Ground Water Monitoring&Remediation

Simultaneous Gamma Prediction Limits for Ground Water Monitoring Applications

by Robert D. Gibbons and Dulal K. Bhaumik

Abstract

Common problems in the analysis of environmental monitoring data are nonnormal distributions (i.e., right skewed such as gamma and lognormal) and the presence of moderate to large numbers of nondetects (i.e., data below a detection or quantification limit). When new monitoring measurements are compared to background (e.g., comparison of a new downgradient ground water measurement to a series of background or upgradient ground water monitoring measurements), prediction intervals are often the statistical method of choice. A limitation of the usual application of normal prediction limits in the analysis of environmental data is the assumption of normality, which is often violated by both extreme concentrations (in background) and the presence of censored data (i.e., nondetects). While nonparametric alternatives are available, they often require larger numbers of background samples than are typically available in routine practice. This paper extends the literature on normal and nonparametric simultaneous prediction intervals to the case of the gamma distribution, which can accommodate a wide variety of nonnormal distributions (with skewed right tails) and the presence of nondetects. Gamma prediction limits are excellent candidates for routine application to ground water monitoring networks at waste disposal facilities and/or other relevant environmental monitoring applications. The method is illustrated using example ground water detection monitoring data. The paper includes a series of tables that can be used for routine application of the statistical methodology.

Introduction

A critical problem in the application of statistical methods to environmental monitoring data is the simultaneous presence of nonnormal distribution of constituent concentrations and the presence of nondetects. Nondetects are the result of a measured concentration being below the instrument's limit of detection (Currie 1968). In many cases, the majority of the measurements can be reported as nondetects, making traditional application of statistical methods difficult at best. A leading statistical tool for environmental detection monitoring programs is the prediction limit (Gibbons 1994). A prediction limit is a statistical tool that specifies the upper (or lower) bound on the concentrations distribution that has a probability less than α of being exceeded by the next single measurement drawn from the distribution. For example, in ground water monitoring programs at waste disposal facilities, background data are often collected from hydraulically upgradient ground water monitoring wells, a 95% confidence prediction limit is computed, and each new chemical measurement from a well located hydraulically downgradient of the facility is then compared to the upper prediction limit (UPL). If the measured concentration in the downgradient well is greater than the UPL, then a statistically significant exceedance is declared and further investigation is required. Over the years, statistical researchers have extended the use of UPLs to include simultaneous comparisons of multiple constituents and monitoring wells, resampling plans, nonnormal distributions, and nonparametric alternatives (see Davis and McNichols 1994, and Gibbons 1994, for a review of this work). When the data are both nonnormal and censored (i.e., consist of a mixture of detected concentrations and nondetects), nonparametric prediction limits are typically the method of choice (Gibbons 1990, 1991, 1994; Davis and McNichols 1999; Gibbons and Coleman 2001). However, there are many cases in which the number of available background measurements is insufficient to ensure an adequate overall confidence level using nonparametric prediction limits. In these cases (i.e., when there is a large number of low values and/or nondetect values), Poisson prediction limits (Gibbons 1987) have been used as a somewhat viable alternative; however, Poisson prediction limits have limited statistical power to detect real contamination when it is present and are not invariant with respect to transformation of scale (e.g., different limits are obtained if the data are expressed in mg/L vs. μg/L).

It should be noted that in general, prediction intervals are most useful for comparison of new measurements to background. This distinction is important as it underlies why prediction limits have received considerably less attention in long-term site assessments, and corrective action monitoring, where interest is more focused on assessing long-term trends and comparisons to regulatory standards (see Gibbons and Coleman 2001, and long-term monitoring optimization methods such as the MAROS system, Aziz et al. 2004).

Recently, Bhaumik and Gibbons (2005) derived simultaneous prediction limits based on the gamma distribution that can be easily adapted to the problem of nonnormally distributed monitoring constituents with a wide variety of detection frequencies. Given the parametric form of these prediction limits, they can be used regardless of the background sample size and even when the majority of the data are not detected. In the following sections, we (1) discuss the gamma distribution and corresponding gamma prediction limits; (2) present a relevant illustration of their use; (3) examine their statistical power characteristics; (4) compare them to normal and nonparametric alternatives; and (5) provide tabulations that can be used for routine application of this statistical methodology.

The Gamma Distribution

The gamma distribution has been used extensively in the physical sciences. For example, in industrial engineering, Davis (1952) and Barlow and Proschan (1965) pointed out the importance of a gamma distribution for the failure times of complex systems under continuous repair and maintenance. The use of a gamma distribution is more appropriate than a normal distribution when the data have a skewed distribution with a long right tail and when variability and concentration are related as they are in the case of many environmental constituents (Gibbons and Coleman 2001). Moreover, a gamma distribution approaches a normal distribution when its shape parameter becomes large. When the underlying distribution is gamma, the use of Student's t distribution and the corresponding assumption of normality are not justified as it is not based on the correct sufficient statistics.

We denote the shape parameter by κ and the scale parameter by θ of a two-parameter gamma distribution. For example, Figure 1 presents four gamma distributions with $\theta = 1$ and $\kappa = 0.5$, 1, 2, and 5, respectively. As shown in Figure 1, when κ is small, the distribution looks like a Poisson distribution with considerable mass at or near zero and a few extreme concentrations. When κ is large (e.g., $\kappa = 5$), the distribution looks normal. Change in the scale parameter (θ), not shown in Figure 1, spreads the distribution out, acting like the variance of a normal distribution.

Figure 1 clearly reveals that the gamma distribution can take on a wide variety of shapes that are relevant for constituent distributions with a wide variety of levels of censoring. Small values of κ are representative of highly censored distributions (i.e., few detected concentrations, e.g., benzene or arsenic), whereas large values of κ are representative of consistently detected constituents (e.g., chloride or conductance). Even if the data are in fact normally distributed, the gamma distribution can be used to model

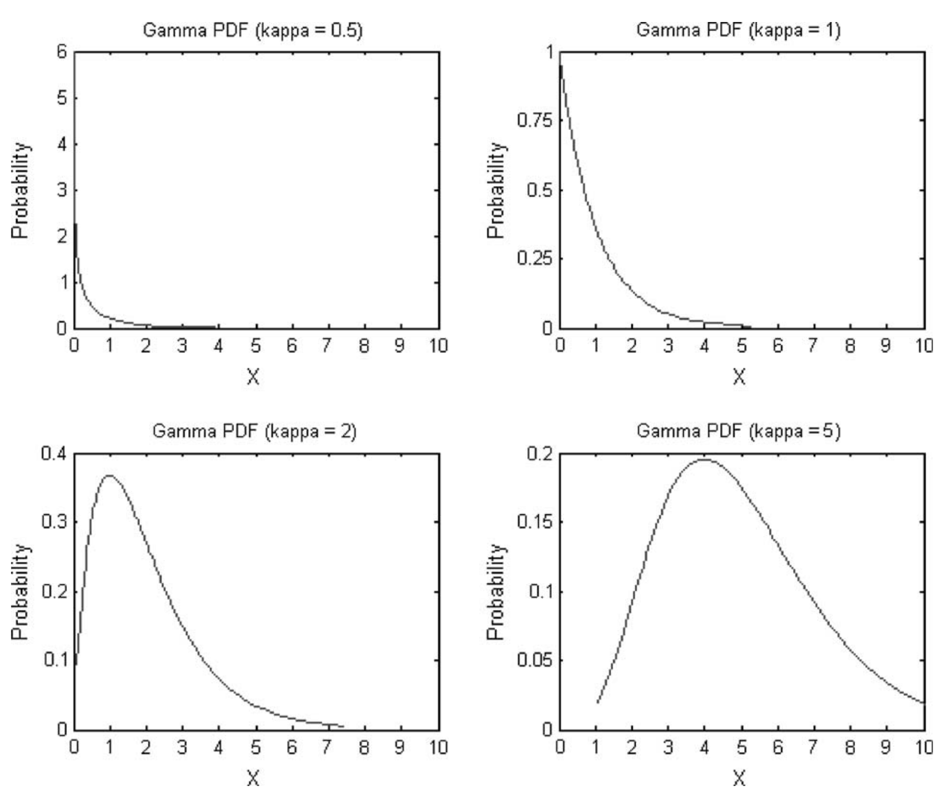

Figure 1. Plot of various gamma distributions.

them. Furthermore, the mean and variance of the gamma distribution are related, a feature that is a signature of environmental data (Gibbons and Coleman 2001).

