Inference on Differences in k Means for Data with Excess Zeros and Detection Limits

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INFORMATION ON DIFFERENCES IN K MEANS FOR DATA WITH EXCESS ZEROS AND DETECTION LIMITS

by

Haolai Jiang

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

Statistics
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Many data have excess zeros or unobservable values falling below detection limit. For example, data on hospitalization costs incurred by members of a health insurance plan will have zeros for the percentage who did not get sick. Benzene exposure measurements on petroleum refinery workers have some exposures fall below the limit of detection. Traditional methods of inference like one-way ANOVA are not appropriate to analyze such data since the point mass at zero violates typical distribution assumptions.

For testing for equality of means of k distributions, we will propose a likelihood ratio test that accounts for excess zeros or detection limits. We will conduct simulations to study finite sample properties of the proposed procedure on both Log-normal distribution and Gamma distribution. One imputation method will be proposed as an alternative approach.
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Haolai Jiang
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CHAPTER I
INTRODUCTION

1.1 Data with Excess Zeros

Data sets with excess zeros are commonly seen in present world. Lachenbruch (2002) indicates that data sets with excess zeros have been recognized to pose potential problems since the mid 1960s or earlier.

There are series of literature citing examples from the real world.

Example 1: (Lachenbruch, 2002) (Hospitalization costs) Data are from studying hospitalization costs in a health insurance plan. Most of the members (90%) of an insurance plan do not have hospitalization costs in a year. The data set contains significant amount of zeros, and some non-zero positive numbers. It may be valuable to determine if the new policy will have impact on the costs and the proportion of people who have been hospitalized.

Example 2: (Neuhauser et. al., 2005) (DNA methylation data) MethyLight technology can be used to measure DNA methylation data. When the test region is not or partially methylated the result is undetectable which is marked as a zero. In contrast, regions that show methylation will have positive values. DNA methylation data with MethyLight data have excess zeros and positive non-zero part.

The above examples offer a peek of the cases in the real world. Traditional methods, such as Analysis of Variance, t test and Kruskal-Wallis test, are not appropriate to analyze such data since the distribution of data violates the typical assumptions.

Two density curves shown in Figure 1.1 provide visualization of the shape of
data with excess zeros, positive non-zero part and also with possible detection limit.

![Figure 1.1: Demonstration of Data with and without Detection Limit](image)

The two curves in Figure 1.1 are generated by assuming that the non-zero part follows Log-normal distribution, with sample size 100, mean and standard deviation of log scale both 1, and the probability of obtaining zero 0.1. The second plot sets up a detection limit of value 1 with a dashed line. We can see clearly that there is a high spike in the distribution at value zero. The count of zeros is even higher for the second plot since additional zeros being added due to the unobservable values falling below detection limit (DL).

Data with excess zeros can be categorized into two cases: one is that the positive part is discrete, and the other one is that the positive part is continuous. Zero-inflated Poisson model (ZIP) is widely used under the assumption that the positive values following a Poisson distribution. For continuous positive part, Log-normal distribution, Gamma distribution and Weibull distribution are often considered. In this dissertation I primarily consider Log-normal distribution as the one for the positive values.

Two-part model is often used due to the mixture of excess zeros and positive part. In general, if the $h(x)$ is the probability density function (p.d.f.) of the distribution of the positive values. The p.d.f. for the mixture distribution (Lachenbruch,
$$f_i(x) = p_i^\delta \times [(1 - p_i) \times h_i(x)]^{1-\delta}$$

where $\delta = 1$ if $x = 0$, $\delta = 0$ if $x > 0$, $p_i$ is the proportion of zeros and $i$ is the group indicator.

It is apparently not appropriate to assume that such data follow a normal distribution. In the case of two independent populations with hypothesis $H_0 : p_1 = p_2$ and $h_1(x) = h_2(x)$ v.s. $H_1 : p_1 \neq p_2$ or $h_1(x) \neq h_1(x)$, Lachenbruch (2001) compares the performance of the two-part models with traditional normal test, Wilcoxon test, and Kolmogrov-Smirnov test. He concludes that the two-part models outperform and at least perform equally well in most of the situations with only one exception.

1.2 Data with Excess Zeros and Detection Limit

In many practical cases, due to the limitation of measurement accuracy there are zeros which are not true zeros. These are unobservable positive values, less than the detection limit (DL). Therefore, in those cases the zeros come from two parts: one is the true zeros, and the other is the values below DL which are unobservable. There are many examples in the literature well demonstrate such situations. Chu (2005) describes that “This is a relevant problem in many cancer prevention trials and HIV studies.”

Example 3: (Aertker and Zaccaro, 2011) (H1N1 vaccination data) Data is the antibody titers in responses to H1N1 vaccination. Zeros are recorded if the antibody titers fall below the lower limit of detection (LLOD). Observations below the LLOD consist of values which are true zeros and nonzero values but are below the LLOD.

Example 4: (Taylor et. al, 2001) (Time-weighted average occupational exposure data) Data are the time-weighted average (TWA) benzene exposure measurements from 38 petroleum refinery workers. Workers’ schedules require operators work in a contamination free environments. Five workers’ exposures fall below the limit of detection (LOD).

Example 5: (Chu et. al, 2005) (Hepatocarcinogenesis data) Hepatocellular
carcinoma (HCC) is one of the most common cancers induced by aflatoxin. This type of cancer is inhibited by oltipraz. Hydroxylated metabolite aflatoxin $M_1$ ($AFM_1$) and non-toxic aflatoxin-mercapturic acid ($AFB-NAC$) are two important factors of oltipraz. The measurement of $AFM_1$ and $AFB-NAC$ can have excess values near zero. Moreover, the measurements are often left censored due to some values falling below DL.

As introduced before, in the case of data with excess zeros and detection limit, in addition to the true zeros there is another source of zeros: positive unobservable values falling below detection limit (DL). Assuming the observed values are from Log-normal distribution, Chu et. al (2006) shows that the p.d.f. of the mixture distribution is

$$f_i(x) = [p_i + (1 - p_i) \times \Phi(\frac{y_L - \mu_i}{\sigma_i})^\delta \times \frac{1 - p_i}{\sigma_i} \times \phi(\frac{y_i - \mu_i}{\sigma_i})]^{1-\delta}$$

where $y_i$ is the logarithm of the original values from Log-normal distribution, $y_L$ is the logarithm of original detection limit, $\mu_i$ and $\sigma_i$ are the mean and standard deviation of log scale, $\Phi(\cdot)$ and $\phi(\cdot)$ are the cumulative distribution function (c.d.f.) and p.d.f. of standard normal distribution, respectively. From the above p.d.f., we see that assuming the positive distribution and the detection limit are known, we could obtain the expected probability of the values falling below the detection limit. Adding the probability of true zeros, the total probability of zeros is $p_i + (1 - p_i) \times \Phi(\frac{y_i - \mu_i}{\sigma_i})$.

### 1.3 Alternative Distributions for Positive Part

Mixture models are typically used to account for the data set with excess zeros and possible detection limit. Such models study zeros part and positive part with different distributions. Apart from using non-parametric methods for the values of positive part, Log-normal distribution is the typical choice for simulating the continuous positive part in many papers. Examples include Zhou et. al. (1997), Taylor et. al. (2001), Chu et. al. (2005, 2006), Nie et. al. (2006), and Daoud (2007).
However, even though Log-normal distribution has nice features that simplifying the calculation procedures, values of the positive part may arise from a distribution other than Log-normal.

As Figure 1.2 shows, Gamma and Weibull distributions could have similar theoretical density curves as Log-normal distribution. Even though the density curves of the three distributions are not always similar, it is still worthwhile considering the situations where their density curves are actually similar and therefore, motivating the consideration of assuming distributions other than Log-normal distribution for the positive part.

![Figure 1.2: Demonstration of Distribution Similarities](image)

### 1.4 Motivation and Dissertation Structure

Daoud (2007) proposes a two-part likelihood ratio test and a two-part Wald test for comparing $p$ and $h(x)$ simultaneously for $K \ (K \geq 3)$ independent populations. Lachenbruch (2001) mentions the potential generalization of two-part models to multiple populations without much details. Zhou and Tu (1999) proposes a likelihood ratio test and a Wald test for comparing overall means of $K$ independent populations. However, none of them considers the detection limit. Chu et. al (2004, 2005 and 2006) considers data with excess zeros and possible detection limits in a series of paper. However, they only focus on the cases of one and two independent
populations.

Motivated by the fact that such type of data are readily available as well as the related studies, I propose a likelihood ratio test for $K$ ($K \geq 3$) independent populations with a detection limit. The simulation and formula derivation will be based on $K = 3$ independent populations, but it could be easily extended to other cases. Furthermore, the robustness and sensitivity of the proposed test will be shown under various combinations of the parameters and under different distributions through simulation studies.

Furthermore, if the number of values below DL could be reasonably estimated, we may remove the detection limit and convert the situation to a typical two-part model. We would like to tentatively explore the imputation techniques for the undetectable values and make recommendation based on that.

