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Statistical Methodology for Data with Multiple Limits of Detection

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STATISTICAL METHODOLOGY FOR DATA WITH MULTIPLE LIMITS OF DETECTION

by

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A dissertation submitted to the Graduate College
in partial fulfillment of the requirements
for the degree of Doctor of Philosophy

Statistics

Western Michigan University

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STATISTICAL METHODOLOGY FOR DATA WITH MULTIPLE LIMITS OF DETECTION

Robert M. Flikkema, Ph.D.

Western Michigan University, 2016

Limitations of instruments used to collect continuous data sometimes lead to obtaining observations lower than a limit of detection. These observations are known as nondetects. They could be zeroes, or positive numbers, but they are too small to be recorded by a measuring device. Nondetects frequently occur in environmental data. Trace amounts of chemicals can exist in soil or groundwater and are undetectable by a machine reading. These observations pose a problem to researchers since the true values are unknown.

Simulations in the literature have led to inconsistent conclusions regarding what estimation technique to use with nondetect data when estimating the population mean. Researchers have used differing distributional assumptions, sample sizes, number of detection limits, and proportions of nondetects when conducting simulations. Many researchers base conclusions on distributional assumptions which are not valid in all environmental datasets. Furthermore, the majority of research involves data with one detection limit and data that is not a mixture of multiple distributions.

The simulations in this research comprehensively investigate lognormal and gamma data with two detection limits as well as non-unimodal lognormal and gamma mixtures. Mean estimation techniques are used to create bootstrap intervals for the population mean. Guidance is given to researchers who wish to estimate a population mean using a dataset from an unknown distribution with multiple detection limits.

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Contents

Acknowledgments	ii
List of Tables	v
List of Figures	v
1 Introduction and Basic Notions	1
1.1 Introduction	1
1.2 Distributions for Modeling Left Censored Environmental Data	2
1.2.1 Lognormal Distribution	2
1.2.2 Gamma Distribution	3
2 Literature Review	4
2.1 Problems with Distribution Selection when Modeling Left-Censored Data	4
2.2 Substitution and Imputation Methods	7
2.2.1 Simple Substitution Methods	7
2.2.2 Substitution of Nondetects by Uniformly Distributed Observations	8
2.2.3 Regression on Order Statistics	8
2.2.4 Imputation of Expected Values	9
2.2.5 Weibull Regression	10
2.3 Estimators Based on Data with Nondetects	11
2.3.1 MLE Estimation	11
2.3.2 Kaplan-Meier Estimation	12
3 Selected Studies on Summary Statistics from Samples with Nondetects	14
3.1 Hewett and Ganser	14
3.2 Clarke	16
3.3 Other Studies	17
3.4 Software for Analyzing Nondetect Data	21
4 Bootstrap Simulation Study	21
4.1 Bootstrap Percentile Interval for the Mean	23
4.2 Bootstrap t Interval for the Mean	24
4.3 Distributions	24
5 Results	25
5.1 Bootstrap Percentile Intervals	27
5.2 Bootstrap t Intervals	28
5.3 Discussion	29
5.4 Real Data Example	37
6 Future Research	40
Appendices	41
A Graphical Results of All Simulations	41
B Numeric Results of All Simulations	57
C R Simulation Code	67

List of Tables

1	Summary of Bootstrap Percentile Interval Results	27
2	Summary of Bootstrap t Interval Results	28
3	Zinc Concentration Data	38
4	Bootstrap Intervals of Zinc Concentration Data	39

List of Figures

1	Lognormal Density Plots	2
2	Gamma Density Plots	3
3	Mixed Lognormal Density Plots	25
4	Mixed Gamma Density Plots	25
5	LN(0, 0.1), N=30 Results	30
6	GAM(9, 0.4), N = 30 Results	30
7	GAM(0.1, 2), N = 50 Results	31
8	LN(0, 0.5), N = 30 Results	32
9	LN(0, 0.25), N = 30 Results	33
10	GAM(2, 0.5), N = 30 Results	33
11	GAM(9, 0.4), N = 30 Results	34
12	70% LN(0, 1), 30% LN(0, 0.25), N = 30 Results	35
13	50% LN(0, 1), 50% LN(0, 0.5), N = 30 Results	35
14	40% GAM(7.5, 1), 60% GAM(2, 2), N = 30 Results	36
15	70% GAM(7.5, 1), 30% GAM(2, 2), N = 30 Results	36
16	Histogram of Zinc Concentration Data	39

1 Introduction and Basic Notions

1.1 Introduction

Left censored observations are present in many research areas and the censoring could happen for various reasons. For example, in environmental research, where the concentration is a very common variable of interest, observations are obtained from measuring devices, which usually have a detection limit(s) and positive values below such limit(s) are recorded as zeros. They could be zeros, but they could also be positive but very small - such values are called non-detects. Every measuring device has its own limit of detection, and two similar devices (even two copies of the same device) might have different limits of detection. If the data are collected using more than one measuring device, they might be subject to multiple detection limits.

Non-detects are usually reported as being less than a given threshold and such observations should never be deleted from the dataset to avoid a strong upward bias in estimating measures of location (Helsel, 2005). Statistical analysis of such data requires special methods, since the assumptions of the standard methodology are either not satisfied or cannot be verified. Practitioners are aware of the problem, an ample literature on handling data with nondetects exists. These papers usually refer to specific problems, and study performance of particular methods using statistical simulations and particular distributions. Helsel (2005) published a research compendium of these methods and drew some general conclusions.

While many methods have been discussed and studied in these publications, comprehensive methodology for analysis of data with multiple methods of detection still needs to be developed. Several authors including Gliet (1985), Clarke (1998), She (1997), and Antweiler (2008), addressed the poor performance of MLE-based methods when distributional assumptions were not satisfied, therefore this dissertation would focus on robust methodology. We will focus on bootstrap estimation of the mean using different imputation methods and nonparametric approaches as researchers would typically not know the distribution an environmental dataset follows. We will study performance of these procedures on different distributions including contaminated (mixed) data, as this is a realistic practical situation. There will be a focus on investigating distributions with different skewness within the same distributional family to see if the best estimation method can differ within one type of distribution. Different sample sizes will also be

tested. The goal is to conduct a comprehensive simulation study that can be used as guidance for researchers with a variety of data.

1.2 Distributions for Modeling Left Censored Environmental Data

Distributions used for modeling environmental data are nonnegative, continuous and skewed to the right and therefore studies often use lognormal and/or gamma models. Some studies also use the Weibull distribution, but it is less common.

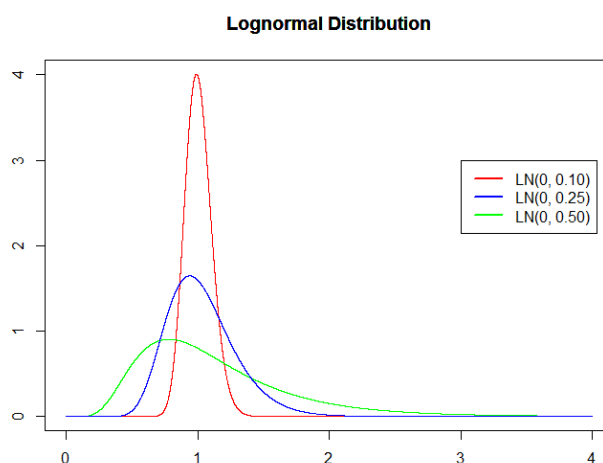
1.2.1 Lognormal Distribution

The most common distribution used for modeling nonnegative data is a lognormal distribution, with density

$$f(x) = \frac{1}{x\sigma\sqrt{2\pi}}e^{-\frac{(\ln x - \mu)^2}{2\sigma^2}}, x > 0. \quad (1)$$

If X is a lognormal random variable with the above density then $Y = \ln X$ has a $N(\mu, \sigma^2)$ distribution. In this research, a lognormal distribution with the above density will be denoted as $LN(\mu, \sigma)$.

Figure 1: Lognormal Density Plots



The three lognormal distributions in the above figure were selected for the simulation study described in Chapters 4 and 5. These distributions were selected due to their difference in

density curves. The $LN(0, 0.10)$ distribution is approximately bell-shaped while the $LN(0, 0.5)$ is extremely right-skewed.

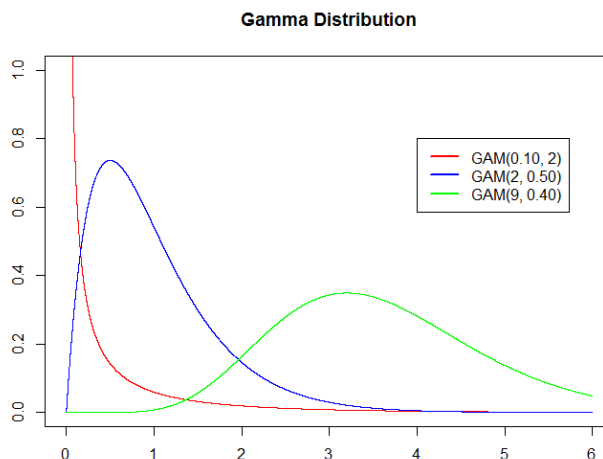
1.2.2 Gamma Distribution

Another distribution frequently used for analysis of environmental data is a gamma distribution. Its density function with the shape parameter k and scale parameter θ is

$$f(x) = \frac{1}{\Gamma(k)\theta^k} x^{k-1} e^{-x/\theta}, x > 0. \quad (2)$$

The shape parameter, k , controls the skewness of the distribution. A smaller value means the density curve will be right skewed. A larger value causes the density function to approach a bell-shape. The scale parameter, θ , controls the scale relative to the x and y-axis of the density curve. Larger θ values will cause the x-axis range of the density curve to increase and the y-axis range to decrease. Smaller values will have a larger y-axis and smaller x-axis. In this research, a gamma distribution with the above density will be denoted as $GAM(k, \theta)$.

Figure 2: Gamma Density Plots



In practice, it can be difficult to differentiate between lognormal and gamma environmental data. Both distributions can be right skewed or nearly bell-shaped depending on the parameter values, and a goodness-of-fit test on environmental data can easily determine that both types of distributions might be reasonable fits (H_0 is not rejected). Myers and Pipin (1990) tested the

robustness of a delta-distribution method that assumes the underlying distribution is lognormal. Simulations were run on lognormal data contaminated with gamma and Weibull observations. The authors concluded that lognormal-based estimators are sensitive to the violation of model assumptions. It must be clearly demonstrated that the uncensored observations follow a lognormal distribution for lognormal-based estimators to be used with confidence. For sample sizes less than 40, the probability of detecting these deviations is low.

One of the goals of this paper is to determine if methods traditionally used for nondetect data can be effective on data from gamma distributions with multiple detection limits. The number of studies investigating this type of data is limited.

2 Literature Review

2.1 Problems with Distribution Selection when Modeling Left-Censored Data

The lognormal distribution is often selected for studies (over other distributions, such as gamma, or Weibull) for convenience. Lognormal data can easily be transformed to normal data and then methods requiring normality assumptions could be applied. While even the Environmental Protection Agency (EPA) recommends the lognormal distribution when investigating environmental data, Singh (1997), and many others (e.g. Blackwood (1992), Reimann (2000), Cho (2004), Mayer (2005), Myers (2000), etc.) call into question the validity of studies that assume the data follows a lognormal distribution.

For example, Blackwood (1992) made the lognormal distribution assumption in radiological monitoring data without any verification. He mentions that the lognormal distribution is commonly chosen because the distribution contains positive, non-zero values that are right skewed and many environmental datasets share these characteristics. However, these properties by themselves do not indicate a lognormal distribution. Blackwood notes that the lognormal distribution is frequently used within literature when data are skewed and do not show a constant variance across groups with different mean values. A logarithmic transformation is used to stabilize the variance and make data symmetrical so that applying normal theory analysis

seems more appropriate. However, it's noted that this will only stabilize the variance if the error term from the underlying model is multiplicative. Blackwood warns against blindly choosing the lognormal distribution as is done so often in the literature and recommends to try other distributions such as gamma and Weibull.

Reimann (2000) conducted a study on geochemical data, testing if variables fit a lognormal distribution. A Shapiro-Wilk normality test was used on the log-transformed variables. Many variables in the dataset had more than 25% observations left-censored. Riemann noted that it was nearly impossible to conclude that those variables were either normal or lognormal so he removed these variables from the dataset. The goodness-of-fit test did not show that the remaining variables followed a normal or lognormal distribution. The variables were also transformed using logarithm, natural logarithm, square root, range, and logit transformations. Goodness-of-fit results showed that no transformation produced a normal distribution fit for more than 20 of 57 variables. This shows that studies selecting methods requiring lognormal and normal assumptions on the basis of data being positive and right skewed, can and should be called into question.

Singh (2001) investigated a generalized log-logistic (GLL) distribution and compared it to the lognormal distribution. The GLL distribution has the following density function:

$$g(x) = \frac{\alpha}{xB(m_1, m_2)} [F(x)]^{m_1} [1 - F(x)]^{m_2}, \quad (3)$$

where

$$F(x) = [1 + e^{-[\beta + \alpha \ln(x)]}]^{-1}, \quad (4)$$

is the log-logistic cumulative distribution function, B is the beta function, m_1 and m_2 are positive integers, $\alpha > 0$, and $\beta > 0$. Note that if $m_1 = m_2 = 1$, $GLL(m_1, m_2)$ reduces to the log-logistic distribution.

The GLL distribution is an extension of the log-logistic distribution, it is similar in shape to the lognormal distribution. The conclusion was that the GLL was a good alternative to the lognormal distribution and outperformed it in some situations. The GLL is typically not used in other research and it's unclear if the results are related to this specific type of data. The

datasets used in Singh (2001) included mercury concentrations in swordfish.

Cho (2004) conducted a study on tropical rainfall and concluded that both lognormal and gamma distributions fit the data relatively well. The gamma distribution fit the data better in rainy regions, while the lognormal was the better fit in dry regions. The gamma distribution underestimated high and light rain rates while the lognormal distribution underestimated intermediate rain rates. This shows that within a single type of data, both distributions can provide a reasonable fit under different circumstances. A researcher unsure of the distribution of a dataset might be wise to test both lognormal and gamma assumptions.

Mayer (2005) investigated how well distributions fit data of fish counts in estuaries. Lognormal, gamma, Poisson, and negative binomial distributions were compared. No single distribution was found to provide a good fit to the right skewed data. But the lognormal distribution was demonstrated to be a reasonable fit under any tested dataset. Mayer claims that the lognormal distribution is the safest choice when the distribution is unknown. However, it's unclear if this conclusion applies only to fishery data since other types were not investigated.

Myers (2000) compared lognormal and gamma distributions using time series datasets involving the number of fish in an area. The conclusion was that either distribution could provide a better fit in a given dataset and none provides a universally better fit than the other.

Wiens (1999) explored a clinical dataset in which the estimate of the mean differed under lognormal and gamma distributional assumptions. He explored reasons for the difference and concluded that while large outliers affected gamma distribution more than lognormal distribution, the substitution of constant values for censored observations had a larger impact on lognormal distribution than gamma distribution. Wiens suggests analyzing a dataset assuming a lognormal distribution, then conducting another analysis assuming the gamma distribution to determine if the results depend on the underlying distribution. If so, then non-parametric methods may be necessary.

Kundu and Manglick (2005) used simulated data to study how well the original lognormal and gamma data could be determined. They obtained asymptotic distributions of the ratio of the maximum likelihoods and used them to determine the minimum sample size required to discriminate between the two distributions for user specified probability of correct selection

and tolerance limit. The results showed that lognormal distributions had a 73% probability of correctly being identified as such with a sample size of 40. The gamma distribution had a similar probability of 66% based on the same sample size (40). However these probabilities would be less for data with nondetects.

Dick (2004) used Akaike information criterion (AIC) to rank candidate models for lognormal, gamma, Weibull, log-logistic, and inverse Gaussian data. His conclusion was that given a sample size larger than 50, AIC is effective at identifying the data-generating distribution.

2.2 Substitution and Imputation Methods

An approach to analysis of the data with nondetects which is definitely not recommended is to ignore the values that are below the detection limit. Instead, such observations could be replaced. In an imputation method a different value is assigned to each nondetect observation. Several imputations done with datasets with values below the detection limit(s) were proposed in the literature by various authors.

2.2.1 Simple Substitution Methods

The most common substitution method replaces all nondetected observations with a single value such as 0, the detection limit DL , half of the detection limit $DL/2$, and $DL/\sqrt{2}$. Once these values are included in a data set, standard statistical formulas can be applied to calculate the descriptive statistics. It is obvious that the choice of an imputation method would have an impact on the value of these statistics. Helsel (2006) commented that studies in which substitution by constants was used often had questionable results. Barringer (2005) conducted a study in which any variable composed by 20% or more of nondetects was dropped from the study, while for less than 20% of nondetected observations, the substitution method was applied and the value of half the detection limit was used. Her conclusion was that Mercury concentrations were higher in residential areas than in undeveloped land, but it's impossible to know if the way she handled nondetects influenced the results of her study. Substituting 0 or the detection limit could have

led to different results.

McCarthy (1994) used a ‘sliding scale’ model where a value for the substitution was related to the percentage of nondetects in the dataset, $DL(1-p)$, where p is the proportion of nondetect observations in the data. If 40% of the data are nondetects, then $0.6DL$ would be substituted for every missing observation. The theoretical basis for using this substitution method is somewhat unclear and Helsel (2005) notes that the accuracy of values of resulting statistics is unknown.

2.2.2 Substitution of Nondetects by Uniformly Distributed Observations

Clarke (1998) used two uniform substitution methods in his simulation paper. The first method substitutes n_0 evenly spaced numbers between 0 and the DL for n_0 nondetects in the dataset. The second method substitutes randomly selected uniform variables $U(0, DL)$ for the censored observations. Samples of data with a single DL set at the 20, 40, 60, 80, and 95th percentiles of the overall distribution were tested. The results of this study are discussed in Section 3.2.

2.2.3 Regression on Order Statistics

Regression on order statistics is an imputation method that substitutes nondetects based on least-squares regression on a probability plot (Helsel, 2005). For $n = n_0 + n_1$ independent normally distributed with a common mean μ and variance σ^2 , n_0 observations are below the detection limit DL ($y_i, i = 1, 2, \dots, n_0$) and n_1 are observed and larger than detection limit DL ($y_i = n_0 + 1, \dots, n_0 + n_1$). Since

$$y_i = \mu + \sigma\Phi^{-1}(P_i), \quad (5)$$

where $P_i = P(Y_i \leq y_i)$ and $\Phi^{-1}(\cdot)$ denotes the inverse cdf of a $N(0, 1)$ distribution, the intercept and slope from a regression on the normal scores would yield inverse transformed adjusted order statistics.

The procedure typically replaces probabilities with adjusted ranks, so that the regression equation becomes

$$y_i = \hat{\mu} + \hat{\sigma}\Phi^{-1}\left(\frac{i - 3/8}{n + 1/4}\right) + \epsilon_i, \quad (6)$$

where $i = n_0 + 1, n_0 + 2, \dots, n_0 + n_1$, and $\hat{\mu}$ and $\hat{\sigma}$ are least squares estimates of μ and σ . The residual errors ϵ_i are assumed to have equal variance and to be uncorrelated. The $\Phi^{-1}\left(\frac{i-3/8}{n+1/4}\right)$ component of the equation is the normal score calculated by Altman's formula. The literature is unclear on what is used for the variance of $\hat{\mu}$. Shumway (2002) suggests the following jackknife estimator.

Let $\hat{\theta}$ be an estimator of some parameter θ . The jackknife estimator computes n pseudoes-
timators, by deleting one observation at a time and redoing the estimation. Let $\theta_{[-i]}$ denote the
estimator with observation i deleted, for $i = 1, 2, \dots, n$. Let

$$\bar{\theta}_{[-\cdot]} = n^{-1} \sum_{i=1}^n \theta_{[-i]}, \quad (7)$$

be the average of these estimators. The Quenouille-Tukey Jackknife estimator is defined as

$$\tilde{\theta} = n\hat{\theta} - (n-1)\bar{\theta}_{[-\cdot]}, \quad (8)$$

and it can be shown that it eliminates a bias term of order $1/n$. An estimator for the variance
of the jackknife estimator is

$$\hat{\sigma}^2(\tilde{\theta}) = \frac{n-1}{n} \sum_{i=1}^n (\theta_{[-i]} - \bar{\theta}_{[-\cdot]})^2. \quad (9)$$

2.2.4 Imputation of Expected Values

This method assumes the underlying distribution of the dataset is normal or lognormal. If n_0
nondetects exist in a dataset, the expectations of the first n_0 order statistics conditional on being
below the detection limit are substituted. Since these expected values depend on the unknown
mean and variance, this procedure must be run iteratively on a computer. The algorithm, given
by Gliet (1985), is as follows.

1. Select any initial convenient guesses for the mean and variance.
2. On the basis of our tentative current values for the mean and variance, calculate the
expected values for the first p order statistics conditional on being less than DL . The
density of the k th order statistic is as follows.

$$f_k(x) = n f(x) \binom{n-1}{k-1} F(x)^{k-1} (1-F(x))^{n-k}. \quad (10)$$

The conditional density of the k th order statistic is given below.

$$f_k(x|X \leq DL) = \frac{g_k(x)}{F_k(DL)} \quad (11)$$

where $g_k(x) = f_k(x)$ for all $x \leq DL$ and 0 otherwise. $F_k(x) = \int_{-\infty}^x f_k(t) dt$.

Finally, the expected value is calculated as:

$$\int_{-\infty}^{\infty} x f_k(x|X \leq DL) dx. \quad (12)$$

3. Now that the first p data points are “known”, we can compute the mean and variance using the standard formulas. These are the updated estimates.
4. If the current and updated values are close, end the procedure. Otherwise, go back to step 2 using the updated versions as the current values.

In practice, this algorithm converged rapidly when “close” was defined by 10^{-6} . Gleit uses this method to handle nondetects and compares it to the MLE and substitution methods.

2.2.5 Weibull Regression

Weibull regression fits a parametric regression model between a dependent variable and one or more independent variables. This model can be used to estimate the survival function of the data. Once the survival function is estimated, the area under the curve is calculated to estimate the mean. This method is typically used with right censored data. Like with the K-M method, nondetect data must be transformed to right-censored data in order to apply this method. The regression model fit is as follows,

$$\log(X_i) = \beta_0 + \beta_1 z_{i1} + \dots + \beta_p z_{ip} + \sigma \epsilon_i \quad (13)$$

where β_0, \dots, β_p are the regression coefficients of interest, σ is a scale parameter, and ϵ_i is an error term. The survival function is estimated as follows:

$$S(t|z) = e^{-[te^{-z^T\beta}]^{\frac{1}{\alpha}}}, \quad (14)$$

where $\beta = (\beta_0, \dots, \beta_p)^T$ is the vector of regression coefficients.

2.3 Estimators Based on Data with Nondetects

2.3.1 MLE Estimation

This method of estimation of population parameters requires that the distribution type is known. In the most general case with left and right censored data in the data set, likelihood L has a form:

$$L = \prod f(x) \prod F(DL_L) \prod S(DL_U), \quad (15)$$

where $f(x)$ is the density (or pdf) of the underlying distribution, $F(x)$ is its cdf, and $S(x) = 1 - F(x)$ is the survival function. Moreover DL_L , and DL_U are lower and upper detection limits, respectively.

For data with the lower limit of detection only (left-censored), two values: x_i and δ_i represent each measurement. The value for the measurement, or for the reporting limit, is given by x . The δ value is an indicator variable that is set to 0 when the value falls below the detection limit and is 1 when the variable is detected (Helsel, 2005). The likelihood function for data with nondetects is

$$L = \prod [f(x_i)]^{\delta_i} \cdot [F(x_i)]^{1-\delta_i}. \quad (16)$$

or

$$L = F(DL)^{n_0} \prod_{i=n_0+1}^n f(x_i), \quad (17)$$

where the dataset is as in Subsection 2.2.3. After substituting in the above equations and setting the partial derivatives of $\ln(L)$ equal to 0, the nonlinear equations are solved by iterative

approximation using the Newton-Raphson method. This provides estimates of the mean and standard deviation for the distribution that best matches both the pdf and the cumulative distribution function estimated from the data (Helsel, 2005). The main drawback of using MLE estimation is that the distribution has to be known or tested. However, testing would most likely be inconclusive if there is a small number of observations in a dataset.

2.3.2 Kaplan-Meier Estimation

The Kaplan-Meier (K-M) method is often used for estimating descriptive statistics in medical and industrial sciences. It is a nonparametric method designed to incorporate data with multiple censoring levels and does not require an assumed distribution (Helsel, 2005). Originally this method was proposed for analysis of right censored survival data. In order for this method to be applicable to left censored nondetect data, the observations must be “flipped” by subtracting them from a large constant. In the original form, the K-M method estimates the survival function, the probability of an individual surviving beyond time x . That is,

$$S(x) = Pr(X > x) = \int_x^\infty f(t) dt \quad (18)$$

where $f(x)$ is a probability density function. The K-M estimator, also called the Product-Limit estimator, takes the form of

$$\hat{S}(t) = \begin{cases} 1 & t < t_1 \\ \prod_{t_i \leq t} (1 - \frac{d_i}{Y_i}) & t_1 \leq t \end{cases} \quad (19)$$

where d_i is the number of events occurring at or before time t_i and Y_i is the number of individuals who are at risk at time t_i . The variance of the Product-Limit estimator can be estimated by Greenwood’s formula (Greenwood, 1926):

$$\hat{V}(\hat{S}(t)) = \hat{S}(t)^2 \sum_{t_i \leq t} \frac{d_i}{Y_i(Y_i - d_i)}. \quad (20)$$

To apply the K-M method to nondetect data, we must first transform the data so that it becomes right censored. Consequently

$$x'_i = M - x_i, \quad (21)$$

where M is an arbitrary number that is larger than the maximum observation in the dataset. If the K-M method is applied to transformed data x'_1, \dots, x'_n then $S = P(x'_i > y) = P(x_i < M - y)$. The latter expression shows that survival probabilities are also the cumulative probabilities of the original data. After transforming the data, the uncensored observations are ranked from small to large, accounting for the number of censored data in between each detected observation. The “number at risk”, b , equals the number of observations, both detected and censored, at and below each detected concentration. The number of uncensored observations at that concentration is d , where d is greater than 1 for tied values. The incremental survival probability is the probability of “surviving” to the next lowest uncensored concentration, given the number of data at and below that concentration, or $(b - d)/b$. The survival function probability is the product of the k incremental probabilities to that point, going from high to low concentration for the k uncensored observations.

$$S = \prod_{j=1}^k \frac{b_j - d_j}{b_j}, \quad (22)$$

which is the product of the $j = 1$ to k probabilities to that point, b_j is the number of people at risk at that point, and d_j is the number of detected observations at that concentration.