Statistically, let $x_1, x_2, \ldots, x_n$ be a random sample of size n drawn from a gamma population for which we want to estimate the unknown parameters κ and θ. Let us denote the arithmetic and geometric means (the exponential of the mean of the natural log-transformed data) based on this random sample by $\bar{x}$ and $\tilde{x}$, respectively. The maximum likelihood estimators of θ and κ denoted by $\hat{\theta}$ and $\hat{\kappa}$ are solutions to the following equations:

$$\ln(\hat{\kappa}) - \psi(\hat{\kappa}) = \ln(\bar{x}/\tilde{x}), \text{and } \hat{\kappa}\hat{\theta} = \bar{x} \qquad (1)$$

where ψ denotes a digamma or Euler's psi function. For a complete description of statistical results on a gamma distribution, see Johnson et al. (1994). The mean and variance of x are:

$$\mathrm{E}(x) = \kappa\theta, \text{and } \mathrm{V}(x) = \kappa\theta^2 \qquad (2)$$

For convenience, our tabled values of prediction limit factors do not require computation of κ or θ.

Simultaneous Gamma Prediction Limits

Following Davis and McNichols' (1987) result for the normal distribution, and Gibbons' 1990, 1991, 1994, and Davis and McNichols' (1999) result for the nonparametric case, Bhaumik and Gibbons (2005) derived simultaneous gamma prediction limits for the next p of m samples at each of r locations. The p represents the number of samples required to be less than the prediction limit (at a given sampling location for a given constituent) in order to pass, and m represents the total number of samples that are collected at each monitoring location for each constituent. For example, if in the presence of an initial exceedance, a single verification resample is obtained and statistical failure is only recorded if both the initial sample and the resample exceed the prediction limit, then $p = 1$ and $m = 2$. If two resamples are taken and failure is indicated only if both resamples (and the initial sample) exceed the UPL, then $p = 1$ and $m = 3$. Finally, if two resamples are collected in the presence of an initial exceedance and failure is indicated if either resample exceeds the UPL, then $p = 2$ and $m = 3$. In the present context, r is the number of monitoring locations. To adjust for multiple monitoring constituents, we would adjust the perconstituent type I error rate (i.e., false-positive rate) to $\alpha = \alpha^*/d$, where d is the number of constituents and α^* is the overall site-wide type I error rate (e.g., $\alpha^* = .05$). For example, with $d = 10$ constituents, $\alpha = .05/10 = .005$.

To ensure ease of use, Bhaumik and Gibbons (2005) derived approximate upper gamma prediction limits based on a scaled standard deviation from the sample mean. Let $S = \sqrt{\hat{\kappa}}\hat{\theta}$, where S is an estimate of the population standard deviation. Thus, the right-sided UPL for a single future observation X coming from the aforementioned gamma distribution is expressed as $\bar{x} + kS$ for a k. Bhaumik and Gibbons (2005) derived a general method for obtaining constants k for different values of κ, θ, r, p, m, and n.

It should be noted that the derivation does not incorporate correlation of the multiple constituents being compared. In general, (1) this correlation is unknown; (2) the available number of samples is too small to provide a good estimate of the intercorrelations among all constituents; and (3) there is no reason to believe that the same correlation applies under uncontaminated and contaminated conditions. As such, the adjustment for multiple comparisons due to multiple constituents is conducted under the assumption of independence, leading to a conservative test. The test is conservative in that it will lead to slightly smaller prediction limits than would be obtained had we known the true correlation among the analytes, therefore leading to an environmentally conservative decision rule.

Simulation Study

To examine the accuracy of the gamma prediction limits and to compare their accuracy to normal and nonparametric alternatives, we conducted the following simulation study. In our study, we set $\theta = 1.0$ and considered values of κ equal to 0.25, 0.5, 1.0, 1.5, 2.0, and 5.0. Background sample sizes of $n = 8$, 20, 50, and 100 were examined. Studies were performed for $r = 1$, 10, and 25 locations. Finally, we examined three sampling plans (1) $p = 1$ and $m = 2$; (2) $p = 1$ and $m = 3$; and (3) $p = 2$ and $m = 3$. Results of the simulation study are presented in Table 1. Table 1 reveals that in all cases, the gamma prediction limits are close to achieving their intended nominal error rates. Even for small sample size ($n = 8$), large values of κ, and $r = 25$, the overall type I error rate never exceeded 16%. As sample size increased to 20 and larger, the gamma prediction limits were close to attaining the nominal 5% rate in all cases, whereas bias in the normal prediction limit was not attenuated by increasing sample size (Table 1). Results for $p = 1$ and $m = 3$ provided the best overall results, whereas the infrequently used $p = 2$ and $m = 3$ provided the worst overall results. By contrast, overall type I error rates were as high as 40% for normal prediction limits and almost 50% for nonparametric prediction limits. However, for a single location (i.e., $r = 1$), type I error rates for normal limits were in many cases <1%, particularly for $p = 1$ and $m = 3$. As expected, type I error rates for nonparametric prediction limits were highly dependent on background sample size n and the number of monitoring locations r. While the confidence level is easily predicted from theory, practitioners often set the prediction limit equal to the maximum background concentration regardless of n, p, m, or r, and as a result, the wide range in overall type I error rates observed in Table 1 is characteristic of routine practice.

Statistical Power

The previous section reveals that gamma prediction limits provide excellent control over type I error rates but provide no evidence that they are effective at controlling type II error (i.e., false-negative) rates. To investigate the statistical power (i.e., one minus the false-negative rate) of

Table 1
Simulation Study of Gamma and Normal Simultaneous UPLs

Sampling Plan (*p* of *m*)	*n*	*κ*	Type I Error Rate Gamma	Normal	Nonparametric
$\theta = 1.0$ and $r = 1$ location					
1 of 2	8	0.25	.048	.038	.023
1 of 2	20	0.25	.037	.019	.001
1 of 2	50	0.25	.047	.024	.003
1 of 2	100	0.25	.061	.021	.000
1 of 2	8	0.50	.072	.064	.031
1 of 2	20	0.50	.049	.035	.003
1 of 2	50	0.50	.046	.023	.000
1 of 2	100	0.50	.049	.026	.000
1 of 2	8	1.00	.040	.036	.020
1 of 2	20	1.00	.042	.041	.008
1 of 2	50	1.00	.050	.031	.000
1 of 2	100	1.00	.052	.037	.000
1 of 2	8	1.50	.059	.047	.022
1 of 2	20	1.50	.059	.050	.006
1 of 2	50	1.50	.045	.037	.000
1 of 2	100	1.50	.039	.024	.000
1 of 2	8	2.00	.067	.055	.030
1 of 2	20	2.00	.043	.033	.003
1 of 2	50	2.00	.064	.048	.000
1 of 2	100	2.00	.047	.044	.000
1 of 2	8	5.00	.061	.053	.029
1 of 2	20	5.00	.061	.052	.004
1 of 2	50	5.00	.061	.056	.000
1 of 2	100	5.00	.050	.043	.001
1 of 3	8	0.25	.051	.014	.003
1 of 3	20	0.25	.048	.004	.000
1 of 3	50	0.25	.049	.007	.000
1 of 3	100	0.25	.035	.007	.000
1 of 3	8	0.50	.054	.029	.015
1 of 3	20	0.50	.055	.017	.000
1 of 3	50	0.50	.052	.009	.000
1 of 3	100	0.50	.046	.009	.000
1 of 3	8	1.00	.054	.035	.009
1 of 3	20	1.00	.045	.016	.000
1 of 3	50	1.00	.045	.019	.000
1 of 3	100	1.00	.049	.019	.000
1 of 3	8	1.50	.056	.038	.008
1 of 3	20	1.50	.061	.029	.000
1 of 3	50	1.50	.058	.029	.001
1 of 3	100	1.50	.056	.026	.000
1 of 3	8	2.00	.048	.037	.008
1 of 3	20	2.00	.058	.036	.001
1 of 3	50	2.00	.074	.041	.000
1 of 3	100	2.00	.050	.024	.000
1 of 3	8	5.00	.059	.042	.007
1 of 3	20	5.00	.048	.036	.000
1 of 3	50	5.00	.049	.034	.000
1 of 3	100	5.00	.056	.035	.000
2 of 3	8	0.25	.045	.065	.043
2 of 3	20	0.25	.042	.034	.005
2 of 3	50	0.25	.050	.026	.002
2 of 3	100	0.25	.042	.024	.000
2 of 3	8	0.50	.071	.090	.068
2 of 3	20	0.50	.043	.039	.014
2 of 3	50	0.50	.043	.033	.002
2 of 3	100	0.50	.055	.047	.001
2 of 3	8	1.00	.074	.078	.061
2 of 3	20	1.00	.062	.060	.008
2 of 3	50	1.00	.040	.040	.001
2 of 3	100	1.00	.056	.053	.002
2 of 3	8	1.50	.067	.072	.054
2 of 3	20	1.50	.063	.060	.013
2 of 3	50	1.50	.043	.046	.004
2 of 3	100	1.50	.066	.064	.001
2 of 3	8	2.00	.075	.065	.055
2 of 3	20	2.00	.071	.071	.014
2 of 3	50	2.00	.071	.067	.001
2 of 3	100	2.00	.040	.038	.000