This dissertation is organized as follows. Chapter Two gives the review of the relevant literature. We will introduce the proposed likelihood ratio test for $K$ ($K \geq 3$) independent populations in Chapter Three. Simulation studies will be conducted in Chapter Four. Chapter Five will explore imputation methods for the values below DL. And Chapter Six will include conclusions and potential future research directions.
CHAPTER II
LITERATURE REVIEW

Lachenbruch (2001) proposes a two-part model with density as \( f_i(x) = p_i^\delta \times [(1 - p_i) \times h_i(x)]^{1-\delta} \) where \( \delta = 1 \) if \( x \) is 0 and \( p_i \) is the probability of zeros. The model assumes that data has a clump at zero and the non-negative part is continuously distributed. Since the probability density function has two parts, the null hypothesis of testing two independent populations also includes two parts: \( H_0 : p_1 = p_2 \) and \( h_1(x) = h_2(x) \). For testing the null hypothesis, it includes a chi-square distribution with 1 degree of freedom (d.f.) for equality of proportion of zeros and a chi-square distribution with 1 d.f. for equality of non-negative distribution. He states that when the sample size is large enough, the test statistic is a summation of two components and follows a chi-square distribution with 2 d.f.. Lachenbruch (2001) introduces the formula of the test statistic:

\[
\chi^2_{(2)} = \left( \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{\hat{p}(1 - \hat{p})(\frac{1}{n_1} + \frac{1}{n_2})}} \right)^2 + U^2
\]

where \( \hat{p} = \frac{n_1 \hat{p}_1 + n_2 \hat{p}_2}{n_1 + n_2} \). He introduces several options for \( U \), including z test, t test, Wilcoxon test and Kolmogorov-Smirnov test.

Under alternative hypothesis, the test statistic follows a non-central chi-square distribution with 2 d.f. and a non-centrality parameter \( \lambda \), which is defined by

\[
\lambda = \frac{(p_1 - p_2)^2 n_1 n_2}{\hat{p}(1 - \hat{p})(\frac{1}{n_1} + \frac{1}{n_2})} + \frac{(\mu_1 - \mu_2)^2}{\sigma^2(\frac{1}{n_1(1 - p_1)} + \frac{1}{n_2(1 - p_2)})}
\]

Lachenbruch fixes sample size \( n_1 = n_2 = 100 \), \( \sigma = 1 \) and \( \mu = 0 \), and
assumes that the non-negative part of data follows a Log-normal distribution and uses Wilcoxon as the choice of $U$ in the test statistic. The predicted power varies from 0.378 to 0.952 over different combinations of $p_1, p_2, \mu_1 - \mu_2$. The predicted powers are calculated based on the non-central chi-square distribution with 2 d.f.. The observed powers are generated from the Monte Carlo simulations.

Lachenbruch (2001) compares the two-part model, proposed in another paper in 2001, with other competitor models. These competitor models include Smirnov test, the t-test with equal variances, and the Wilcoxon rank sum test. Binomial test for proportion of zeros is used for all two-part models. In the paper, the author tries to address three questions: whether those tests retain size 0.05 for type I error probability; whether they have the appropriate null distribution; and comparing the observed powers of the tests in various situations.

Lachenbruch runs simulations in various situations and finds that if the populations differ only in the proportions, but not in the conditional distributions, all of the tests perform poorly with low power. If the populations differ only in the means of the Log-normal distributions, but not the proportion of zeros, the picture is unclear, and the results depend on the proportion of zeros. When differences occur in both the proportion of zeros and the conditional distributions, Smirnov test and Wilcoxon rank sum test perform well.

Unlike the regular two-part zero-inated model $f_i(y) = (p_i)^{\delta}[\times g_i(y)]^{1-\delta}$, Chu, Nie, & Cole (2006) considers the differences between true zeros and the left-censored values due to the detection limits. The authors use a mixture model in the form of $f_i(y) = [p_i + (1 - p_i) \times G_i(y_L)]^{\delta}[\times g_i(y)]^{1-\delta}$, where $i = 1, 2$, $y_L$ is the detection limit, $p_i$ is the proportion of true zeros and $g_i(\cdot), G_i(\cdot)$ are the p.d.f and c.d.f., respectively.

The hypothesis of primary interested in Chu et. al. (2006) is $H_0 : \mu_1 = \mu_2$ vs. $\mu_1 \neq \mu_2$. They derived formulas of sample size and power under the assumptions of equal variances and unequal variances separately. The authors use a Bernoulli/Log-normal mixture model to apply on an example. They specify the percentage of true zeros and the detection limit. They also use the Maximum Likelihood Estimates
(MLEs) from the data to set up \( p_1, p_0, \mu_1, \mu_0, \sigma_0 \) and \( \sigma_1 \).

Chu et al., (2006) then conducts two sets of Monte Carlo simulations under different combinations of the probability of true zeros and percentage of the left-censored values, under the assumptions of equal and unequal variances separately. For each condition, 20,000 trials are generated.

The authors conclude that under equal variances assumption, the results show the expected power, 0.8, if assuming \( p_1 \neq p_0 \). The sample size is overestimated when \( p_1 = p_0 \). Under the assumption of unequal variances, the empirical power is slightly under the expected power, 0.8. The sample size is overestimated.

Nie, Chu, & Cole (2006) indicates that when conducting a medical research it is often assumed that, in the data a proportion of individuals coming from a Log-normal distribution, while the remaining individuals have true zeros because they were not exposed to the disease. Due to the detection limit, there may be some exposed individuals whose values fall below the detection limit, which are indistinguishable from the individuals with true zeros. Therefore, the observed data follow the mixture distribution with a probability density function

\[
 f_i(y) = \left[ p + (1 - p) \times \Phi \left( \frac{y_L - \mu_i}{\sigma_i} \right) \right]^\delta \times \left[ \frac{1 - p}{\sigma_i} \times \phi \left( \frac{y_L - \mu_i}{\sigma_i} \right) \right]^{1-\delta}
\]

where \( y \) is the nature logarithm of the measurement, \( \Phi(.) \) and \( \phi(.) \) are the standard normal cumulative distribution function (c.d.f.) and probability density function (p.d.f.), respectively. \( y_L \) is the detection limit on the log scale, and \( i = 1 \) indicates the treatment group while \( i = 0 \) indicates control group.

Nie et. al (2006) provides a general approach for sample size estimation for comparing the mean differences of two independent groups with equal proportion of true zeros, which is \( p_0 = p_1 = p_2 \).

Under the equal variances case, \( \sigma_0 = \sigma_1 = \sigma \), via maximum likelihood estimates (MLEs), they propose a formula for the optimal sample size by

\[
 n = \min_{Q_0} \left\{ \sqrt{\Sigma_0 \Phi^{-1}(1 - c^{-1} \alpha)} + \sqrt{\Sigma_1 \Phi^{-1}(1 - \beta)} \right\} (\mu_1 - \mu_0)^{-2}
\]
where \( n = n_0 + n_1 \), \( Q_0 = \frac{n_0}{n} \), \( \Sigma_0 \) is the variance of \( \sqrt{n}(\hat{\mu}_0 - \hat{\mu}_1) \) under null hypothesis, \( H_0 : \mu_0 = \mu_1 \), \( \Sigma_1 \) is the variance of \( \sqrt{n}(\hat{\mu}_0 - \hat{\mu}_1) \) under alternative hypothesis, \( H_1 : \mu_0 \neq \mu_1 \) and \( c = 1 \) or \( 2 \) indicating one-sided or two-sided test. The likelihood ratio test (LRT) follows a standard chi-square distribution with one degree of freedom.

1. Monte Carlo simulations are conducted for comparing the proposed sample size calculation to the naïve method which is simply inflating the sample size to compensate the information loss through left-censoring. Simulations are based on different combinations of the parameters: the proportion of true zeros, \( P = 0.4, 0.2 \), and probabilities of values under detection limit for control and treatment groups \( (0.1, 0.03), (0.2, 0.075), (0.3, 0.13), (0.4, 0.197) \), respectively. By setting significance level \( \alpha = 0.05 \) and the desired power \( \gamma = 0.8 \), the results indicate that the naïve approach tends to consistently underestimate the sample size. The observed power of the proposed method yields higher powers than those from the naïve approach. It is observed that the sample size increases much when the censored proportion increases. Nie et al. (2006) claims that this is due to the small decreases of the Fisher information for \( \mu \) as the censoring proportion increases.

Neuhauser and Jockel (2005) builds a two-part permutation test based on Lanchenbruch’s two-part model. Lanchenbruch’s two-part model is in the form of \( X^2 = B^2 + W^2 \), where \( B \) is the Binomial test for testing the proportion of zeros and \( W \) is Wilcoxon sum rank test. The second part could use other tests, such as student’s \( t \) test, Kolmogorov-Smirnov test and so on. One of the reasons to use Wilcoxon sum rank test is “Non-parametric tests based on ranks are more appropriate for non-normally distributed data such as microarry data” according to the authors.

The authors carry out the permutation test based on the sum statistics \( X^2 \) since it is not necessary to determine the permutation distributions of the summands \( B^2 \) and \( W^2 \) to calculate the p-values of the univariate tests related to \( B^2 \) and \( W^2 \). The authors use a simple random sample of 20,000 permutations to determine the p-values of the two-part permutation test.
Using a simulation study to actual microarray data, the results show that the p-values of two-part permutation test are smaller than Lancenbruch’s two-part model, which corresponds to a higher power.

Neuhauser and Jockel claim that the two-part permutation test has several advantages: “First, it avoids the use of any asymptotic distribution and, therefore, can safely be applied in case of small sample sizes that are common in microarray experiments. Second, it reduces without any loss of power to the exact Wilcoxon test if there were no zero values. Thus, it can be used in routine analysis. Third the permutation test opens the possibility to use other tests to construct the two-part test.”

However, the proposed two-part permutation test has one disadvantage, namely, it can be computer-intensive if the sample size is not too small.

Taylor, Kupper, Rappaport and Lyles (2001) compares censored Log-normal mixture model (mixture model) and left-truncated normal distribution and finds the Maximum Likelihood estimates of $\mu_y$ and $\sigma^2_y$, where $y$ is the logarithm of the values from Log-normal distribution, are the same for both the mixture model and the left-truncated normal distribution. Therefore, they emphasizes: “observations falling below the LOD contribute no information toward the estimation of $\mu_y$ and $\sigma^2_y$. LOD is the acronym of limit of detection. The quoted statement fails when the LOD varies across groups.