The standard error of S is (Helsel, 2005)

$$s.e.(S) = S \sqrt{\sum_{j=1}^k \frac{d_j}{b_j(b_j - d_j)}}. \quad (23)$$

The K-M estimate of the mean can be found by integrating under the K-M survival curve. The estimate of the mean will be used in the simulations described in Chapter 4.

3 Selected Studies on Summary Statistics from Samples with Nondetects

This section discusses and summarizes other studies which focused on estimating summary statistics of data with nondetects. The majority of these studies used simulated data to evaluate estimation methods.

3.1 Hewett and Ganser

Hewett and Ganser (2007) conducted a study comparing the performance of several methods for estimating the 95th percentile and the mean of right skewed occupational exposure data. The methods investigated were: maximum likelihood estimation, regression on order statistics (ROS), substitution methods, several nonparametric quantile methods for the 95th percentile and the Kaplan-Meier method.

The three substitution methods Hewett chose to compare are substitution of the detection limit, one half the detection limit, and the detection limit divided by $\sqrt{2}$. The latter substitution has been used occasionally in the literature, including in Hornung and Reed (1990). Hewett also investigates regression on order statistics. This method is described in Subsection 2.2.3. The standard MLE method is tested along with two MLE variations proposed by Kroll and Stedinger (1996) and Succop (2004). Finally, the Kaplan-Meier method is applied to estimate the quantile and mean.

Hewett investigated various datasets in this simulation. Three separate simulations were performed which varied the sample size, proportion of nondetects, and geometric standard deviation (GSD).

- Simulation 1: n ranged between 20 and 100, the true percent censored ranged between 1% and 50% and the true geometric standard deviation (GSD) ranged between 1.2 and 4.
- Simulation 2: n ranged between 20 and 100, the true percent censored ranged between 50% and 80% and the true GSD ranged between 1.2 and 4.
- Simulation 3: n ranged between 5 and 19, the true percent censored ranged between 1%

and 50% and the true GSD ranged between 1.2 and 4.

The geometric standard deviation is as follows.

$$\sigma_g = \exp\left(\sqrt{\frac{\sum_{i=1}^n (\ln \frac{A_i}{\mu_g})^2}{n}}\right) \quad (24)$$

where μ_g is the geometric mean of the dataset. The geometric mean of n observations is the n th root of the product of the observations, $\sqrt[n]{x_1 x_2 \dots x_n}$. For each of those simulations, Hewett devised the following 4 scenarios:

- Scenario I: a single lognormal distribution and a single limit of detection (DL)
- Scenario II: a single lognormal distribution and three DLs
- Scenario III: a mixture of two lognormal distributions and a single DL
- Scenario IV: a mixture of two lognormal distributions and three DLs

The substitution methods performed poorly overall. The DL/2 and DL/ $\sqrt{2}$ were in the top half of methods tested with respect to root mean square error (RMSE) when estimating the 95th percentile of the distribution. RMSE is a measure frequently used as an error metric for numerical estimation. If n $\hat{\theta}$ estimators are produced using an estimation method for a parameter, θ , the RMSE is as follows:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (\theta - \hat{\theta}_i)^2}. \quad (25)$$

The researchers' opinion of the substitution methods was that the DL substitution should be avoided altogether, but there were situations where the other two constant substitutions performed adequately when estimating the percentile. The ROS method, which was introduced in Subsection 2.2.3, tended to be in the middle to top half of the bias and RMSE rankings when sample sizes ranged from 20 to 100 and percent censored ranged from 1% to 80%. This method performed well when tested with multiple DLs and/or contaminated distributions. The ROS methods performed poorly when estimating the 95th percentile using small datasets. MLE methods performed well in the single distribution scenarios and were generally robust in the

multiple DL and contaminated distribution scenarios. The K-M nonparametric methods were consistently in the middle to bottom half of the bias and RMSE rankings when estimating the 95th percentile. The K-M method was among the worst methods whenever there was a single DL. Hewett and Ganser refutes Helsel's claim that the K-M method should be used for estimating the mean when the percent of censored observations is $< 50\%$. This study showed that the K-M was among the worst methods under these conditions. Hewett and Ganser conclude that the MLE methods are superior to other methods when estimating the mean or 95th percentile. It's worth noting that gamma data was not investigated.

3.2 Clarke

Clarke (1998) used various mean comparison methods for very small sample sizes of $n < 10$. The methods he investigated included substitution methods, MLE estimation of the mean and standard deviation, and ROS methods. He then ran simulations on normal, lognormal, and gamma data and used Fisher's Least Significant Difference test to investigate type I error rate and power for the methods when comparing two means. The LSD test is typically used with post-hoc ANOVA hypothesis testing. Clarke's conclusion was that the simple substitution methods outperformed the more advanced methods. However, only sample sizes of 10 or less were investigated. This study could be expanded and larger sample sizes could be investigated. Clarke used SAS to generate 674 groups of populations. Parameters were specified for normal, lognormal, and gamma-probability distributions. The reason these three distributions were chosen is that they are considered likely distributions for chemical concentration data in the environment. For each of the 674 groups, one population was generated to represent a reference sediment, and one to three additional populations were created to represent dredged sediment treatments which would be compared to the reference. The reference means were all set to 1 and the reference standard deviation was set to 0.1, 0.5, 1, 2, or a random number between 0.1 and 2. This encompassed nearly the entire range of coefficients of variation (CVs) calculated for 530 samples of uncensored sediment or tissue contaminant concentration data from several sediment evaluation projects. Some of the simulated treatment populations had their means set to 1, the same as the reference population, and were used to assess the type 1 error rate of the various methods.

For other treatment populations, means were set to values greater than 1 to assess the power of the methods as the treatment population means differed from the reference mean in these instances. Clarke tested various standard deviations of the treatment populations. Some were set equal to the reference standard deviation, some were set equal to the treatment population means, others were set equal to a random mixture of values between 0.1 and 2.

Simulations were conducted using 500 random samples drawn from each population. Sample sizes were of size n less than 10 and a detection limit was imposed at either the 20, 40, 60, 80, or 95th percentile. The 10 procedures investigated were substitution using: the detection limit (DL), half the detection limit (DL/2), 0, evenly spaced numbers between 0 and DL, and random numbers selected from the $U(0, DL)$ distribution. He also used regression on order statistics using the lognormal and normal distributions, MLE estimation of the mean and standard deviation using the lognormal, normal, and Weibull distributions. He then applied the LSD test to investigate type I error rates and power.

The percent of censored data seemed to have the largest impact on the results. The power of the ROS methods declined rapidly as the percentage of censored data increased. When censoring percentage was 80% or less, one or more substitution methods at least tied for the highest power in 60% of simulations. Several methods including the uniform distribution and MLE methods were tied for the highest power at 20-40% censoring. Type I error rates generally remained acceptable (less than 0.1) for most methods until nondetects exceeded 60%. All tests were conducted with a nominal type I Error rate of $\alpha = 0.05$. This study did not investigate data with multiple DLs or sample sizes over 10 and these results cannot be expanded to those situations.

3.3 Other Studies

Gliet (1985) conducted a study comparing the MLE method, the expected value method, and the three substitution methods using normally distributed data. The substitutions investigated were: 0, half the detection limit (DL/2), and the detection limit (DL) for sample sizes of 5, 10, and 15. The bias and variance of the estimators produced by each method were compared. The expected value method performed much better than the substitution and MLE methods.

The MLE method is known to perform poorly with small sample sizes and had large bias and variance. Gliet does not explore large sample sizes so it is possible the MLE could perform better with larger sample sizes. This study did not test gamma or lognormal data.

Helsel (2006) showed that substitution methods performed much worse than methods specifically designed to handle nondetect data. Helsel used a normal distribution so the MLE method was easily applicable. A sample size of 50 was used for the study. Because the data distribution was known and the sample size was relatively large, one would expect the MLE method to outperform the substitution method, which it did.

Shumway (2002) investigated methodology for estimating mean concentrations of toxic pollutants in water. Simulated samples of size 20 and 50 were used that had 50 or 80% nondetects. The MLE estimation method was tested on data that was transformed using the Box-Cox transformation. ROS was also tested on data with and without the Box-Cox transformation. The formula for the Box-Cox transformation is given below:

$$x'_\lambda = \frac{x^\lambda - 1}{\lambda}, \quad (26)$$

where λ is the transformation parameter that is chosen based on the correlation between the transformed data and a normal probability plot. The purpose of the Box-Cox transformation is to transform a dataset into having a normal distribution. Shumway concludes that none of the methods are consistently better than the other methods based on bias and coverage properties of 95% confidence intervals of the mean.

She (1997) performed a simulation study on the MLE estimation method, ROS, Kaplan-Meier and the one-half substitution method using lognormal and gamma data. The data was transformed to right censored data in order to apply the Kaplan-Meier estimator. The conclusion was that the Kaplan-Meier performed consistently well on data from both the lognormal and gamma distributions. The MLE performed well for the lognormal distribution when it had a low skew but performed poorly with a high skew. A sample size of 21 was used in this study.

Antweiler (2008) did a comparison study on descriptive statistics using the substitution methods, MLE, ROS, and Kaplan-Meier techniques on chemical concentration datasets collected by the U.S. Geological Survey. The datasets used ranged in sample sizes from 34 to 841 and in

percentage of censored data from 13.7% to 94.5%. The nondetects in the datasets were reported as values larger than zero. The conclusion was that the Kaplan-Meier technique performed best with datasets that had less than 70% nondetect observations. For datasets with over 70%, no technique performed well, with MLE and substitution performing particularly poorly.

Sinha (2006) used Monte Carlo simulations to evaluate statistical methods for estimating 95% upper confidence limits (UCL) of means for left-censored lognormal data. The nonparametric Chebyshev Theorem was used to calculate the UCLs because it could be applied to all the imputation methods. The formula for the Chebyshev UCL is as follows:

$$UCL = \bar{x} + \frac{s\sqrt{1/\alpha}}{\sqrt{n}}, \quad (27)$$

where $1 - \alpha$ is a confidence level.

Sample size and percentage of nondetect data was allowed to vary randomly. A first set of simulations with data having between 15% to 50% nondetects evaluated the following mean estimation methods: trimmed mean, Winsorization, Aitchinson's and ROS. The trimmed mean method removes points from the lower and upper ends of the data. If the lowest 5% of the data is nondetects, then these observations are removed along with the largest 5%. Winsorization replaces data in both tails of a dataset with the next less extreme value. Aitchinson's method calculates summary statistics for only the detected data. To estimate the mean, the sample mean of uncensored observations is collected and is multiplied by the proportion of uncensored observations. The ROS method was recommended for samples having a percentage of nondetects within these limits. A second set of simulations containing between 51% and 80% nondetects indicated that random uniform substitution was better for samples with a larger percentage of nondetects.

As shown here, even though a lot of research has been published about analysis of data with nondetects, there is no clear consensus on how to effectively analyze such data. Researchers select different sample sizes, different percentiles as limits of detection for simulated data or they use real-world datasets. For example, Helsel (2005) claimed the K-M method should be used to estimate the mean with data that has less than 50% nondetects but Hewett and Ganser refute this claim (2007) and concludes that ROS should be used. Clarke (1998) concluded that the

method used depends on the percentage of censored observations, but his study was conducted on samples of 10 or less. Gliet (1985) concluded the expected value method was the best when estimating the mean but his study was conducted on normally distributed data. Shumway (2002) concluded that neither the MLE or ROS methods was consistently better when estimating the mean. She (1997) concluded that the K-M method performed consistently well on lognormal and gamma data and that the MLE method performed well on lognormal data with a low skew. Antweiler (2008) concluded the K-M method performed best when a dataset had less than 70% nondetects and no technique performed well when the percentage of nondetects exceeded 70%. Sinha (2006) recommends ROS when the percentage of nondetects is between 15% and 50% and random uniform substitution when the percentage of nondetects exceeds 50%. However the trimmed mean, Winzorization, and Aitchinson's methods which are compared to ROS in the study seem to be primitive and outdated as they are rarely mentioned in the literature.

Especially contradicting are conclusions related to the distributional assumption. Many researchers used lognormal or gamma assumptions and MLE methods, however it is difficult to identify the correct distribution with real-world data unless an extremely large dataset can be obtained. Oftentimes, a real dataset will have 50 or less observations and a goodness-of-fit test will not be able to distinguish between lognormal and gamma data. Many studies that tested if data belonged to a specific type of distribution ended with the researcher concluding that no distribution fit the data better than others being tested. This was demonstrated in Reimann (2000), Cho (2004), Mayer (2005), Wiens (1999), and Dick (2004).

Furthermore, relatively little work has been done on datasets with multiple detection limits in comparison to data with a single DL. The one thing the literature did agree on was that constant substitution methods perform poorly with nondetect data.

The simulations in this study will focus on datasets with 20, 30, and 50 observations with two DLs. If a researcher has data from an unknown distribution with two DLs, how will common nondetect methods perform when estimating the mean? The four most common nondetect methods in the literature will be tested: substitution by a constant, substitution by $U(0, DL)$, ROS, and Kaplan-Meier. Bootstrap confidence intervals will be obtained from data after applying these four methods. Bootstrap percentile and t intervals will be used as they do not

require any distributional assumptions. The specific bootstrap confidence intervals used will be discussed in Chapter 4.

3.4 Software for Analyzing Nondetect Data

There are two software packages in R that were built to analyze data with nondetects. The NADA (2013) and EnvStats (2015) packages.

In 2005, Lee and Helsel published a paper discussing S-language software for regression on order statistics. This package supports data with multiple DLs. It has then been implemented into the NADA package. The NADA package also contains a function to perform Kaplan-Meier on left-censored data. It also includes several environmental datasets with a varying level of nondetects, Lee (2013).

The EnvStats package, created by Millard in 2013, has a number of functions to estimate the parameters of a specified distribution from a sample with nondetects and to create confidence intervals for the mean. It also contains functions for estimating the quantiles of these distributions as well as performing goodness-of-fit tests. The nondetect functions are a small part of this package and advanced imputation techniques such as ROS are not implemented.

An additional R package called zCompositions exists which conducts analysis on nondetect composition data. Each observation in this type of data is a vector and conveys relative information about parts of a whole. As this type of data differs from the data discussed in this research, the zCompositions package was not used in the simulations. This package was written by Palarea-Albaladejo and Martn-Fernndez in 2015.

Croghan (2003) published SAS code to perform constant substitution, ROS and maximum likelihood estimation on data with nondetects. The code was written for data with one DL.

The NADA package was used in the simulations in this study as it has the capability to run estimation techniques on data with multiple DLs.

4 Bootstrap Simulation Study

The purpose of this study is to investigate the effectiveness of imputation methods and Kaplan Meier for estimating the mean in a comprehensive way that would provide guidance for practicing

researchers analyzing data with nondetects. The four methods investigated are: substitution by $DL/\sqrt{3}$, substitution by a uniform random value between 0 and the DL, regression on order statistics, and Kaplan-Meier estimation. These methods were chosen as most frequent in the literature. The $DL/\sqrt{2}$, 0, DL, and $DL/2$ substitutions have been extensively tested in the literature and constant substitution has been universally found to be one of the worst imputation methods except in sample sizes of less than 10. The $DL/\sqrt{3}$ value was chosen for the constant value for these simulations. The study was designed with the following situation in mind. Suppose a researcher has a sample of data with two detection limits and wants to estimate the population mean. The sample size is too small (≤ 50) for the researcher to accurately determine if the data originated from a lognormal, gamma, or mixed distribution. Based on this information, can the researcher choose an estimation method and obtain a bootstrap interval with good coverage?

There are multiple types of bootstrap intervals. DiCiccio and Efron (1996) discussed the theory behind three such types. BC_a (bias corrected accelerated), bootstrap-t and ABC (approximate bootstrap confidence intervals). The bootstrap-t was used in this study but the other two could be looked at in future simulations. The BC_a estimator of θ is defined as

$$\hat{\theta}_{BC_a}[\alpha] = \hat{G}^{-1}\Phi\left(z_0 + \frac{z_0 + z^{(\alpha)}}{1 - a(z_0 + z^{(\alpha)})}\right), \quad (28)$$

where $\hat{G}(c)$ is the cumulative distribution function of B bootstrap replications,

$$\hat{G}(c) = \#\{\hat{\theta}^*(b) \leq c\}/B. \quad (29)$$

Φ is the standard normal cdf, and a is an acceleration parameter estimated by

$$\hat{a} = \frac{1}{6}(\sum(x_i - \bar{x})^3 / [\sum(x_i - \bar{x})^2]^{3/2}). \quad (30)$$

The acceleration parameter, a , is a measurement of how quickly the standard error is changing.

The ABC estimator of θ is defined as:

$$\widehat{\theta}_{ABC}[\alpha] = \hat{\theta} + \frac{w}{(1 - \hat{a}w)^2} \sqrt{\hat{\theta}}, \quad (31)$$

where

$$w = \hat{z}_0 + z^{(\alpha)}. \quad (32)$$

Simulations in this study will focus on two types of bootstrap intervals used in conjunction with four methods of imputation. The goal will be to determine which of the methods best estimate the mean of a sample with nondetects by calculating the proportion of coverage. Three lognormal and three gamma distributions with different shapes and additionally two lognormal mixtures and two gamma mixtures will be used. Sample sizes of 20, 30, and 50 will be generated from all the distributions. Each sample size will be tested with all combinations of two detection limits from out of quantiles of order 0.2, 0.4, and 0.6 respectively. One thousand bootstrap intervals will be calculated, each bootstrap interval will be obtained based on 300 bootstrap estimates. The proportion of intervals containing the population mean will be reported. The two types of intervals used are described in the next subsection. The number of bootstrap estimates was chosen after considering the number of simulations to be conducted and available computing power. After running test simulations with 300 and 1000 bootstrap estimates, it was determined that the difference in results was minimal and 300 was appropriate for the simulations when considering the computational time between the two values.

4.1 Bootstrap Percentile Interval for the Mean

The simulation algorithm for calculating a $100 * (1 - \alpha)\%$ bootstrap percentile interval for the mean is as follows.

- Generate a random sample of data of size n from a given distribution.
- Apply detection limits to the data with p_1 and p_2 being the two proportions of nondetects and DL_1 , DL_2 being quantiles of order p_1 , p_2 respectively. If any of the first $n/2$ observations in the sample fall below DL_1 , set them as nondetects. If any of the second $n/2$ observations fall below DL_2 , set them as nondetects.
- Generate a bootstrap sample by taking a sample of size n with replacement from the original sample and calculate the sample mean after applying an imputation method.

Repeat B times to obtain B bootstrap estimates of the mean.

- Order the B estimates from smallest to largest and take the $100 * [\alpha/2]th$ and $100 * [(1 - \alpha)/2]th$ percentiles to obtain a $100 * (1 - \alpha)\%$ bootstrap percentile interval.

For the simulations in the following section, B was set as 300 and the number of intervals calculated for each combination of detection limits was 1,000. The nominal coverage was set at 95%.

4.2 Bootstrap t Interval for the Mean

To calculate a bootstrap t interval, B bootstrap estimates, $\hat{\theta}_i^*, i = 1, \dots, B$, are obtained in the same manner as the bootstrap percentile interval. The following formula will produce a bootstrap t interval.

$$SE_{BOOT} = \sqrt{\frac{1}{B} \sum_{j=1}^B (\hat{\theta}_j^* - \hat{\theta}_{BOOT})^2} \quad (33)$$

where

$$\hat{\theta}_{BOOT} = \frac{1}{B} \sum_{j=1}^B \hat{\theta}_j^* \text{ is an average of all } \hat{\theta}_j^*, j = 1, 2, \dots, B$$

A $100 * (1 - \alpha)\%$ confidence interval for θ is then

$$\hat{\theta} \pm t_{\alpha/2, n-1} \times SE_{BOOT} \quad (34)$$

4.3 Distributions

The three lognormal distributions used for the simulations are shown in Figure 1 in Subsection 1.2.1. The distributions were chosen because of their difference in the shape of density functions and because the means and variances of the distributions were similar to those of the distributions used and discussed in the literature. The $LN(0, 0.1)$ distribution approaches a symmetric bell shape, while the $LN(0, 0.5)$ distribution is extremely right skewed.

The three gamma distributions used are shown in Figure 2 in Subsection 1.2.2. All three are right skewed but have different levels of skew.

In addition, two mixed lognormal and two mixed gamma distributions were used in simulations. One lognormal unimodal, one lognormal non-unimodal, and two non-unimodal gamma distributions were selected. These non-unimodal distributions were deliberately chosen to investigate the impact the shape of the density function had on the results.

Figure 3: Mixed Lognormal Density Plots

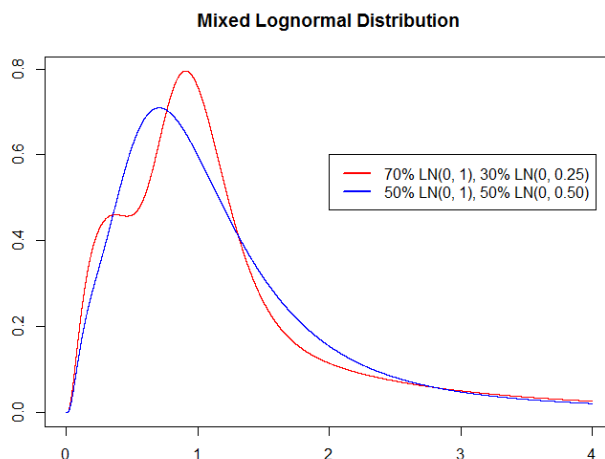
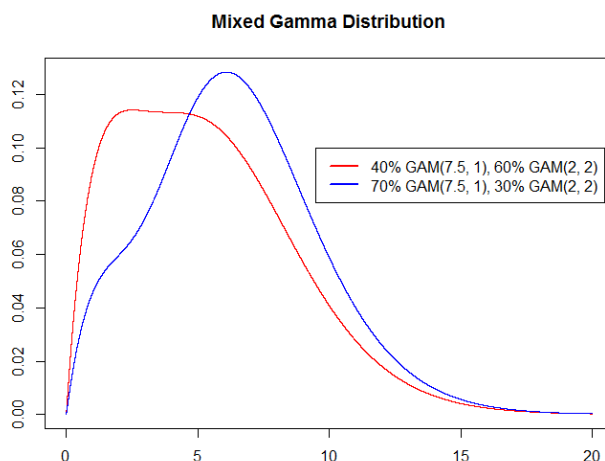


Figure 4: Mixed Gamma Density Plots



5 Results

The tables given on the subsequent pages summarize the methods that performed best in the simulations. The methods were judged based on coverage and width of the bootstrap intervals.

Intervals with high coverage and low widths are desired. If one interval had slightly lower coverage than a second interval but a slightly lower width, the intervals were considered to have approximately equal effectiveness when estimating the population mean. The results of each simulation are represented graphically in Appendix A. Two intervals that are approximately equidistant from the top left corner of a frame would be considered to have equal effectiveness when estimating the population mean. If a cell contains the word “All” it means all methods performed equally well in that simulation.

5.1 Bootstrap Percentile Intervals

N = 20						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/KM	ROS	ROS	ROS	ROS	ROS
LN(0, 0.25)	K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.50)	K-M	K-M	ROS/K-M	K-M	ROS	Constant/ROS
GAM(0.1, 2)	All	All	All	All	All	All
GAM(2, 0.5)	K-M	ROS/K-M	Constant/ROS	ROS/K-M	Constant/ROS	Constant
GAM(9, 0.4)	K-M	K-M/ROS	Constant/ROS	ROS/K-M	Constant/ROS	Constant/ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	Constant
50% LN(0, 1), 50% LN(0, 0.50)	K-M	K-M	K-M	K-M	Constant/ROS/K-M	Constant
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	K-M/ROS	Constant/ROS	ROS	Constant/ROS	Constant
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	ROS	ROS	ROS	Constant
N = 30						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/K-M	ROS	ROS/K-M	ROS	ROS	ROS
LN(0, 0.25)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.50)	K-M	K-M	ROS/K-M	K-M	ROS	Constant/ROS
GAM(0.1, 2)	All	All	All	All	All	K-M
GAM(2, 0.5)	ROS/K-M	ROS/K-M	Constant/ROS	ROS/K-M	Constant/ROS	Constant
GAM(9, 0.4)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	Constant
50% LN(0, 1), 50% LN(0, 0.50)	K-M	K-M	K-M	K-M	K-M	Constant
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	ROS	Constant/ROS	Constant/ROS
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	Constant/ROS	Constant/ROS	Constant
N = 50						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.25)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.50)	K-M	ROS/K-M	ROS/K-M	ROS/K-M	ROS	Constant/ROS
GAM(0.1, 2)	All	All	All	All	ROS	K-M
GAM(2, 0.5)	ROS/K-M	ROS/K-M	Constant/ROS/K-M	ROS/K-M	Constant/ROS	Constant
GAM(9, 0.4)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	Constant
50% LN(0, 1), 50% LN(0, 0.50)	ROS/K-M	K-M	Constant/ROS/K-M	K-M	K-M	Constant
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	Constant/ROS	Constant/ROS	Constant
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	Constant/ROS	Constant/ROS	Constant