Table 1 (Continued)
Simulation Study of Gamma and Normal Simultaneous UPLs

Sampling Plan (*p* of *m*)	*n*	*κ*	Type I Error Rate Gamma	Normal	Nonparametric
2 of 3	8	5.00	.079	.064	.067
2 of 3	20	5.00	.050	.049	.012
2 of 3	50	5.00	.053	.049	.003
2 of 3	100	5.00	.051	.050	.000
$\theta = 1.0$ and $r = 10$ locations					
1 of 2	8	0.25	.066	.165	.165
1 of 2	20	0.25	.043	.083	.033
1 of 2	50	0.25	.049	.063	.007
1 of 2	100	0.25	.055	.065	.001
1 of 2	8	0.50	.065	.136	.150
1 of 2	20	0.50	.054	.102	.041
1 of 2	50	0.50	.064	.086	.011
1 of 2	100	0.50	.051	.074	.003
1 of 2	8	1.00	.096	.134	.169
1 of 2	20	1.00	.069	.106	.046
1 of 2	50	1.00	.047	.068	.002
1 of 2	100	1.00	.040	.065	.000
1 of 2	8	1.50	.079	.100	.152
1 of 2	20	1.50	.065	.097	.038
1 of 2	50	1.50	.050	.087	.009
1 of 2	100	1.50	.049	.073	.004
1 of 2	8	2.00	.098	.103	.176
1 of 2	20	2.00	.060	.083	.033
1 of 2	50	2.00	.050	.070	.007
1 of 2	100	2.00	.060	.078	.002
1 of 2	8	5.00	.117	.104	.172
1 of 2	20	5.00	.080	.086	.050
1 of 2	50	5.00	.058	.070	.010
1 of 2	100	5.00	.061	.076	.006
1 of 3	8	0.25	.043	.061	.042
1 of 3	20	0.25	.046	.034	.007
1 of 3	50	0.25	.035	.014	.000
1 of 3	100	0.25	.051	.018	.000
1 of 3	8	0.50	.062	.067	.048
1 of 3	20	0.50	.054	.047	.004
1 of 3	50	0.50	.054	.026	.001
1 of 3	100	0.50	.051	.028	.000
1 of 3	8	1.00	.078	.084	.052
1 of 3	20	1.00	.057	.051	.006
1 of 3	50	1.00	.055	.038	.001
1 of 3	100	1.00	.047	.029	.000
1 of 3	8	1.50	.070	.062	.046
1 of 3	20	1.50	.060	.050	.004
1 of 3	50	1.50	.060	.039	.001
1 of 3	100	1.50	.060	.041	.000
1 of 3	8	2.00	.069	.061	.051
1 of 3	20	2.00	.052	.047	.004
1 of 3	50	2.00	.057	.046	.001
1 of 3	100	2.00	.041	.032	.000
1 of 3	8	5.00	.080	.057	.047
1 of 3	20	5.00	.052	.044	.004
1 of 3	50	5.00	.058	.052	.001
1 of 3	100	5.00	.049	.043	.000
2 of 3	8	0.25	.068	.232	.266
2 of 3	20	0.25	.067	.189	.096
2 of 3	50	0.25	.040	.127	.019
2 of 3	100	0.25	.057	.124	.003
2 of 3	8	0.50	.104	.225	.304
2 of 3	20	0.50	.071	.172	.092
2 of 3	50	0.50	.056	.147	.021
2 of 3	100	0.50	.066	.144	.004
2 of 3	8	1.00	.097	.180	.305
2 of 3	20	1.00	.067	.153	.088
2 of 3	50	1.00	.055	.138	.027
2 of 3	100	1.00	.044	.129	.005
2 of 3	8	1.50	.123	.156	.307
2 of 3	20	1.50	.086	.164	.113
2 of 3	50	1.50	.060	.125	.027
2 of 3	100	1.50	.056	.127	.008
2 of 3	8	2.00	.125	.144	.299

Table 1 (Continued)
Simulation Study of Gamma and Normal Simultaneous UPLs

Sampling Plan (p of m)	n	κ	Type I Error Rate Gamma	Normal	Nonparametric
2 of 3	20	2.00	.064	.132	.082
2 of 3	50	2.00	.062	.126	.026
2 of 3	100	2.00	.056	.119	.006
2 of 3	8	5.00	.115	.083	.273
2 of 3	20	5.00	.080	.104	.088
2 of 3	50	5.00	.056	.107	.018
2 of 3	100	5.00	.048	.103	.006
$\theta = 1.0$ and $r = 25$ locations					
1 of 2	8	0.25	.064	.255	.290
1 of 2	20	0.25	.060	.188	.100
1 of 2	50	0.25	.046	.119	.017
1 of 2	100	0.25	.050	.084	.004
1 of 2	8	0.50	.086	.192	.263
1 of 2	20	0.50	.071	.176	.101
1 of 2	50	0.50	.069	.146	.022
1 of 2	100	0.50	.044	.096	.003
1 of 2	8	1.00	.093	.175	.292
1 of 2	20	1.00	.062	.134	.078
1 of 2	50	1.00	.061	.123	.029
1 of 2	100	1.00	.047	.114	.002
1 of 2	8	1.50	.125	.156	.299
1 of 2	20	1.50	.072	.138	.081
1 of 2	50	1.50	.064	.128	.018
1 of 2	100	1.50	.053	.122	.009
1 of 2	8	2.00	.122	.136	.283
1 of 2	20	2.00	.072	.121	.083
1 of 2	50	2.00	.062	.119	.017
1 of 2	100	2.00	.064	.125	.004
1 of 2	8	5.00	.124	.098	.274
1 of 2	20	5.00	.073	.099	.096
1 of 2	50	5.00	.065	.105	.014
1 of 2	100	5.00	.063	.095	.004
1 of 3	8	0.25	.088	.143	.125
1 of 3	20	0.25	.057	.063	.015
1 of 3	50	0.25	.046	.029	.003
1 of 3	100	0.25	.052	.021	.000
1 of 3	8	0.50	.068	.108	.092
1 of 3	20	0.50	.053	.065	.009
1 of 3	50	0.50	.049	.043	.000
1 of 3	100	0.50	.053	.039	.000
1 of 3	8	1.00	.077	.091	.091
1 of 3	20	1.00	.052	.063	.010
1 of 3	50	1.00	.063	.059	.003
1 of 3	100	1.00	.059	.050	.000
1 of 3	8	1.50	.090	.099	.101
1 of 3	20	1.50	.069	.073	.013
1 of 3	50	1.50	.063	.067	.000
1 of 3	100	1.50	.045	.045	.001
1 of 3	8	2.00	.082	.081	.100
1 of 3	20	2.00	.078	.086	.017
1 of 3	50	2.00	.049	.054	.000
1 of 3	100	2.00	.052	.056	.000
1 of 3	8	5.00	.105	.073	.103
1 of 3	20	5.00	.071	.066	.008
1 of 3	50	5.00	.059	.060	.000
1 of 3	100	5.00	.043	.044	.000
2 of 3	8	0.25	.122	.404	.487
2 of 3	20	0.25	.059	.301	.191
2 of 3	50	0.25	.063	.216	.050
2 of 3	100	0.25	.063	.203	.016
2 of 3	8	0.50	.089	.292	.452
2 of 3	20	0.50	.079	.281	.199
2 of 3	50	0.50	.060	.236	.048
2 of 3	100	0.50	.057	.196	.010
2 of 3	8	1.00	.133	.229	.449
2 of 3	20	1.00	.061	.223	.179
2 of 3	50	1.00	.076	.218	.053
2 of 3	100	1.00	.059	.198	.014
2 of 3	8	1.50	.125	.179	.453
2 of 3	20	1.50	.085	.183	.177
2 of 3	50	1.50	.064	.205	.059
2 of 3	100	1.50	.064	.193	.014
2 of 3	8	2.00	.120	.146	.447
2 of 3	20	2.00	.090	.185	.201
2 of 3	50	2.00	.050	.174	.043
2 of 3	100	2.00	.041	.167	.010
2 of 3	8	5.00	.164	.131	.461
2 of 3	20	5.00	.090	.129	.190
2 of 3	50	5.00	.068	.137	.049
2 of 3	100	5.00	.060	.144	.017

the procedure and to compare it against normal and nonparametric alternatives, a second simulation study was performed. The background distribution was gamma with $\kappa = 0.5$, 1.0, 2.0, and, 5.0 and $\theta = 0.2$. The $n = 20$ background measurements were generated and $m = 2$ future measurements generated for each of $r = 13$ locations. The $r = 13$ was selected because the 95% confidence nonparametric prediction limit for pass 1 of 2 samples in each of 13 locations is defined as the maximum of $n = 20$ background measurements. The alternative hypothesis was generated by sampling the future samples out of a distribution with the same value of κ as the background distribution and $\theta = .4$, .6, .8, and 1.0. The resulting power curves are displayed in Figures 2a through 2d. Figures 2a through 2d reveal that both the gamma and the nonparametric prediction limits achieve their nominal type I error rate of 5% (at $\theta = .2$) for smaller values of κ and come close for large values of $\kappa = 5.0$. By contrast, the normal limit has a type I error rate of >10%, which becomes slightly smaller for larger values of κ. This is consistent with the fact that the gamma distribution tends toward the normal distribution as κ increases in magnitude. In terms of power, the normal limit is most powerful, but at the expense of an inflated type I error rate. The gamma prediction limit achieves its preselected error rate of 5% and has increased power relative to the nonparametric alternative throughout the range of effect sizes. Note that for $\kappa = 5.0$, the scale of the x-axis is restricted to a maximum value of θ of 0.5 (Figure 2d) instead of 1.0 (as in Figures 2a through 2c) because the test is much more powerful for larger values of κ and we wanted to provide a more visually interpretable depiction of the comparison of the power curves for the three methods.

