Practical Stats Newsletter for November 2015
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## In-person courses:

## Permutation Tests

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## Applied Environmental Statistics

St. Paul, MN Feb 1-5, $2016 \quad \$ 950$ (it's a bargain! Limited seats available.)
Organized by the Univ. of Minnesota Extension https://drive.google.com/file/d/0B2ukVHiz4qEKYkN5Y213QXNqam8/view?pli=1

## Webinars:

Nondetects And Data Analysis
Spring 2016. A series of 4 webinars. Schedule coming soon.
2. How to Compute Percentiles with Both Greater Thans and Less Thans

Censored data are values known only to be either below (nondetects) or above ('too numerous to count') a threshold. A single number is not available. What statistical methods exist for data that contains both types of censoring in the same dataset-sometimes called "doubly censored"?

Coliform bacteria data in surface water can be doubly censored. Values such as $<1$ and $>2400$ are both present in this example. The question is "How should percentiles -median or the $75^{\text {th }}$ percentile -- be computed with such data?" In the survival analysis sections of commercial software, both parametric and nonparametric methods are available to do that. For the parametric method, first find a reasonable fitting distribution to use as the model. The usual parametric method to compute characteristics is Maximum Likelihood Estimation or MLE, but there is also one using regression on probability plots. The nonparametric method is called Turnbull, and is an extension of the Kaplan-Meier procedure. See Helsel (2012) for more detail on these methods, or sign up for our Spring 2016 webinar series. Here we perform MLE using Minitab ${ }^{\circledR}$ as representative of commercial software capabilities. The survival package in R also has these capabilities.

The data were put into the interval-censored format (see Helsel, 2012) -- two columns are used to represent each value, the low end and high end of values bracketing each observation. Nondetects such as $<1$ have a value of 0 for the low end and the detection limit for the upper end. Greater-thans such as $>2400$ had a value of 2400 for the low end and ' $*$ ', the missing value indicator, for the upper end (there is no upper limit estimated). Detected values of 25 had the value of 25 in both columns. Data in this format can be input to either MLE or Turnbull methods.

Data are input in their original units. Using 0 as the low endpoint of nondetects is fine even for distributions like the lognormal that cannot incorporate true zeros - the interval does not include the lower endpoint value, only approaches it. However, the example data had several "detected zeros", where zero was in both the lower and upper columns. The scientist believed they saw no colonies in the dish. Logs cannot be taken of "detected zeros", but can be incorporated into the analysis in at least three ways. The first (and best in my opinion) is to call them $<1$ s. This simply acknowledges that coliforms could be present in the original sample but at a level difficult to observe with the small aliquot tested. The best fitting distribution is then selected as the model. A second method is to only consider distributions that can incorporate zeros. Power transformations such as the cube or fourth root have the benefit that their transform of a zero value is still zero. Invertebrate biologists often use the fourth root (data^1/4), but the root that most closely approximates a normal distribution should be used. This would be an excellent method (assuming the root-transformed data looked approximately like a normal distribution) if current coliform regulations did not specify the use of logarithms. Third, a three-parameter lognormal distribution could be used to model the data. This distribution adds a constant threshold to the data prior to computing logs, so that $\mathrm{y}=\log (\mathrm{x}-\mathrm{t})$, where t is the threshold. If fitted with a statistics package, the threshold is adjusted to best fit the data. Scientists often arbitrarily add 1 prior to taking logs (so
$t=-1$ ). This may not be the best fitting value, and using different constants will produce different results. Letting the data establish the best fitting constant is a far preferable method to always using $t=-1$. We'll show the results of methods 1 to 3 below.

Method 1. Zeros as $<1$ s.
Distributions were tested to see which best fit the data shape. Using methods for censored data insure that nondetetcts and greater-thans are included in the fitting procedure. Figure 1 shows the fit of data to four common distributions. The Weibull and lognormal distributions, both skewed distributions, fit best as shown by the straight pattern on their probability plots and lowest Anderson-Darling statistics. Censored values on both ends are not plotted as individual points, but they are used to define the percentile position in the dataset for plotting on the graph. For example, in each plot the lowest dot is at a coliform value of just below 1 near the $10^{\text {th }}$ percentile. This is because 225 of the 1028 values ( $22 \%$ ) are nondetects, some of which have detection limits higher than, and some less or equal to, the lowest detected value. We select the lognormal distribution here because it has the best fit (lowest AD statistic), and also because the USEPA recreational bathing beach criteria specify the use of the geometric mean in their regulation. Note that these plots do not substitute a value for nondetects or greater thans. They simply count the proportion of each in determining percentiles for the entire data set, and then plot the detected observations at their computed percentiles.