5.2 Bootstrap t Intervals

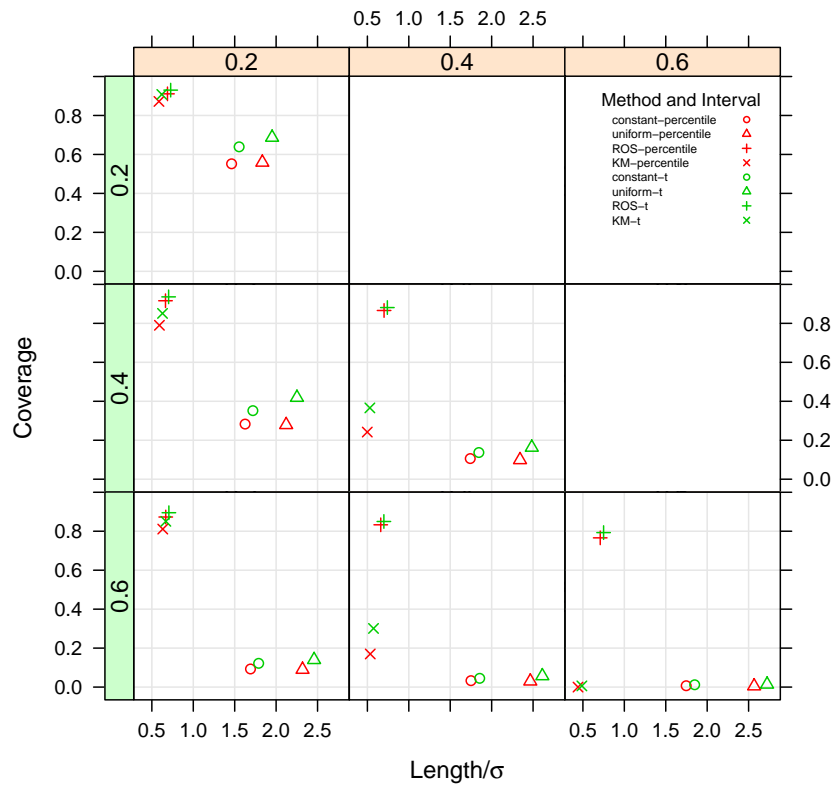
N = 20						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.25)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.50)	K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
GAM(0.1, 2)	All	All	All	All	All	All
GAM(2, 0.5)	ROS/K-M	ROS/K-M	Constant/ROS	K-M	K-M	Constant/ROS
GAM(9, 0.4)	K-M	ROS/K-M	Constant/ROS	K-M	ROS	Constant/ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	K-M
50% LN(0, 1), 50% LN(0, 0.50)	K-M	K-M	K-M	K-M	K-M	Constant
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	ROS/K-M	ROS	Constant/ROS
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	ROS	ROS	ROS	Constant/ROS
N = 30						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.25)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.50)	K-M	K-M	ROS/K-M	K-M	ROS/K-M	Constant/ROS
GAM(0.1, 2)	All	All	All	All	All	K-M
GAM(2, 0.5)	ROS/K-M	ROS/K-M	Constant/ROS	K-M	Constant/ROS	Constant/ROS
GAM(9, 0.4)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	K-M
50% LN(0, 1), 50% LN(0, 0.50)	K-M	K-M	K-M	K-M	K-M	Constant/K-M
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	ROS	Constant/ROS	Constant/ROS
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	ROS	ROS	Constant/ROS	Constant/ROS
N = 50						
Distribution	$(DL_1 = 0.2, DL_2 = 0.2)$	(0.2, 0.4)	(0.2, 0.6)	(0.4, 0.4)	(0.4, 0.6)	(0.6, 0.6)
LN(0, 0.10)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
LN(0, 0.25)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	Constant/ROS
LN(0, 0.50)	K-M	K-M	ROS/K-M	ROS/K-M	ROS	Constant/ROS
GAM(0.1, 2)	All	All	All	All	All	K-M
GAM(2, 0.5)	ROS/K-M	ROS/K-M	Constant/K-M	K-M	Constant/ROS	Constant/ROS
GAM(9, 0.4)	ROS/K-M	ROS/K-M	ROS/K-M	ROS	ROS	ROS
70% LN(0, 1), 30% LN(0, 0.25)	K-M	K-M	K-M	K-M	K-M	K-M
50% LN(0, 1), 50% LN(0, 0.50)	K-M	K-M	K-M	K-M	K-M	Constant/K-M
40% GAM(7.5, 1), 60% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS	Constant/ROS	Constant/ROS	Constant
70% GAM(7.5, 1), 30% GAM(2, 2)	ROS/K-M	ROS/K-M	Constant/ROS/K-M	Constant/ROS	Constant/ROS	Constant/ROS

5.3 Discussion

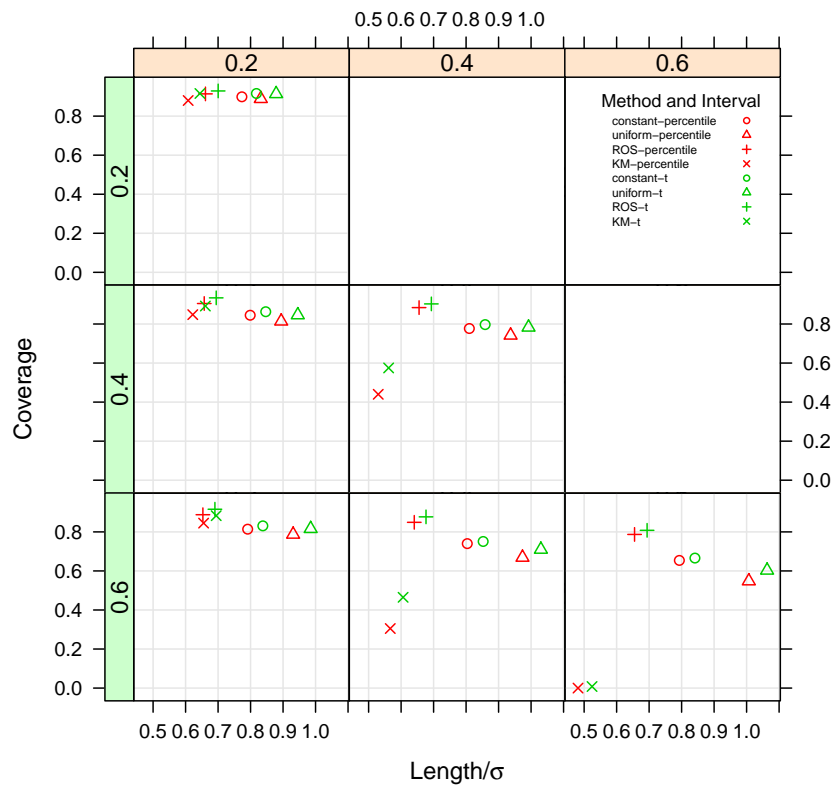
While studies in the literature reach conclusions that are generalized for distribution types or levels of detection (DL), the results show that the best method can vary within both of these factors. The best method for a skewed gamma distribution is not necessarily the best method for a more symmetrical gamma distribution. Likewise, the best method for a particular distribution can be different with a 40% DL and a 60% DL.

One observation from these results is that the ROS method performs better than the other methods with symmetrical distributions. Given below is a graphical representation of the results for the most-symmetrical lognormal and gamma distributions with the $N = 30$ sample size. A complete set of graphs can be found in Appendix A. Each frame represents a set of two detection limits used in that simulation. The y-axis of the cell represents the coverage of each method and the x-axis represents the width of the interval given in population standard deviations. The coverage and width of the eight confidence intervals are plotted within a frame. Methods that perform well will be near the top left of the frame because they have large coverage and small width.

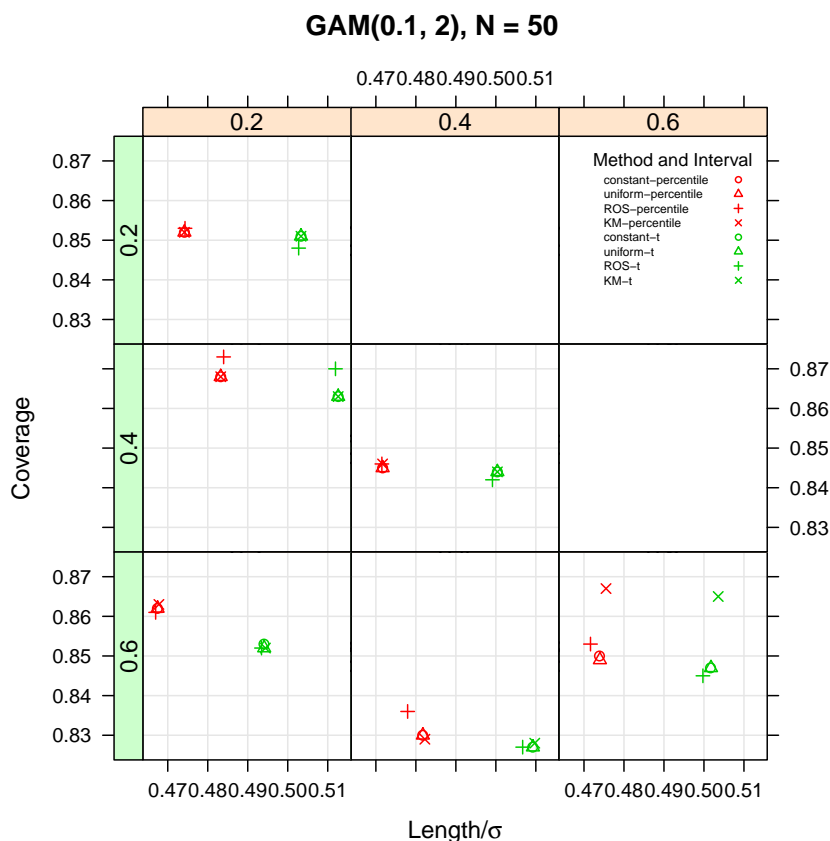
LN(0, 0.1), N = 30



GAM(9, 0.4), N = 30



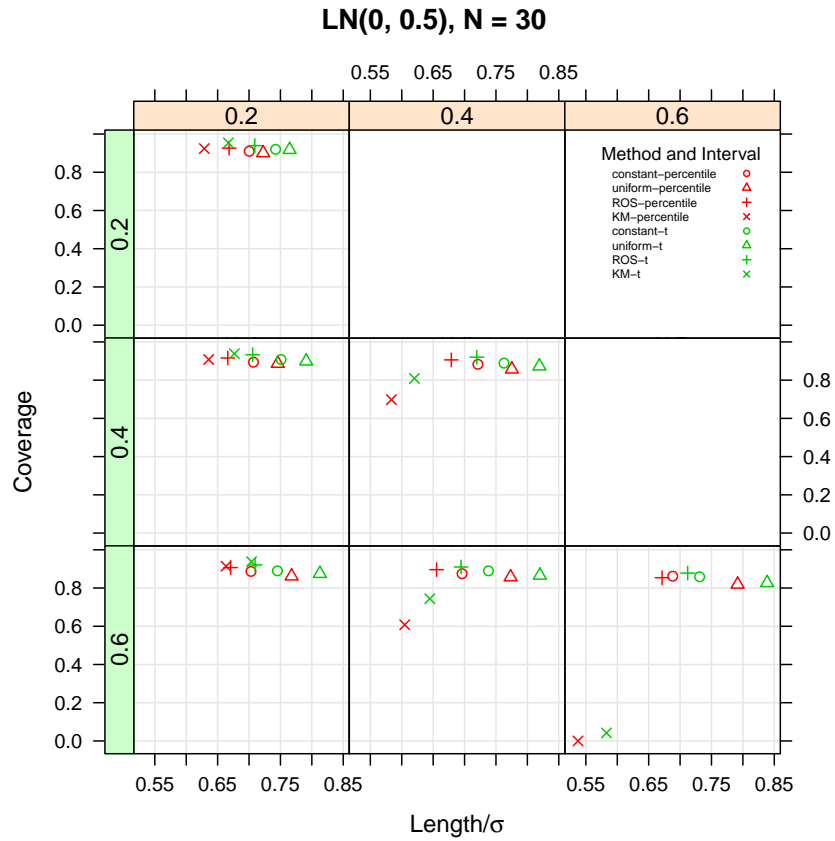
For the samples with lower DLs, the ROS and K-M methods equally outperform the constant and uniform substitution methods when considering both coverage and width. However, K-M starts to perform poorly once the percentage of nondetects exceeds 40%. At this point, ROS clearly outperforms the other three methods. The excellent performance of ROS in somewhat symmetrical distributions was consistent for all three sample sizes tested.



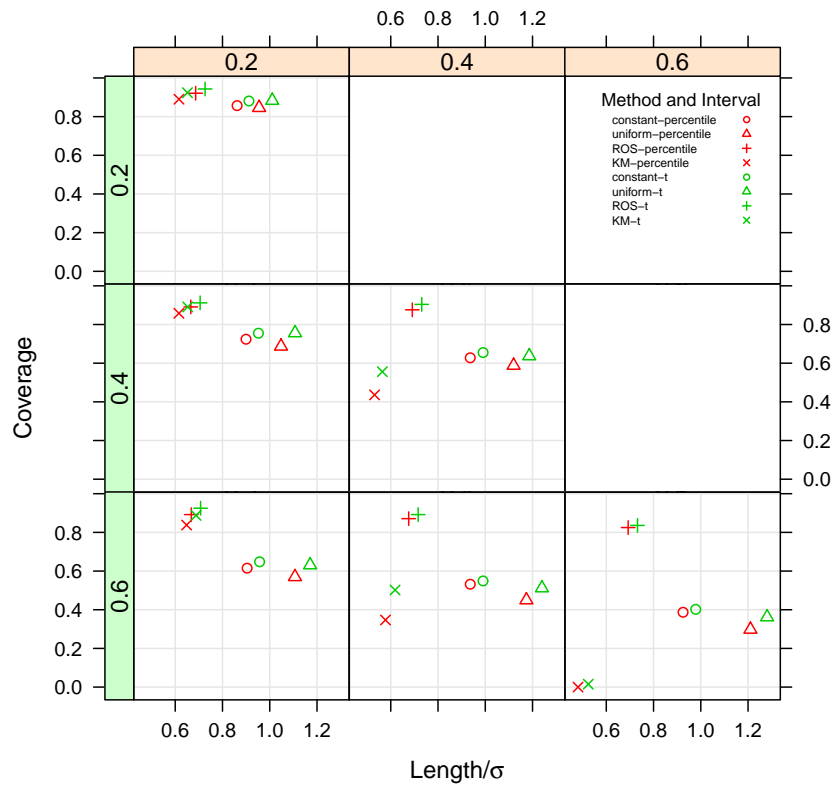
For the gamma distribution with the most skew, $GAM(0.1, 2)$, all the methods performed relatively equally until the percentage of nondetects reached 60%. At this point, K-M started to outperform the other methods. This contrasts with the more symmetric distributions where K-M performed poorly with large DLs. It suggests that if a researcher is confronted with a dataset that is highly skewed and contains a large number of nondetects, K-M should be considered when estimating the population mean. If the dataset was symmetrical, K-M should be avoided.

For the moderately skewed distributions, the result depended on the percentage of nondetects in the sample. For samples composed of less than 40% nondetects, K-M performed equally well as ROS and both were better estimation methods than constant or uniform substitution. However,

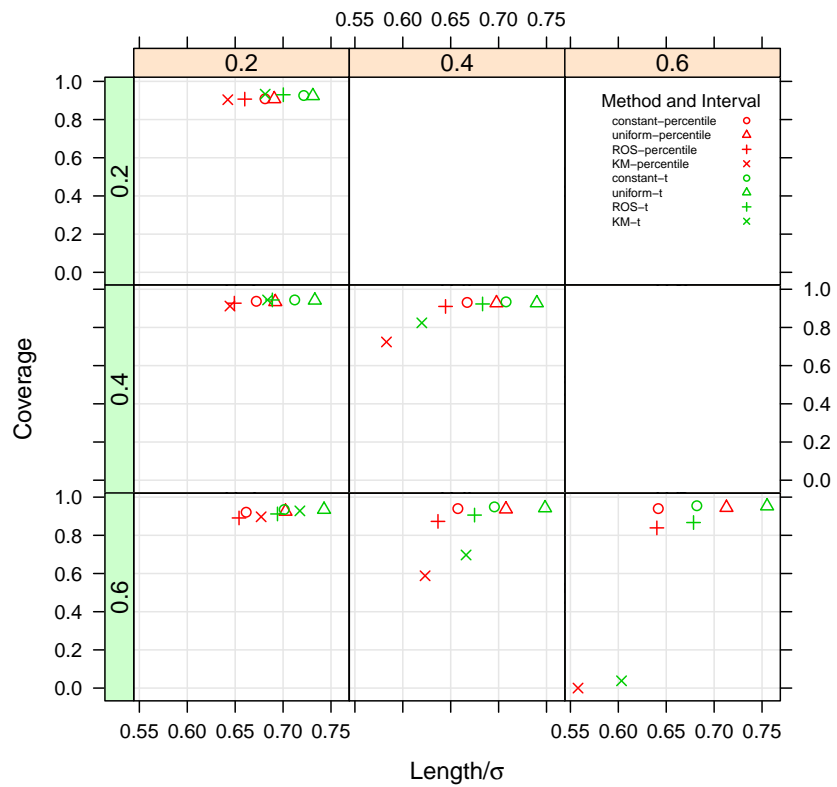
once the percentage of nondetects exceeded 40%, the ROS started to outperform K-M. Somewhat surprisingly, the constant substitution method performed equally well as ROS for some of the moderately skewed distributions when the percentage of nondetects exceeded 60%. However, it is a riskier choice compared to ROS as unlike ROS, it did not perform well in all of these simulations.



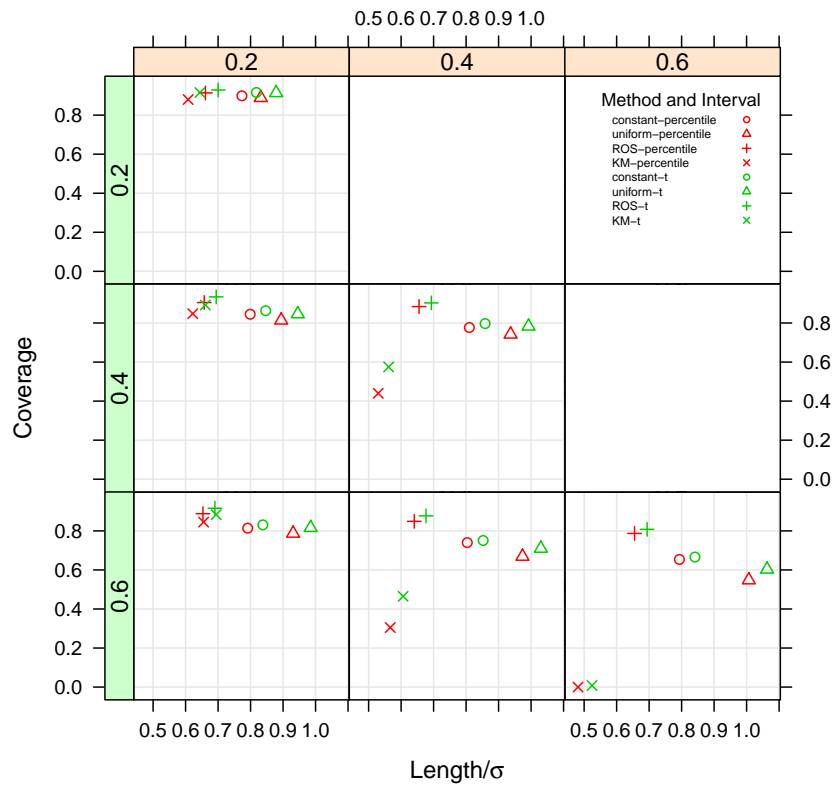
LN(0, 0.25), N = 30



GAM(2, 0.5), N = 30



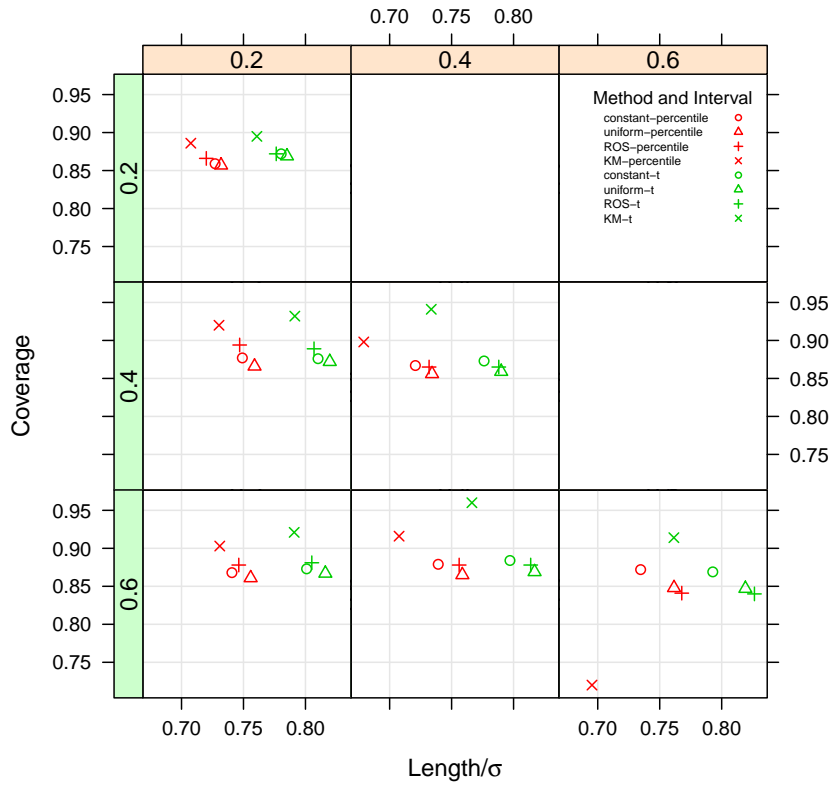
GAM(9, 0.4), N = 30



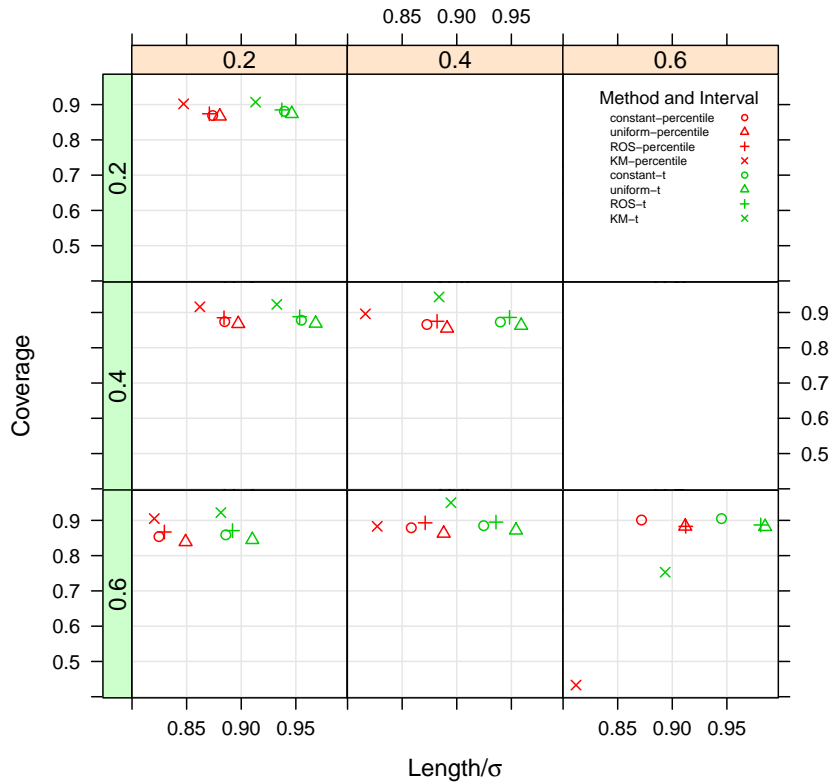
If a researcher has skewed data, the researcher should consider both the amount of skew as well as the percentage of nondetects. If the dataset has an extreme amount of skew and a low percentage of nondetects, any of the four methods would likely produce similar results. If the percentage of nondetects is very large, the K-M method should be used. For a dataset with a more moderate amount of skew, ROS or K-M should be used with a smaller percentage of nondetects but if that percentage exceeds 40%, ROS should be considered more than K-M.

For mixed distributions the results differed between the lognormal and gamma mixtures.

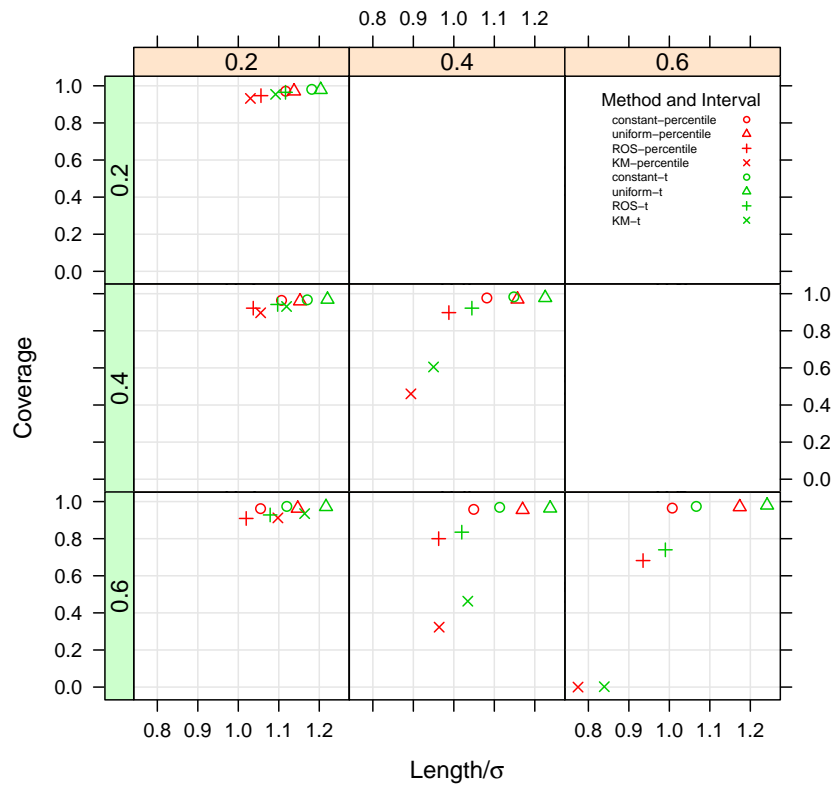
70% LN(0, 1), 30% LN(0, 0.25), N = 30



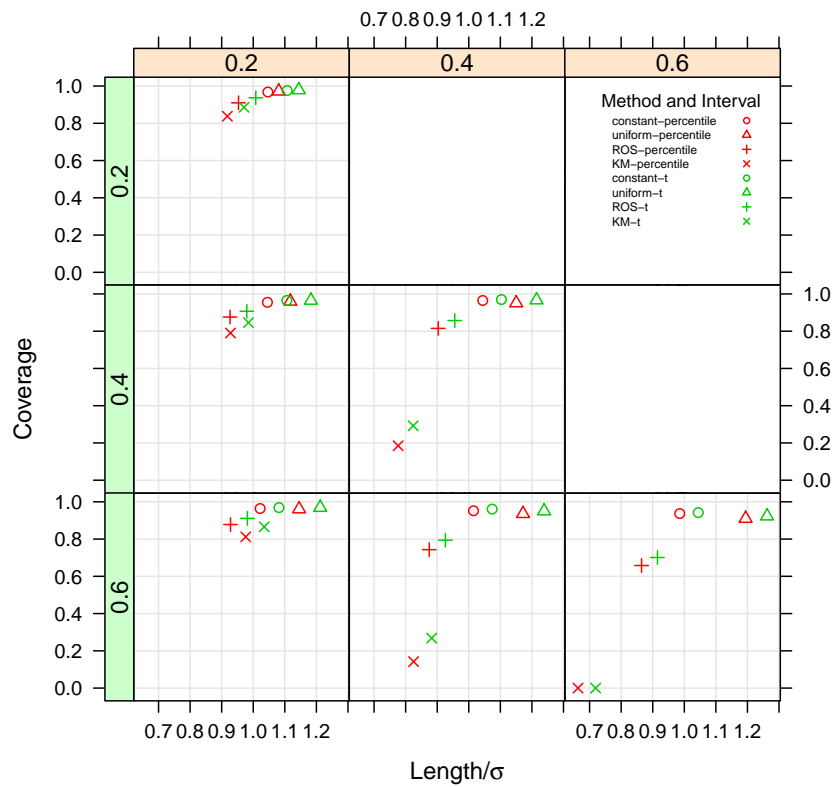
50% LN(0, 1), 50% LN(0, 0.5), N = 30



40% GAM(7.5, 1), 60% GAM(2, 2), N = 30



70% GAM(7.5, 1), 30% GAM(2, 2), N = 30



The K-M method performed better than the other methods with the lognormal mixtures in the majority of simulations. For the gamma mixtures, ROS and K-M outperformed the other two methods when the percentage of nondetects was less than 40%. Once this threshold was met, ROS and constant substitution performed better. Once the 60% threshold was hit, constant substitution outperformed the other three methods with the percentile intervals. Note that the density curves of the gamma mixtures had a larger x-axis range than the lognormal mixtures. The lognormal densities approached zero around a value of four while the gamma mixtures approached zero around a value of 20. For a more compact non-unimodal mixture, K-M should be considered. For flatter mixtures with more skew, ROS and K-M should be used with lower DLs while ROS or constant substitution should be used with higher DLs.