The estimated proportion of true zeros, denoted $\hat{\omega}$, has a upper limit $n_0/n$, where $n_0$ is the number of zeros and $n$ is the total sample size. The value of $\hat{\omega}$ falls below zero when $n_0 < n\Phi(\hat{\epsilon})$, where $\Phi(.)$ is the c.d.f. of standard normal distribution, and $\hat{\epsilon} = \frac{LOD - \hat{\mu}_y}{\hat{\sigma}_y}$. Taylor et.al. (2001) proposes a mixture model with restriction of $\hat{\omega} > 0$. They tests $H_0: \mu_x \geq C$ v.s. $H_1: \mu_x \leq C$, where $x$ follows a Log-normal distribution and $C$ is a constant, by Likelihood Ratio (LR) test with test statistic $\hat{T} = 2\{lnL_m(\hat{\tau}_1) - lnL_m(\hat{\tau}_0)\}$, where $\hat{\tau} = \{\hat{\omega}, \hat{\mu}_y, \hat{\sigma}^2_y\}$. Taylor et. al. claims that $\hat{T}$ asymptotically follows a 50-50 mixture of a chi-square distribution with 1 degree of freedom and a point mass at zero. Additionally, they uses a two-step test for testing the appropriateness of censored model. First step tests $H_0: \omega = 0$ v.s. $H_1: \omega > 0$, 


and then the next step tests the sample mean.

Taylor et.al. (2001) conducts a simulation study for the one-sided LR test under different settings for comparing the type I error and power of censored model, mixture model, restricted mixture model and two-step procedure. They concludes that “Asymptotically, imposing the restriction \( \hat{\omega} \geq 0 \) has no consequence on ML estimation or hypothesis testing for a mixture model with true \( \omega > 0 \). And they also conclude that “Test accuracy can be improved somewhat by performing a two-step procedure where one reduces to the censored data model if an initial one-sided LR test of \( H_0 : \omega = 0 \) v.s. \( H_1 : \omega > 0 \) is not rejected at the 0.05 significance level.”

Zhou and Tu (1999) proposes a likelihood ratio test for testing the overall mean equality of several independent populations that contain zeros and values from Log-normal distribution. Their null hypothesis of interest is \( H_0 : M_1 = \cdots = M_K \), where \( M_j = E(Y_{ij}) \), and \( Y_{ij} \) are random sample from jth population, for \( j = 1, \ldots, K \). Since there is no closed-form solution for the maximum likelihood estimators under the null hypothesis \( H_0 \), they use numerical method, Davidon-Fletcher-Powell (DFP) algorithm, for finding the maximum likelihood estimates (MLEs). In the paper they conclude that the proposed test performs very well in terms of power and Type I error.

Daoud (2007) proposes two-part likelihood ratio test (LRT) and two-part Wald test for testing hypothesis of \( K (K \geq 3) \) independent populations.

\[
H_0 : p_1 = \cdots = p_k \cap m_1 = \cdots = m_k
\]

vs.

\[
H_1 : p_i \neq p_{i'} \cup m_j \neq m_{j'}
\]

for some \( i \neq i' \) or \( j \neq j' \), where \( p_i \) and \( m_j \) are the proportion of zeros and the mean of Log-normal distribution, respectively. Daoud’s Two-part likelihood ratio model tests the proportion of zeros, \( p_i \), and the Log-normal part separately by the regular LRT. Each part of LRT follows chi-square distribution with \( k - 1 \) degrees of
freedom asymptotically and the two parts are independent. Combining two LRTs together, the overall two-part LRT test statistics asymptotically follows a chi-square distribution with $2(k - 1)$ degrees of freedom. The same concepts apply to two-part Wald test. Daoud (2007) concludes that the two-part LRT and two-part Wald test perform very well in terms of size and power of test, compared to the existing tests under large sample. However, both tests do not perform well under small sample size.

Chu et al (2008) proposed a Bayesian approach to estimate the treatment effects for data with excess zeros and detection limits. They compare the performance of the proposed approach with maximum likelihood method via Markov chain Monte Carlo (MCMC) method on small to moderate sample size. They conclude that both approaches provided similar inference of the real example in the article. However, the paper indicates that “simulation studies with small-to-moderate sample sizes suggest that Bayesian approach provides better coverage probabilities than the frequentist approach via the maximum likelihood method since it is ‘exact’ conditional on the data without relying on asymptotic approximation or ‘plug-in’ principle.”

Helsel and Cohn (1988) introduce two methods called LR and MR to estimate $\mu$ and $\sigma^2$ for data with single and multiple detection limits, respectively. They conduct simulation study to compare Mean Square Error (MSE) and bias with other commonly used methods, and concluded that MR is a “robust and efficient method.” Due to the nature of the method, MR method was later named Regression on Order Statistics (ROS).
CHAPTER III
METHODOLOGY

The proposed model is based on a likelihood ratio test for testing the hypothesis

\[ H_0 : M_1 = M_2 = \cdots = M_k \text{ vs. } H_1 : M_i \neq M_{i'} \text{ for some } i \neq i' \]

where \( M_i \) is the mean of the positive part of \( i \)th population \( i = 1 \cdots k \).

We can apply different distributions here. If we assume the positive parts are from Log-normal distribution with \( \mu_i \) and \( \sigma_i \) as mean and standard deviation on the log scale, then \( M_i = e^{\mu_i + \frac{\sigma_i^2}{2}} \). When we assume \( \sigma_i \) is equal for all independent populations, it is equivalent to test \( H_0 : \mu_1 = \mu_2 = \cdots = \mu_k \text{ vs. } H_1 : \mu_i \neq \mu_{i'} \text{ for some } i \neq i' \).

If the positive parts are from Gamma distribution with \( \alpha \) as shape parameter and \( \beta \) as scale parameter, the mean is \( M_i = \alpha \beta \). On the other hand, if we use Weibull distribution with scale parameter \( \lambda \) and shape parameter \( k \) to simulate positive values, the mean is \( M_i = \lambda \Gamma(1 + \frac{1}{k}) \), where \( \Gamma(\cdot) \) is gamma function.

Now we use Log-normal distribution for testing the hypothesis in the above equation. Assuming the standard deviation, \( \sigma \), and the probability of true zeros, \( p \), are equal for all populations, the probability density function of one population is

\[
f(y_i|\theta^*) = \{P + (1 - P) \times \Phi\left(\frac{y_{L,i} - \mu_i}{\sigma}\right)\}^{m_i} \times \prod_{j=m_i+1}^{n_i} \left\{\frac{1-P}{\sigma} \times \phi\left(\frac{y_{ij} - \mu_i}{\sigma}\right)\right\}
\]

where \( \theta^* = (\mu_i, \sigma, P) \) are the unknown parameters vector, \( y_{L,i} \) is the detection limit in the log scale, \( \phi(\cdot) \) and \( \Phi(\cdot) \) are the p.d.f. and c.d.f. of standard normal distribution.

Without loss of generality, we assume that the first \( m_i \) values in the \( i \)th population
are below the DL \( y_L \) and let \( n_i \) be the total sample size of the \( i \)th population. From the above p.d.f., all parameters are continuous, so it is apparently that the following likelihood function is continuous and differentiable.

Let \( y_{ij} (i = 1, 2, \ldots, k \text{ and } j = 1, 2, \ldots, n_i) \) be the Log-transformed values for the \( j \)th observation in the \( i \)th population. Since we assume the positive part following a Log-normal distribution, \( y_{ij} \) follows a normal distribution. The likelihood function for \( k \) populations is

\[
L_m(\mu_1, \mu_2, \ldots, \mu_k, \sigma, P, \ldots) = \prod_{i=1}^{k} \left\{ P + (1 - P) \times \Phi \left( \frac{y_L - \mu_i}{\sigma} \right) \right\}^{n_i} \times \prod_{j=m_i+1}^{n_i} \left\{ \frac{1 - P}{\sigma} \times \phi \left( \frac{y_{ij} - \mu_i}{\sigma} \right) \right\}
\]

Similar to Taylor et al. (2001) and Nie et al. (2006) for two independent sample case, we derive the equations to obtain the maximum likelihood estimate (MLE) of \( \theta = (\mu_1, \ldots, \mu_k, \sigma, P) \). We need to solve the following equations,

\[
\frac{m_i \times (1 - P) \phi(\varepsilon_i)}{\sigma \times [P + (1 - P) \times \Phi(\varepsilon_i)]} + \frac{\sum_{j=m_i+1}^{n_i} (y_{ij} - \mu_i)}{\sigma^2} = 0
\]

\[
\sum_{i=1}^{k} \left\{ \frac{m_i \times (1 - P) \times (-\varepsilon_i) \times \phi(\varepsilon_i)}{P + (1 - P) \times \Phi(\varepsilon_i)} - \frac{n_i - m_i}{\sigma} + \frac{\sum_{j=m_i+1}^{n_i} (y_{ij} - \mu_i)^2}{\sigma^3} \right\} = 0
\]

\[
\sum_{i=1}^{k} \left\{ \frac{m_i \times [1 - \Phi(\varepsilon_i)]}{P + (1 - P) \times \Phi(\varepsilon_i)} - \frac{n_i - m_i}{1 - P} \right\} = 0
\]

where \( \varepsilon_i = \frac{y_L - \mu_i}{\sigma} \), \( \sigma_1 = \sigma_2 = \cdots = \sigma_k = \sigma \) and \( i = 1, 2, \ldots, k \).

