetects, let us assume that there are two DLs, namely, $DL_1 = 35$ and $DL_2 = 43$, in alkalinity concentration data in Example 1. The original data in Table 4 with six nondetects are arranged as in Table 11.

There are two nondetects below $DL_1 = 35$ and four nondetects below $DL_2 = 45$. After taking cube-root transformation of the above data and cube-root transformation of the DLs, we computed the MLEs $\hat{\mu}_0 = 3.7826$ and $\hat{\sigma}_0 = .4852$. The 95% UCL for the mean calculated using Algorithm 3 with 100,000 runs as 64.95. Notice that this UCL is very close to the UCL 65.12, which is based on the uncensored samples in Table 4. We also computed 90% CIs for the mean as (50.36, 64.95), for the shape parameter as (3.79, 11.24) and for the scale parameter as (5.10, 15.44).

Using Algorithm 4 with 100,000 runs, we estimated 95% UPLs for the means of samples of sizes 5, 10, and 15 as 76.7, 72.2, and 70.1, respectively. This means that, for example, the mean concentration in a future sample of size 15 will be no more than 70.1 with confidence 95%. We also notice that all these UPLs are close to the corresponding UPLs 75.6, 71.4, and 69.6 based on the uncensored sample in Example 1.

Furthermore, using Algorithm 5, we found a 95% UCL for the 90th percentile as 102.90, which is larger than the UCL 97.71 based on the uncensored sample in Example 1.

Example 5. To illustrate the methods for data with nondetects, let us suppose that there are three detection limits $DL_1 = .5$, $DL_2 = 1$ and $DL_3 = 1.4$ in vinyl chloride data in Table 5. The data with nondetects are as shown in Table 12.

TABLE 9 Coverage probabilities of 95% UPLs that contain at least l of m observations at each of r locations

$n = 12$				a						a		
(PDL_1, PDL_2)	r	m	l	.5	1	2	r	m	l	.5	1	2
(.1, .2)	1	3	1	.95	.95	.95	4	2	1	.93	.94	.95
(.1, .3)				.95	.94	.95	4	3	1	.95	.95	.95
(.2, .2)				.94	.95	.95	4	4	1	.95	.95	.95
(.2, .3)				.95	.95	.95	4	5	2	.95	.95	.95
(.1, .5)				.95	.96	.95	4	6	2	.95	.95	.95
(.1, .2)	1	4	2	.95	.95	.95	4	2	1	.93	.94	.95
(.1, .3)				.96	.94	.95	4	3	1	.95	.95	.95
(.2, .2)				.95	.95	.95	4	4	1	.95	.95	.95
(.2, .3)				.96	.95	.95	4	5	2	.95	.95	.95
(.1, .5)				.95	.96	.95	4	6	2	.95	.95	.95
(.1, .2)	2	2	1	.94	.95	.95	4	2	1	.93	.94	.95
(.1, .3)				.95	.94	.95	4	3	1	.95	.95	.95
(.2, .2)				.95	.95	.95	4	4	1	.95	.95	.95
(.2, .3)				.96	.95	.95	4	5	2	.95	.95	.95
(.1, .5)				.95	.96	.95	4	6	2	.95	.95	.95
(.1, .2)	2	5	2	.94	.95	.95	4	2	1	.93	.94	.95
(.1, .3)				.95	.94	.95	4	3	1	.95	.95	.95
(.2, .2)				.95	.95	.95	4	4	1	.95	.95	.95
(.2, .3)				.96	.95	.95	4	5	2	.95	.95	.95
(.1, .5)				.95	.96	.95	4	6	2	.95	.95	.95
(.1, .2)	5	10	6	.94	.95	.95	4	2	1	.93	.94	.95
(.1, .3)				.95	.94	.95	4	3	1	.95	.95	.95
(.2, .2)				.95	.95	.95	4	4	1	.95	.95	.95
(.2, .3)				.96	.95	.95	4	5	2	.95	.95	.95
(.1, .5)				.95	.96	.95	4	6	2	.95	.95	.95

P_{DL_i} = probability that a concentration is less than the detection limit DL_i.