The results were fairly consistent for the sample sizes tested. This indicates that sample sizes between 20 and 50 do not have a significant impact on the best method to use. It's worth noting that the uniform substitution method consistently performed poorest out of the four methods. The method did achieve large coverage in many of the simulations, but consistently had the largest width by a wide margin.

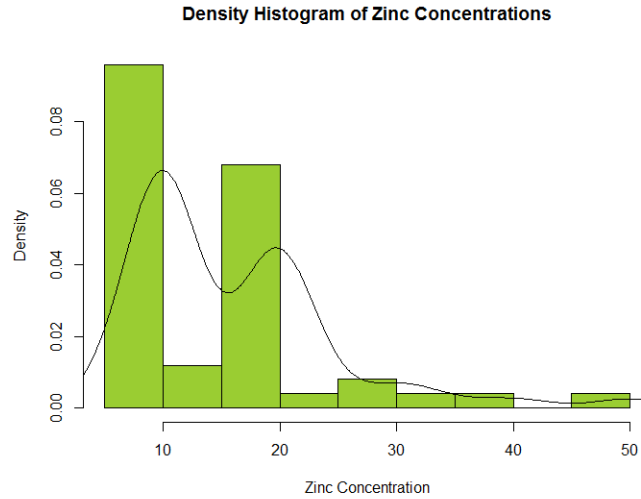
The bootstrap percentile intervals consistently had a smaller width and lower coverage than the bootstrap t intervals. In the majority of simulations, the coverage difference was fairly insignificant but the width difference was fairly large. For symmetric distributions the intervals performed similarly, but for skewed distributions the percentile interval started to perform better than the t interval.

5.4 Real Data Example

The following dataset is taken from a paper by Millard (1988). The dataset contains groundwater zinc concentrations ($\mu\text{g}/L$) from a zone within the San Joaquin Valley in California. The dataset contains two DLs, 10 and 3. If a value in the dataset is a nondetect, the DL is displayed.

Zinc Concentration	Nondetect?	Zinc Concentration	Nondetect?
10	Yes	9	No
5	No	18	No
10	Yes	12	No
10	No	11	No
11	No	19	No
8	No	3	Yes
10	Yes	10	Yes
10	No	10	No
10	No	10	No
10	Yes	10	No
10	Yes	10	No
10	Yes	10	No
10	Yes	10	No
10	No	20	No
20	No	10	Yes
20	No	20	No
20	No	10	Yes
10	No	20	No
40	No	50	No
33	No	10	No
20	No	10	No
10	No	10	No
30	No	20	No
10	No	20	No
20	No	20	No
10	Yes	20	No
23	No	17	No
10	No	10	Yes
10	No	20	No
29	No	20	No
10	Yes	10	No
10	Yes	10	No
7	No	10	Yes

A histogram of the data with the nondetects removed is given below overlapped with the R density function output of the data.



The data appears to be fairly bimodal so we might conclude that it's a mixed distribution. Suppose the researcher is interested in calculating a confidence interval for the average zinc concentration within the zone. The 95% bootstrap confidence intervals for the four methods investigated in the simulations are given below. Each interval is calculated from 300 bootstrap samples of the data.

Method	95% Percentile CI	Width	95% t CI	Width
Constant Substitution	(11.55, 15.52)	3.97	(11.35, 15.52)	4.17
Uniform Substitution	(11.31, 15.40)	4.09	(11.11, 15.41)	4.30
ROS	(11.40, 15.75)	4.35	(11.39, 15.64)	4.25
Kaplan-Meier	(11.80, 15.92)	4.12	(11.68, 15.90)	4.22

If we compare the density functions to those used in the previous section, it can be concluded that this data appears to be similar to the non-unimodal mixed distributions. Furthermore, the data matches up more to the gamma mixtures than to the lognormal mixtures. This is apparent when comparing the height and width of the density curve. The gamma mixtures tested did not reach as high of a density on the y-axis as the lognormal mixtures did and covered a wider range on the x-axis. In other words, the gamma mixtures are more skewed than the lognormal mixtures.

The K-M and ROS methods performed better than the other two methods with a similar

proportion of nondetects to this sample of data (24.2%). The K-M method produced intervals with a slightly smaller width and smaller coverage at this level of nondetects in the simulations. The widths of the above intervals are consistent with this. It's likely a matter of personal preference of the researcher on which method to use. If the researcher values the width of the interval more than the coverage, then the K-M interval should be used. If the researcher values a higher coverage, then the ROS interval should be used. Note that in general, the bootstrap percentile intervals outperformed the bootstrap t-intervals with skewed data and therefore, the percentile intervals would be preferred in this situation.

6 Future Research

The simulations conducted in this study produced two specific types of bootstrap intervals. Additional bootstrap intervals such as BC_a , and ABC have been discussed in the literature and could be tested in future simulations.

This study tested lognormal and gamma data. Another distribution mentioned occasionally in environmental data literature is Weibull. Simulations involving this distribution could be added.

Additional mixed distributions could be tested. Different parameters could be used or lognormal and gamma data could have data from a normal distribution added to it. Sample sizes larger than 50 could also be tested.

A statistic occasionally mentioned in nondetect literature is the 95th percentile. The simulations in this study could be repeated for this statistic.

This study tested data with two detection limits but additional DLs could be present in environmental data. Simulations of data with three DLs could be conducted.

The simulations in this study estimated a single mean. Hypothesis testing for the difference between multiple means could be tested as well.

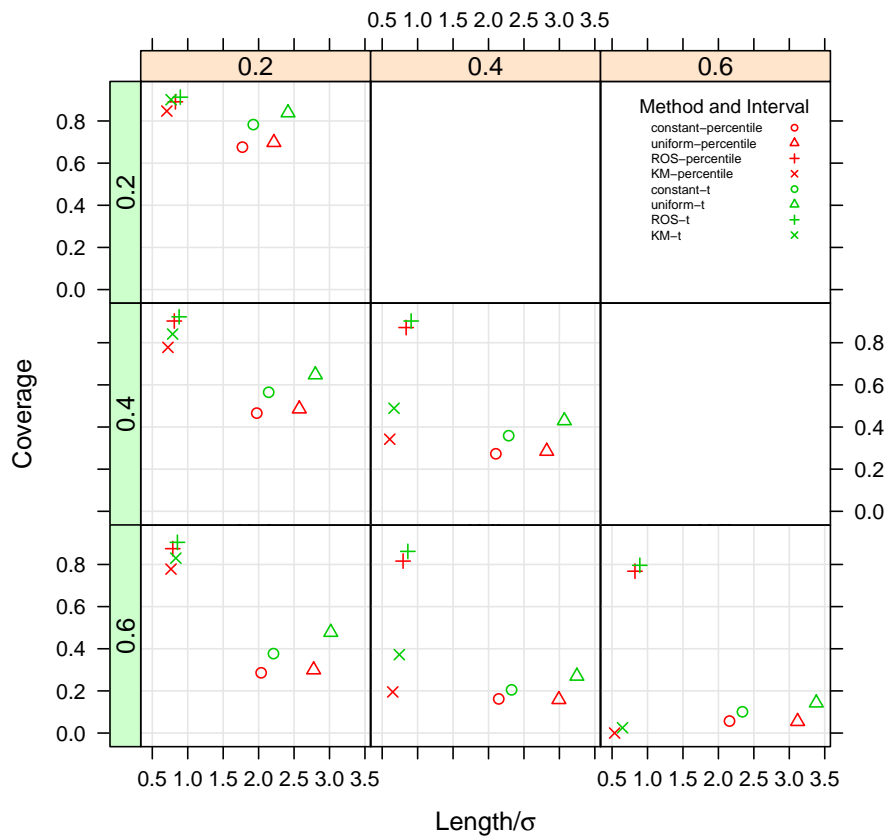
Appendices

A Graphical Results of All Simulations

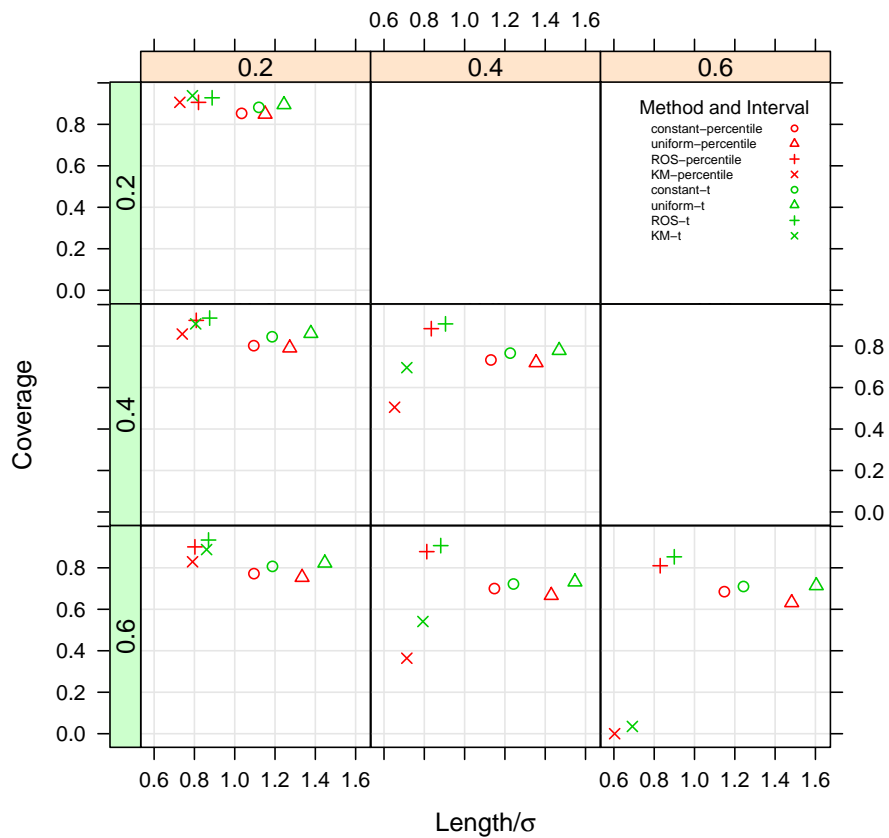
The graphs below are a representation of the numerical results in Appendix A. In each table, each frame represents a combination of two detection limits. The coverage of each interval is given on the y-axis and the average width in population standard deviations of each interval is given on the x-axis. Intervals in the top left of each frame performed well in the simulation as they had high coverage and a low width.