There exists no closed-form solution for MLEs, so we rely on numerical methods to find the solution. Among numerous numerical methods, we purposely choose L-BFGS-B method since “L-BFGS-B is a limited-memory algorithm for solving large nonlinear optimization problems subject to simple bounds on the variables.” (Zhou et. al., 1997). L-BFGS-B method is an extension of Limited-memory Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. The objective of algorithm L-BFGS-B is to minimize a nonlinear function of \( n \) variables (Zhou et. al., 1997).

The nuisance parameters in our likelihood function needed to be constrained
when searching for optimal values: the standard deviation \( \sigma \geq 0 \) and the probability of zeros \( 0 < p < 1 \).

\( H_0 \) is equivalent to \( H'_0 : \mu_1 = \mu_2 = \cdots = \mu_k \) when \( \sigma_1 = \sigma_2 = \cdots = \sigma_k = \sigma \).

We are only interested in parameter \( \mu_i \). We treat parameters \( \sigma \) and \( P \) as nuisance parameters. Let the parameters under the null hypothesis be \( \theta_0 = (\mu, \mu, \ldots, \mu, \sigma, P) \), and the parameters under the alternative hypothesis be \( \theta = (\mu_1, \ldots, \mu_k, \sigma, P) \). The likelihood function under \( H_0 \) is

\[
L_m(\mu, \mu, \ldots, \mu, \sigma, P) = \prod_{i=1}^{k} \left( P + (1 - P) \times \Phi \left( \frac{y_{L_i} - \mu}{\sigma} \right) \right)^{m_i} \times \\
\prod_{j=m_i+1}^{n_i} \left\{ \frac{1-P}{\sigma} \times \phi \left( \frac{y_{ij} - \mu}{\sigma} \right) \right\}
\]

Let \( \varepsilon = \frac{y_{L} - \mu}{\sigma} \). To find the MLE under \( H_0 \), similarly we need to solve the following equations

\[
\sum_{i=1}^{k} \left\{ \frac{m_i \times (1 - P) \times \phi(\varepsilon)}{\sigma \times \left[ P + (1 - P) \times \Phi(\varepsilon) \right]} + \frac{\sum_{j=m_i+1}^{n_i} (y_{ij} - \mu)}{\sigma^2} \right\} = 0
\]

\[
\sum_{i=1}^{k} \left\{ \frac{m_i \times (1 - P) \times (-\varepsilon) \times \phi(\varepsilon)}{P + (1 - P) \times \Phi(\varepsilon)} - \frac{n_i - m_i}{\sigma} + \frac{\sum_{j=m_i+1}^{n_i} (y_{ij} - \mu)^2}{\sigma^3} \right\} = 0
\]

\[
\sum_{i=1}^{k} \left\{ \frac{m_i \times (1 - \Phi(\varepsilon))}{P + (1 - P) \times \Phi(\varepsilon)} - \frac{n_i - m_i}{1 - P} \right\} = 0
\]

The likelihood ratio is

\[
\lambda(\theta) = \frac{L_m(\mu, \mu, \ldots, \mu, \sigma, P)}{L_m(\mu_1, \mu_2, \ldots, \mu_k, \sigma, P)}
\]

And the test statistics \( T = -2 \times \ln \lambda(\theta) \) follows a \( \chi^2 \) distribution with degrees of freedom \( k - 1 \). \( k \) is number of independent populations which is three in the present study.
CHAPTER IV
SIMULATIONS AND RESULTS

In this chapter, we will conduct a set of Monte Carlo simulations by the proposed Likelihood ratio model in Chapter 3. Type I error and statistical power will be evaluated and compared. We will treat standard deviation, $\sigma$, and the probability of true zeros, $p$, as nuisance parameters which are not of our primary interest in this study. Our primary interest is on mean comparison of the positive part for $K$ ($K \geq 3$) independent populations. Each combination of parameters will run 5000 simulations to obtain respective observed size and power.

As will show below, there are over 10000 different combinations in the total of observed size and power, and each combination will run 5000 simulations, it is computation intensive and requires large computing resources. Due to the heavy computation requirement, we run all the programs on Amazon Elastic Compute Cloud (EC2). The server on Amazon EC2 has 16 CPUs, 30GB of Memory, and 2x160 GB SSD Storage. All the R codes are paralleled to utilize all 16 CPUs simultaneously on server. The computation time is significantly reduced by conducting parallel computation with cloud computing, compared to using personal computer. All the program codes are written in RStudio version 0.98.1049 using R version 3.1.1 on Linux Ubuntu (64-bit) 14.04LTS platform.
4.1 Log-normal Distribution

4.1.1 Settings

Specifically, in the simulation study of this chapter we compare the equality of the means in log scale of positive part in three independent populations. For comparing type I error we compare the combinations of parameters $\mu$ and $\sigma$ in log scale, $p$, $\sigma$, Detection limit (DL) $y_L$ and group size $n$. The range of parameters $\mu$ and $\sigma$ in log scale is from 0.5 to 5, incremented by 0.5. The probability of true zeros $p$ has range \{0.1, 0.2, 0.3, 0.4, 0.5\}. We set the probability under DL as \{0.01, 0.1, 0.2, 0.3, 0.4\} and group size as \{100, 200, 500\}, so that the actual values of $y_L$ vary by different combination of $\mu$ and $\sigma$, with small, medium and large sample. The significance level is $\alpha = 0.05$. Under such setting, there will be $10 \times 10 \times 5 \times 5 \times 5 = 7500$ different combinations of $\mu, \sigma, p, y_L$ and $n$.

As introduced before, the mean and standard deviation in the log scale, $\mu$ and $\sigma$, range from 0.5 to 5 with increment of 0.5. The actual mean and standard deviation of Log-normal distribution are $e^{\mu + \frac{\sigma^2}{2}}$ and $\sqrt{(e^{\sigma^2-1})e^{2\mu + \sigma^2}}$, respectively. Therefore, the range of mean for the Log-normal distribution is $[1.868, 39824784]$, and the range of standard deviation for the Log-normal distribution is $[1.284, 6.48 \times 10^{12}]$. We think the above range is sufficiently large for the case of present study.

For observed power, all the settings keep the same as in observed size with exception of $\mu$. We keep all $\mu$ identical for observed size, but we vary $\mu$ for comparing observed power. The differences in $\mu$ are decided by the convention introduced by Cohen (1988). Small, medium and large effect size are 0.2, 0.5 and 0.8, respectively. By the formula of $\frac{\max \mu\text{ difference}}{\sigma} = \text{effect size}$, we can calculate the maximum difference of $\mu$ among all populations. Since we use three independent populations in the simulations, without loss of generality we set the difference between $\mu_1$ and $\mu_2$ equals to the maximum difference from the convention, and $\mu_3$ is set to equal to $\mu_1$, $\mu_2$ and $\frac{\mu_1 + \mu_2}{2}$ in three combinations, respectively. However, the above procedure for power will no longer guarantee $\mu$ to fall in the range of 0.5 and 5.

Since we should set different values of $\mu$ to obtain observed power, consid-
ering the effect size convention and the selection of values of mean for the third population, there are at least \(7500 \times 3 = 22500\) combinations to obtain observed power. In order to save resources and for the sake of parsimony, we categorize each of the parameters \(\mu, \sigma, p\) into small, medium and large size. \(\mu = \{0.5, 1.0, 1.5, 2.0\}, \sigma = \{0.5, 1.0, 1.5, 2.0\}, p = \{0.1, 0.2, 0.3\}\) are set as small; \(\mu = \{2.5, 3.0, 3.5\}, \sigma = \{2.5, 3.0, 3.5\}, p = 0.3\) are set as medium; and \(\mu = \{4.0, 4.5, 5.0\}, \sigma = \{4.0, 4.5, 5.0\}, p = \{0.4, 0.5\}\) are set as large. Therefore, under each \(n\) and \(y_L\), we choose different combinations of \(\mu, \sigma\) and \(p\) with observed sizes between 0.49 and 0.51.

There are two steps to generate the data. First, based on the sample size we generate number of true zeros for each population by Binomial distribution. Second, the rest of the data for each population are generated from a Log-normal distribution. We will later use data generated from Gamma distribution to evaluate the performance of the proposed model. Third, values below the DL are censored and combined with the true zeros as the total number of zeros. The restricted Maximum likelihood Estimates (MLEs) under \(H_0: \mu_1 = \mu_2 = \mu_3\) and unrestricted MLEs under \(H_1: \mu_i \neq \mu_j, \text{ for some } i, j\) are calculated using L-BFGS-B method with parameter restrictions in OPTIM function in R software.

4.1.2 Results

Tables 4.1-4.3 show the observed size from simulation for \(n = 100, 200\) and \(500\). The full table of observed size consists of 500 rows, we show a random sample of 50 rows as an example. The full tables are Table 7.1-7.3 in Appendix A.

Each row in the tables shows mean \(\mu\) in log scale, standard deviation \(\sigma\) in log scale, probability of true zeros \(p\), and the observed sizes under different detection limits. For example, \(DL0.01\) stands for the probability of a positive values falling under DL, which is \(P(y \leq DL) = 0.01\), where \(y\) is the random variables from Log-normal distribution. The means of three populations are equal for size calculation, so we show only one \(\mu\) instead of three.

The standard error of observed size in the present study is \(se = \sqrt{\frac{0.05(1-0.05)}{5000}} = 0.00308\). We consider the observed sizes within \(3 \times se\) as an acceptable range, which
is $0.05 \pm 0.0092 \approx [0.041, 0.059]$. From Tables 4.1-4.3 and, we see a general pattern that as $P(y \leq DL)$ increases, the observed size becomes larger. However, the pattern is clear if comparing sizes of column $DL0.001$ and column $DL0.4$. This finding concurs with the expectation because when $P(y \leq DL)$ becomes large, there are more positive values falling below $DL$, which means we have less available positive observed information. The result, observed size, will become less accurate.