Illustration

To illustrate the problem, consider the following vinyl chloride–detected concentrations (originally presented by Bhaumik and Gibbons 2005) obtained from upgradient background monitoring wells displayed in Table 2. The original data represent all upgradient ground water quality samples in the state of California collected by Waste Management Inc. from 1989 to 1992. The data included 350

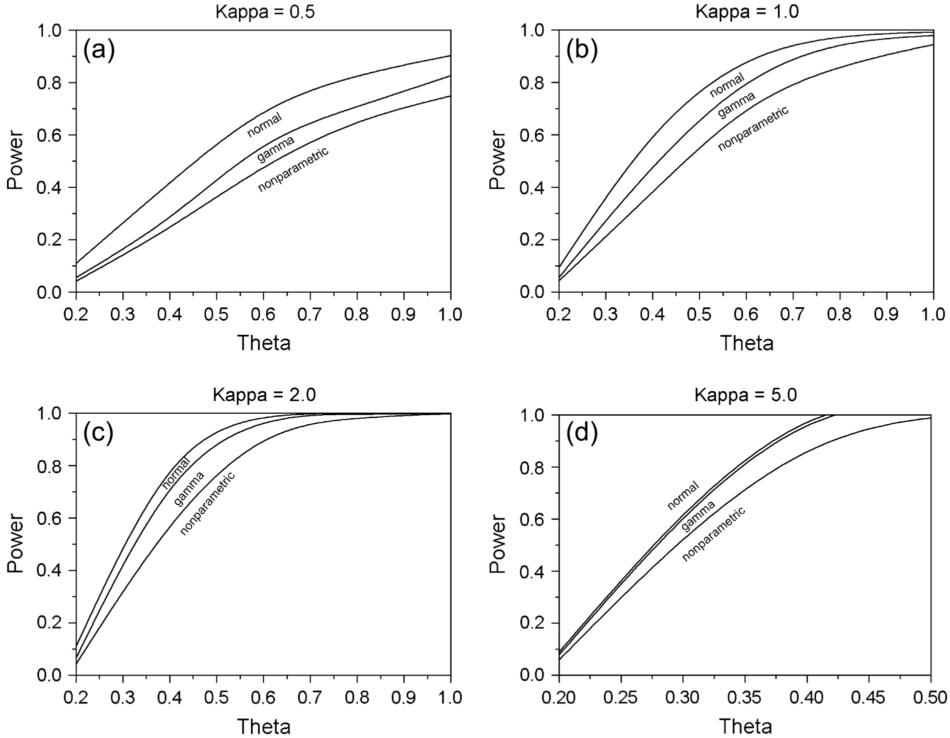

Figure 2. (a) Power curves for gamma, normal, and nonparametric UPLs (κ = 0.5). (b) Power curves for gamma, normal, and nonparametric UPLs (κ = 1.0). (c). Power curves for gamma, normal, and nonparametric UPLs (κ = 2.0). (d) Power curves for gamma, normal, and nonparametric UPLs (κ = 5.0).

samples from 38 upgradient monitoring wells from 11 waste disposal facilities. All analyses were performed using SW846 Method 8240. The data presented here represent the detected concentrations only. An important assumption of the method is that there is no significant trend during the background period.

Figure 3 presents a gamma probability plot corresponding to the data displayed in Table 2. Figure 3 reveals an excellent fit of these data to the gamma distribution. Note that since vinyl chloride is not naturally occurring, it should never be detected in upgradient background monitoring wells, but this is clearly not true in practice.

To begin constructing the UPL, note that we have $n =$ 34 vinyl chloride measurements with mean $\bar{x} = 1.879$ µg/L and standard deviation (S) = 1.823 µg/L. Our estimates of κ and θ are $\hat{\kappa} = 1.063$ and $\hat{\theta} = 1.769$. Now suppose that we have a site with a single future monitoring location $r = 1$ and that in the event of an initial exceedance of the prediction limit, a single verification resample is permitted, failure being indicated only if both the initial and resample both exceed the prediction limit. This is the same as requiring that at least $p = 1$ out of $m = 2$ samples are in bounds. In this case, the 95% confidence UPL is obtained as $\bar{x} + 0.576S = 2.929$ µg/L. Now consider the same sampling scheme, but increase the number of monitoring locations to $r = 10$. In this case, the 95% confidence UPL is obtained as $\bar{x} + 1.835S = 5.224$ µg/L. Shifting the resampling program to including one of two resamples in bounds in the event of an initial exceedance (i.e., $p = 1$ and $m = 3$) decreases the prediction limit to $\bar{x} + 0.901S = 3.521$ µg/L. Finally, increasing the number of resamples in bounds from one to two (i.e., $p = 2$ and $m = 3$) increases the prediction limit to $\bar{x} + 2.441S = 6.330$ µg/L.

To determine the accuracy of the computed prediction limits, we computed actual confidence levels via simulation. Using the estimated aforementioned parameters, we simulated 34 new background measurements from a gamma distribution with parameters $\kappa = 1.063$ and $\theta = 1.769$. For each of the aforementioned scenarios, (1) $r = 1$, $p = 1$, $m = 2$; (2) $r = 10$, $p = 1$, $m = 2$; (3) $r = 10$, $p = 1$, $m = 3$; and (4) $r = 10$, $p = 2$, $m = 3$; prediction limits were computed for the simulated background data ($n = 34$). Based on the specific conditions listed in 1 to 4, m new downgradient monitoring measurements were generated at each of r locations. If fewer than p of m of those generated measurements were in bounds at any of the r locations, a failure was recorded. This process was then repeated 10,000 times and the simulated confidence levels were

Table 2
Detected Vinyl Chloride Concentrations from Upgradient Background Ground Water Monitoring Wells in g/L

5.1	1.2	1.3	0.6	0.5
2.4	0.5	1.1	8.0	0.8
0.4	0.6	0.9	0.4	2.0
0.5	5.3	3.2	2.7	2.9
2.5	2.3	1.0	0.2	0.1
0.1	1.8	0.9	2.0	4.0
6.8	1.2	0.4	0.2	

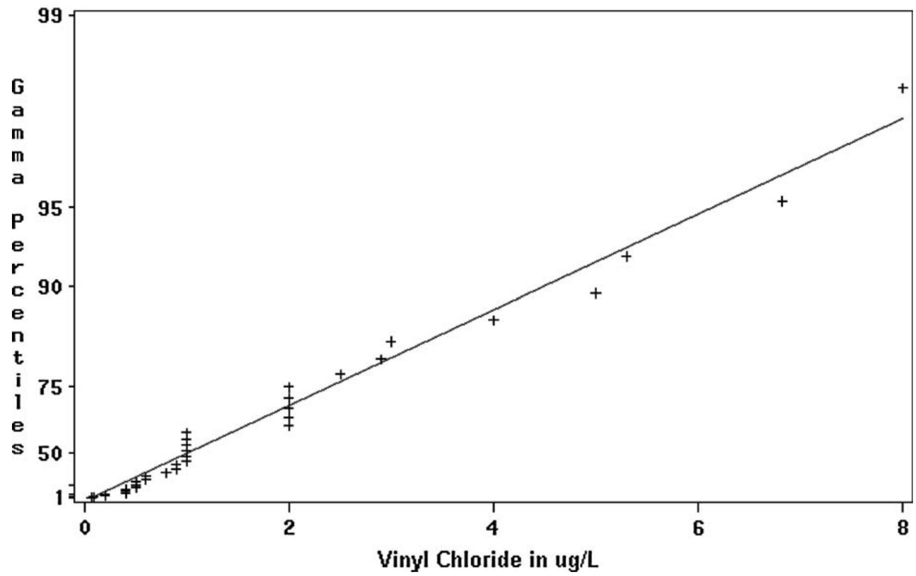

Figure 3. Gamma probability plot for vinyl chloride data.

computed. Simulated confidence levels were .9511, .9408, .9506, and .9417 for conditions 1 to 4, respectively. These results indicate that the prediction limits achieve their intended confidence levels.