Bootstrap Simulation Results, N = 20

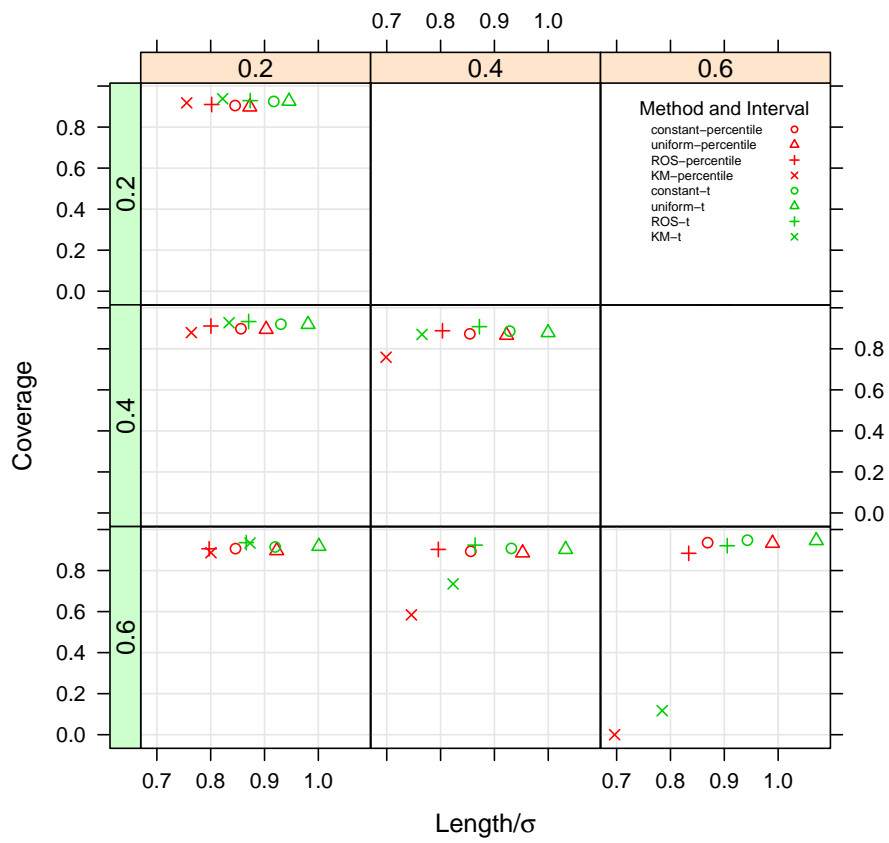
LN(0, 0.1), N = 20



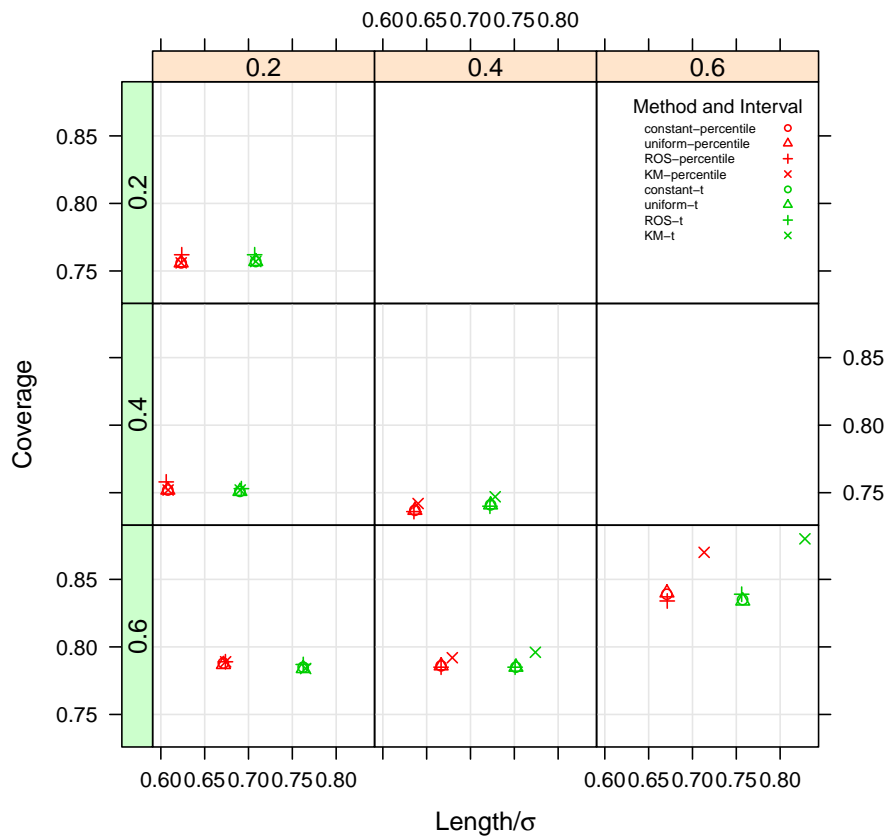
LN(0, 0.25), N = 20



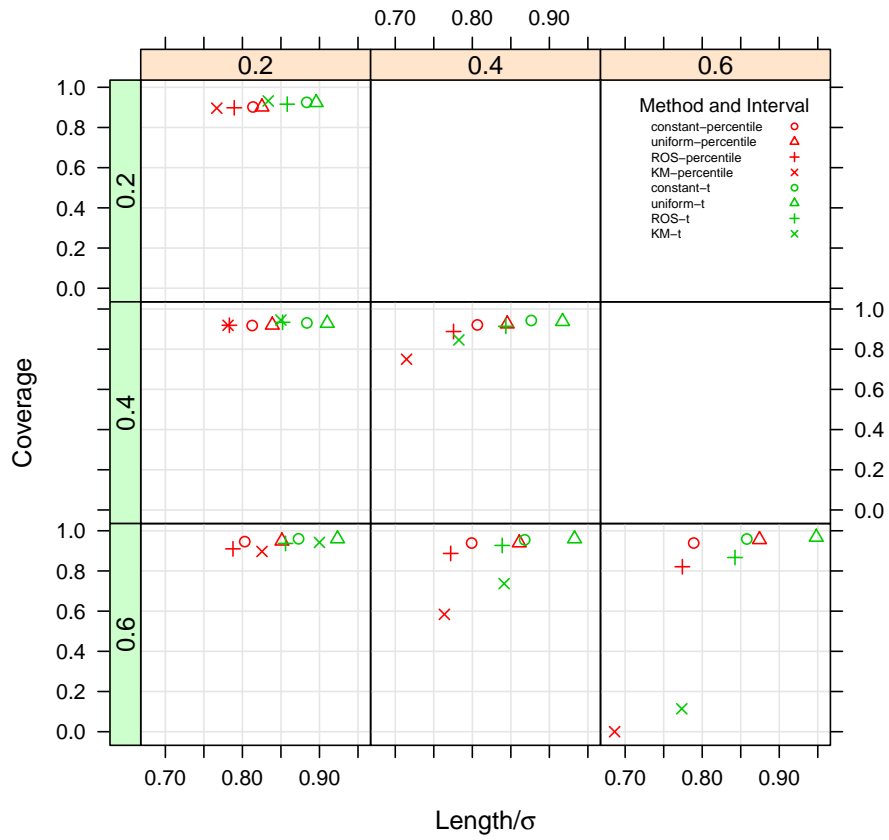
LN(0, 0.5), N = 20



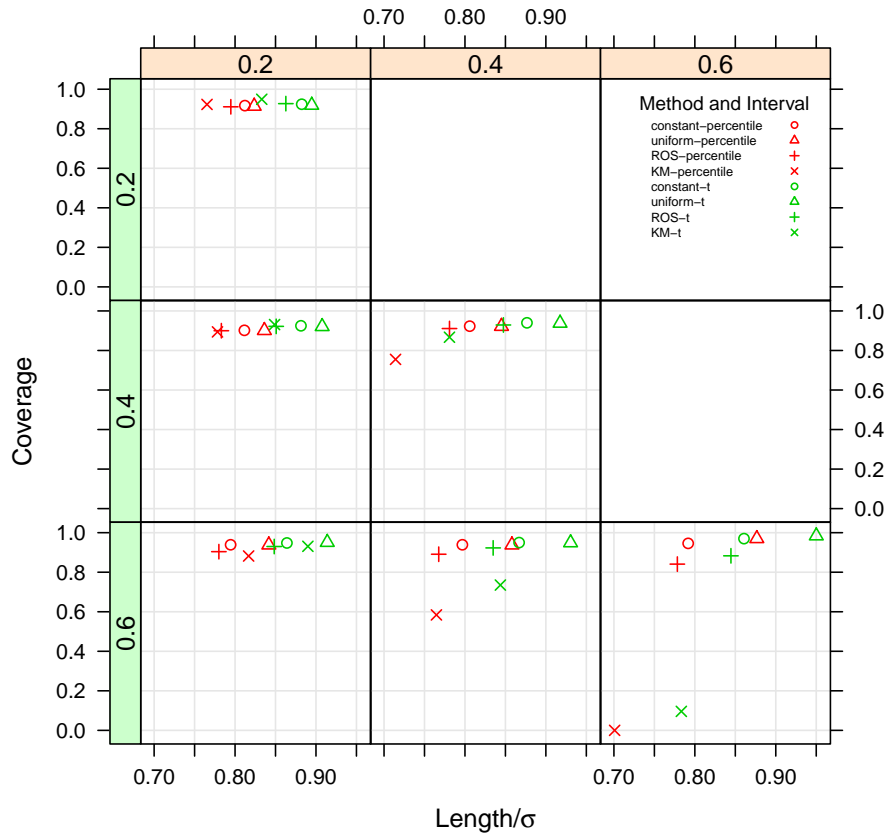
GAM(0.1, 2), N = 20



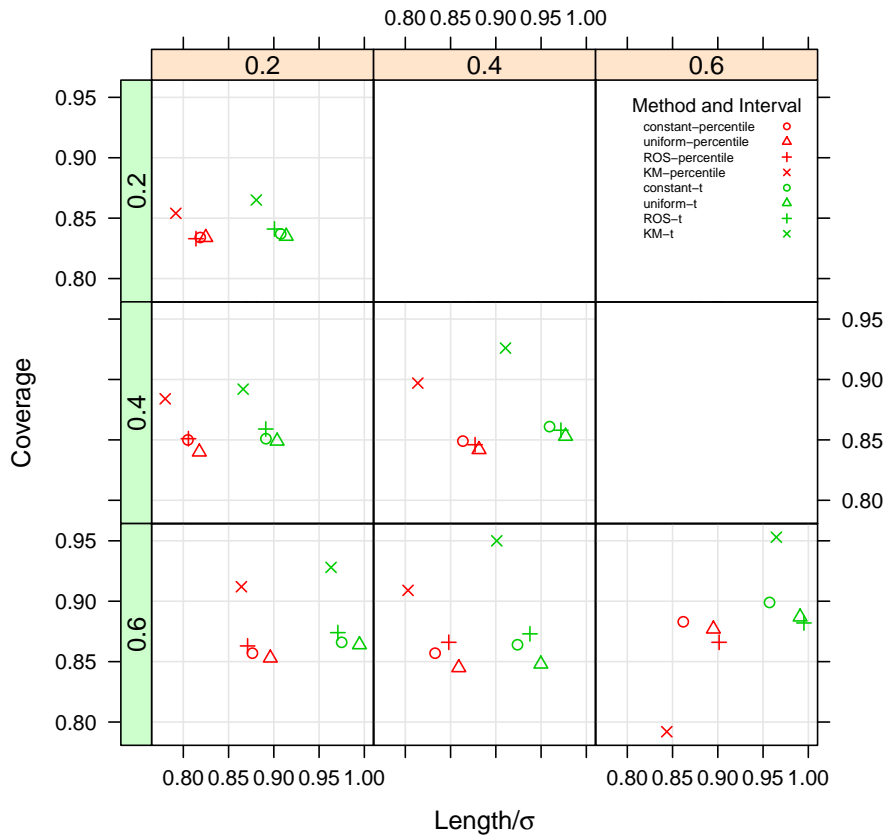
GAM(2, 0.5), N = 20



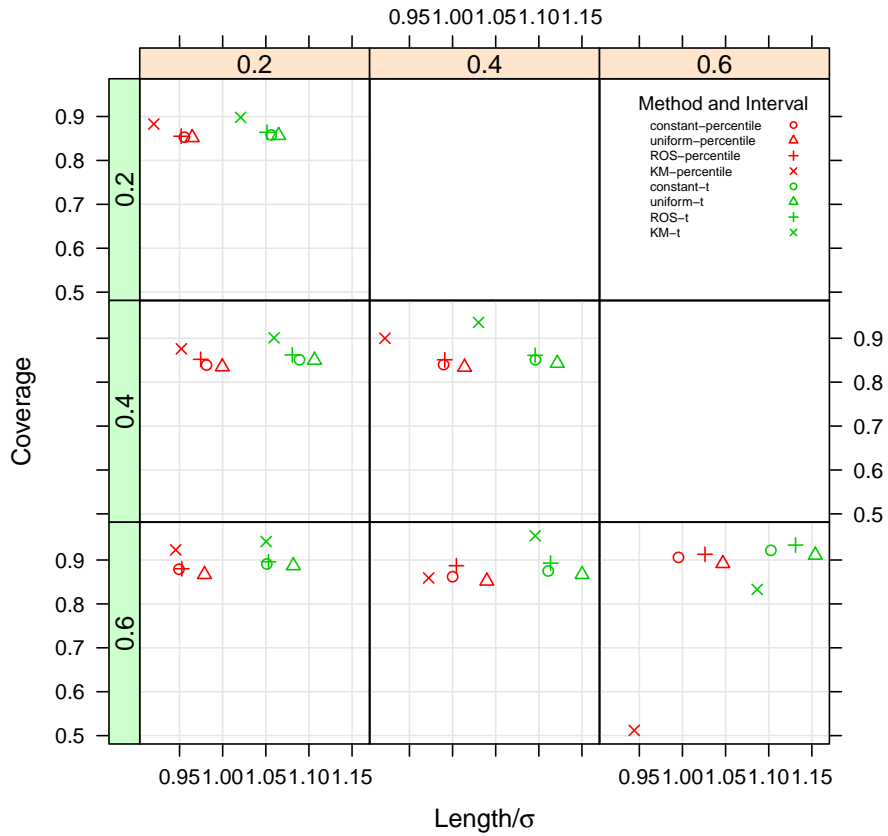
GAM(9, 0.4), N = 20



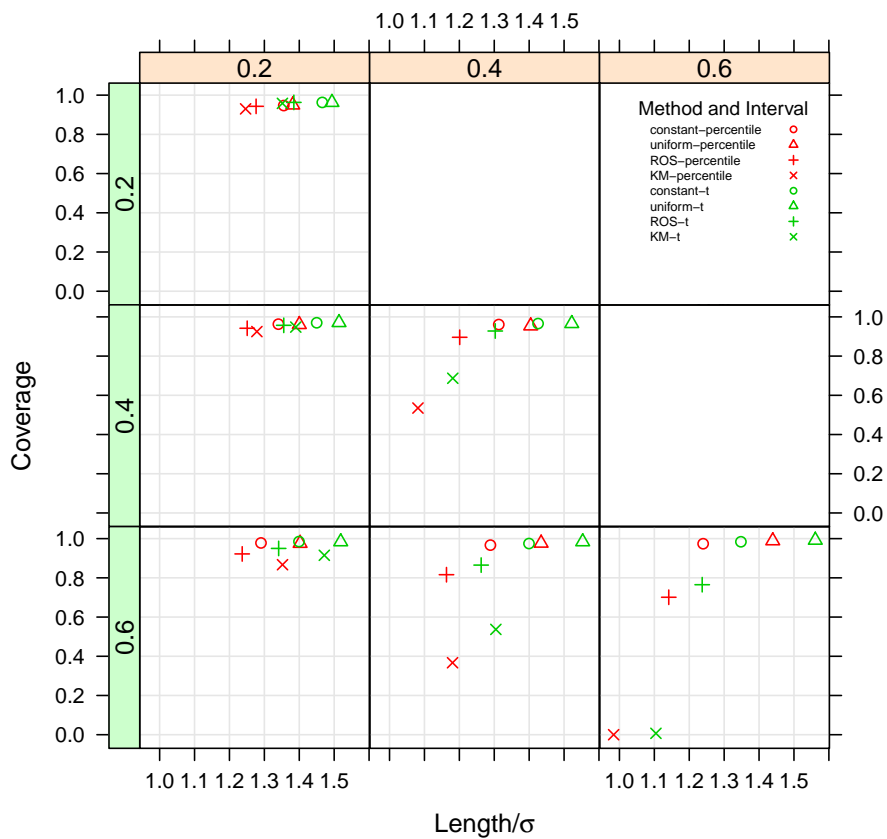
70% LN(0, 1), 30% LN(0, 0.25), N = 20



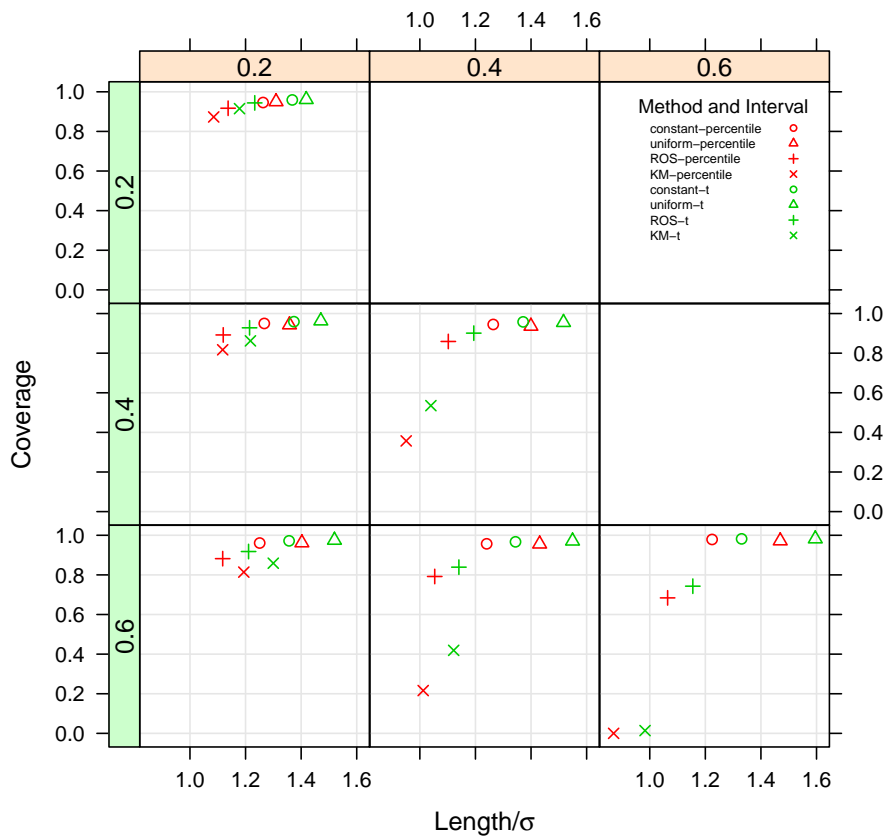
50% LN(0, 1), 50% LN(0, 0.50), N = 20



40% GAM(7.5, 1), 60% GAM(2, 2), N = 20

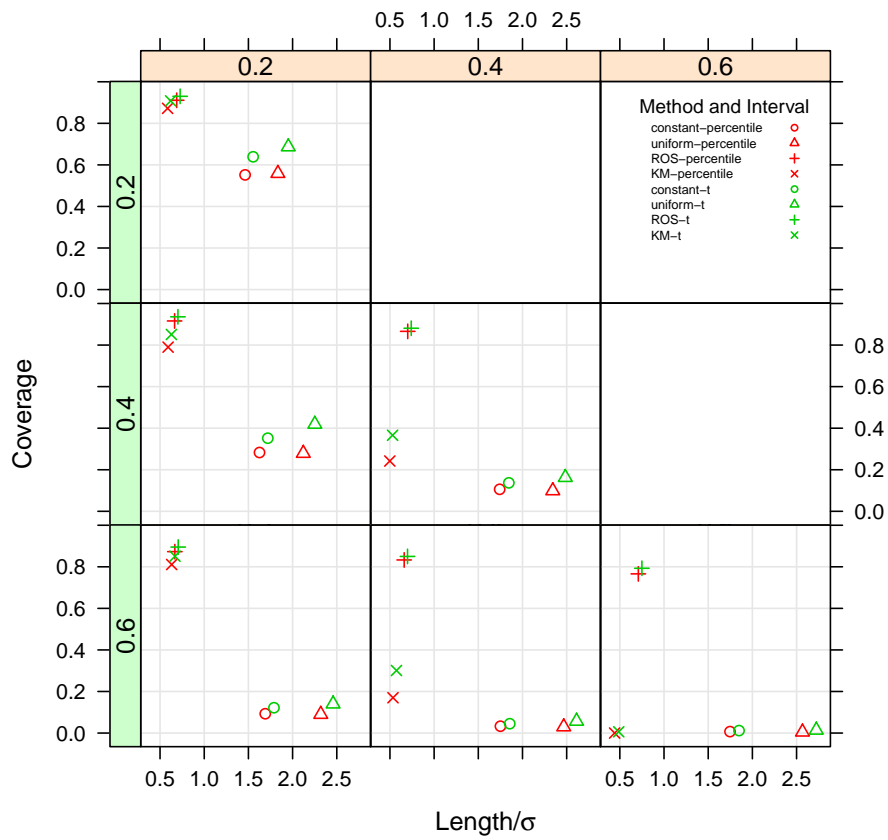


70% GAM(7.5, 1), 30% GAM(2, 2), N = 20

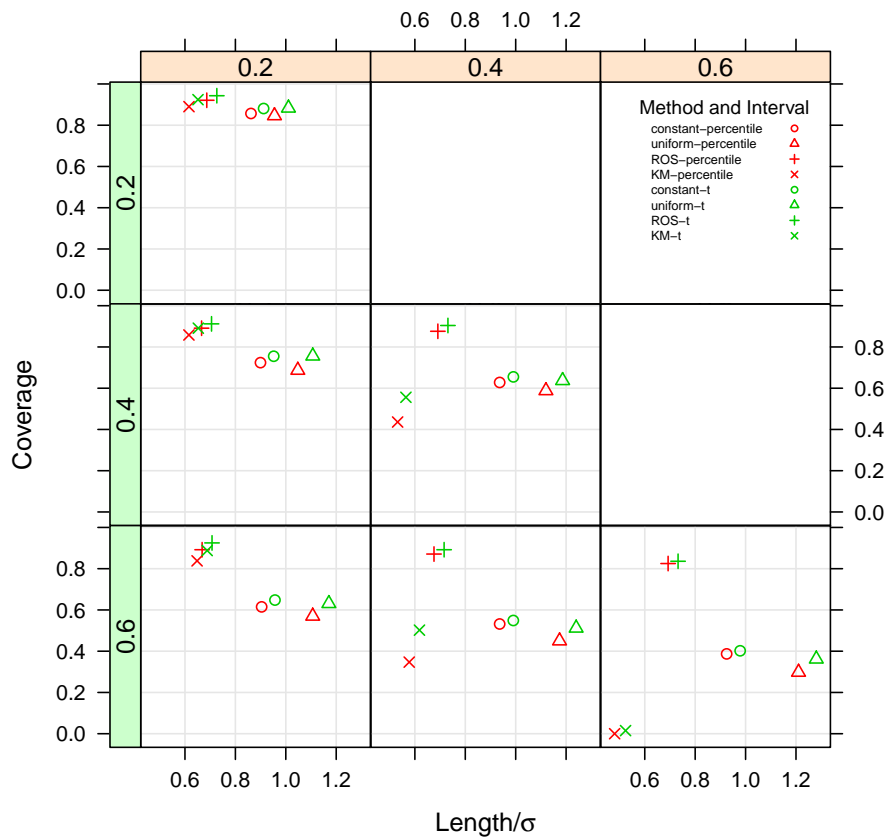


Bootstrap Simulation Results, N = 30

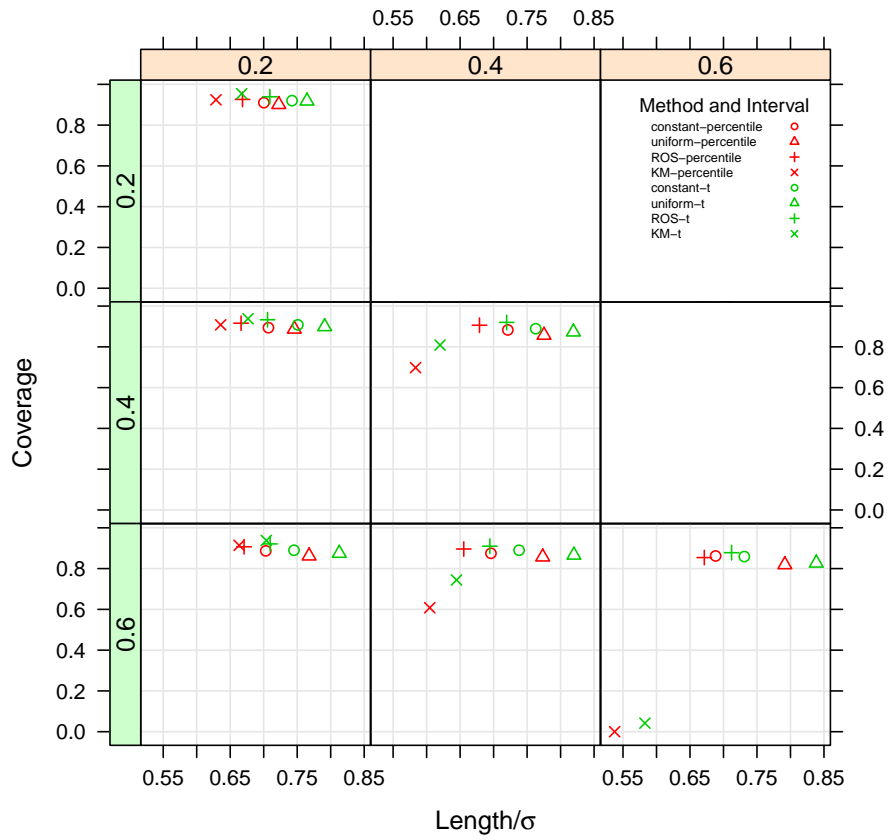
LN(0, 0.1), N = 30



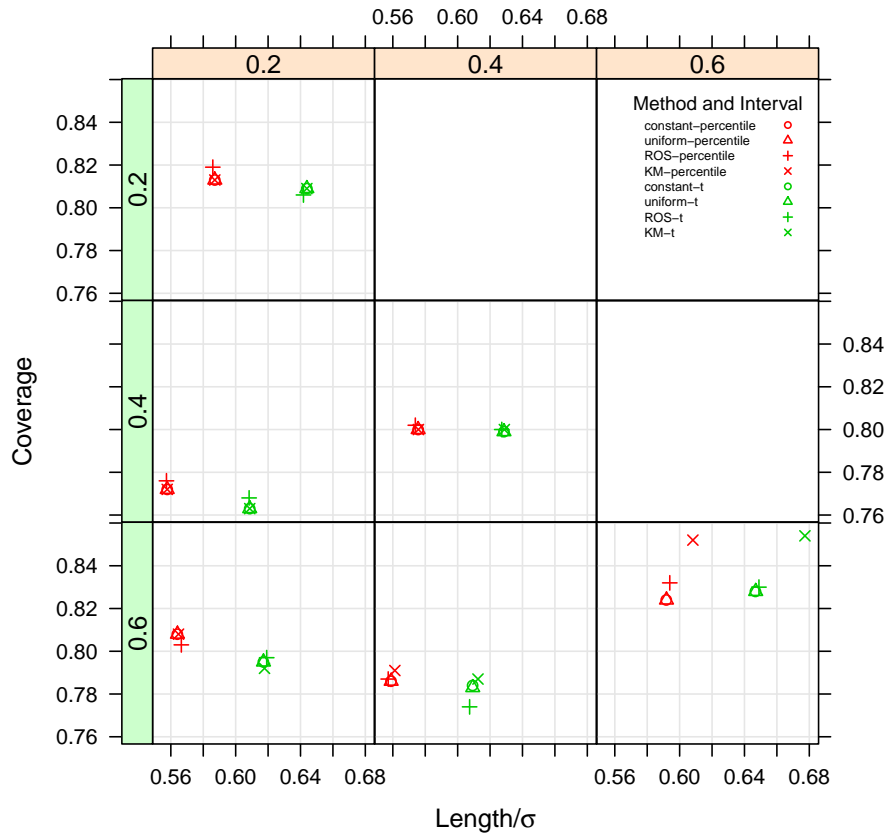
LN(0, 0.25), N = 30



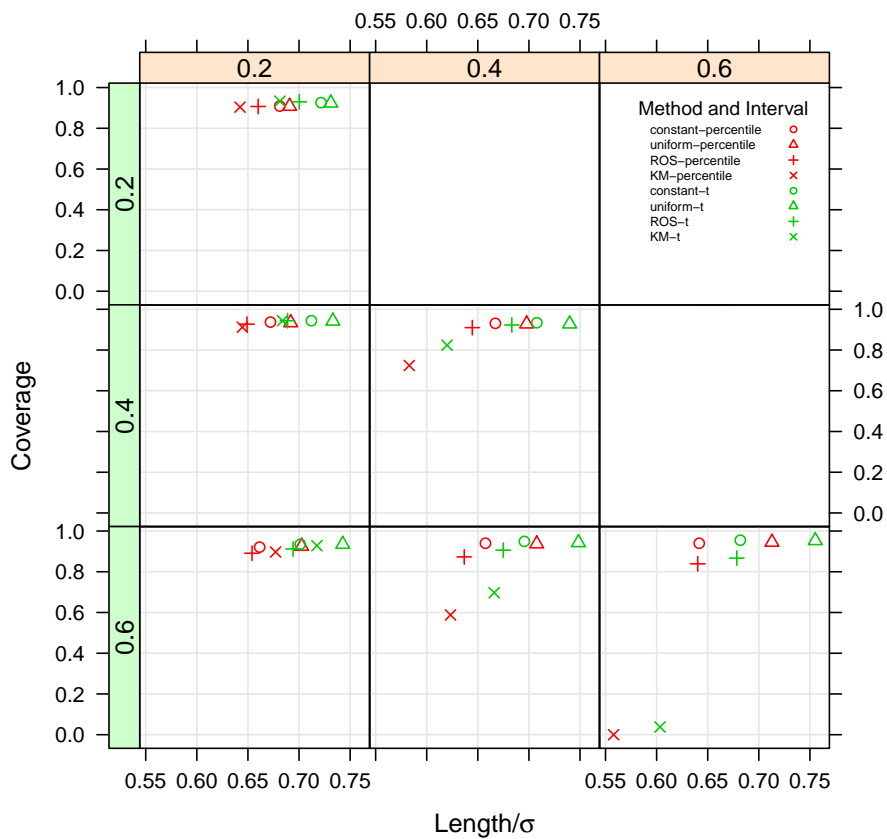
LN(0, 0.5), N = 30



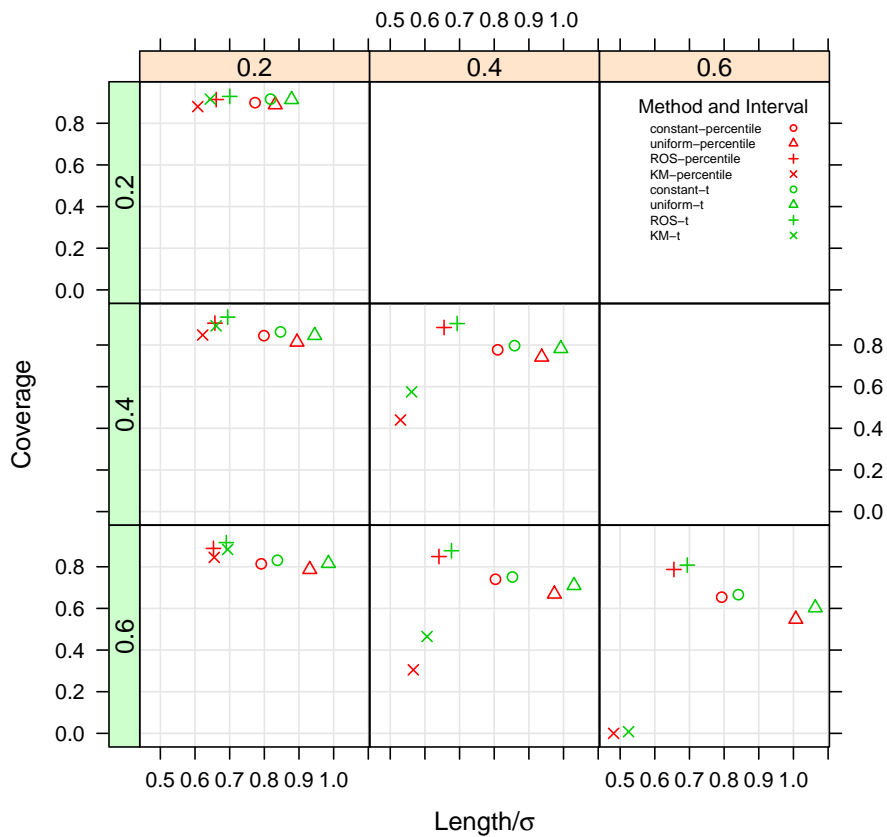
GAM(0.1, 2), N = 30



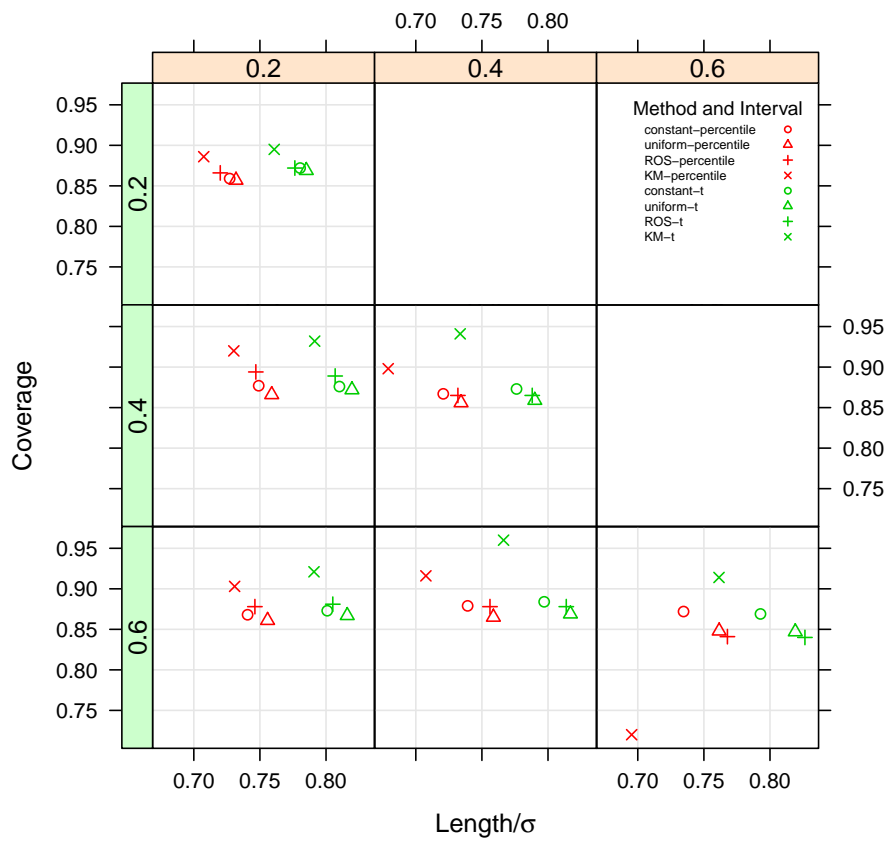
GAM(2, 0.5), N = 30



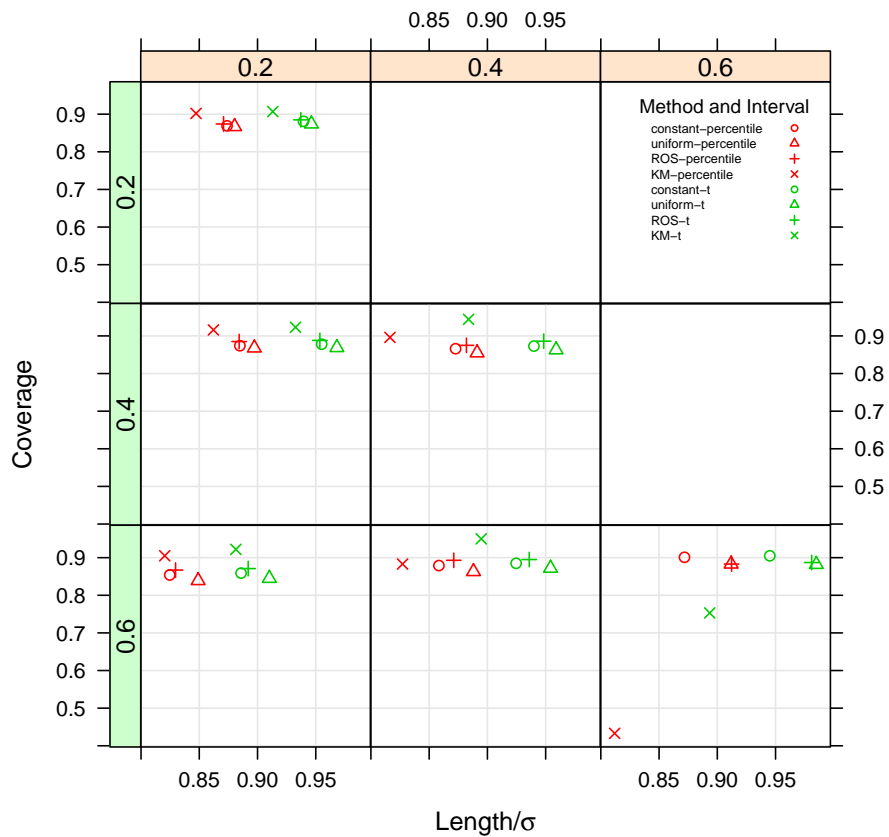
GAM(9, 0.4), N = 30



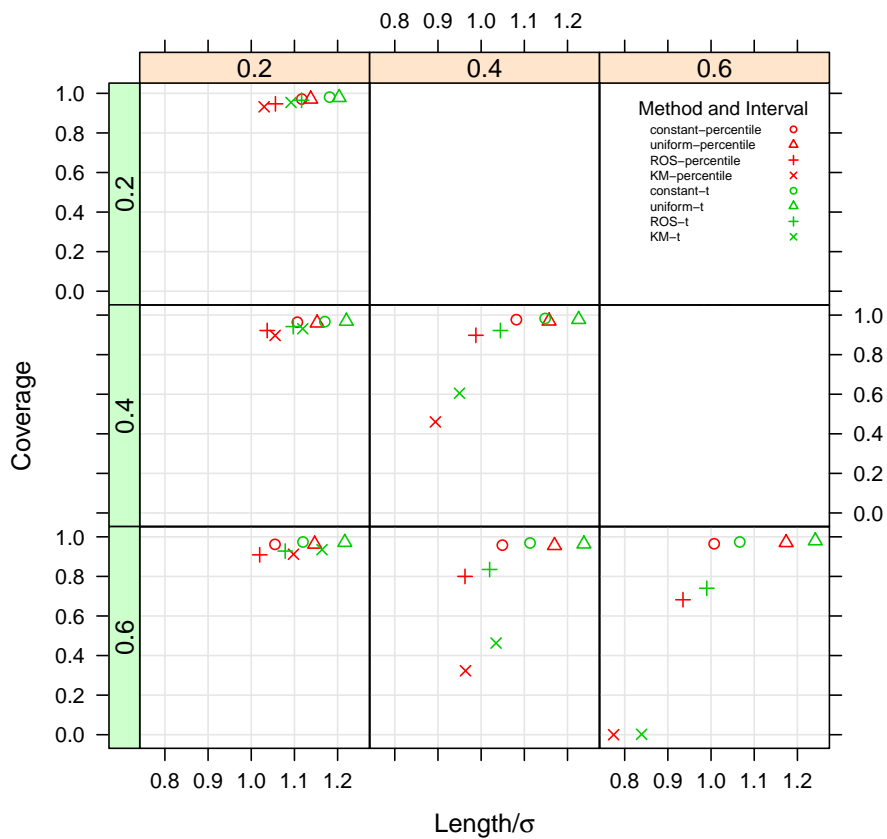