When comparing across three population sizes, $n = 100, 200$ and $500$, we found under the same combination of $\mu, \sigma$ and $p$, large group size will tend to have a better observed size with minor fluctuations, which is close to $0.05$. This finding is intuitive that more data are available, more accurate the test will be.

From Table 4.1, we found the observed sizes tend to be large when the probability of true zeros $p = 0.4$ or $0.5$. This finding implies that when group sizes are small, $n = 100$ for example, large $p$ will reduce the number of observed positive values, and the situation becomes even worse under large values of $P(y \leq DL)$. The sizes are out of the normal range $[0.041, 0.059]$ if $P(y \leq DL) = 0.4$, such as rows 1, 2, 5, 12, 14, 18 and 20. Table 7.1 of Appendix A with complete cases also supports the above finding. This finding is relaxed a little when the group size increases as in Table 4.2 and 4.3. We see that some cases with $p = 0.3$ or $0.2$ have observed sizes out of the normal range, such as rows 9, 12, and 37 in Table 4.2 and rows 27 in Table 4.3. Table 7.2 and 7.3 in Appendix A have more rows of this situation.

Looking further on finding the combinations of parameters that have large observed sizes, we found that $P(y \leq DL), n$ and $p$ are three dominant factors. From Tables 4.1-4.3 and Tables 7.1-7.3, observed sizes are out of the range for the combinations of large $P(y \leq DL)$, small $n$ and large $p$. In those cases, the observed sizes are bad. Moreover, we find that when $p, n$ and $P(y \leq DL)$ fixed, the combinations of small $\mu$ and large $\sigma$ tend to have worse observed size than the combinations of large $\mu$ and small $\sigma$.

In summary, across all 7500 combinations of $\mu, \sigma, p, P(y \leq DL)$ and $n$, the proposed likelihood ratio test maintains good observed sizes. The observed sizes increases as $P(y \leq DL)$ increases and it decreases as group size increases. And
$P(y \leq DL)$, $n$ and $p$ are three dominant parameters in that large $P(y \leq DL)$, small $n$ and large $p$ will always lead to bad observed sizes. And also, the combinations of large $\mu$ and small $\sigma$ tend to have better sizes than those of small $\mu$ and large $\sigma$.

Table 4.1: Example of Observed Size Comparison for $n=100$

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$\sigma$</th>
<th>$p$</th>
<th>DL0.01</th>
<th>DL0.1</th>
<th>DL0.2</th>
<th>DL0.3</th>
<th>DL0.4</th>
</tr>
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<tbody>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>0.5</td>
<td>0.051</td>
<td>0.057</td>
<td>0.053</td>
<td>0.060</td>
<td>0.065</td>
</tr>
<tr>
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<td>1.0</td>
<td>0.4</td>
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<td>0.053</td>
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<td>0.064</td>
</tr>
<tr>
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<td>0.3</td>
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<td>0.051</td>
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<tr>
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<td>0.057</td>
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As introduced in section 4.1.1, there are 7500 different combinations of parameters for observed size calculation. However, there will be much more combinations to vary mean \( \mu \) for observed power calculation. In order to save resources, we categorize \( \mu, \sigma \) and \( p \) into small, medium and large, and select the combinations where they have observed size around 0.05 to see those parameter combinations performances on observed power.

The following Table 4.4 is the partial table of observed power with \( n = 100, P(y \leq DL) = 0.1 \). The observed powers under other combinations of parameters are Table 7.4-7.17 in Appendix B. We only show \( \mu_1 \), the largest mean of three \( \mu \)'s, in the table, but one can indirectly calculate the smallest \( \mu \) using Cohen (1988)'s convention and \( \sigma \). However, we set the third mean, \( \mu_3 \), to be equal to either largest mean \( \mu_1 \), smallest mean \( \mu_2 \) or \( \frac{\mu_1 + \mu_2}{2} \). We find that the observed power is the smallest out of three situations when \( \mu_3 = \frac{\mu_1 + \mu_2}{2} \). In order to be conservative, under each combination of \( \mu_1 \) and \( \mu_2 \) we select the power with \( \mu_3 = \frac{\mu_1 + \mu_2}{2} \) only.

From Table 4.4 and Table7.4-7.17 we find that generally speaking the proposed likelihood ratio test have good powers under large effect size while setting the size around 0.05. More specifically, all but a few parameter combinations yielded powers above 0.8. The powers decreases when effect size decreases and \( P(y \leq DL) \) increases. The powers for small effect size are bad, usually below 0.3 for small and medium group size, \( n = 100 \) or 200. When \( n = 500 \) the power could reach above 0.4 when \( P(y \leq DL) = 0.4 \), and for smaller \( P(y \leq DL) \) the power could reach above 0.6.

In summary, we follow the convention of Cohen (1988) to set 0.2, 0.5 and 0.8 as small, medium and large effect size. From Table 4.4 and Tables 7.4-7.17 in Appendix B we find the proposed likelihood ratio test performs very well on observed

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<th>( n )</th>
<th>( \mu )</th>
<th>( \sigma )</th>
<th>( p )</th>
<th>( P(y \leq DL) )</th>
<th>( P(y \leq DL) )</th>
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power when maximum difference in mean, $max|\mu_1 - \mu_2| = 0.8\sigma$. When $n$ is small, $P(y \leq DL)$ is large and $max|\mu_1 - \mu_2| = 0.2\sigma$, the power is bad. However, power could reach above 0.6 even though $max|\mu_1 - \mu_2| = 0.2\sigma$ and $P(y \leq DL)$ is large.

### Table 4.4: Observed Power with Various Effect Size for n=100

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<th>$p$</th>
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### 4.2 Gamma Distribution

The above conclusions are drawn based on the assumption that data are from a Log-normal distribution. This is a common assumption in many literature. However, there are a few other probability distributions that could have very similar density shapes to Log-normal distribution, as an example, Gamma distribution. The following a few figures show the similarity of Log-normal and Gamma distributions under
certain values of parameters. We set the coefficient of variation to be equal in order to match the parameters.

Figure 4.1: Similarity Between Log-normal and Gamma Distribution

Figure 4.1 includes the density curves of Log-normal distributions with parameters \((\mu, \sigma) = (0.5, 0.1), (0.5, 0.3), (0, 0.1), (0, 0.3), (0.25, 0.1)\) and \((0.25, 0.3)\), respectively. And it also includes the density curves of Gamma distribution with shape parameters \(\alpha\) and scale parameter \(s\), \((\alpha, s) = (99.5, 0.017), (10.62, 0.16), (99.5, 0.01), (10.62, 0.1), (99.5, 0.013), \) and \((10.62, 0.126)\), respectively, with the form of \(p.d.f\) as \(f(x; \alpha, s) = \frac{1}{\Gamma(\alpha)s^\alpha}x^{\alpha-1}e^{-\frac{x}{s}}\). We match parameters of Log-normal distribution with Gamma distribution by matching the square of Coefficient of Variation. The details
are as follow:

The mean and variance of Long-normal distribution are \( e^{\mu + \frac{\sigma^2}{2}} \) and \( e^{2\mu + \sigma^2}(e^{\sigma^2} - 1) \), \( CV^2 = \frac{\text{var}(Y)}{\text{E}(Y)^2} = e^{\sigma^2} - 1 \), and the mean and variance of Gamma distribution are \( \alpha \beta \) and \( \alpha \beta^2 \), \( CV^2 = \frac{\text{var}(Y)}{\text{E}(Y)^2} = \frac{1}{\alpha} \), where \( \alpha \) is the shape parameter and \( \beta \) is the scale parameter. By matching \( CV^2 \), we have the corresponding parameters of Gamma distribution.

\[
\begin{align*}
\alpha &= \frac{1}{e^{\sigma^2} - 1} \\
\beta &= e^{\mu + \frac{\sigma^2}{2}}(e^{\sigma^2} - 1)
\end{align*}
\]

The shape parameter \( \alpha \) is related to \( \sigma \) only, and we know that the shape of Gamma distribution will be strictly decreasing when \( \alpha \leq 1 \). So by the above formula, in order to have similarity with Gamma distribution, \( \sigma \) has to meet the criterion \( \alpha = \frac{1}{e^{\sigma^2} - 1} > 1 \Rightarrow \sigma < 0.83 \).

We are interested in if the likelihood ratio test proposed in Chapter Three perform well when the data are from a Gamma distribution, instead of a Log-normal distribution. In another word, we would like to see the robustness of the proposed likelihood ratio test, which is generated based on Log-normal distribution, using data from a Gamma distribution. The results are as follows using the parameters from above figure.

Table 4.5 shows the observed size comparison between Log-normal distribution and Gamma distribution. The first five columns are the parameters of Log-normal and corresponding Gamma distribution. The last four columns are sizes of Long-normal and Gamma distribution under \( P(y_i \leq DL) = 0.1 \) and \( 0.4 \), respectively. We see that sizes of both distributions are close and it is hard to decide which is constantly better than the other one. The majority of them are within the normal range \([0.041, 0.059]\) for \( P(y_i \leq DL) = 0.1 \). And there are more sizes out of the range when the detection limit becomes larger, \( P(y_i \leq DL) = 0.4 \).