TABLE 10 Concentrations of triphenyltin

51	29	71	69	34	56	83	<2	<2
107	35	<2	26	4	10	<2	2	<2

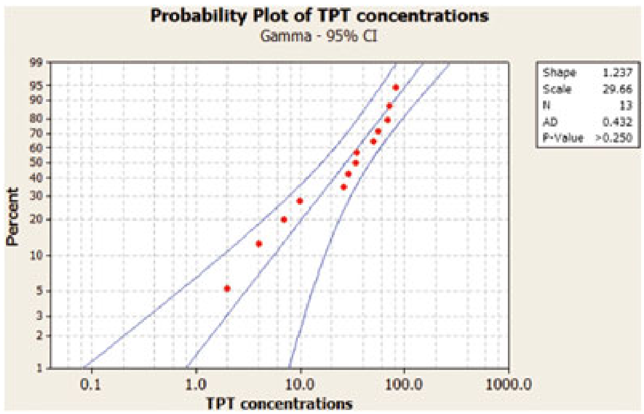

FIGURE 1 At each of the 160 locations, we plot the parameter estimates for three selected variables: air temperature, the cloud contrast, and turbulent kinetic energy

Notice that there are nine nondetects, which means the sample includes a little over 25% nondetects. After taking cube-root transformation of the data and DLs, we calculated the MLEs $\hat{\mu}_0 = 1.0736$ and $\hat{\sigma}_0 = .43297$. Using Algorithm 3 with 100,000 runs, the 95% UCL for the mean vinyl concentration was estimated as 2.63. The 95% UCL for the 90th percentile (using Algorithm 4 with 100,000 runs) is 6.42. These two UCLs are larger than the corresponding UCLs 2.53 and 5.81 based on the complete uncensored sample of 34 measurements. Recall that the smaller UCLs are better in terms of precision. Thus, the loss of information due to nondetects caused a little reduction in precision.

Using Algorithm 5, we also calculated 95% UPLs for the means of future samples of sizes 5, 10, and 15 as 3.90, 3.40, and 3.17, respectively. These three UPLs are close to the corresponding UPLs 3.66, 3.20, and 3.02 based on uncensored sample in Example 2.

Finally, for some selected values of (r,l,m), we computed 95% UPLs that include at least l of m vinyl chloride concentrations from each of r locations. These UPLs for the censored and uncensored cases are given in Table 13. The UPLs for the uncensored case are taken from Krishnamoorthy *et al.* (2008), and the UPLs for the censored case were computed using Algorithm 6 with 100,000 runs. Note that the UPLs based on censored and censored samples are very close when (r,l,m) = (1,1,2) and (10, 1, 3). To interpret the results in Table 13,

TABLE 11 Alkalinity concentrations: censored sample obtained from data in Table 4

58	**82**	**<43**	**<35**	**118**	**96**	**49**	**54**	**<43**	**51**	**66**	**89**	**<43**	**51**
54	55	59	<43	39	40	60	63	59	70	<35	52	79	

TABLE 12 Vinyl chloride concentrations: censored sample obtained from data in Table 5

5.1	**2.4**	**<.5**	**.5**	**2.5**	**<.5**	**6.8**	**1.2**	**<1.4**	**<1**	**5.3**	**2.3**
1.8	1.2	1.3	<1.4	.9	3.2	1.0	.9	<.5	.6	8.0	.4
2.7	.2	2.0	<.5	.5	<1.4	2.0	2.9	<.5	4.0		

TABLE 13 95% UPLs that include at least l of m vinyl chloride concentrations from each of r locations based on uncensored and censored and censored samples

r	l	m	Uncensored	Censored
1	1	2	2.89	2.95
10	1	2	5.20	5.59
10	1	3	3.48	3.55
10	2	3	6.37	6.96

note that the 95% UPL is 6.37 when $(r,l,m) = (10,2,3)$. This means that at least 2 in a future sample of 3 concentrations from each of 10 locations are no more than 6.37 with confidence 95%.

5 | CONCLUDING REMARKS

Most of the methods proposed in the literature for estimation and prediction involving a gamma distribution are likelihood-based. Even though the MLEs are not in closed-form, and they are calculated using some iterative scheme, the likelihood-based methods are not difficult to use. Krishnamoorthy *et al.* (2008) have presented simple methods for finding tolerance limits and prediction limits, which are essentially normal-based methods applied to cube-root-transformed samples. In this article, we proposed fiducial method that can be used to find approximate solutions to all the problems considered in Krishnamoorthy *et al.* (2008), in addition to the problems of estimating the mean and predicting the mean of a future sample. Furthermore, the fiducial method can be readily applied to handle samples with multiple DLs. For the uncensored case, the proposed methods require only the arithmetic mean and standard deviation of the cube root transformed samples to find approximate solutions, which makes the proposed methods more appealing. However, the methods for the censored case involve repeated calculation of the MLEs of the normal parameters. In order to help environmentalists and practitioners in other areas of sciences, we provided R codes as a supplemental materials and also posted at http://www.ucs.louisiana.edu/~kxk4695/. Furthermore, we have evaluated the coverage probabilities of all approximate methods for their accuracy. Overall, our coverage studies indicate that the methods are accurate, and they can be safely used in application as long as the shape parameter is not too small.

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SUPPORTING INFORMATION

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