70% LN(0, 1), 30% LN(0, 0.25), N = 30



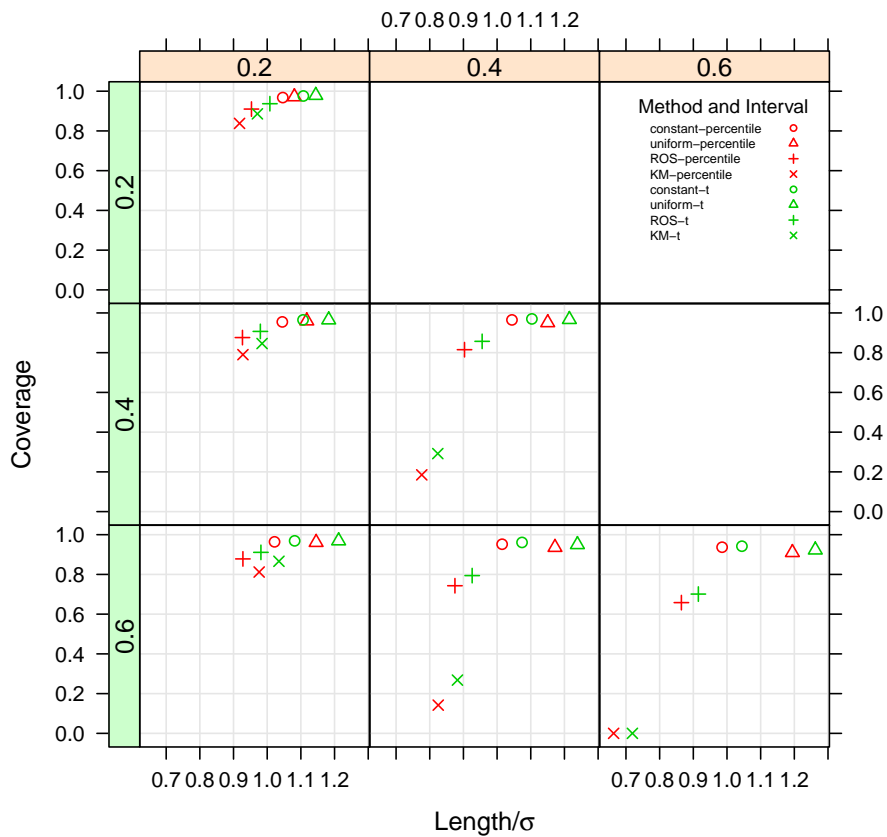
50% LN(0, 1), 50% LN(0, 0.5), N = 30



40% GAM(7.5, 1), 60% GAM(2, 2), N = 30

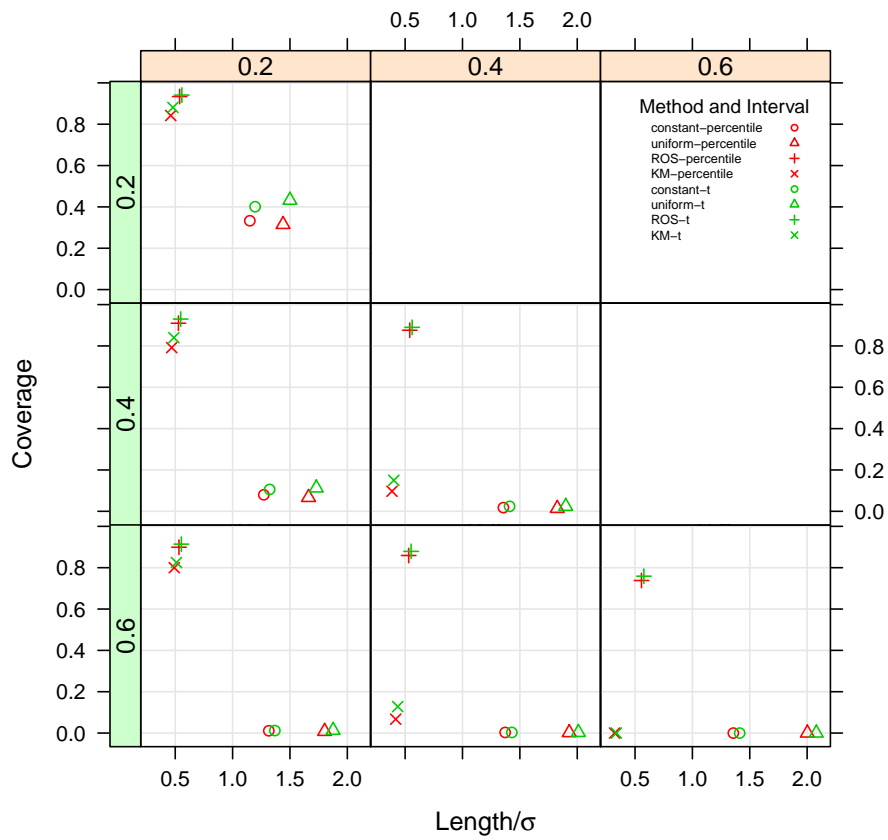


70% GAM(7.5, 1), 30% GAM(2, 2), N = 30

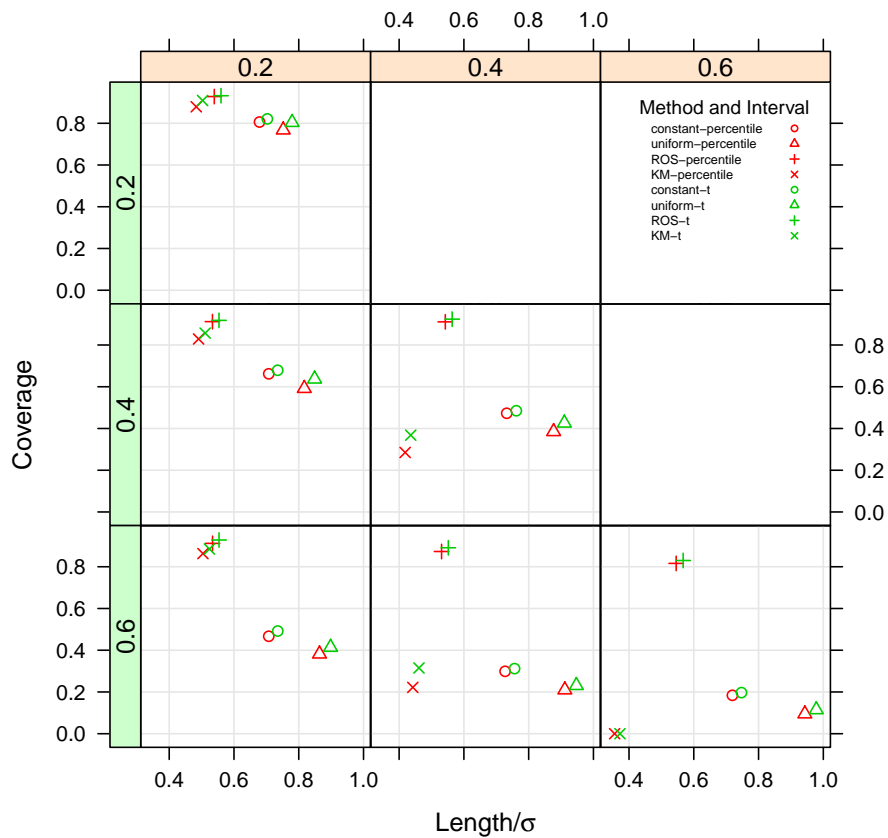


Bootstrap Simulation Results, N = 50

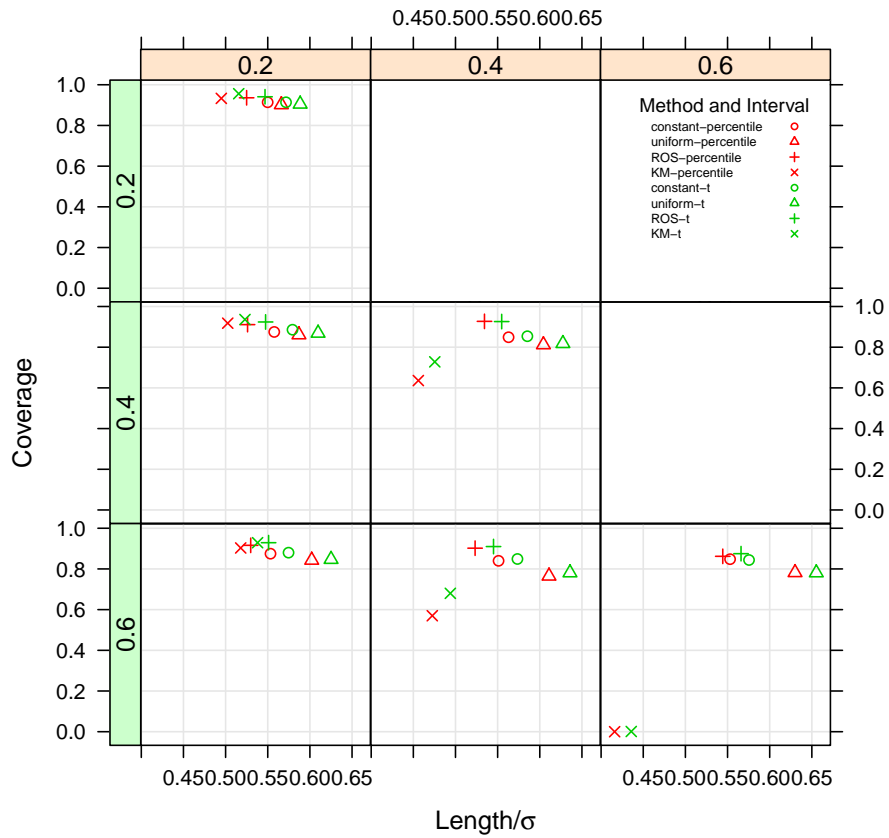
LN(0, 0.1), N = 50



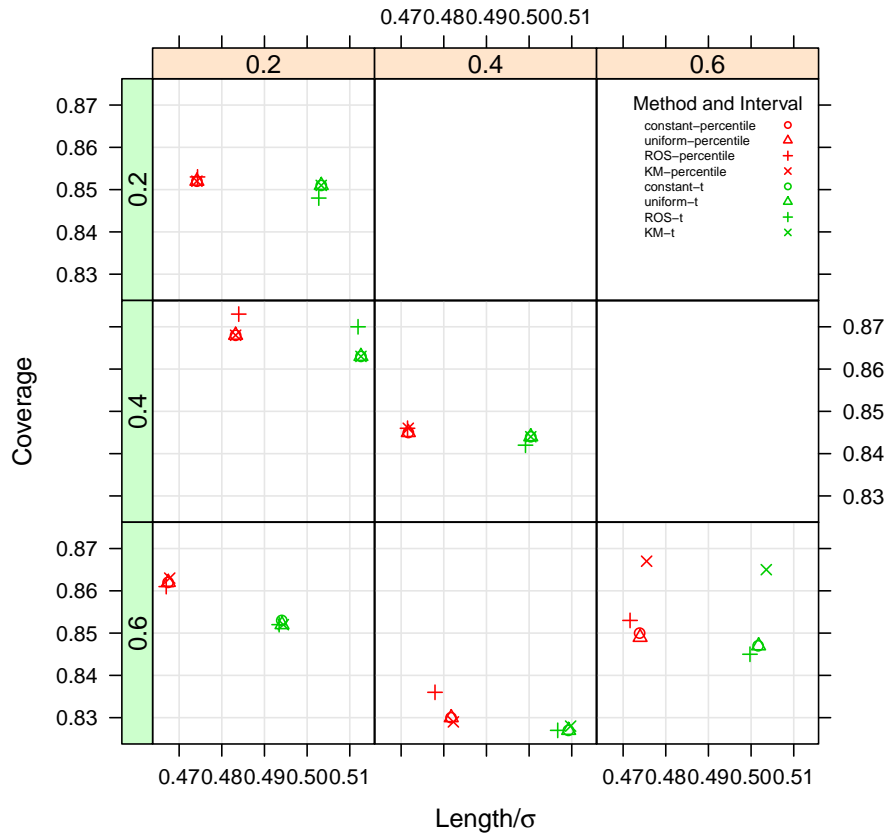
LN(0, 0.25), N = 50



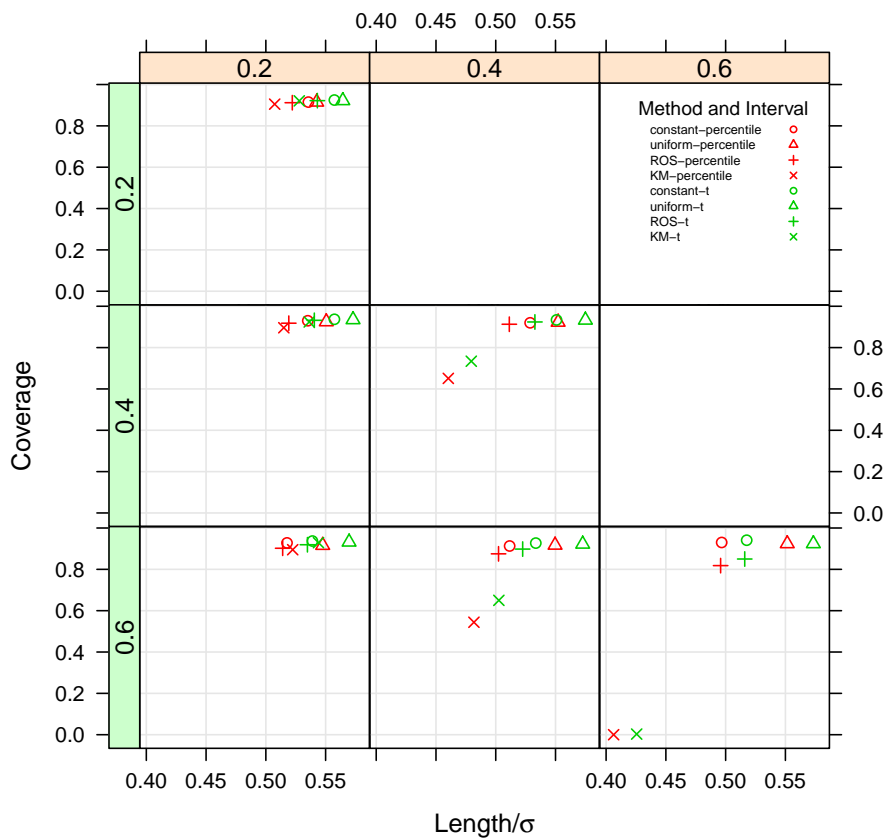
LN(0, 0.5), N = 50



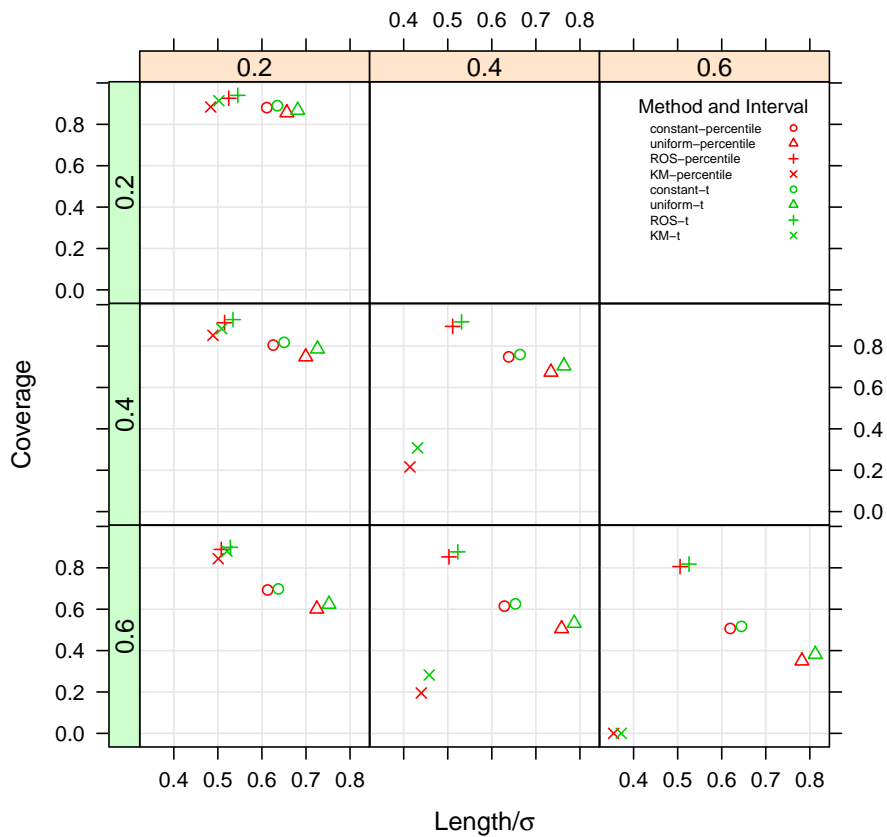
GAM(0.1, 2), N = 50



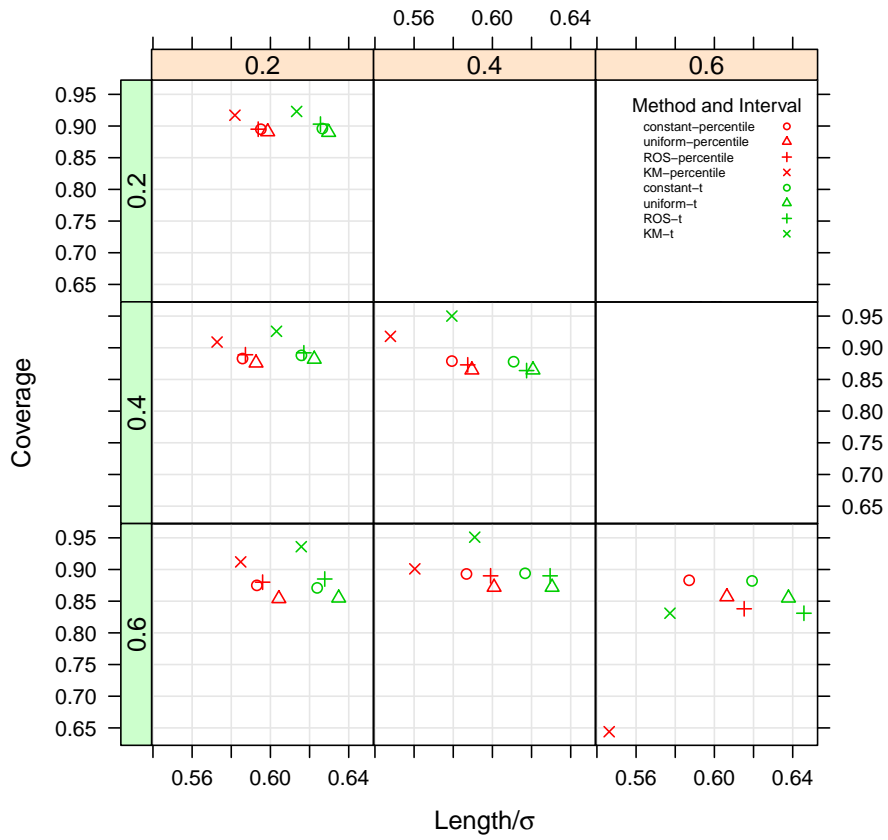
GAM(2, 0.5), N = 50



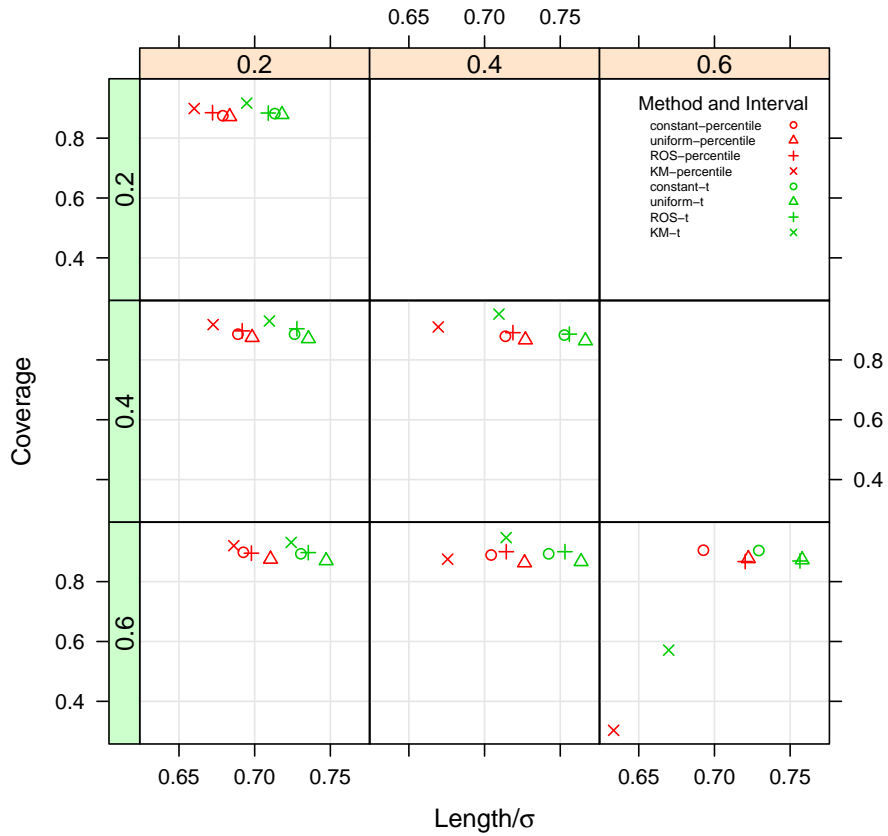
GAM(9, 0.4), N = 50



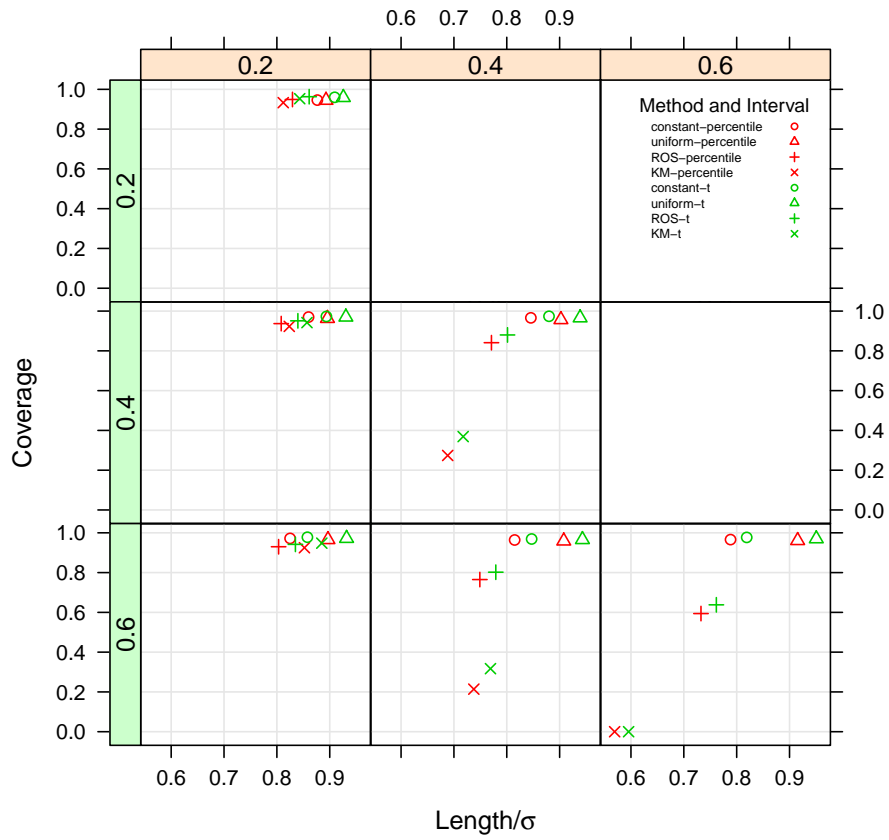
70% LN(0, 1), 30% LN(0, 0.25), N = 50



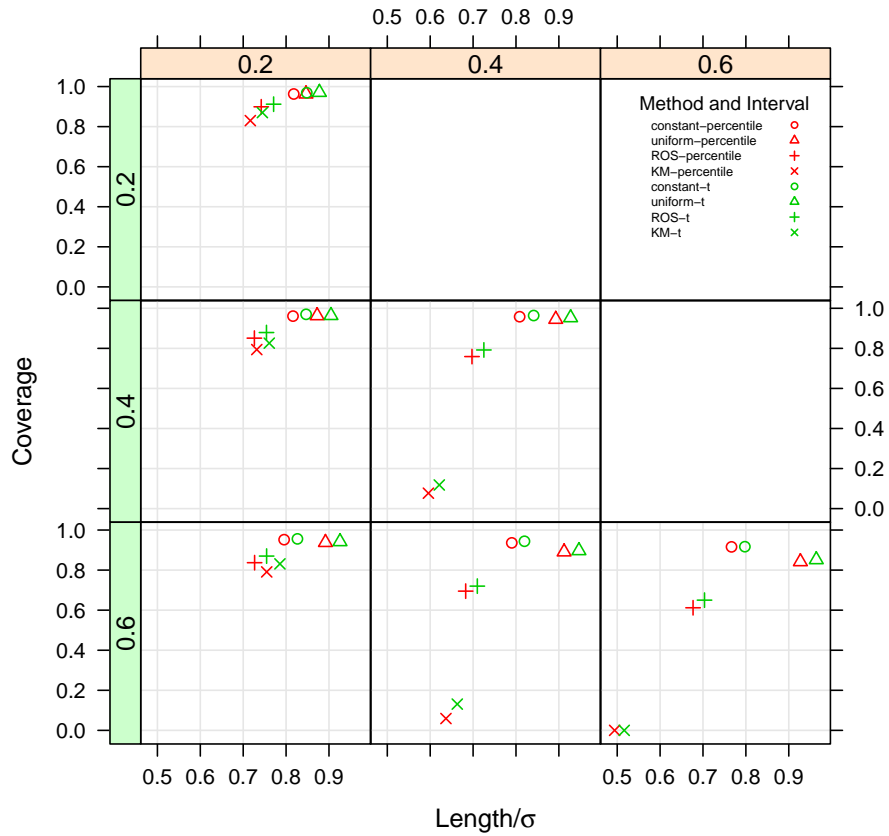
50% LN(0, 1), 50% LN(0, 0.5), N = 50



40% GAM(7.5, 1), 60% GAM(2, 1) N = 50



70% GAM(7.5, 1), 30% GAM(2, 1) N = 50



B Numeric Results of All Simulations

Two numbers are given for each interval. The first number is the proportion out of 1000 confidence intervals that contained the population mean. The second number is the average width of the confidence intervals given in population standard deviations.