On the observed statistical power side, we use sample size \( n = 100 \) and DL is \( P(y_i \leq DL) = 0.1 \) in Table 4.6 and we sort it ascendingly by \( \sigma \) and \( \mu_1 \), descendingly by \( \mu_2 \), and We see that both distributions perform well on large effect size and poor
Table 4.5: Size Comparison of Log-normal vs Gamma Distributions, $n = 100$

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<th>Gamma0.1</th>
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<td>0.060</td>
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<td>0.056</td>
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on small effect size. Another finding is that Log-normal distribution is sensitive to
the probability of true zero $p$. The power drops when $p$ increases. However, Gamma
distribution does not show this pattern. In addition, the power changes only slightly
for Gamma distribution on the same level of effect size when $p$ increases. But power
of Log-normal changes much more as $p$ increases. We think the reason is that the
scale parameter $\beta$ changes much smaller compared to the changes of $\mu$. For example,
from row 10–18 in the table, $\beta$ changes 0.0003 when $\mu$ changes 0.03, and tiny changes
offset the increment of $p$.

In summary, if the true data are from a Gamma distribution, the proposed
Log-normal based likelihood ratio test still maintain relatively good observed size.
The test have high powers for both distributions on large effect size. On the same
level of effect size, the test on Gamma distribution tends to maintain the power well
as $p$ increases.
Table 4.6: Observed Power Comparison of Log-normal vs Gamma Distributions

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<th>$\mu_1$</th>
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<th>$p$</th>
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CHAPTER V
IMPUTATION METHODS

When non-detect values exist, a typical way is simply substituting all values below DL with \( \frac{DL}{2}, \frac{2DL}{3}, \frac{DL}{\sqrt{2}}, \) or \( DL \). However, Chu et al. (2008) points out that such substitution has two potential drawbacks: (1) some of these values may come from a special distribution, and (2) it fails to take left censoring models into account. Moreover, Krishnamoorthy et al. (2009) indicates that such approach is the worst with respect to mean squared error criterion.

In our study, we propose a new imputation method to obtain the distribution parameters. However, there are two primary challenges need to be addressed in the study:

1. Estimate number of values below the DL, and separate them from true zeros. Notice that we are not able to distinguish true zeros from the values below DL in the original observations.

2. Impute the values below the DL, “fill in” the observed values, and finally obtain the parameter estimates.

We first look at one population case. Let us recall that there are two parts of the observations: one is observed positive values, and the other part is zeros, and we are not able to distinguish the values below DL from all zeros.

Our ideas of the imputation method could be demonstrated by the following steps:

1. Obtain initial estimates \( \hat{\mu}_0 \) and \( \hat{\sigma}_0 \) from observed positive values.
2. Fit a Log-normal distribution \( f_0(\cdot) \) in terms of \( \hat{\mu}_0 \) and \( \hat{\sigma}_0 \).

3. Calculate the probability of \( f_0(\cdot) \) under DL, \( \hat{p}_+ \).

4. Calculate the expected number of values falling below DL, based on the equation of 
\[
\frac{\hat{p}_+}{1 - \hat{p}_+} = \frac{\hat{n}_+}{n - m} \Rightarrow \hat{n}_+ = (n - m) \times \frac{\hat{p}_+}{1 - \hat{p}_+}, \text{ where } \hat{n}_+ \text{ is the estimated number of values falling below DL, } n \text{ is the total group sample size, and } m \text{ is the number of observed zeros.}
\]

5. Generate \( \hat{n}_+ \) values from \( f_0(\cdot) \) falling below DL by rejection method.

6. Combine \( \hat{n}_+ \) new generated values with the \( n - m \) observed values as a “complete” data set. Calculate updated estimated \( \hat{\mu}_1 \) and \( \hat{\sigma}_1 \).

7. Fit an updated Log-normal distribution \( f_1(\cdot) \) in terms of \( \hat{\mu}_1 \) and \( \hat{\sigma}_1 \).

8. Repeat Steps 4 - 6 until the \( \hat{\mu}_i - \hat{\mu}_{i-1} \) and \( \hat{\sigma}_i - \hat{\sigma}_{i-1} \) converge.

The above algorithm has a natural drawback of overestimating the number of values under DL since the initial estimates \( \hat{\mu}_0 \) and \( \hat{\sigma}_0 \) are expected to be greater than the true values. After each iteration, the estimates of mean \( \mu \) will be “dragged” smaller and standard deviation \( \sigma \) will be larger and hence \( \hat{n}_+ \) increases. Essentially, it is highly likely that the number of values under DL is overestimated and ultimately all zeros (both true and not-true) will be treated as values under DL. This results in underestimate of \( \mu \) and overestimate of \( \sigma \).

The R codes for the above algorithm is in Appendix C.

Another imputation method is called Regression on Order Statistics (ROS). It is first introduced by Helsel and Cohn (1988) as MR method, and after series of modifications, the ROS formed. ROS method use the unobserved values collectively to obtain the summary statistics, not assigning them to individual observations. More powerfully, ROS could address the data with multiple detection limit. However, such case is not under consideration in the present study.

ROS assumes the number of values under DL is known and replaces those values by the DL. In the present study, the issue is that we do not know that
number. In order to implement ROS, we use the estimate from Step 4 above, \( \hat{n}_+ \), to be the estimate of number of values below DL. However, \( \hat{n}_+ \) has different values for each iteration, and it tends to be under-estimated in the initial iteration and over-estimated in the last iteration. In the present study, we use \( \hat{n}_+ \) from the last iteration.

The following Figures 5.1 - 5.3 show the estimated \( \mu \) and \( \sigma \) compared to their true values. The DL is always set to be \( P(y \leq DL) = 0.1 \). The true values of mean \( \mu \), standard deviation \( \sigma \), and probability of true zeros \( p \) are listed in the figure captions respectively. There are totally 1000 iterations and under each iteration the estimate of \( \mu \) and \( \sigma \) will be obtained with a group of size \( n = 100 \). The pink line, \textit{m.combin}, stands for the combination of the proposed imputation method in this chapter and ROS, and the blue line, \textit{m.impt}, stands for the estimates from using the proposed method alone.

We see from the figures that \textit{m.impt} tends to have unstable estimates, both on mean and standard deviation.

In order to make the conclusion more comprehensive, we need to see the comparison under different combinations of \( \mu, \sigma \), and \( p \). Our current recommendation is that when the sample size is more than 100, Regression on Order Statistics (ROS) using the estimate of number of values under DL from the proposed imputation method is recommended for obtaining summary statistics for the data with undetectable values.
Mean comparison between Iterative Imputation and combined method

SD comparison between Iterative Imputation and combined method

Figure 5.1: Estimates under $\mu = 1$, $\sigma = 0.5$, $p = 0.5$, $n = 100$
Figure 5.2: Estimates under $\mu = 0.5, \sigma = 0.3, p = 0.1, n = 100$
Mean comparison between Iterative Imputation and combined method

SD comparison between Iterative Imputation and combined method

Figure 5.3: Estimates under $\mu = 1.5, \sigma = 1, p = 0.3, n = 100$
CHAPTER VI
CONCLUSIONS

The present study proposed a likelihood ratio test for \( K \geq 3 \) independent populations with a detection limit. The simulation and formula derivation will be based on \( K = 3 \) independent populations. Furthermore, the robustness (observed power) and sensitivity (observed size) of the proposed test was shown under various combinations of the parameters and under Log-normal distribution and Gamma distribution through simulation studies.

We found that generally speaking the proposed likelihood ratio test maintains good observed sizes. The observed sizes increases as \( P(y \leq DL) \) increases and it decreases as group size increases. And \( P(y \leq DL) \), \( n \) and \( p \) are three dominant parameters that large \( P(y \leq DL) \), small \( n \) and large \( p \) will always lead to bad observed sizes. Moreover, the combinations of large \( \mu \) and small \( \sigma \) tend to have better sizes than those of small \( \mu \) and large \( \sigma \). As for the observed power side, the proposed likelihood ratio test performs very well on observed power when maximum difference in mean, \( \max|\mu_1 - \mu_2| = 0.8\sigma \). When \( n \) is small, \( P(y \leq DL) \) is large and \( \max|\mu_1 - \mu_2| = 0.2\sigma \), the power is bad. However, power could reach above 0.6 even though \( \max|\mu_1 - \mu_2| = 0.2\sigma \) and \( P(y \leq DL) \) is large.

When data is actually from a Gamma distribution with a similar density curve as Log-normal distribution, the proposed Log-normal based likelihood ratio test still maintain relatively good observed size. The test have high powers for both distributions on large effect size. On the same level of effect size, the test on Gamma distribution tends to maintain the power well as \( p \) increases.

The imputation methods may be another direction to test the hypothesis
with data with excess zeros and detection limits. Our recommendation is that the combination of the proposed imputation method and Regression on Order Statistics outperform the proposed imputation method alone.

The work presented in the current study could be extended in the following directions:

First, evaluate and improve the test performance under small group size ($n < 100$).

Second, investigate the performance of the test under large detection limit case, for example $P(y \leq DL) \geq 0.5$.

Third, if the underlying distribution is other than Log-normal or Gamma distribution, the performance of the test.

Fourth, derive a likelihood ratio test directly on Gamma distribution.