The Problem of Nondetects

A potential complication of the methodology described thus far is that it is common for a proportion of the analytic measurements to be reported as less than a limit of detection (Currie 1968). Even if every effort is made to limit the censoring of the data by reporting all measured concentrations, there will still be instances where the analyte is simply not detected in the sample and no concentration estimate is available. In such cases, the U.S. EPA (1992) has advised that either one-half of the detection limit be imputed for the nondetected measurements or that under the assumption of normality or lognormality either Aitchison's (1955) adjustment or Cohen's (1959, 1961) estimator be used to provide estimates of the mean and variance of the censored distribution. The adjusted mean and variance are then used in computing normal or lognormal prediction limits with only limited success (Gibbons 1994, pp. 214–215). Alternatively, when censoring is 50% or more, the U.S. EPA has advocated the use of nonparametric prediction limits as described by Gibbons (1990, 1991) and Davis and McNichols (1999). Since the volatile organic compounds used to illustrate the use of simultaneous gamma prediction limits in this paper are plagued with problems of nondetects, we studied the behavior of these prediction limits for various degrees of censoring. In a limited simulation study based on the vinyl chloride data in the previous example for $r = 1$, $p = 1$, and $m = 2$, we studied the effects of 10%, 25%, 50%, and 75% censoring on the simulated confidence levels obtained over 10,000 simulations. As in the previous illustration, the complete data ($n = 34$ measurements) were generated from a gamma distribution with parameters $\kappa = 1.063$ and $\theta = 1.769$. Given these population parameters, to achieve 10%, 25%, 50%, and 75% censoring, the data were censored at the following cutpoints: 0.2209, 0.5745, 1.3341, and 2.6053. A separate simulation study was performed for each cutpoint (i.e., level of censoring). Any simulated measurement below one of these censoring points was replaced by one-half of the value of the censoring point. This is consistent with the U.S. EPA's use of imputation of one-half of the detection limit for nondetects. Results of the study revealed that the simultaneous gamma prediction limits are, in fact, remarkably robust to both modest and more extreme levels of censoring. Simulated confidence levels were 0.951 for 10% censoring, 0.950 for 25% censoring, 0.947 for 50% censoring, and 0.962 for 75% censoring.

To ensure that the robustness of the method to the presence of censored data generalized to other values of the population parameters, we repeated the simulation study for gamma distributions with parameters $\kappa = 0.5$ and $\theta = 1.0$, and $\kappa = 0.25$ and $\theta = 1.0$ (Table 3). Table 3 reveals that the robustness observed for the original example data generalizes to other values of κ and θ as well.

Finally, it is common to encounter data sets with multiple censoring points. In these cases, imputation of half of each of the different detection limits should provide quite similar results to those obtained here. To test this conjecture, we resimulated data from the original example using 25% censoring, but rather than imputing one-half of a single censoring point, we imputed two different censoring points, one equal to the detection limit and the other equal to one-half of the detection limit, in equal proportions. Results of this simulation with two different censoring points provided an overall confidence level of 0.955, indicating that gamma prediction limits are also robust to the presence of more than one censoring point, a condition that is quite common in environmental data.

The net result is that the routine use of gamma prediction limits for data that contain nondetected concentrations will yield unbiased prediction limit estimates with the

Table 3
Cutpoints and the Corresponding Simulated Confidence Levels for Various Combinations of Gamma Parameters at Different Censoring Levels

Parameters	Censoring Levels			
	10%	25%	50%	75%
$\kappa = 1.063, \theta = 1.769$	0.2209[1] (0.951)[2]	0.5745 (0.950)	1.3341 (0.947)	2.6053 (0.962)
$\kappa = 0.5, \theta = 1.0$	0.0079 (0.952)	0.0508 (0.953)	0.2274 (0.955)	0.6617 (0.974)
$\kappa = 0.25, \theta = 1.0$	0.0000675 (0.953)	0.0026 (0.955)	0.0438 (0.959)	0.2606 (0.969)

[1]Cutpoints.
[2]Simulated confidence levels.

intended nominal type I error rate. For routine practice, this is a major advantage of this methodology.

Tabled Values

To aid in application, we have constructed Table 4, which contains gamma prediction limit factors k for various combinations of n, r, p, m, and $\hat{\kappa}$ that are commonly encountered in practice. The three panels of Table 4 provide prediction limit factors for $\alpha = 0.05$, 0.005, and 0.002, which provide adjustment for 1, 10, and 25 constituents, respectively. Using the values of k found in Table 4, the prediction limit $\bar{x} + kS$ can be computed directly. Furthermore, the values of $\hat{\kappa}$ (5.16, 1.14, 0.62, 0.43, and 0.34) correspond to values of $\bar{x}/\tilde{x}$ equal to .10, .50, 1.00, 1.50, and 2.00, respectively. As such, only the statistics $\bar{x}$, $\tilde{x}$, and S are required to compute the gamma prediction limits. In terms of the sampling plan, Table 4 provides values of k for $p = 1$ and $m = 2$, $p = 1$ and $m = 3$, and $p = 2$ and $m = 3$, which are the three primary sampling plans used in most environmental monitoring programs. The table includes background sample sizes of $n = 8$, 16, 32, and 48, and $r =$ 1, 2, 4, 8, 16, 32, and 64 locations. These values of n, r, p, m, α, and $\hat{\kappa}$ should cover a great many routine applications and can be easily interpolated to include others. For example, a prediction limit for a site with $r = 64$ wells that monitors 25 constituents $\alpha = 0.05/25 = 0.002$ can be constructed using the tabled values. Should other values of k be required, the reader is referred to the original paper by Bhaumik and Gibbons (2005).

Inspection of Table 4 reveals several interesting features. First, for $p = 1$ and $m = 3$, some of the values of k are negative. This indicates that when we only require one of three measurements in bounds, the gamma prediction limit can be less than the arithmetic mean for certain combinations of n, r, and $\hat{\kappa}$. Second, the largest values of k are found for the smallest values of n and $\hat{\kappa}$. Third, as expected, increasing the number of future comparisons r increases k. Finally, of the three sampling plans, one of three in bounds produces the smallest prediction limits, followed by one of two in bounds, followed by two of three in bounds.

It should be noted that when n, κ, and α are small, and the number of monitoring wells is large, the gamma prediction limit factors k can be too large to be of practical value. In these cases, pass 1 of 3 resampling plans should be used, and the number of background samples should be increased if possible. In the interim, $\alpha = 0.05$ could be used as a conservative measure. In general, use of factors of $k > 5$ should be avoided. Using $p = 1$ and $m = 3$, one should generally be able to obtain a value of $k < 5$ for most monitoring programs.

A fundamental difference between normal and gamma prediction limits is that the multiplier k is different for each constituent in the case of a gamma distribution because the multiplier depends on κ. This is not the case for normal prediction limits where the multiplier only depends on n, p, m, r, and α. For this reason, each constituent will have a different multiplier k, when using gamma prediction limits. The values of k in Table 4 are exact for interwell comparisons (i.e., upgradient vs. downgradient), but only approximate for intrawell comparisons (i.e., comparison of each well with its own history). The reason is that the repeated comparison of each of r downgradient monitoring wells to a common upgradient background is directly incorporated into the computation of the prediction limit factor. In intrawell monitoring, there is no correlation because the new monitoring data for each well are compared to that well's own historical background; therefore, the comparisons are independent. The effect of this statistical misspecification is that the prediction limits will be slightly conservative for intrawell monitoring applications (i.e., too small) and will actually provide more than an overall 95% confidence level.