Bootstrap Simulation Results, $N = 20$

LN(0, 0.1)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.676	1.771	0.783	1.925								
	Uniform	0.698	2.215	0.839	2.415								
	ROS	0.891	0.826	0.913	0.895								
	K-M	0.847	0.705	0.901	0.765								
0.4	Constant	0.466	1.974	0.565	2.142	0.273	2.104	0.359	2.284				
	Uniform	0.486	2.574	0.648	2.800	0.285	2.821	0.430	3.070				
	ROS	0.903	0.810	0.923	0.879	0.872	0.838	0.903	0.908				
	K-M	0.778	0.721	0.841	0.787	0.342	0.607	0.489	0.667				
0.6	Constant	0.286	2.036	0.377	2.209	0.162	2.144	0.205	2.326	0.057	2.157	0.101	2.339
	Uniform	0.300	2.776	0.478	3.018	0.159	2.992	0.270	3.247	0.055	3.117	0.143	3.381
	ROS	0.875	0.789	0.905	0.854	0.816	0.795	0.862	0.862	0.768	0.823	0.796	0.891
	K-M	0.778	0.764	0.830	0.832	0.195	0.649	0.372	0.742	0.000	0.536	0.025	0.648

LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.853	1.034	0.882	1.120								
	Uniform	0.849	1.151	0.895	1.245								
	ROS	0.906	0.820	0.928	0.888								
	K-M	0.906	0.728	0.938	0.790								
0.4	Constant	0.802	1.095	0.845	1.186	0.733	1.131	0.766	1.226				
	Uniform	0.791	1.273	0.861	1.378	0.720	1.355	0.779	1.469				
	ROS	0.924	0.809	0.935	0.876	0.884	0.835	0.907	0.905				
	K-M	0.858	0.740	0.907	0.806	0.505	0.652	0.696	0.713				
0.6	Constant	0.772	1.095	0.807	1.187	0.700	1.148	0.722	1.242	0.685	1.148	0.710	1.243
	Uniform	0.754	1.334	0.823	1.447	0.667	1.430	0.732	1.548	0.632	1.482	0.714	1.604
	ROS	0.901	0.802	0.934	0.870	0.878	0.812	0.907	0.881	0.810	0.830	0.853	0.900
	K-M	0.829	0.791	0.888	0.860	0.364	0.713	0.541	0.793	0.000	0.604	0.035	0.692

LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.905	0.845	0.925	0.917								
	Uniform	0.898	0.873	0.926	0.945								
	ROS	0.910	0.802	0.929	0.873								
	K-M	0.918	0.755	0.938	0.822								
0.4	Constant	0.898	0.856	0.920	0.930	0.873	0.854	0.886	0.928				
	Uniform	0.895	0.903	0.919	0.981	0.866	0.923	0.879	1.000				
	ROS	0.911	0.800	0.933	0.871	0.888	0.804	0.908	0.872				
	K-M	0.879	0.764	0.927	0.834	0.759	0.699	0.870	0.765				
0.6	Constant	0.907	0.846	0.915	0.920	0.894	0.856	0.908	0.931	0.936	0.869	0.948	0.943
	Uniform	0.897	0.923	0.918	1.001	0.886	0.952	0.903	1.032	0.933	0.990	0.946	1.071
	ROS	0.906	0.797	0.936	0.866	0.903	0.796	0.924	0.864	0.884	0.834	0.921	0.905
	K-M	0.887	0.801	0.934	0.873	0.584	0.746	0.735	0.823	0.000	0.696	0.117	0.785

GAM(0.1, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.756	0.623	0.757	0.708								
	Uniform	0.756	0.623	0.757	0.708								
	ROS	0.762	0.624	0.762	0.707								
	K-M	0.756	0.623	0.757	0.708								
0.4	Constant	0.752	0.608	0.751	0.690	0.737	0.637	0.741	0.723				
	Uniform	0.752	0.608	0.751	0.690	0.737	0.637	0.741	0.723				
	ROS	0.758	0.606	0.753	0.692	0.736	0.635	0.740	0.722				
	K-M	0.752	0.608	0.752	0.691	0.742	0.640	0.747	0.728				
0.6	Constant	0.788	0.671	0.785	0.762	0.786	0.666	0.785	0.752	0.839	0.671	0.835	0.757
	Uniform	0.787	0.671	0.784	0.762	0.786	0.667	0.785	0.752	0.840	0.671	0.834	0.757
	ROS	0.789	0.674	0.787	0.762	0.785	0.666	0.785	0.751	0.834	0.671	0.839	0.756
	K-M	0.789	0.674	0.784	0.765	0.792	0.679	0.796	0.774	0.870	0.713	0.880	0.828

GAM(2, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.902	0.814	0.925	0.883								
	Uniform	0.902	0.825	0.924	0.896								
	ROS	0.898	0.789	0.916	0.858								
	K-M	0.896	0.767	0.932	0.833								
0.4	Constant	0.918	0.813	0.931	0.884	0.921	0.806	0.943	0.876				
	Uniform	0.920	0.839	0.929	0.910	0.926	0.845	0.938	0.917				
	ROS	0.919	0.783	0.934	0.852	0.888	0.776	0.914	0.844				
	K-M	0.919	0.781	0.945	0.850	0.750	0.715	0.846	0.783				
0.6	Constant	0.946	0.803	0.960	0.873	0.939	0.799	0.955	0.868	0.939	0.789	0.959	0.858
	Uniform	0.949	0.851	0.960	0.923	0.940	0.861	0.960	0.933	0.956	0.874	0.968	0.948
	ROS	0.910	0.788	0.937	0.856	0.887	0.772	0.927	0.839	0.821	0.774	0.867	0.843
	K-M	0.897	0.825	0.942	0.900	0.584	0.764	0.737	0.841	0.000	0.686	0.114	0.773

GAM(9, 0.4)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.917	0.812	0.924	0.882								
	Uniform	0.914	0.824	0.919	0.895								
	ROS	0.911	0.795	0.927	0.863								
	K-M	0.923	0.765	0.949	0.833								
0.4	Constant	0.902	0.812	0.925	0.881	0.923	0.806	0.940	0.877				
	Uniform	0.901	0.836	0.921	0.908	0.922	0.845	0.938	0.918				
	ROS	0.900	0.783	0.922	0.851	0.911	0.781	0.929	0.848				
	K-M	0.894	0.778	0.931	0.849	0.755	0.714	0.867	0.781				
0.6	Constant	0.939	0.795	0.948	0.864	0.939	0.797	0.950	0.867	0.946	0.792	0.970	0.861
	Uniform	0.938	0.842	0.951	0.914	0.938	0.858	0.949	0.931	0.970	0.877	0.984	0.950
	ROS	0.904	0.780	0.930	0.848	0.891	0.768	0.923	0.835	0.841	0.778	0.883	0.845
	K-M	0.882	0.817	0.931	0.890	0.584	0.765	0.735	0.844	0.000	0.701	0.096	0.783

70 % LN(0, 1), 30 % LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.834	0.819	0.837	0.908								
	Uniform	0.834	0.825	0.835	0.914								
	ROS	0.833	0.814	0.841	0.901								
	K-M	0.854	0.792	0.865	0.881								
0.4	Constant	0.850	0.805	0.851	0.891	0.849	0.864	0.861	0.959				
	Uniform	0.840	0.818	0.849	0.904	0.842	0.881	0.853	0.977				
	ROS	0.851	0.806	0.859	0.891	0.846	0.877	0.858	0.972				
	K-M	0.884	0.780	0.892	0.866	0.897	0.814	0.926	0.911				
0.6	Constant	0.857	0.876	0.866	0.975	0.857	0.833	0.864	0.924	0.883	0.862	0.899	0.957
	Uniform	0.853	0.896	0.864	0.995	0.845	0.859	0.848	0.950	0.877	0.895	0.887	0.991
	ROS	0.863	0.871	0.874	0.971	0.866	0.848	0.873	0.938	0.866	0.901	0.882	0.995
	K-M	0.912	0.864	0.928	0.963	0.909	0.803	0.950	0.901	0.792	0.844	0.953	0.965

50 % LN(0, 1), 50 % LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.853	0.956	0.858	1.056								
	Uniform	0.852	0.965	0.857	1.065								
	ROS	0.855	0.952	0.864	1.051								
	K-M	0.883	0.920	0.898	1.021								
0.4	Constant	0.839	0.981	0.851	1.089	0.840	0.990	0.851	1.096				
	Uniform	0.835	1.000	0.85	1.106	0.834	1.014	0.843	1.121				
	ROS	0.852	0.975	0.862	1.081	0.851	0.991	0.861	1.096				
	K-M	0.876	0.952	0.901	1.060	0.900	0.922	0.936	1.030				
0.6	Constant	0.879	0.949	0.891	1.051	0.862	1.000	0.875	1.111	0.906	0.995	0.922	1.103
	Uniform	0.867	0.979	0.887	1.082	0.852	1.040	0.867	1.150	0.892	1.047	0.911	1.154
	ROS	0.880	0.953	0.896	1.053	0.887	1.004	0.893	1.114	0.913	1.026	0.934	1.131
	K-M	0.923	0.946	0.942	1.050	0.859	0.972	0.955	1.096	0.512	0.944	0.833	1.087

40 % GAM(7.5, 1), 60 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.947	1.356	0.963	1.466								
	Uniform	0.950	1.381	0.963	1.494								
	ROS	0.943	1.276	0.963	1.384								
	K-M	0.930	1.246	0.958	1.352								
0.4	Constant	0.963	1.340	0.970	1.450	0.961	1.313	0.966	1.426				
	Uniform	0.961	1.400	0.971	1.514	0.954	1.404	0.966	1.522				
	ROS	0.942	1.251	0.957	1.356	0.896	1.201	0.928	1.303				
	K-M	0.925	1.279	0.948	1.390	0.535	1.081	0.687	1.181				
0.6	Constant	0.978	1.290	0.985	1.399	0.967	1.289	0.975	1.400	0.974	1.240	0.984	1.348
	Uniform	0.976	1.402	0.984	1.519	0.977	1.434	0.984	1.553	0.989	1.439	0.992	1.561
	ROS	0.922	1.237	0.950	1.341	0.816	1.163	0.865	1.262	0.701	1.141	0.765	1.237
	K-M	0.867	1.352	0.915	1.472	0.367	1.180	0.537	1.305	0.000	0.983	0.007	1.105

40 % GAM(7.5, 1), 60 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.946	1.263	0.959	1.368								
	Uniform	0.950	1.310	0.961	1.418								
	ROS	0.917	1.137	0.944	1.233								
	K-M	0.873	1.085	0.915	1.178								
0.4	Constant	0.950	1.267	0.959	1.374	0.945	1.264	0.958	1.372				
	Uniform	0.943	1.358	0.963	1.471	0.936	1.400	0.955	1.517				
	ROS	0.892	1.120	0.928	1.214	0.859	1.102	0.901	1.194				
	K-M	0.817	1.118	0.862	1.218	0.357	0.951	0.535	1.040				
0.6	Constant	0.961	1.251	0.972	1.357	0.957	1.240	0.967	1.344	0.979	1.224	0.982	1.330
	Uniform	0.962	1.403	0.975	1.520	0.956	1.431	0.971	1.549	0.972	1.469	0.982	1.596
	ROS	0.882	1.118	0.918	1.211	0.792	1.054	0.839	1.140	0.684	1.064	0.743	1.155
	K-M	0.814	1.194	0.859	1.300	0.216	1.012	0.419	1.122	0.000	0.870	0.014	0.983

Bootstrap Simulation Results, N = 30

LN(0, 0.1)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.552	1.462	0.639	1.553								
	Uniform	0.559	1.834	0.687	1.951								
	ROS	0.911	0.688	0.930	0.727								
	K-M	0.872	0.586	0.908	0.620								
0.4	Constant	0.283	1.626	0.352	1.719	0.106	1.742	0.137	1.846				
	Uniform	0.279	2.121	0.419	2.252	0.099	2.343	0.163	2.485				
	ROS	0.916	0.665	0.936	0.702	0.866	0.701	0.881	0.741				
	K-M	0.790	0.591	0.851	0.629	0.242	0.499	0.366	0.530				
0.6	Constant	0.093	1.691	0.122	1.789	0.033	1.750	0.045	1.856	0.007	1.747	0.012	1.849
	Uniform	0.090	2.319	0.140	2.458	0.030	2.467	0.057	2.612	0.005	2.567	0.014	2.723
	ROS	0.873	0.668	0.895	0.705	0.833	0.661	0.850	0.699	0.766	0.709	0.793	0.750
	K-M	0.811	0.632	0.851	0.669	0.170	0.535	0.301	0.574	0.000	0.441	0.006	0.488

LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.857	0.862	0.881	0.912								
	Uniform	0.846	0.955	0.883	1.011								
	ROS	0.921	0.686	0.943	0.726								
	K-M	0.890	0.616	0.924	0.652								
0.4	Constant	0.724	0.90	0.755	0.952	0.628	0.936	0.655	0.991				
	Uniform	0.687	1.048	0.756	1.107	0.588	1.120	0.637	1.186				
	ROS	0.891	0.666	0.912	0.705	0.876	0.691	0.904	0.731				
	K-M	0.858	0.616	0.891	0.653	0.436	0.532	0.556	0.564				
0.6	Constant	0.615	0.904	0.648	0.957	0.532	0.936	0.549	0.991	0.387	0.925	0.402	0.979
	Uniform	0.570	1.107	0.631	1.171	0.450	1.174	0.512	1.240	0.298	1.210	0.362	1.281
	ROS	0.892	0.668	0.925	0.707	0.871	0.676	0.892	0.716	0.825	0.693	0.836	0.732
	K-M	0.838	0.648	0.888	0.688	0.347	0.578	0.502	0.618	0.000	0.48	0.015	0.524

LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.910	0.70	0.920	0.742								
	Uniform	0.901	0.723	0.918	0.765								
	ROS	0.926	0.668	0.939	0.709								
	K-M	0.924	0.629	0.954	0.667								
0.4	Constant	0.894	0.707	0.908	0.751	0.883	0.721	0.889	0.763				
	Uniform	0.887	0.746	0.899	0.791	0.857	0.775	0.873	0.819				
	ROS	0.916	0.666	0.933	0.706	0.906	0.679	0.920	0.720				
	K-M	0.908	0.636	0.938	0.677	0.698	0.584	0.809	0.620				
0.6	Constant	0.887	0.703	0.890	0.745	0.875	0.696	0.890	0.738	0.862	0.688	0.859	0.731
	Uniform	0.862	0.768	0.875	0.813	0.857	0.773	0.866	0.820	0.819	0.792	0.827	0.839
	ROS	0.907	0.671	0.921	0.710	0.896	0.655	0.910	0.694	0.854	0.671	0.878	0.712
	K-M	0.914	0.663	0.938	0.704	0.608	0.605	0.744	0.645	0.000	0.538	0.042	0.583

GAM(0.1, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.813	0.587	0.809	0.644								
	Uniform	0.813	0.587	0.809	0.644								
	ROS	0.819	0.586	0.806	0.642								
	K-M	0.813	0.587	0.809	0.644								
0.4	Constant	0.772	0.558	0.763	0.609	0.800	0.576	0.799	0.629				
	Uniform	0.772	0.558	0.763	0.609	0.800	0.576	0.799	0.629				
	ROS	0.776	0.557	0.768	0.608	0.802	0.574	0.800	0.627				
	K-M	0.772	0.558	0.763	0.609	0.800	0.576	0.800	0.629				
0.6	Constant	0.808	0.564	0.795	0.617	0.786	0.559	0.784	0.609	0.824	0.592	0.828	0.647
	Uniform	0.808	0.564	0.795	0.617	0.786	0.559	0.783	0.609	0.824	0.592	0.828	0.647
	ROS	0.803	0.566	0.797	0.619	0.787	0.557	0.774	0.607	0.832	0.594	0.830	0.649
	K-M	0.808	0.565	0.792	0.618	0.791	0.561	0.787	0.613	0.852	0.608	0.854	0.677

GAM(2, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.909	0.681	0.926	0.722								
	Uniform	0.908	0.691	0.924	0.731								
	ROS	0.907	0.660	0.930	0.700								
	K-M	0.904	0.642	0.933	0.681								
0.4	Constant	0.937	0.672	0.944	0.712	0.931	0.667	0.934	0.708				
	Uniform	0.934	0.692	0.942	0.733	0.928	0.698	0.928	0.740				
	ROS	0.927	0.649	0.944	0.689	0.910	0.645	0.923	0.683				
	K-M	0.912	0.645	0.944	0.684	0.724	0.583	0.824	0.620				
0.6	Constant	0.921	0.661	0.935	0.701	0.940	0.657	0.949	0.696	0.940	0.642	0.955	0.682
	Uniform	0.925	0.703	0.935	0.743	0.937	0.708	0.943	0.748	0.945	0.713	0.953	0.755
	ROS	0.891	0.654	0.912	0.694	0.873	0.637	0.906	0.675	0.839	0.640	0.867	0.678
	K-M	0.897	0.677	0.928	0.718	0.588	0.623	0.697	0.666	0.000	0.558	0.038	0.603

GAM(9, 0.4)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.899	0.773	0.916	0.818								
	Uniform	0.889	0.832	0.914	0.879								
	ROS	0.914	0.661	0.929	0.700								
	K-M	0.880	0.608	0.916	0.644								
0.4	Constant	0.845	0.799	0.863	0.847	0.777	0.810	0.797	0.859				
	Uniform	0.814	0.894	0.846	0.945	0.742	0.937	0.783	0.992				
	ROS	0.905	0.657	0.934	0.694	0.884	0.655	0.903	0.693				
	K-M	0.848	0.622	0.892	0.661	0.440	0.530	0.575	0.562				
0.6	Constant	0.814	0.791	0.831	0.838	0.740	0.804	0.751	0.853	0.654	0.793	0.666	0.841
	Uniform	0.787	0.931	0.816	0.985	0.669	0.974	0.710	1.030	0.548	1.007	0.603	1.063
	ROS	0.888	0.653	0.916	0.690	0.849	0.641	0.877	0.677	0.787	0.655	0.808	0.694
	K-M	0.845	0.655	0.883	0.694	0.305	0.567	0.465	0.606	0.000	0.481	0.008	0.524

70 % LN(0, 1), 30 % LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.859	0.727	0.872	0.78								
	Uniform	0.857	0.732	0.869	0.785								
	ROS	0.866	0.720	0.872	0.776								
	K-M	0.886	0.708	0.895	0.761								
0.4	Constant	0.877	0.749	0.876	0.810	0.867	0.721	0.873	0.776				
	Uniform	0.866	0.759	0.872	0.820	0.856	0.734	0.859	0.790				
	ROS	0.894	0.747	0.889	0.807	0.865	0.732	0.865	0.788				
	K-M	0.920	0.730	0.932	0.791	0.898	0.679	0.941	0.734				
0.6	Constant	0.868	0.741	0.873	0.801	0.879	0.739	0.884	0.797	0.872	0.735	0.869	0.793
	Uniform	0.861	0.756	0.867	0.816	0.865	0.759	0.869	0.817	0.848	0.762	0.847	0.819
	ROS	0.878	0.746	0.881	0.805	0.878	0.756	0.878	0.814	0.841	0.768	0.840	0.826
	K-M	0.903	0.731	0.921	0.791	0.916	0.708	0.960	0.766	0.720	0.695	0.914	0.761

50 % LN(0, 1), 50 % LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.869	0.874	0.881	0.940								
	Uniform	0.867	0.880	0.874	0.946								
	ROS	0.874	0.871	0.885	0.937								
	K-M	0.902	0.847	0.907	0.913								
0.4	Constant	0.874	0.885	0.878	0.955	0.866	0.873	0.873	0.940				
	Uniform	0.868	0.897	0.869	0.968	0.855	0.891	0.863	0.959				
	ROS	0.885	0.884	0.888	0.954	0.875	0.882	0.886	0.948				
	K-M	0.916	0.862	0.923	0.933	0.896	0.816	0.944	0.884				
0.6	Constant	0.854	0.825	0.859	0.886	0.879	0.858	0.885	0.925	0.901	0.872	0.905	0.945
	Uniform	0.839	0.849	0.845	0.910	0.863	0.888	0.872	0.954	0.883	0.912	0.882	0.985
	ROS	0.867	0.830	0.871	0.892	0.893	0.871	0.895	0.936	0.883	0.912	0.887	0.981
	K-M	0.905	0.820	0.922	0.881	0.883	0.827	0.950	0.895	0.433	0.812	0.753	0.893

40 % GAM(7.5, 1), 60 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.971	1.117	0.981	1.181								
	Uniform	0.971	1.138	0.979	1.204								
	ROS	0.947	1.056	0.965	1.117								
	K-M	0.932	1.030	0.954	1.092								
0.4	Constant	0.964	1.107	0.967	1.170	0.977	1.082	0.983	1.148				
	Uniform	0.960	1.152	0.969	1.220	0.970	1.157	0.978	1.226				
	ROS	0.922	1.037	0.942	1.097	0.898	0.988	0.922	1.045				
	K-M	0.897	1.055	0.931	1.119	0.460	0.894	0.605	0.950				
0.6	Constant	0.962	1.055	0.974	1.120	0.958	1.049	0.969	1.113	0.965	1.007	0.974	1.066
	Uniform	0.963	1.147	0.972	1.217	0.956	1.170	0.964	1.238	0.971	1.174	0.980	1.241
	ROS	0.909	1.020	0.928	1.079	0.800	0.963	0.835	1.020	0.682	0.935	0.740	0.990
	K-M	0.912	1.098	0.935	1.164	0.323	0.964	0.463	1.035	0.000	0.774	0.002	0.839

70 % GAM(7.5, 1), 30 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.968	1.046	0.976	1.107								
	Uniform	0.972	1.081	0.979	1.144								
	ROS	0.910	0.953	0.937	1.008								
	K-M	0.838	0.918	0.886	0.971								
0.4	Constant	0.955	1.045	0.965	1.106	0.965	1.044	0.967	1.215				
	Uniform	0.960	1.118	0.965	1.183	0.951	1.150	0.965	1.183				
	ROS	0.876	0.927	0.907	0.980	0.815	0.903	0.857	0.956				
	K-M	0.790	0.928	0.846	0.985	0.185	0.776	0.292	0.824				
0.6	Constant	0.964	1.022	0.969	1.082	0.952	1.015	0.961	1.074	0.937	0.986	0.942	1.044
	Uniform	0.961	1.145	0.969	1.212	0.936	1.172	0.950	1.239	0.910	1.194	0.923	1.262
	ROS	0.878	0.928	0.911	0.981	0.743	0.875	0.794	0.926	0.658	0.865	0.701	0.915
	K-M	0.812	0.976	0.866	1.035	0.142	0.825	0.268	0.882	0.000	0.663	0.000	0.719

Bootstrap Simulation Results, N = 50

LN(0, 0.1)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.333	1.150	0.401	1.196								
	Uniform	0.315	1.440	0.432	1.500								
	ROS	0.934	0.538	0.941	0.558								
	K-M	0.842	0.461	0.881	0.480								
0.4	Constant	0.080	1.272	0.106	1.323	0.018	1.357	0.024	1.410				
	Uniform	0.067	1.662	0.113	1.730	0.014	1.826	0.024	1.900				
	ROS	0.910	0.528	0.930	0.548	0.876	0.540	0.890	0.561				
	K-M	0.792	0.469	0.840	0.488	0.097	0.386	0.150	0.402				
0.6	Constant	0.011	1.316	0.012	1.368	0.003	1.372	0.003	1.430	0.000	1.357	0.000	1.412
	Uniform	0.008	1.802	0.013	1.876	0.002	1.930	0.003	2.010	0.000	2.002	0.000	2.080
	ROS	0.899	0.533	0.914	0.553	0.859	0.531	0.879	0.552	0.738	0.556	0.759	0.577
	K-M	0.800	0.492	0.825	0.511	0.067	0.418	0.128	0.436	0.000	0.322	0.000	0.337

LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.806	0.679	0.821	0.703								
	Uniform	0.768	0.752	0.804	0.779								
	ROS	0.928	0.539	0.932	0.560								
	K-M	0.879	0.483	0.909	0.503								
0.4	Constant	0.662	0.707	0.679	0.735	0.473	0.732	0.485	0.762				
	Uniform	0.592	0.817	0.637	0.849	0.385	0.877	0.426	0.910				
	ROS	0.912	0.533	0.918	0.554	0.911	0.543	0.924	0.564				
	K-M	0.829	0.491	0.857	0.511	0.285	0.419	0.368	0.436				
0.6	Constant	0.467	0.707	0.492	0.735	0.299	0.727	0.312	0.756	0.184	0.719	0.197	0.747
	Uniform	0.382	0.864	0.414	0.898	0.210	0.912	0.231	0.947	0.095	0.943	0.115	0.978
	ROS	0.912	0.534	0.928	0.554	0.873	0.531	0.891	0.552	0.816	0.546	0.830	0.567
	K-M	0.863	0.504	0.885	0.524	0.222	0.442	0.315	0.461	0.000	0.356	0.000	0.372

LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.914	0.550	0.914	0.572								
	Uniform	0.902	0.566	0.905	0.588								
	ROS	0.936	0.525	0.941	0.547								
	K-M	0.933	0.495	0.956	0.516								
0.4	Constant	0.875	0.558	0.886	0.579	0.849	0.563	0.854	0.585				
	Uniform	0.861	0.587	0.869	0.610	0.812	0.604	0.818	0.627				
	ROS	0.911	0.526	0.924	0.547	0.927	0.534	0.926	0.555				
	K-M	0.918	0.503	0.936	0.523	0.636	0.456	0.728	0.475				
0.6	Constant	0.875	0.553	0.880	0.575	0.840	0.551	0.849	0.573	0.848	0.553	0.844	0.575
	Uniform	0.843	0.602	0.847	0.625	0.765	0.611	0.781	0.636	0.782	0.630	0.781	0.655
	ROS	0.916	0.530	0.929	0.551	0.902	0.523	0.910	0.545	0.862	0.544	0.875	0.566
	K-M	0.903	0.518	0.929	0.538	0.570	0.472	0.680	0.494	0.000	0.416	0.001	0.436

GAM(0.1, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.852	0.474	0.851	0.503								
	Uniform	0.852	0.474	0.851	0.503								
	ROS	0.853	0.474	0.848	0.503								
	K-M	0.852	0.474	0.851	0.503								
0.4	Constant	0.868	0.483	0.863	0.513	0.845	0.472	0.844	0.500				
	Uniform	0.868	0.483	0.863	0.513	0.845	0.472	0.844	0.500				
	ROS	0.873	0.484	0.870	0.512	0.846	0.471	0.842	0.499				
	K-M	0.868	0.483	0.863	0.513	0.846	0.472	0.844	0.500				
0.6	Constant	0.862	0.467	0.853	0.494	0.830	0.482	0.827	0.509	0.850	0.474	0.847	0.502
	Uniform	0.862	0.467	0.852	0.494	0.830	0.482	0.827	0.509	0.849	0.474	0.847	0.502
	ROS	0.861	0.467	0.852	0.493	0.836	0.478	0.827	0.507	0.853	0.472	0.845	0.500
	K-M	0.863	0.468	0.852	0.494	0.829	0.482	0.828	0.510	0.867	0.476	0.865	0.504

GAM(2, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.915	0.536	0.925	0.557								
	Uniform	0.915	0.543	0.922	0.564								
	ROS	0.912	0.522	0.922	0.543								
	K-M	0.905	0.507	0.921	0.528								
0.4	Constant	0.930	0.535	0.937	0.557	0.920	0.529	0.934	0.551				
	Uniform	0.925	0.551	0.935	0.573	0.923	0.552	0.933	0.575				
	ROS	0.918	0.519	0.932	0.541	0.913	0.511	0.924	0.533				
	K-M	0.896	0.515	0.924	0.536	0.651	0.460	0.734	0.480				
0.6	Constant	0.928	0.518	0.937	0.539	0.913	0.512	0.927	0.534	0.930	0.497	0.941	0.518
	Uniform	0.916	0.548	0.932	0.570	0.917	0.550	0.922	0.573	0.924	0.552	0.924	0.573
	ROS	0.902	0.514	0.919	0.535	0.875	0.502	0.898	0.523	0.818	0.496	0.850	0.516
	K-M	0.895	0.522	0.929	0.544	0.544	0.482	0.650	0.503	0.000	0.406	0.003	0.426

GAM(9, 0.4)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.881	0.611	0.890	0.635								
	Uniform	0.856	0.656	0.868	0.681								
	ROS	0.926	0.525	0.940	0.545								
	K-M	0.884	0.484	0.914	0.502								
0.4	Constant	0.805	0.626	0.818	0.650	0.748	0.638	0.759	0.664				
	Uniform	0.748	0.699	0.786	0.726	0.674	0.734	0.704	0.764				
	ROS	0.913	0.515	0.928	0.534	0.895	0.511	0.917	0.531				
	K-M	0.852	0.489	0.884	0.509	0.216	0.414	0.308	0.432				
0.6	Constant	0.693	0.613	0.698	0.637	0.615	0.628	0.626	0.654	0.507	0.619	0.517	0.645
	Uniform	0.601	0.725	0.624	0.752	0.506	0.758	0.532	0.787	0.350	0.782	0.382	0.812
	ROS	0.889	0.508	0.899	0.528	0.853	0.503	0.877	0.523	0.806	0.506	0.818	0.526
	K-M	0.844	0.501	0.880	0.521	0.195	0.440	0.282	0.458	0.000	0.355	0.000	0.372