Lastly, more sophisticated imputation methods may be developed.
### APPENDIX A

**Tables of Observed Size**

Table 7.1: Observed Size Comparison for n=100

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### APPENDIX B

**Tables of Observed Power**

**Table 7.4: Observed Powers at Various Effect Sizes.** $n=100$, $P(y \leq DL)=0.01$

<table>
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<th>Mu1</th>
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<th>Small Effect</th>
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Table 7.5: Observed Power at Various Effect Sizes. n=100, P(y≤DL)=0.2

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Table 7.6: Observed Power at Various Effect Sizes. \( n=100, P(y \leq DL)=0.3 \)

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Table 7.7: Observed Power at Various Effect Sizes. n=100, P(y≤DL)=0.4

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Table 7.8: Observed Power at Various Effect Sizes. n=200, P(y≤DL)=0.01

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Table 7.13: Observed Power at Various Effect Sizes. n=500, P(y ≤ DL) = 0.01

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Table 7.14: Observed Power at Various Effect Sizes. $n=500$, $P(y \leq DL) = 0.2$

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Table 7.16: Observed Power at Various Effect Sizes. \( n=500, P(y \leq DL)=0.3 \)

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APPENDIX C
Sample R Codes

### Setting ###
library(knitr)
library(ggplot2)
library(xtable)
library(plyr)
library(dplyr)
library(NADA)
set.seed(19851109)

### Demonstration of Data with Excess Zeros and DL ###
para <- c(mu = 1, sigma = 1, p = 0.2, y.1 = 1)
n <- 100
n0 <- rbinom(1, n, para[3])
y <- rlnorm(n-n0, para[1], para[2])

dat1 <- c(rep(0, n0), y)

m <- qplot(dat1, geom="histogram", binwidth = .2)
m_f <- m + geom_histogram(aes(fill = ..count..), binwidth = 0.2) +
theme(axis.title.x = element_blank())

m_f + theme(legend.position = 'none', axis.text= element_text(size=18)

axis.title=element_text(size = 18))

## (b) With detection limit.

y.1 <- para[4]; y1 <- y
dat2 <- c(rep(0, n0 + length(y1[y1 < y.1])), y1[y1 >= y.1])

m2 <- qplot(dat2, geom="histogram", binwidth = .2)
m2_f <- m2 + geom_histogram(aes(fill = ..count..), binwidth = 0.2) +
geom_vline(aes(xintercept=1),colour="#BB0000", linetype="dashed") +

theme(axis.title.x = element_blank())

m2_f + theme(legend.position = 'none',axis.text= element_text(size=18)
### See shape similarity ###

\[ \mu_1 = 0.5; \sigma = 0.25; \]

\[ \text{shape}_\gamma = \frac{1}{(\exp(\sigma^2)-1)}; \text{scale}_\gamma = (\exp(\sigma^2/2)\times(\exp(\sigma^2)-1))\times\exp(\mu_1) \]

\[ \text{scale}_wbl \leftarrow \frac{1}{(\exp(\sigma^2)-1)} \times (\exp(\sigma^2/2)\times(\exp(\sigma^2)-1))\times\exp(\mu_1) / \gamma \left(1+\frac{1}{3.5}\right) \]

\[ \text{ff} \leftarrow \text{ggplot}(\text{NULL}, \text{aes}(x = x, \text{linetype} = g)) \]

\[ \text{ff} + \text{stat}_\text{function}(\text{data}=\text{data.frame}(x = c(0, 10), g = \text{factor}(1)), \text{fun} = \text{dlnorm}, \]

\[ \arg = \text{list} \left( \text{meanlog} = \mu_1, \text{sdlog} = \sigma \right) + \]

\[ \text{stat}_\text{function}(\text{data}=\text{data.frame}(x = c(0, 10), g = \text{factor}(2)), \text{fun} = \text{dgamma}, \]

\[ \arg = \text{list} \left( \text{shape} = \text{shape}_\gamma, \text{scale} = \text{scale}_\gamma \right) + \]

\[ \text{stat}_\text{function}(\text{data}=\text{data.frame}(x = c(0, 10), g = \text{factor}(3)), \text{fun} = \text{dweibull}, \]

\[ \arg = \text{list} \left( \text{shape} = 4.2, \text{scale} = \text{scale}_wbl - 0.25 \right) + \]

\[ \text{scale}_\text{linetype}_\text{manual}(\text{values}=c(1, 2, 6), \text{labels} = c \left( \text{"Log-normal"}, \text{"gamma"}, \text{"weibull"} \right), \text{name} = \text{"Distribution"}) \]

### Size calculation ###

#### All Data are from Log-normal, model is lognormal ####

\[ \text{rm(list} = \text{ls}()) \]

# 1. give parameters under null hypothesis.

\[ \text{Mu} \leftarrow \text{seq}(0.5, 5, 0.5); \text{sigma} \leftarrow \text{seq}(0.5, 5, 0.5) \]

\[ p \leftarrow \text{seq}(0.1, 0.5, 0.1); k \leftarrow 3 \text{ crit_val} \leftarrow \text{qchisq}(0.95, k - 1) \]

\[ R = 5000; n1 \leftarrow n2 \leftarrow n3 \leftarrow 100; \text{perc} \leftarrow 0.1 \text{ # probability under DL.} \]

# Generate a matrix contains all combinations.

\[ \text{sim} \leftarrow \text{expand.grid}(\text{Mu} = \text{Mu}, \text{Mu2} = \text{Mu}, \text{Mu3} = \text{Mu}, \text{sigma} = \text{sigma}, p = p) \]

\[ \text{sim}\text{.df} \leftarrow \text{sim}[\text{sim}\$\text{Mu1} == \text{sim}\$\text{Mu2} \& \text{sim}\$\text{Mu2} == \text{sim}\$\text{Mu3},] \]

\[ y_L \leftarrow \text{qnorm(perc, sim}\text{.df}[, 1], \text{sim}\text{.df}[4]) \]

# This is the DL floating with various combination of Mu and Sigma
\[
si m . y L \leftarrow \text{cbind}(si m . df, y_L = y_L)
\]
\[
si m \leftarrow \text{unnname}(\text{as.list}(\text{as.data.frame}(t(si m . y L)))), \text{force}=T
\]
\[
\text{get_result} \leftarrow \text{function}(\text{para_tru}){
\]
\[
m1_{\text{tru}0} \leftarrow \text{rbinom}(1, n1, \text{para_tru}[5]) \quad \# \text{this is number of true zeros}
\]
\[
m2_{\text{tru}0} \leftarrow \text{rbinom}(1, n2, \text{para_tru}[5])
\]
\[
m3_{\text{tru}0} \leftarrow \text{rbinom}(1, n3, \text{para_tru}[5])
\]
\[
y_L \leftarrow \text{para_tru[6]}
\]
\[
x1 \leftarrow \text{rnorm}(n1 - m1_{\text{tru}0}, \text{para_tru}[1], \text{para_tru}[4]); y1 \leftarrow \text{log}(x1)
\]
\[
x2 \leftarrow \text{rnorm}(n2 - m2_{\text{tru}0}, \text{para_tru}[2], \text{para_tru}[4]); y2 \leftarrow \text{log}(x2)
\]
\[
x3 \leftarrow \text{rnorm}(n3 - m3_{\text{tru}0}, \text{para_tru}[3], \text{para_tru}[4]); y3 \leftarrow \text{log}(x3)
\]
\[
\text{para_init} \leftarrow \text{c(median(y1), median(y2), median(y3), sd(c(y1, y2, y3))},
\]
\[
\left(\frac{m1_{\text{tru}0} + m2_{\text{tru}0} + m3_{\text{tru}0}}{n1 + n2 + n3}\right)
\]
\[
\text{para_null} \leftarrow \text{c(mu = median(c(y1, y2, y3))), sigma = para_init[k + 1],}
\]
\[
p = \text{para_init[k + 2]}
\]
\[
y \leftarrow \text{list}(y1[y1 >= y_L], y2[y2 >= y_L], y3[y3 >= y_L])
\]
\[
m1 \leftarrow m1_{\text{tru}0} + \text{sum}(y1 < y_L)
\]
\[
m2 \leftarrow m2_{\text{tru}0} + \text{sum}(y2 < y_L)
\]
\[
m3 \leftarrow m3_{\text{tru}0} + \text{sum}(y3 < y_L)
\]
\[
\# \text{3. find unrestricted max log-likelihood}
\]
\[
\text{log.like1} \leftarrow \text{function}(\text{para_init}, y){
\]
\[
\mu1 \leftarrow \text{para_init[1]}
\]
\[
\mu2 \leftarrow \text{para_init[2]}
\]
\[
\mu3 \leftarrow \text{para_init[3]}
\]
\[
sigma \leftarrow \text{para_init[4]}
\]
\[
p \leftarrow \text{para_init[5]}
\]
\[
\text{log.lli} \leftarrow m1 \cdot \text{log}(p + (1 - p) \cdot \text{pnorm}((y_L - \mu1) / \sigma))
\]
\[
+ (n1 - m1) \cdot
\]
\[
\quad \text{log}(1 - p) - (n1 - m1) \cdot \text{log}(\sigma) - (n1 - m1) \cdot \text{log}(\sqrt{2 \pi}) -
\]

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\[
\begin{align*}
\text{sum} & \left( (y_1 - \mu_1)^2 / 2 / \sigma^2 + \\
& \quad \mu_2 \log(p + (1 - p) \cdot \text{pnorm}(y_1 - \mu_2 / \sigma)) + \\
& \quad (n_2 - \mu_2) \cdot \log(1 - p) - (n_2 - \mu_2) \cdot \log(\sigma) - (n_2 - \mu_2) \cdot \log(\sqrt{2 \pi}) - \\
& \quad \text{sum}((y_2 - \mu_2)^2 / 2 / \sigma^2 + \\
& \quad \mu_3 \log(p + (1 - p) \cdot \text{pnorm}(y_1 - \mu_3 / \sigma)) + \\
& \quad (n_3 - \mu_3) \cdot \log(1 - p) - (n_3 - \mu_3) \cdot \log(\sigma) - (n_3 - \mu_3) \cdot \log(\sqrt{2 \pi}) - \\
& \quad \text{sum}((y_3 - \mu_3)^2 / 2 / \sigma^2)
\right)
\end{align*}
\]

\text{return}(-\log.lii)

\}

\text{opt1 <- optim(par}_\text{a-init, log-like1, y = y, hessian= F,}
\qquad \text{lower = c(-Inf, -Inf, -Inf, 10^{-5}, 10^{-5})},
\qquad \text{upper = c(Inf, Inf, Inf, Inf, 1 - 10^{-5}), method = "L-BFGS-B")}