Discussion

Simultaneous gamma prediction limits should provide a useful addition to the arsenal of statistical methods that are useful in ground water monitoring applications in particular and environmental statistics in general. The methodology presented here extends earlier work for the normal distribution (Davis and McNichols 1987) and nonparametric alternatives (Gibbons 1990, 1991; Davis and McNichols 1999) to the case of a gamma distributed random variable. Use of the gamma distribution permits association between the mean and the variance of the distribution, a phenomenon that is commonly observed in practice. Furthermore, the gamma distribution permits analysis of skewed distributions, only some of which were

Table 4

Gamma Prediction Limit Factors k as a Function of n, r, p, m, and $\hat{\kappa}$

			k						k		
n	r	$\hat{\kappa}$	$p = 1$, $m = 2$	$p = 1$, $m = 3$	$p = 2$, $m = 3$	n	r	$\hat{\kappa}$	$p = 1$, $m = 2$	$p = 1$, $m = 3$	$p = 2$, $m = 3$
Prediction limit $= \bar{x} + kS$, $\alpha = 0.05$ (i.e., 1 constituent)											
8	1	5.16	0.896	0.396	1.387	32	1	5.16	0.735	0.253	1.171
8	1	1.14	0.844	0.248	1.518	32	1	1.14	0.602	0.081	1.130
8	1	0.62	0.773	0.130	1.578	32	1	0.62	0.485	−0.036	1.059
8	1	0.43	0.702	0.039	1.611	32	1	0.43	0.388	−0.117	0.984
8	1	0.34	0.641	−0.025	1.626	32	1	0.34	0.313	−0.169	0.920
8	2	5.16	1.239	0.661	1.738	32	2	5.16	1.034	0.481	1.469
8	2	1.14	1.306	0.558	2.051	32	2	1.14	0.960	0.320	1.520
8	2	0.62	1.321	0.456	2.273	32	2	0.62	0.870	0.195	1.506
8	2	0.43	1.313	0.365	2.450	32	2	0.43	0.783	0.100	1.469
8	2	0.34	1.296	0.293	2.586	32	2	0.34	0.713	0.033	1.429
8	4	5.16	1.585	0.932	2.079	32	4	5.16	1.328	0.709	1.755
8	4	1.14	1.815	0.903	2.608	32	4	1.14	1.335	0.574	1.914
8	4	0.62	1.966	0.845	3.035	32	4	0.62	1.292	0.456	1.972
8	4	0.43	2.071	0.782	3.414	32	4	0.43	1.235	0.357	1.990
8	4	0.34	2.158	0.727	3.749	32	4	0.34	1.183	0.282	1.990
8	8	5.16	1.919	1.192	2.410	32	8	5.16	1.613	0.927	2.032
8	8	1.14	2.351	1.264	3.185	32	8	1.14	1.717	0.833	2.312
8	8	0.62	2.678	1.283	3.868	32	8	0.62	1.738	0.733	2.457
8	8	0.43	2.965	1.277	4.492	32	8	0.43	1.727	0.640	2.545
8	8	0.34	3.204	1.263	5.093	32	8	0.34	1.706	0.566	2.597
8	16	5.16	2.247	1.447	2.732	32	16	5.16	1.888	1.137	2.300
8	16	1.14	2.899	1.641	3.776	32	16	1.14	2.105	1.096	2.712
8	16	0.62	3.460	1.765	4.724	32	16	0.62	2.204	1.024	2.958
8	16	0.43	3.970	1.849	5.672	32	16	0.43	2.256	0.948	3.131
8	16	0.34	4.423	1.909	6.573	32	16	0.34	2.280	0.882	3.246
8	32	5.16	2.566	1.695	3.055	32	32	5.16	2.156	1.340	2.561
8	32	1.14	3.479	2.029	4.378	32	32	1.14	2.499	1.362	3.117
8	32	0.62	4.301	2.281	5.654	32	32	0.62	2.692	1.328	3.478
8	32	0.43	5.084	2.487	6.958	32	32	0.43	2.815	1.278	3.742
8	32	0.34	5.834	2.663	8.187	32	32	0.34	2.896	1.229	3.938
8	64	5.16	2.881	1.933	3.360	32	64	5.16	2.417	1.538	2.816
8	64	1.14	4.067	2.428	4.997	32	64	1.14	2.896	1.630	3.525
8	64	0.62	5.167	2.827	6.598	32	64	0.62	3.195	1.644	4.010
8	64	0.43	6.302	3.190	8.250	32	64	0.43	3.406	1.630	4.381
8	64	0.34	7.365	3.502	9.974	32	64	0.34	3.561	1.604	4.662
16	1	5.16	0.788	0.300	1.242	48	1	5.16	0.717	0.237	1.146
16	1	1.14	0.679	0.133	1.251	48	1	1.14	0.578	0.064	1.091
16	1	0.62	0.572	0.014	1.214	48	1	0.62	0.458	−0.052	1.011
16	1	0.43	0.479	−0.072	1.163	48	1	0.43	0.360	−0.131	0.930
16	1	0.34	0.406	−0.128	1.115	48	1	0.34	0.286	−0.182	0.862
16	2	5.16	1.102	0.542	1.559	48	2	5.16	1.011	0.461	1.439
16	2	1.14	1.069	0.395	1.687	48	2	1.14	0.924	0.295	1.467
16	2	0.62	1.004	0.273	1.732	48	2	0.62	0.828	0.171	1.435
16	2	0.43	0.936	0.176	1.746	48	2	0.43	0.738	0.077	1.386
16	2	0.34	0.875	0.105	1.741	48	2	0.34	0.665	0.011	1.338
16	4	5.16	1.413	0.783	1.864	48	4	5.16	1.300	0.684	1.719
16	4	1.14	1.485	0.678	2.133	48	4	1.14	1.287	0.541	1.844
16	4	0.62	1.490	0.572	2.288	48	4	0.62	1.231	0.420	1.875
16	4	0.43	1.473	0.478	2.392	48	4	0.43	1.165	0.321	1.871
16	4	0.34	1.446	0.403	2.457	48	4	0.34	1.105	0.246	1.854
16	8	5.16	1.716	1.017	2.159	48	8	5.16	1.578	0.897	1.988
16	8	1.14	1.915	0.969	2.589	48	8	1.14	1.654	0.790	2.223
16	8	0.62	2.015	0.896	2.874	48	8	0.62	1.652	0.682	2.329
16	8	0.43	2.074	0.819	3.094	48	8	0.43	1.624	0.587	2.381
16	8	0.34	2.106	0.754	3.258	48	8	0.34	1.590	0.511	2.405
16	16	5.16	2.010	1.242	2.446	48	16	5.16	1.848	1.101	2.249
16	16	1.14	2.358	1.269	3.052	48	16	1.14	2.024	1.040	2.603
16	16	0.62	2.576	1.243	3.489	48	16	0.62	2.091	0.956	2.794
16	16	0.43	2.736	1.200	3.851	48	16	0.43	2.113	0.873	2.915
16	16	0.34	2.848	1.156	4.132	48	16	0.34	2.114	0.803	2.989
16	32	5.16	2.295	1.461	2.729	48	32	5.16	2.109	1.299	2.503
16	32	1.14	2.809	1.574	3.522	48	32	1.14	2.398	1.293	2.985
16	32	0.62	3.167	1.612	4.132	48	32	0.62	2.543	1.240	3.271
16	32	0.43	3.454	1.616	4.648	48	32	0.43	2.627	1.178	3.470
16	32	0.34	3.679	1.610	5.075	48	32	0.34	2.673	1.119	3.603
16	64	5.16	2.579	1.675	3.005	48	64	5.16	2.364	1.491	2.752
16	64	1.14	3.271	1.887	3.999	48	64	1.14	2.775	1.548	3.371
16	64	0.62	3.784	1.999	4.797	48	64	0.62	3.008	1.534	3.759

Table 4 (Continued)
Gamma Prediction Limit Factors k as a Function of n, r, p, m, and $\hat{\kappa}$