Figure 1. Fit of data to four common distributions


Figure 2. Lognormal Probability Plot for the Coliform Data
The listed median of 41.295 is the geometric mean. It is the mean of the logarithms (3.72) transformed back to original units (here in natural logs), estimating the median of data in original units. The software also provides a large table of percentiles, along with their $95 \%$ confidence intervals:

|  |  | Standard | 95.0\% Normal CI |  |
| :---: | :---: | :---: | :---: | :---: |
| Percent | Percentile | Error | Lower | Upper |
| 1 | 0.0684499 | 0.0139093 | 0.0459627 | 0.101939 |
| 2 | 0.144941 | 0.0268636 | 0.100793 | 0.208427 |
| 5 | 0.446598 | 0.0712489 | 0.326677 | 0.610541 |
| 10 | 1.21380 | 0.167606 | 0.925996 | 1.59105 |
| 20 | 4.07347 | 0.468935 | 3.25069 | 5.10452 |
| 25 | 6.45247 | 0.694765 | 5.22484 | 7.96853 |
| 30 | 9.75253 | 0.992775 | 7.98854 | 11.9060 |
| 40 | 20.5631 | 1.92442 | 17.1170 | 24.7030 |
| 50 | 41.2950 | 3.68884 | 34.6625 | 49.1965 |
| 60 | 82.9288 | 7.36965 | 69.6725 | 98.7073 |
| 70 | 174.855 | 16.1969 | 145.824 | 209.664 |
| 75 | 264.283 | 25.4887 | 218.763 | 319.273 |
| 80 | 418.629 | 42.6760 | 342.812 | 511.214 |
| 90 | 1404.91 | 170.405 | 1107.65 | 1781.94 |
| 98 | 11765.3 | 1946.50 | 8506.99 | 16271.6 |
| 99 | 24912.7 | 4552.02 | 17413.7 | 35641.2 |
| 99.9 | 203911 | 47618.6 | 129021 | 322269 |

The nonparametric Turnbull method will similarly produce estimates, without assuming the data follow a lognormal or other distributional shape.

Method 2. Transforming data to normality with a power function such as the fourth-root. Raising data to a power less than 1 will transform right-skewed data to something more like a normal distribution, as does the log transformation. The primary benefit of a power transform is that zero values remain zero -- logarithms cannot be computed for a value of zero. Transforming the low and high columns for censored data by the fourth root, for example, a value of $<10$ becomes $<\left(10^{\wedge} 0.25\right)$, or $<1.78$. A censored normal distribution is then fit to the transformed values. Choose the power that most closely produces values that can be fit well by a normal distribution.

The fourth root is often used by biologists, so we start there. The transformed values are not fit very well by a normal distribution (Figure 3). As the exponent of the transform gets closer to zero, the result is more like a log transformation. Using the tenth root ( $x^{\wedge} 1 / 10$ ), a normal distribution is more closely approximated (Figure 4). The percentiles of the tenth-root transformed data are computed and re-transformed by raising them to a power of 10 , resulting in the estimates in original units, below.


Figure 3. Fit of the fourth-root transform to a normal distribution


| Table of Statistics |  |
| :--- | ---: |
| Mean | 1.46904 |
| StDev | 0.473010 |
| Median | 1.46904 |
| IQR | 0.638081 |
| AD $^{+}$ | 1.450 |

Figure 4. Fit of the tenth-root transform to a normal distribution

| Estimated | percentiles in original |  |  |
| ---: | ---: | ---: | ---: | ---: |
| Percent | Percentile | Lower CI | Upper CI |
| 1.0 | 0.0000 | 0.0000 | 0.0002 |
| 2.0 | 0.0009 | 0.0003 | 0.0029 |
| 5.0 | 0.0248 | 0.0114 | 0.0511 |
| 10.0 | 0.2288 | 0.1339 | 0.3803 |
| 20.0 | 1.9847 | 1.3858 | 2.8071 |
| 25.0 | 4.0457 | 2.9574 | 5.4820 |
| 30.0 | 7.3645 | 5.5680 | 9.6669 |
| 40.0 | 19.989 | 15.820 | 25.1218 |
| 50.0 | 46.811 | 38.093 | 57.2854 |
| 60.0 | 102.544 | 84.787 | 123.5798 |
| 70.0 | 222.808 | 185.477 | 266.7712 |
| 75.0 | 334.102 | 278.202 | 399.9154 |
| 80.0 | 514.952 | 428.011 | 617.4756 |
| 90.0 | 1481.37 | 1217.00 | 1796.3537 |
| 95.0 | 3282.29 | 2660.87 | 4031.4070 |
| 98.0 | 7494.90 | 5979.35 | 9347.8186 |
| 99.0 | 12542.0 | 9900.6 | 15801.5754 |
| 99.9 | 46751.4 | 35903.1 | 60465.5588 |