\text{lrt1 <- -opt1$value}

\# 4. find max log-likelihood under null hypothesis.
\text{log-like0 <- function(par}_\text{a-null, y)(}
\qquad \text{mu1 <- mu2 <- mu3 <- par}_\text{a-null}[1]
\qquad \text{sigma <- par}_\text{a-null}[2]
\qquad \text{p <- par}_\text{a-null}[3]
\qquad \text{log.li0 <- m1 * log(p + (1 - p) * \text{pnorm}(y_1 - \mu_1 / \sigma))}
\qquad \quad + (n1 - m1) \cdot 
\qquad \quad \log(1 - p) - (n1 - m1) \cdot \log(\text{sigma}) - (n1 - m1) \cdot \log(\sqrt{2 \pi}) - \\
\qquad \quad \text{sum}((y_1 - \mu_1)^2 / 2 / \sigma^2 + \\
\qquad \quad \mu_2 \log(p + (1 - p) \cdot \text{pnorm}(y_1 - \mu_2 / \sigma)) + \\
\qquad \quad (n2 - \mu_2) \cdot \log(1 - p) - (n2 - \mu_2) \cdot \log(\text{sigma}) - (n2 - \mu_2) \cdot \log(\sqrt{2 \pi}) - \\
\qquad \quad \text{sum}((y_2 - \mu_2)^2 / 2 / \sigma^2 + \\
\qquad \quad \mu_3 \log(p + (1 - p) \cdot \text{pnorm}(y_1 - \mu_3 / \sigma)) + \\
\qquad \quad (n3 - \mu_3) \cdot \log(1 - p) - (n3 - \mu_3) \cdot \log(\text{sigma}) - (n3 - \mu_3) \cdot \log(\sqrt{2 \pi}) -
\}

90
\[
\text{sum}((y[3]) - mu3)^2 / 2 / \text{sigma}^2
\]

return(-log.lik0)
}

opt0 <- optim(par=null, log.like0, y = y, hessian = F, lower = c(-Inf, 10^-5, 10^-5),
               upper = c(Inf, Inf, 1 - 10^-5), method = "L-BFGS-B")
lrt0 <- opt0$value
num <- (2 * (lrt1 - lrt0)) > crit_val
return(num)
}

get.size <- function(para.tru) mean(replicate(R, get_result(para.tru)))
res <- c(0, unlist(mclapply(sim, get.size, mc.cores = 16)))[-1]
sim.xtable <- cbind(sim.y1, obs.size=res)
sim.xtable <- arrange(sim.xtable, obs.size)
sim.dis <- xtable(sim.xtable, caption="Simulate 5000 times, prob <= y_L is 0.1",
                  digits=c(0,1,1,1,1,2,3,3))
print.xtable(sim.dis, type="html", file="simxtable.html")
save(sim.dis, sim.xtable, file="abc.RData")

### Graphics from Proposed Method and Combined Method ###

para.true <- c(Mu = 1.5, Sigma = 1, P = 0.3)  # parameter could be changed accordingly
n <- 100; perc <- 0.1
DL <- pnorm(perc, para.true[1], para.true[2])
max<- 1000
m.impt <- sd.impt <- m.combin <- sd.combin <- numeric(max)
loglike <- function(Mu, Sigma, P, y = y){
    log.li <- m * log(P + (1 - P) * pnorm(DL, Mu, Sigma)) + (n - m)
    * log(1 - P) -(n - m) * log(Sigma) -
    (n - m) * log(sqrt(2 * pi)) -sum((y - Mu)^2) / 2 / Sigma^2
    return(-log.li)
}

max.iter <- 500
iter <- 0
```r

tol <- 0.0001
logli_1 <- 0
logli_0 <- 1
for(i in 1:max){
  m00 <- rbinom(1, n, para_true[3])
  x <- rlnorm(n - m00, para_true[1], para_true[2])
  y_all <- log(x)
  y <- y_all[y_all >= DL]
  y_org <- y
  m <- m00 + sum(y_all < DL)
  Mu_hat0 <- mean(y)
  Sigma_hat0 <- sd(y)
  P_hat_0 <- m/n
  #2. get estimate of mean and sigma.
  repeat{
    iter <- iter + 1
    Mu_hat <- Mu_hat0
    Sigma_hat <- Sigma_hat0
    P_hat_plus <- pnorm(DL, Mu_hat, Sigma_hat)
    P_hat <- P_hat_0
    if(abs(logli_1 - logli_0) / abs(logli_0) > tol &
      iter < max.iter){
      #3. impute values below DL.
      n_to <- ceiling((n - m) * P_hat_plus /
        (1 - P_hat_plus))
      n_to_impute <- min(c(n_to, m))
      seat <- numeric(n_to_impute)
      tt <- rnorm(1000, Mu_hat, Sigma_hat)
      t <- tt[tt < DL]
      seat <- t[1:n_to_impute]
      logli_0 <- loglike(Mu_hat, Sigma_hat, P_hat_0, y)
      y <- c(y_org, seat)
      Mu_hat0 <- mean(y)
      Sigma_hat0 <- sd(y)
      P_hat_0 <- (n - length(y))/n
    }
  }
```
logli_1 <- loglike(Mu_hat0, Sigma_hat0,
          , P_hat_0, y)
}
else break

### ROS and combined ###
oo <- rep(F, length(y.org))
uu <- rep(T, n_to_impute)
y_test <- c(rep(DL, n_to_impute), y.org)
cri <- c(uu, oo)
myros = ros(y_test, cri)
mean_ROS <- mean(myros)
sd_ROS <- sd(myros)

### Compare ###
m.impt[i] <- Mu_hat0
m.combin[i] <- mean_ROS
sd.impt[i] <- Sigma_hat0
sd.combin[i] <- sd_ROS

Mu_impt = mean(m.impt)
Mu_ros = mean(m.combin)
sd_impt = mean(sd.impt)
sd_ros = mean(sd.combin)

ddd <- data.frame(m.impt, m.combin, index = seq(1, max, by = 1))
p1 <- ggplot(ddd, aes(index)) +
        geom_line(aes(y=m.impt, colour = 'm.impt')) +
        geom_line(aes(y=m.combin, colour = 'm.combin')) +
        geom_hline(yintercept = para_true[1]) +
        ggtitle("Mean comparison between Iterative Imputation and combined method") +
        ylab('Means') +
        scale_shape_discrete(name="") + labs(fill="")

eee <- data.frame(sd.impt, sd.combin, index = seq(1, max, by = 1))
p2 <- ggplot(eee, aes(index)) +
        geom_line(aes(y=sd.impt, colour = 'sd.impt')) +
        geom_line(aes(y=sd.combin, colour = "sd.combin")) +
        geom_hline(yintercept = para_true[2]) +
ggtile('SD\_comparison\_between\_Iterative\_Imputation\_and\_combined\_method') +
  ylab('Standard\_Deviations')

### Draw multiple plots in ggplots, found online ###
multiplot <- function(..., plotlist=NULL, file, cols=1, layout=NULL) {
  require(grid)
  # Make a list from the ... arguments and plotlist
  plots <- c(list(...), plotlist)
  numPlots = length(plots) # If layout is NULL, then use 'cols' to
determine layout
  if (is.null(layout)) {
    # Make the panel
    # ncol: Number of columns of plots
    # nrow: Number of rows needed, calculated from # of cols
    layout <- matrix(seq(1, cols * ceiling(numPlots/cols)),
                     ncol = cols, nrow = ceiling(numPlots/cols))
  }
  if (numPlots==1) {
    print(plots[[1]])
  }
  else {
    # Set up the page
    grid.newpage()
    pushViewport(viewport(layout = grid.layout(nrow(layout), ncol(layout))
                  )))
    # Make each plot, in the correct location
    for (i in 1:numPlots) {
      # Get the i,j matrix positions of the
      # regions that contain this subplot
      matchidx <- as.data.frame(
        which(layout == i, arr.ind = TRUE))
      print(plots[[i]], vp = viewport(layout.pos.row = matchidx$\row,
                                       layout.pos.
                                       col = matchidx$col))
    }
  }
}
multiplot(p1, p2)
APPENDIX D
R Session Information

R version 3.1.1 (2014-07-10)
Platform: x86_64-pc-linux-gnu (64-bit)
locale:
[1] LC_CTYPE=en_US.UTF-8
[2] LC_NUMERIC=C
[3] LC_TIME=en_US.UTF-8
[4] LC_COLLATE=en_US.UTF-8
[5] LC_MONETARY=en_US.UTF-8
[6] LC_MESSAGES=en_US.UTF-8
[7] LC_PAPER=en_US.UTF-8
[8] LC_NAME=C
[9] LC_ADDRESS=C
[10] LC_TELEPHONE=C
[12] LC_IDENTIFICATION=C
attached base packages:
[1] splines stats graphics grDevices utils
[6] datasets methods base parallel
other attached packages:
[1] knitr_1.6.18 dplyr_0.2 plyr_1.8.1
[4] NADA_1.5-6 survival_2.37-7 xtable_1.7-3
[7] ggplot2_1.0.0
loaded via a namespace (and not attached):
[1] assertthat_0.1 colorspace_1.2-4 digest_0.6.4
[4] evaluate_0.5.5 formatR_1.0 grid_3.1.1
[7] gtable_0.1.2 MASS_7.3-34 munsell_0.4.2
[10] parallel_3.1.1 proto_0.3-10 Rcpp_0.11.2
[13] reshape2_1.4 scales_0.2.4 stringr_0.6.2
[16] tools_3.1.1
Bibliography


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