			k						k		
n	r	$\hat{\kappa}$	$p=1$, $m=2$	$p=1$, $m=3$	$p=2$, $m=3$	n	r	$\hat{\kappa}$	$p=1$, $m=2$	$p=1$, $m=3$	$p=2$, $m=3$
16	64	0.43	4.217	2.067	5.487	48	64	0.43	3.162	1.498	4.043
16	64	0.34	4.575	2.110	6.087	48	64	0.34	3.266	1.458	4.246
Prediction limit $= \bar{x} + kS$, $\alpha = 0.005$ (i.e., 10 constituents)											
8	1	5.16	2.197	1.470	2.598	32	1	5.16	1.808	1.118	2.137
8	1	1.14	2.880	1.711	3.629	32	1	1.14	1.995	1.073	2.477
8	1	0.62	3.489	1.878	4.629	32	1	0.62	2.075	0.999	2.668
8	1	0.43	4.074	2.008	5.672	32	1	0.43	2.110	0.922	2.795
8	1	0.34	4.618	2.110	6.741	32	1	0.34	2.122	0.855	2.877
8	2	5.16	2.428	1.598	2.940	32	2	5.16	1.993	1.218	2.405
8	2	1.14	3.305	1.920	4.326	32	2	1.14	2.264	1.203	2.887
8	2	0.62	4.142	2.166	5.788	32	2	0.62	2.405	1.148	3.192
8	2	0.43	4.991	2.378	7.427	32	2	0.43	2.490	1.081	3.414
8	2	0.34	5.791	2.544	9.097	32	2	0.34	2.538	1.022	3.575
8	4	5.16	2.767	1.862	3.283	32	4	5.16	2.261	1.421	2.668
8	4	1.14	3.991	2.379	5.084	32	4	1.14	2.667	1.476	3.305
8	4	0.62	5.223	2.827	7.107	32	4	0.62	2.909	1.464	3.735
8	4	0.43	6.590	3.262	9.452	32	4	0.43	3.081	1.429	4.069
8	4	0.34	7.947	3.650	11.961	32	4	0.34	3.200	1.391	4.324
8	8	5.16	3.110	2.121	3.625	32	8	5.16	2.523	1.619	2.925
8	8	1.14	4.710	2.862	5.857	32	8	1.14	3.074	1.752	3.728
8	8	0.62	6.428	3.578	8.504	32	8	0.62	3.439	1.795	4.301
8	8	0.43	8.483	4.298	11.716	32	8	0.43	3.710	1.801	4.765
8	8	0.34	10.607	4.991	15.399	32	8	0.34	3.910	1.793	5.127
8	16	5.16	3.449	2.386	3.969	32	16	5.16	2.781	1.814	3.179
8	16	1.14	5.460	3.373	6.673	32	16	1.14	3.491	2.033	4.157
8	16	0.62	7.807	4.406	10.018	32	16	0.62	3.988	2.140	4.885
8	16	0.43	10.650	5.523	14.375	32	16	0.43	4.375	2.199	5.496
8	16	0.34	13.687	6.628	19.109	32	16	0.34	4.684	2.230	5.981
8	32	5.16	3.782	2.644	4.308	32	32	5.16	3.035	2.005	3.429
8	32	1.14	6.242	3.917	7.530	32	32	1.14	3.914	2.319	4.595
8	32	0.62	9.244	5.281	11.737	32	32	0.62	4.554	2.499	5.493
8	32	0.43	13.005	6.849	17.186	32	32	0.43	5.084	2.620	6.267
8	32	0.34	17.229	8.530	23.728	32	32	0.34	5.500	2.700	6.903
8	64	5.16	4.112	2.896	4.647	32	64	5.16	3.285	2.193	3.676
8	64	1.14	7.079	4.466	8.439	32	64	1.14	4.344	2.608	5.040
8	64	0.62	10.814	6.228	13.433	32	64	0.62	5.146	2.871	6.122
8	64	0.43	15.534	8.327	19.996	32	64	0.43	5.829	3.064	7.084
8	64	0.34	21.433	10.607	28.233	32	64	0.34	6.386	3.204	7.889
16	1	5.16	1.936	1.232	2.287	48	1	5.16	1.767	1.080	2.087
16	1	1.14	2.258	1.264	2.818	48	1	1.14	1.914	1.015	2.370
16	1	0.62	2.463	1.241	3.205	48	1	0.62	1.961	0.928	2.511
16	1	0.43	2.610	1.200	3.519	48	1	0.43	1.967	0.844	2.593
16	1	0.34	2.715	1.156	3.769	48	1	0.34	1.959	0.773	2.637
16	2	5.16	2.135	1.342	2.582	48	2	5.16	1.946	1.177	2.347
16	2	1.14	2.573	1.416	3.316	48	2	1.14	2.169	1.137	2.755
16	2	0.62	2.879	1.424	3.886	48	2	0.62	2.266	1.066	2.989
16	2	0.43	3.114	1.408	4.393	48	2	0.43	2.312	0.989	3.144
16	2	0.34	3.298	1.382	4.814	48	2	0.34	2.332	0.923	3.248
16	4	5.16	2.425	1.565	2.870	48	4	5.16	2.206	1.374	2.601
16	4	1.14	3.057	1.741	3.824	48	4	1.14	2.546	1.393	3.145
16	4	0.62	3.533	1.829	4.617	48	4	0.62	2.729	1.357	3.482
16	4	0.43	3.940	1.880	5.346	48	4	0.43	2.844	1.304	3.722
16	4	0.34	4.267	1.906	5.993	48	4	0.34	2.915	1.253	3.894
16	8	5.16	2.712	1.783	3.154	48	8	5.16	2.461	1.565	2.850
16	8	1.14	3.553	2.077	4.352	48	8	1.14	2.930	1.652	3.537
16	8	0.62	4.230	2.266	5.401	48	8	0.62	3.209	1.659	3.986
16	8	0.43	4.843	2.400	6.395	48	8	0.43	3.403	1.638	4.325
16	8	0.34	5.364	2.502	7.298	48	8	0.34	3.535	1.608	4.575
16	16	5.16	2.997	2.000	3.435	48	16	5.16	2.710	1.753	3.094
16	16	1.14	4.067	2.424	4.891	48	16	1.14	3.316	1.913	3.932
16	16	0.62	4.976	2.731	6.228	48	16	0.62	3.703	1.971	4.504
16	16	0.43	5.829	2.977	7.554	48	16	0.43	3.987	1.988	4.951
16	16	0.34	6.600	3.173	8.758	48	16	0.34	4.192	1.987	5.289
16	32	5.16	3.279	2.214	3.713	48	32	5.16	2.955	1.936	3.334
16	32	1.14	4.595	2.782	5.460	48	32	1.14	3.708	2.177	4.332
16	32	0.62	5.771	3.224	7.107	48	32	0.62	4.210	2.293	5.038
16	32	0.43	6.930	3.613	8.771	48	32	0.43	4.595	2.357	5.603
16	32	0.34	7.947	3.927	10.344	48	32	0.34	4.887	2.389	6.047
16	64	5.16	3.559	2.425	3.996	48	64	5.16	3.198	2.116	3.573
16	64	1.14	5.140	3.148	6.044	48	64	1.14	4.103	2.444	4.736

Table 4 (Continued)
Gamma Prediction Limit Factors *k* as a Function of *n*, *r*, *p*, *m*, and $\hat{\kappa}$