70 % LN(0, 1), 30 % LN(0, 0.25)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.895	0.595	0.896	0.627								
	Uniform	0.891	0.599	0.890	0.630								
	ROS	0.895	0.594	0.903	0.626								
	K-M	0.917	0.582	0.923	0.613								
0.4	Constant	0.883	0.586	0.888	0.616	0.879	0.579	0.878	0.611				
	Uniform	0.876	0.593	0.882	0.622	0.865	0.590	0.865	0.621				
	ROS	0.889	0.587	0.892	0.617	0.873	0.587	0.864	0.617				
	K-M	0.909	0.573	0.926	0.603	0.918	0.548	0.950	0.579				
0.6	Constant	0.875	0.593	0.871	0.624	0.893	0.587	0.894	0.617	0.883	0.587	0.882	0.619
	Uniform	0.854	0.604	0.855	0.635	0.872	0.601	0.872	0.630	0.857	0.606	0.855	0.638
	ROS	0.880	0.596	0.885	0.628	0.890	0.599	0.890	0.629	0.838	0.615	0.831	0.646
	K-M	0.912	0.585	0.936	0.616	0.901	0.560	0.951	0.591	0.644	0.546	0.831	0.577

50 % LN(0, 1), 50 % LN(0, 0.5)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.875	0.679	0.882	0.713								
	Uniform	0.872	0.683	0.879	0.718								
	ROS	0.885	0.672	0.884	0.709								
	K-M	0.899	0.660	0.917	0.695								
0.4	Constant	0.886	0.689	0.886	0.726	0.879	0.714	0.883	0.753				
	Uniform	0.875	0.698	0.871	0.736	0.867	0.727	0.864	0.767				
	ROS	0.897	0.692	0.904	0.728	0.891	0.719	0.886	0.756				
	K-M	0.918	0.673	0.930	0.710	0.910	0.669	0.953	0.710				
0.6	Constant	0.898	0.693	0.893	0.731	0.889	0.704	0.893	0.742	0.905	0.693	0.904	0.729
	Uniform	0.875	0.710	0.870	0.747	0.863	0.726	0.867	0.764	0.877	0.722	0.873	0.758
	ROS	0.895	0.698	0.897	0.735	0.900	0.714	0.900	0.753	0.867	0.720	0.869	0.756
	K-M	0.920	0.686	0.931	0.724	0.875	0.676	0.947	0.714	0.303	0.633	0.571	0.670

40 % GAM(7.5, 1), 60 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.946	0.877	0.960	0.909								
	Uniform	0.945	0.893	0.959	0.926								
	ROS	0.949	0.829	0.963	0.861								
	K-M	0.933	0.812	0.953	0.843								
0.4	Constant	0.970	0.860	0.973	0.894	0.966	0.846	0.974	0.880				
	Uniform	0.963	0.896	0.970	0.931	0.957	0.902	0.966	0.939				
	ROS	0.937	0.808	0.951	0.840	0.841	0.771	0.880	0.801				
	K-M	0.923	0.823	0.942	0.857	0.274	0.688	0.369	0.717				
0.6	Constant	0.972	0.825	0.978	0.858	0.964	0.815	0.969	0.847	0.966	0.788	0.977	0.819
	Uniform	0.966	0.897	0.972	0.932	0.959	0.908	0.966	0.943	0.961	0.915	0.970	0.951
	ROS	0.930	0.803	0.942	0.835	0.765	0.749	0.802	0.779	0.594	0.732	0.638	0.762
	K-M	0.925	0.852	0.948	0.885	0.214	0.738	0.317	0.769	0.000	0.569	0.000	0.596

70 % GAM(7.5, 1), 30 % GAM(2, 2)

p_0	Method	0.2				0.4				0.6			
		percentile		t		percentile		t		percentile		t	
0.2	Constant	0.963	0.818	0.969	0.848								
	Uniform	0.963	0.846	0.971	0.878								
	ROS	0.899	0.742	0.912	0.771								
	K-M	0.830	0.717	0.870	0.745								
0.4	Constant	0.961	0.816	0.970	0.847	0.958	0.809	0.964	0.841				
	Uniform	0.963	0.872	0.964	0.905	0.945	0.893	0.953	0.927				
	ROS	0.851	0.726	0.879	0.754	0.759	0.697	0.792	0.725				
	K-M	0.794	0.732	0.826	0.761	0.077	0.596	0.118	0.621				
0.6	Constant	0.952	0.795	0.956	0.826	0.936	0.790	0.944	0.820	0.916	0.767	0.917	0.798
	Uniform	0.938	0.892	0.942	0.926	0.891	0.912	0.897	0.947	0.842	0.927	0.852	0.964
	ROS	0.837	0.727	0.870	0.755	0.695	0.683	0.720	0.710	0.612	0.677	0.650	0.704
	K-M	0.791	0.755	0.831	0.786	0.059	0.637	0.131	0.663	0.000	0.494	0.000	0.516

C R Simulation Code

Given below is the R code used to run the simulations. There are three main functions that were used, a function to generate the bootstrap estimates, a function to calculate the bootstrap intervals, and a function to calculate the coverage and width (in standard deviations) of the intervals. The bootstrap estimate function is given for all four distribution types to demonstrate how the data was created, but the latter two functions are only given for the lognormal simulations as they were virtually identical for the other three distribution types.

Lognormal Simulations

```

library(NADA)
library(xtable)
lnorm.2DL <- function(meanlog, sdlog, dl1p, dl2p, n, n.BOOT) {
  n2 <- n%/%2
  cen1 <- cen2 <- replicate(n2,FALSE)

repeat{
  dl1 <- qlnorm(dl1p, meanlog=meanlog, sdlog=sdlog)
  dl2 <- qlnorm(dl2p, meanlog=meanlog, sdlog=sdlog)

  obs1 <- rlnorm(n2, meanlog=meanlog, sdlog=sdlog)
  obs2 <- rlnorm(n2, meanlog=meanlog, sdlog=sdlog)

  obs1a <- ifelse(obs1 < dl1, dl1, obs1)
  obs2a <- ifelse(obs2 < dl2, dl2, obs2)

  cen1 <- ifelse(obs1 < dl1, TRUE, FALSE)
  cen2 <- ifelse(obs2 < dl2, TRUE, FALSE)

  cenind1 <- ifelse(obs1 > dl1, 1, 0) #IF UNCENSORED, 1, ELSE 0
  cenind2 <- ifelse(obs2 > dl2, 1, 0)

  n.uncen1 <- sum(cenind1)
  n.uncen2 <- sum(cenind2)

  if (n.uncen1 > 2 & n.uncen2 > 2) {break} #AT LEAST 2 UNCENSORED VALUES FROM EACH SAMPLE
}

data <- data.frame(obs=c(obs1a, obs2a), cen=c(cen1, cen2))

mean.const <- mean.unif <- mean.ros <- mean.km <- sd.const <- sd.unif <- sd.ros <- sd.km <- numeric(n.BOOT)

#ROS
data0 <- data
samp.ros <- ros(data0$obs, data0$cen)
data.out <- as.data.frame(samp.ros)$modeled

for (i in 1:n.BOOT){

#TAKE RESAMPLE OF ORIGINAL DATA OF SIZE n USED TO CALCULATE MEAN AND SD USING EACH OF THE THREE METHODS
databoot <- data[sample(n, size=n, replace=TRUE),]
dummyobs <- numeric(n)
#CONSTANT ESTIMATE

dummyobs <- ifelse(databoot$cen, databoot$obs*1/sqrt(3), databoot$obs)

```

```

mean.const[i] <- mean(dummyobs)
sd.const[i] <- sd(dummyobs)

#UNIFORM ESTIMATE

dummyobs <- ifelse(databoot$cen, runif(n, 0, databoot$obs), databoot$obs)

mean.unif[i] <- mean(dummyobs)
sd.unif[i] <- sd(dummyobs)

ros.boot <- data.out[sample(n, size=n, replace=TRUE)]

mean.ros[i] <- mean(ros.boot)
sd.ros[i] <- sd(ros.boot)

#KM
obs = databoot$obs
censored = as.logical(databoot$cen)
mycenfit = cenfit(obs, censored)
mean.km[i] <- mean(mycenfit)[1]
sd.km[i] <- sd(mycenfit)
}

#ACTUAL MEAN
mean.real <- replicate(n.BOOT, exp(meanlog+(sdlog^2)/2))

estimates <- data.frame(mean.const, mean.unif, mean.ros, mean.km, mean.real, sd.const, sd.unif, sd.ros, sd.km, row.names=NULL)
names(estimates) = c("Constant", "Uniform", "ROS", "KM", "Actual_Mean", "ConstSD", "UnifSD", "ROSsd", "KMsd")
estimates
}

lnorm.bootint <- function(meanlog, sdlog, d1p, d12p, n, n.int, n.BOOT){

#STORES THE BOOTSTRAP QUANTILE INTERVAL ESTIMATES
const.low.quant <- const.up.quant <- unif.low.quant <- unif.up.quant <- ros.low.quant <- ros.up.quant <- km.low.quant <- km.up.quant <- numeric(n.int)

#STORES THE BOOTSTRAP T INTERVAL ESTIMATES
const.low.t <- const.up.t <- unif.low.t <- unif.up.t <- ros.low.t <- ros.up.t <- km.low.t <- km.up.t <- numeric(n.int)

for (i in 1:n.int){
#CALCULATE THE N MEAN ESTIMATES USED FOR EACH BOOTSTRAP INTERVAL
estimates <- lnorm.2DL(meanlog, sdlog, d1p, d12p, n, n.BOOT)
const.boot <- estimates$Constant
unif.boot <- estimates$Uniform
ros.boot <- estimates$ROS
km.boot <- estimates$KM

#SAVE THE 95% LOWER AND UPPER QUANTILE CONFIDENCE INTERVAL LIMITS
const.low.quant[i] <- quantile(const.boot, 0.025)
const.up.quant[i] <- quantile(const.boot, 0.975)

unif.low.quant[i] <- quantile(unif.boot, 0.025)
unif.up.quant[i] <- quantile(unif.boot, 0.975)

ros.low.quant[i] <- quantile(ros.boot, 0.025)
ros.up.quant[i] <- quantile(ros.boot, 0.975)

km.low.quant[i] <- quantile(km.boot, 0.025)
km.up.quant[i] <- quantile(km.boot, 0.975)

#SAVE THE 95% LOWER AND UPPER T CONFIDENCE INTERVAL LIMIT
pointest <- mean(estimates$Constant)
se.const <- sqrt((sum((estimates$Constant - pointest)^2))/n.BOOT)
const.low.t[i] <- pointest + qt(0.025, n - 1)*se.const
const.up.t[i] <- pointest + qt(0.975, n - 1)*se.const

#SAVE THE 95% LOWER AND UPPER T CONFIDENCE INTERVAL LIMITS
pointest <- mean(estimates$Uniform)
se.unif <- sqrt((sum((estimates$Uniform - pointest)^2))/n.BOOT)
unif.low.t[i] <- pointest + qt(0.025, n - 1)*se.unif
unif.up.t[i] <- pointest + qt(0.975, n - 1)*se.unif

#SAVE THE 95% LOWER AND UPPER T CONFIDENCE INTERVAL LIMITS
pointest <- mean(estimates$ROS)
se.ros <- sqrt((sum((estimates$ROS - pointest)^2))/n.BOOT)
ros.low.t[i] <- pointest + qt(0.025, n - 1)*se.ros
ros.up.t[i] <- pointest + qt(0.975, n - 1)*se.ros

#SAVE THE 95% LOWER AND UPPER T CONFIDENCE INTERVAL LIMITS
pointest <- mean(estimates$KM)
se.km <- sqrt((sum((estimates$KM - pointest)^2))/n.BOOT)
km.low.t[i] <- pointest + qt(0.025, n - 1)*se.km
km.up.t[i] <- pointest + qt(0.975, n - 1)*se.km
}

interval.ests <- data.frame(const.low.quant, const.up.quant, unif.low.quant, unif.up.quant,
ros.low.quant, ros.up.quant, km.low.quant, km.up.quant, const.low.t, const.up.t,
unif.low.t, unif.up.t, ros.low.t, ros.up.t, km.low.t, km.up.t, row.names=NULL)
interval.ests
}

#THIS FUNCTION TAKES THE BOOTSTRAP INTERVALS AND CALCULATES PROPORTIONS OF INTERVALS THAT INCLUDE THE TRUE MEAN
lnmean.props <- function(meanlog, sdlog, d1p, d12p, n, n.int, n.BOOT){

#REAL MEAN
x <- exp(meanlog + (sdlog^2)/2)
intervals <- lnorm.bootint(meanlog=meanlog, sdlog=sdlog, d1p=d1p, d12p=d12p, n=n, n.int=n.int, n.BOOT=n.BOOT)

for (i in 1:n.int){

```

```

const.quant.ind <- ifelse(x < intervals$const.low.quant | x > intervals$const.up.quant, 0, 1)
unif.quant.ind <- ifelse(x < intervals$unif.low.quant | x > intervals$unif.up.quant, 0, 1)
ros.quant.ind <- ifelse(x < intervals$ros.low.quant | x > intervals$ros.up.quant, 0, 1)
km.quant.ind <- ifelse(x < intervals$km.low.quant | x > intervals$km.up.quant, 0, 1)

const.t.ind <- ifelse(x < intervals$const.low.t | x > intervals$const.up.t, 0, 1)
unif.t.ind <- ifelse(x < intervals$unif.low.t | x > intervals$unif.up.t, 0, 1)
ros.t.ind <- ifelse(x < intervals$ros.low.t | x > intervals$ros.up.t, 0, 1)
km.t.ind <- ifelse(x < intervals$km.low.t | x > intervals$km.up.t, 0, 1)
}

const.quant.prop <- mean(const.quant.ind)
unif.quant.prop <- mean(unif.quant.ind)
ros.quant.prop <- mean(ros.quant.ind)
km.quant.prop <- mean(km.quant.ind)

const.t.prop <- mean(const.t.ind)
unif.t.prop <- mean(unif.t.ind)
ros.t.prop <- mean(ros.t.ind)
km.t.prop <- mean(km.t.ind)

sd <- sqrt((exp(sdlog^2) - 1)*exp(2*meanlog + sdlog^2))

const.quant.width <- mean(intervals$const.up.quant - intervals$const.low.quant)/sd
unif.quant.width <- mean(intervals$unif.up.quant - intervals$unif.low.quant)/sd
ros.quant.width <- mean(intervals$ros.up.quant - intervals$ros.low.quant)/sd
km.quant.width <- mean(intervals$km.up.quant - intervals$km.low.quant)/sd

const.t.width <- mean(intervals$const.up.t - intervals$const.low.t)/sd
unif.t.width <- mean(intervals$unif.up.t - intervals$unif.low.t)/sd
ros.t.width <- mean(intervals$ros.up.t - intervals$ros.low.t)/sd
km.t.width <- mean(intervals$km.up.t - intervals$km.low.t)/sd

props <- data.frame(const.quant.prop, unif.quant.prop, ros.quant.prop, km.quant.prop, const.t.prop, unif.t.prop, ros.t.prop, km.t.prop,
  const.quant.width, unif.quant.width, ros.quant.width, km.quant.width, const.t.width, unif.t.width, ros.t.width, km.t.width)
props
}

```

Gamma Simulations

```

gamma.2DL <- function(shape, scale, dl1p, dl2p, n, n.BOOT) {
  n2 <- n/2
  cen1 <- cen2 <- replicate(n2, FALSE)
  cen1 <- cen2 <- replicate(n2, FALSE)

  repeat{
    dl1 <- qgamma(dl1p, shape=shape, scale=scale)
    dl2 <- qgamma(dl2p, shape=shape, scale=scale)

    obs1 <- rgamma(n2, shape=shape, scale=scale)
    obs2 <- rgamma(n2, shape=shape, scale=scale)

    obs1a <- ifelse(obs1 < dl1, dl1, obs1)
    obs2a <- ifelse(obs2 < dl2, dl2, obs2)

    cen1 <- ifelse(obs1 < dl1, TRUE, FALSE)
    cen2 <- ifelse(obs2 < dl2, TRUE, FALSE)

    cenind1 <- ifelse(obs1 > dl1, 1, 0) #IF UNCENSORED, 1, ELSE 0
    cenind2 <- ifelse(obs2 > dl2, 1, 0)

    n.uncen1 <- sum(cenind1)
    n.uncen2 <- sum(cenind2)

    if (n.uncen1 > 2 & n.uncen2 > 2) {break} #AT LEAST 2 UNCENSORED VALUES FROM EACH SAMPLE
  }

  data <- data.frame(obs=c(obs1a, obs2a), cen=c(cen1, cen2))

  mean.const <- mean.unif <- mean.ros <- mean.km <- sd.const <- sd.unif <- sd.ros <- sd.km <- numeric(n.BOOT)

  #ROS
  data0 <- data
  samp.ros <- ros(data0$obs, data0$cen)
  data.out <- as.data.frame(samp.ros)$modeled

  for (i in 1:n.BOOT){
    #TAKE RESAMPLE OF ORIGINAL DATA OF SIZE n USED TO CALCULATE MEAN AND SD USING EACH OF THE THREE METHODS
    databoot <- data[sample(n, size=n, replace=TRUE),]
    dummyobs <- numeric(n)
    #CONSTANT ESTIMATE
    dummyobs <- ifelse(databoot$cen, databoot$obs*1/sqrt(3), databoot$obs)

    mean.const[i] <- mean(dummyobs)
    sd.const[i] <- sd(dummyobs)

    #UNIFORM ESTIMATE
    dummyobs <- ifelse(databoot$cen, runif(n, 0, databoot$obs), databoot$obs)

    mean.unif[i] <- mean(dummyobs)
    sd.unif[i] <- sd(dummyobs)

    #ROS
    ros.boot <- data.out[sample(n, size=n, replace=TRUE)]
  }
}

```

```

mean.ros[i] <- mean(ros.boot)
sd.ros[i] <- sd(ros.boot)

#KM
obs = databoot$obs
censored = as.logical(databoot$cen)
mycenfit = cenfit(obs, censored)
mean.km[i] <- mean(mycenfit)[1]
sd.km[i] <- sd(mycenfit)
}

#ACTUAL MEAN
mean.real <- replicate(n.BOOT, shape*scale)

estimates <- data.frame(mean.const, mean.unif, mean.ros, mean.km, mean.real, sd.const, sd.unif, sd.ros, sd.km, row.names=NULL)
names(estimates) = c("Constant", "Uniform", "ROS", "KM", "Actual_Mean", "ConstSD", "UnifSD", "ROSsd", "KMsd")
estimates
}

```

Mixed Lognormal Simulations

```

lnorm.2DL <- function(meanlog, sdlog, dl1p, dl2p, n, n.BOOT, p.cont) {
  n2 <- n%/2
  cen1 <- cen2 <- replicate(n2, FALSE)
  #DETERMINE DLS USING A SAMPLE OF 10,000 OBS
  dlsamp1 <- rlnorm(10000*p.cont, meanlog=0, sdlog=0.25)
  dlsamp2 <- rlnorm(10000*(1-p.cont), meanlog=meanlog, sdlog=sdlog)
  dlsamp <- c(dlsamp1, dlsamp2)

  dl1 <- quantile(dlsamp, dl1p)
  dl2 <- quantile(dlsamp, dl2p)

  repeat{
    obs1x <- rlnorm(ceiling(n2*(1-p.cont)), meanlog=meanlog, sdlog=sdlog)
    obs1y <- rlnorm(floor(n2*p.cont), meanlog=0, sdlog=0.25)
    obs1 <- c(obs1x, obs1y)
    obs2x <- rlnorm(ceiling(n2*(1-p.cont)), meanlog=meanlog, sdlog=sdlog)
    obs2y <- rlnorm(floor(n2*p.cont), meanlog=0, sdlog=0.25)
    obs2 <- c(obs2x, obs2y)

    obs1a <- ifelse(obs1 < dl1, dl1, obs1)
    obs2a <- ifelse(obs2 < dl2, dl2, obs2)

    cen1 <- ifelse(obs1 < dl1, TRUE, FALSE)
    cen2 <- ifelse(obs2 < dl2, TRUE, FALSE)

    cenind1 <- ifelse(obs1 > dl1, 1, 0) #IF UNCENSORED, 1, ELSE 0
    cenind2 <- ifelse(obs2 > dl2, 1, 0)

    n.uncen1 <- sum(cenind1)
    n.uncen2 <- sum(cenind2)

    if (n.uncen1 > 2 & n.uncen2 > 2) {break} #AT LEAST 2 UNCENSORED VALUES FROM EACH SAMPLE AND AT LEAST 1 CENSORED VALUE
  }

  data <- data.frame(obs=c(obs1a, obs2a), cen=c(cen1, cen2))

  mean.const <- mean.unif <- mean.ros <- mean.km <- sd.const <- sd.unif <- sd.ros <- sd.km <- numeric(n.BOOT)

  #ROS
  data0 <- data
  samp.ros <- ros(data0$obs, data0$cen)
  data.out <- as.data.frame(samp.ros)$modeled

  for (i in 1:n.BOOT){
    #TAKE RESAMPLE OF ORIGINAL DATA OF SIZE n USED TO CALCULATE MEAN AND SD USING EACH OF THE THREE METHODS
    databoot <- data[sample(n, size=n, replace=TRUE),]
    dummyobs <- numeric(n)
    #CONSTANT ESTIMATE

    dummyobs <- ifelse(databoot$cen, databoot$obs*1/sqrt(3), databoot$obs)

    mean.const[i] <- mean(dummyobs)
    sd.const[i] <- sd(dummyobs)

    #UNIFORM ESTIMATE
    dummyobs <- ifelse(databoot$cen, runif(n, 0, databoot$obs), databoot$obs)

    mean.unif[i] <- mean(dummyobs)
    sd.unif[i] <- sd(dummyobs)

    ros.boot <- data.out[sample(n, size=n, replace=TRUE)]

    mean.ros[i] <- mean(ros.boot)
    sd.ros[i] <- sd(ros.boot)

    #KM
    obs = databoot$obs
    censored = as.logical(databoot$cen)
    mycenfit = cenfit(obs, censored)
    mean.km[i] <- mean(mycenfit)[1]
    sd.km[i] <- sd(mycenfit)
  }

  #ACTUAL MEAN

```

```

mean.real <- replicate(n.BOOT, (exp(meanlog+(sdlog^2)/2))*(1-p.cont) + exp(0+(0.25^2)/2)*(p.cont))

estimates <- data.frame(mean.const, mean.unif, mean.ros, mean.km, mean.real, sd.const, sd.unif, sd.ros, sd.km, row.names=NULL)

names(estimates) = c("Constant", "Uniform", "ROS", "KM", "Actual_Mean", "ConstSD", "UnifSD", "ROSsd", "KMsd")
estimates
}

```

Mixed Gamma Simulations

```

gamma.2DL <- function(shape, scale, dl1p, dl2p, n, n.BOOT, p.cont) {
  n2 <- n%%2
  cen1 <- cen2 <- replicate(n2,FALSE)
  #DETERMINE DLS USING A SAMPLE OF 10,000 OBS
  dlsamp1 <- rgamma(10000*p.cont, shape=2, scale=2)
  dlsamp2 <- rgamma(10000*(1-p.cont), shape=shape, scale=scale)
  dlsamp <- c(dlsamp1, dlsamp2)

  dl1 <- quantile(dlsamp, dl1p)
  dl2 <- quantile(dlsamp, dl2p)

  repeat{

    obs1x <- rgamma(ceiling(n2*(1-p.cont)), shape=shape, scale=scale)
    obs1y <- rgamma(floor(n2*p.cont), shape=2, scale=2)
    obs1 <- c(obs1x, obs1y)
    obs2x <- rgamma(ceiling(n2*(1-p.cont)), shape=shape, scale=scale)
    obs2y <- rgamma(floor(n2*p.cont), shape=2, scale=2)
    obs2 <- c(obs2x, obs2y)

    obs1a <- ifelse(obs1 < dl1, dl1, obs1)
    obs2a <- ifelse(obs2 < dl2, dl2, obs2)

    cen1 <- ifelse(obs1 < dl1, TRUE, FALSE)
    cen2 <- ifelse(obs2 < dl2, TRUE, FALSE)

    cenind1 <- ifelse(obs1 > dl1, 1, 0) #IF UNCENSORED, 1, ELSE 0
    cenind2 <- ifelse(obs2 > dl2, 1, 0)

    n.uncen1 <- sum(cenind1)
    n.uncen2 <- sum(cenind2)

    if (n.uncen1 > 2 & n.uncen2 > 2) {break} #AT LEAST 2 UNCENSORED VALUES FROM EACH SAMPLE AND AT LEAST 1 CENSORED VALUE
  }

  data <- data.frame(obs=c(obs1a, obs2a), cen=c(cen1, cen2))

  mean.const <- mean.unif <- mean.ros <- mean.km <- sd.const <- sd.unif <- sd.ros <- sd.km <- numeric(n.BOOT)

  #ROS
  data0 <- data
  samp.ros <- ros(data0$obs, data0$cen)
  data.out <- as.data.frame(samp.ros)$modeled

  for (i in 1:n.BOOT){
    #TAKE RESAMPLE OF ORIGINAL DATA OF SIZE n USED TO CALCULATE MEAN AND SD USING EACH OF THE THREE METHODS
    databoot <- data[sample(n, size=n, replace=TRUE),]
    dummyobs <- numeric(n)
    #CONSTANT ESTIMATE

    dummyobs <- ifelse(databoot$cen, databoot$obs*1/sqrt(3), databoot$obs)

    mean.const[i] <- mean(dummyobs)
    sd.const[i] <- sd(dummyobs)

    #UNIFORM ESTIMATE

    dummyobs <- ifelse(databoot$cen, runif(n, 0, databoot$obs), databoot$obs)

    mean.unif[i] <- mean(dummyobs)
    sd.unif[i] <- sd(dummyobs)

    #ROS, data.out is code from earlier that is the ROS method obs run on original data
    ros.boot <- data.out[sample(n, size=n, replace=TRUE)]

    mean.ros[i] <- mean(ros.boot)
    sd.ros[i] <- sd(ros.boot)

    #KM
    obs = databoot$obs
    censored = as.logical(databoot$cen)
    mycenfit = cenfit(obs, censored)
    mean.km[i] <- mean(mycenfit)[1]
    sd.km[i] <- sd(mycenfit)
  }

  #ACTUAL MEAN
  mean.real <- replicate(n.BOOT, shape*scale*(1-p.cont) + 2*2*p.cont)

  estimates <- data.frame(mean.const, mean.unif, mean.ros, mean.km, mean.real, sd.const, sd.unif, sd.ros, sd.km, row.names=NULL)

  names(estimates) = c("Constant", "Uniform", "ROS", "KM", "Actual_Mean", "ConstSD", "UnifSD", "ROSsd", "KMsd")
  estimates
}

```

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