The "detected zeros" plot in Figure 4 as an outlier at zero, and may strongly influence the estimate of a mean. The biggest downside of using the power transform procedure is that computation of a mean in the original units is difficult. You would need the equation for that power (here the $10^{\text {th }}$ root) that modifies the re-transformed median to a value for the mean. Or, the 'smearing estimator' could be used (Helsel and Hirsch, 2002). Means do not translate across scales, while percentiles in transformed units can be directly retransformed back to original units.

Method 3. Using a 3-parameter lognormal and leaving zeros as zeros.
As shown below, the 3-parameter lognormal or other skewed distribution fits the data well (small A-D statistic), and gives similar results to Method 1.


Figure 5. Fit of data to four 3-parameter distributions
The estimates of percentiles with the 3-parameter lognormal are quite similar to Method 1 where zeros were treated as $<1 \mathrm{~s}$ and a standard 2-parameter lognormal was fit to the data. An abbreviated table for the 3-parameter model gives results for several percentiles:

| Table of (selective) | Percentiles |  |  |  |
| ---: | ---: | ---: | ---: | ---: |
| Standard | 95.0\% Normal CI |  |  |  |
| Percent | Percentile | Error | Lower | Upper |
| 10 | 0.890139 | 0.149142 | 0.597826 | 1.18245 |
| 25 | 5.28919 | 0.666681 | 3.98252 | 6.59586 |
| 50 | 38.1749 | 3.70755 | 30.9082 | 45.4415 |
| 75 | 275.375 | 28.5325 | 219.452 | 331.298 |
| 90 | 1630.25 | 222.189 | 1194.77 | 2065.73 |
| 95 | 4725.63 | 766.211 | 3223.88 | 6227.38 |
| 99 | 34792.0 | 7531.71 | 20030.1 | 49553.9 |
| 99.9 | 326076 | 91874.9 | 146004 | 506147 |

The problem with simply adding a 1 to data for the 3-parameter threshold, as is commonly done by some biologists, is that the choice is arbitrarily made. It will likely not fit the data as well as the Method 3 solution, and so produce less accurate estimates of means and percentiles. Let the data select the threshold instead.

Conclusion: the three methods produce estimates of medians that are within the $95 \%$ confidence intervals of the other methods. Methods 1 and 3 estimates of medians are
geometric means, meeting regulatory guidelines. The power transform (Method 2) estimate of median does not use logarithms, so is not a geometric mean.

| Method: | 1. 0s as <s | 2. Power transform | 3. 3-param dist |
| :--- | ---: | ---: | ---: | ---: |
| Estimate of | 41.2950 | 46.811 | 38.1749 |

Using one of the three methods shown here to compute descriptive statistics for doublycensored data should be the norm in environmental analysis. Perhaps someday they will. Learn more about methods for censored data in our upcoming 2016 webinars.
3. Updates for Minitab macros

We provide free Minitab macros online for methods in the textbook Statistics for Censored Environmental Data using Minitab and $R$ (the NADA macros for censored data), and for routines for general environmental statistics to students who take our Applied Environmental Statistics course. Minitab altered some of its commands in its latest version (17.2), changing how they work from that in 17.1, which disrupted the use of a few of our macros. If you are using our trend analysis macros from the Applied Environmental Statistics course with Minitab 17.2, email us at ask@practicalstats.com (stating the time and place you took our AES class) and we'll send you the macros that produce correct plots with 17.2. The freely-available NADA macros on our Downloads web page http://practicalstats.com/downloads/
work with both 17.1 and 17.2 of Minitab. We regret the hassles, but changes to commands like this usually occur only in major revisions of software. We updated our macros when version 17 was released. We were surprised when these changes were included in this 'minor' recent 17.2 update of Minitab.
'Til next time,
Practical Stats
-- Make sense of your data