			k						*k*		
n	*r*	$\hat{\kappa}$	$p = 1, m = 2$	$p = 1, m = 3$	$p = 2, m = 3$	*n*	*r*	$\hat{\kappa}$	$p = 1, m = 2$	$p = 1, m = 3$	$p = 2, m = 3$
16	64	0.62	6.619	3.751	8.048	48	64	0.62	4.732	2.624	5.589
16	64	0.43	8.102	4.298	10.127	48	64	0.43	5.228	2.740	6.286
16	64	0.34	9.462	4.767	12.046	48	64	0.34	5.614	2.813	6.838
Prediction limit = $\bar{x} + kS$, $\alpha = 0.002$ (i.e., 25 constituents)											
8	1	5.16	2.888	2.225	3.063	32	1	5.16	2.347	1.684	2.491
8	1	1.14	4.259	3.092	4.613	32	1	1.14	2.800	1.845	3.025
8	1	0.62	5.720	3.974	6.307	32	1	0.62	3.085	1.910	3.369
8	1	0.43	7.365	4.931	8.250	32	1	0.43	3.288	1.933	3.630
8	1	0.34	9.097	5.879	10.344	32	1	0.34	3.432	1.938	3.820
8	2	5.16	2.888	1.953	3.413	32	2	5.16	2.347	1.487	2.753
8	2	1.14	4.243	2.554	5.411	32	2	1.14	2.800	1.566	3.443
8	2	0.62	5.687	3.106	7.749	32	2	0.62	3.082	1.571	3.921
8	2	0.43	7.304	3.665	10.529	32	2	0.43	3.284	1.550	4.298
8	2	0.34	8.998	4.168	13.687	32	2	0.34	3.432	1.520	4.589
8	4	5.16	3.232	2.219	3.752	32	4	5.16	2.608	1.684	3.008
8	4	1.14	4.997	3.072	6.242	32	4	1.14	3.212	1.844	3.870
8	4	0.62	7.009	3.921	9.324	32	4	0.62	3.616	1.908	4.498
8	4	0.43	9.452	4.814	13.185	32	4	0.43	3.930	1.931	5.014
8	4	0.34	12.132	5.705	17.937	32	4	0.34	4.168	1.934	5.421
8	8	5.16	3.568	2.483	4.101	32	8	5.16	2.865	1.877	3.262
8	8	1.14	5.801	3.616	7.118	32	8	1.14	3.633	2.127	4.301
8	8	0.62	8.504	4.822	11.032	32	8	0.62	4.176	2.259	5.090
8	8	0.43	11.864	6.210	16.320	32	8	0.43	4.615	2.337	5.759
8	8	0.34	15.677	7.646	22.523	32	8	0.34	4.958	2.385	6.308
8	16	5.16	3.906	2.746	4.442	32	16	5.16	3.118	2.068	3.510
8	16	1.14	6.638	4.177	8.034	32	16	1.14	4.059	2.415	4.744
8	16	0.62	10.112	5.823	12.967	32	16	0.62	4.754	2.626	5.712
8	16	0.43	14.818	7.819	19.996	32	16	0.43	5.338	2.770	6.552
8	16	0.34	20.441	9.974	28.233	32	16	0.34	5.801	2.871	7.265
8	32	5.16	4.249	3.008	4.795	32	32	5.16	3.369	2.254	3.760
8	32	1.14	7.573	4.789	9.059	32	32	1.14	4.493	2.708	5.197
8	32	0.62	11.991	6.914	15.041	32	32	0.62	5.363	3.006	6.367
8	32	0.43	18.145	9.650	23.855	32	32	0.43	6.100	3.229	7.412
8	32	0.34	25.064	12.674	34.788	32	32	0.34	6.713	3.393	8.292
8	64	5.16	4.594	3.266	5.171	32	64	5.16	3.616	2.439	4.010
8	64	1.14	8.492	5.411	10.120	32	64	1.14	4.938	3.005	5.673
8	64	0.62	13.932	8.110	17.316	32	64	0.62	5.992	3.400	7.058
8	64	0.43	21.760	11.572	27.851	32	64	0.43	6.917	3.710	8.327
8	64	0.34	31.176	15.677	43.062	32	64	0.34	7.701	3.949	9.435
16	1	5.16	2.524	1.859	2.678	48	1	5.16	2.290	1.627	2.431
16	1	1.14	3.222	2.201	3.485	48	1	1.14	2.672	1.737	2.883
16	1	0.62	3.776	2.434	4.142	48	1	0.62	2.886	1.762	3.148
16	1	0.43	4.251	2.610	4.716	48	1	0.43	3.026	1.752	3.331
16	1	0.34	4.647	2.744	5.216	48	1	0.34	3.116	1.731	3.458
16	2	5.16	2.521	1.639	2.963	48	2	5.16	2.290	1.437	2.682
16	2	1.14	3.222	1.854	4.006	48	2	1.14	2.672	1.478	3.273
16	2	0.62	3.767	1.975	4.898	48	2	0.62	2.885	1.455	3.645
16	2	0.43	4.240	2.053	5.730	48	2	0.43	3.026	1.412	3.920
16	2	0.34	4.633	2.103	6.465	48	2	0.34	3.116	1.367	4.116
16	4	5.16	2.809	1.857	3.249	48	4	5.16	2.543	1.627	2.930
16	4	1.14	3.728	2.197	4.548	48	4	1.14	3.055	1.737	3.666
16	4	0.62	4.493	2.426	5.704	48	4	0.62	3.369	1.761	4.158
16	4	0.43	5.196	2.600	6.849	48	4	0.43	3.592	1.751	4.530
16	4	0.34	5.791	2.733	7.869	48	4	0.34	3.749	1.730	4.814
16	8	5.16	3.090	2.074	3.531	48	8	5.16	2.790	1.813	3.173
16	8	1.14	4.251	2.550	5.106	48	8	1.14	3.445	1.999	4.064
16	8	0.62	5.267	2.912	6.576	48	8	0.62	3.868	2.076	4.680
16	8	0.43	6.233	3.211	8.065	48	8	0.43	4.187	2.108	5.169
16	8	0.34	7.103	3.449	9.462	48	8	0.34	4.418	2.117	5.540
16	16	5.16	3.373	2.287	3.813	48	16	5.16	3.035	1.996	3.413
16	16	1.14	4.799	2.917	5.679	48	16	1.14	3.838	2.264	4.466
16	16	0.62	6.093	3.425	7.496	48	16	0.62	4.385	2.403	5.219
16	16	0.43	7.396	3.880	9.403	48	16	0.43	4.805	2.483	5.835
16	16	0.34	8.620	4.267	11.245	48	16	0.34	5.127	2.528	6.317
16	32	5.16	3.654	2.499	4.095	48	32	5.16	3.276	2.175	3.651
16	32	1.14	5.362	3.294	6.289	48	32	1.14	4.234	2.532	4.874
16	32	0.62	6.985	3.974	8.504	48	32	0.62	4.911	2.737	5.777
16	32	0.43	8.645	4.608	10.899	48	32	0.43	5.451	2.873	6.532
16	32	0.34	10.281	5.163	13.264	48	32	0.34	5.871	2.964	7.135
16	64	5.16	3.932	2.708	4.387	48	64	5.16	3.514	2.351	3.888

Table 4 (Continued)
Gamma Prediction Limit Factors k as a Function of n, r, p, m, and $\hat{\kappa}$

			k						k		
n	r	$\hat{\kappa}$	$p = 1$, $m = 2$	$p = 1$, $m = 3$	$p = 2$, $m = 3$	n	r	$\hat{\kappa}$	$p = 1$, $m = 2$	$p = 1$, $m = 3$	$p = 2$, $m = 3$
16	64	1.14	5.942	3.688	6.945	48	64	1.14	4.639	2.803	5.298
16	64	0.62	7.956	4.560	9.617	48	64	0.62	5.457	3.082	6.367
16	64	0.43	10.072	5.398	12.574	48	64	0.43	6.129	3.282	7.274
16	64	0.34	12.132	6.184	15.537	48	64	0.34	6.656	3.420	8.025

previously amenable to computation based on lognormal assumption. Results of a limited simulation study revealed that in contrast to simultaneous gamma prediction limits, simultaneous normal prediction limits do not achieve their intended nominal type I error rate when applied to data generated from a gamma distribution. Simultaneous nonparametric prediction limits do achieve their intended nominal type I error rate but have reduced statistical power relative to simultaneous gamma prediction limits. Finally, we have shown that the gamma prediction limits are remarkably robust to censoring of the data based on limits of detection, a condition that typifies environmental data in most if not all areas of application.

References

Aitchison, J. 1955. On the distribution of a positive random variable having a discrete probability mass at the origin. *Journal of the American Statistical Association* 50, no. 271: 901–908.

Aziz, J.J., M. Vanderford, C.J. Newell, M.L. Ling, H.S. Rifai, and J.R. Gonzales. 2004. *Monitoring and Remediation Optimization System (MAROS) Software User's Guide*. San Antonio, Texas: Air Force Center for Environmental Excellence.

Barlow, R.E., and F. Proschan. 1965. *Mathematical Theory of Reliability.* New York: John Wiley and Sons.

Bhaumik, D.K., and R.D. Gibbons. 2005. One-sided approximate prediction intervals for at least *p* of *m* observations from a gamma population at each of *r* locations. *Technometrics* 48, no. 1: 112–119.

Cohen, A.C. 1961. Tables for maximum likelihood estimates: Singly truncated and singly censored samples. *Technometrics* 3, no. 4: 535–541.

Cohen, A.C. 1959. Simplified estimators for the normal distribution when samples are singly censored or truncated. *Technometrics* 1, no. 3: 217–237.

Currie, L.A. 1968. Limits for qualitative detection and quantitative determination. *Analytical Chemistry* 40, no. 3: 586–593.

Davis, D.J. 1952. An analysis of some failure data. *Journal of the American Statistical Association* 47, no. 256: 113–150.

Davis, C.B., and R.J. McNichols. 1999. Simultaneous nonparametric prediction limits. *Technometrics* 41, no. 2: 89–101.

Davis, C.B., and R.J. McNichols. 1994. Ground-water monitoring statistics update: I: Progress since 1988. *Ground Water Monitoring and Remediation* 14, 148–158.

Davis, C.B., and R.J. McNichols. 1987. One-sided intervals for at least *p* of *m* observations from a normal population on each of *r* future occasions. *Technometrics* 29, no. 3: 359–370.

Gibbons, R.D. 1994. *Statistical Methods for Ground-Water Monitoring*. New York: John Wiley & Sons.

Gibbons, R.D. 1991. Some additional nonparametric prediction limits for ground-water monitoring at waste disposal facilities. *Ground Water* 29, no. 5: 729–736.

Gibbons, R.D. 1990. A general statistical procedure for Ground-Water Detection Monitoring at waste disposal facilities. *Ground Water* 28, no. 2: 235–243.

Gibbons, R.D. 1987. Statistical models for the analysis of volatile organic compounds in waste disposal sites. *Ground Water* 25, no. 4: 572–580.

Gibbons, R.D., and D.E. Coleman. 2001. *Statistical Methods for Detection and Quantification of Environmental Contamination*. New York: Wiley.

Johnson, N.L., S. Kotz, and N. Balakrishnan. 1994. *Continuous Univariate Distributions-1*, 2nd ed. New York: Wiley.

U.S. EPA. 1992. *Statistical Analysis of Ground-Water Monitoring Data at RCRA Facilities*. Addendum to Interim Final Guidance Document. Washington, D.C.: U.S. EPA.

Biographical Sketches

Robert D. Gibbons*, corresponding author, is the Director of the Center for Health Statistics and Professor of Psychiatry and Biostatistics at the University of Illinois at Chicago. He may be reached at Center for Health Statistics, University of Illinois at Chicago, 1601 West Taylor, Chicago, IL 60612; 312-413-7755; fax 312-996-2113; rdgib@uic.edu.*

Dulal K. Bhaumik *is a member of the Center for Health Statistics and Professor of Psychiatry and Biostatistics at the University of Illinois at Chicago, 1601 West Taylor, Chicago, IL 60612.*