GUIDANCE FOR
DATA QUALITY ASSESSMENT

Practical Methods for
Data Analysis

EPA QA/G-9

QA97 Version
4.6 TRANSFORMATIONS

Most statistical tests and procedures contain assumptions about the data to which they will be applied. For example, some common assumptions are that the data are normally distributed; variance components of a statistical model are additive; two independent data sets have equal variance; and a data set has no trends over time or space. If the data do not satisfy such assumptions, then the results of a statistical procedure or test may be biased or incorrect. Fortunately, data that do not satisfy statistical assumptions may often be converted or transformed mathematically into a form that allows standard statistical tests to perform adequately.

4.6.1 Types of Data Transformations

Any mathematical function that is applied to every point in a data set is called a transformation. Some commonly used transformations include:

Logarithmic ($\log X$ or $\ln X$): This transformation may be used when the original measurement data follow a lognormal distribution or when the variance at each level of the data is proportional to the square of the mean of the data points at that level. For example, if the variance of data collected around 50 ppm is approximately 250, but the variance of data collected around 100 ppm is approximately 1000, then a logarithmic transformation may be useful. This situation is often characterized by having a constant coefficient of variation (ratio of standard deviation to mean) over all possible data values.

The logarithmic base (for example, either natural or base 10) needs to be consistent throughout the analysis. If some of the original values are zero, it is customary to add a small quantity to make the data value non-zero as the logarithm of zero does not exist. The size of the small quantity depends on the magnitude of the non-zero data and the consequences of potentially erroneous inference from the resulting transformed data. As a working point, a value of one tenth the smallest non-zero value could be selected. It does not matter whether a natural (ln) or base 10 (log) transformation is used because the two transformations are related by the expression $\ln(X) = 2.303 \log(X)$. Directions for applying a logarithmic transformation with an example are given in Box 4.6-1.

Square Root ($\sqrt{X}$): This transformation may be used when dealing with small whole numbers, such as bacteriological counts, or the occurrence of rare events, such as violations of a standard over the course of a year. The underlying assumption is that the original data follow a Poisson-like distribution in which case the mean and variance of the data are equal. It should be noted that the square root transformation overcorrects when very small values and zeros appear in the original data. In these cases, $\sqrt{X+1}$ is often used as a transformation.

Inverse Sine (Arcsine $X$): This transformation may be used for binomial proportions based on count data to achieve stability in variance. The resulting transformed data are expressed in radians (angular degrees). Special tables must be used to transform the proportions into degrees.

Box-Cox Transformations: This transformation is a complex power transformation that takes the original data and raises each data observation to the power lambda ($\lambda$). A logarithmic transformation is a special case of the Box-Cox transformation. The rationale is to find $\lambda$ such that the transformed data have the best possible additive model for the variance structure, the errors are normally
distributed, and the variance is as constant as possible over all possible concentration values. The Maximum Likelihood technique is used to find $\lambda$ such that the residual error from fitting the theorized model is minimized. In practice, the exact value of $\lambda$ is often rounded to a convenient value for ease in interpretation (for example, $\lambda = -1.1$ would be rounded to -1 as it would then have the interpretation of a reciprocal transform). One of the drawbacks of the Box-Cox transformation is the difficulty in physically interpreting the transformed data.

### 4.6.2 Reasons for Data Transformations

By transforming the data, assumptions that are not satisfied in the original data can be satisfied by the transformed data. For instance, a right-skewed distribution can be transformed to be approximately Gaussian (normal) by using a logarithmic or square-root transformation. Then the normal-theory procedures can be applied to the transformed data. If data are lognormally distributed, then apply procedures to logarithms of the data. However, selecting the correct transformation may be difficult. If standard transformations do not apply, it is suggested that the data user consult a statistician.

Another important use of transformations is in the interpretation of data collected under conditions leading to an Analysis of Variance (ANOVA). Some of the key assumptions needed for analysis (for example, additivity of variance components) may only be satisfied if the data are transformed suitably. The selection of a suitable transformation depends on the structure of the data collection design; however, the interpretation of the transformed data remains an issue.

While transformations are useful for dealing with data that do not satisfy statistical assumptions, they can also be used for various other purposes. For example, transformations are useful for consolidating data that may be spread out or that have several extreme values. In addition, transformations can be used to derive a linear relationship between two variables, so that linear regression analysis can be applied. They can also be used to efficiently estimate quantities such as the mean and variance of a lognormal distribution. Transformations may also make the analysis of data easier by changing the scale into one that is more familiar or easier to work with.

Once the data have been transformed, all statistical analysis must be performed on the transformed data. No attempt should be made to transform the data back to the original form because this can lead to biased estimates. For example, estimating quantities such as means, variances, confidence limits, and regression coefficients in the transformed scale typically leads to biased estimates when transformed back into original scale. However, it may be difficult to understand or apply results of statistical analysis expressed in the transformed scale. Therefore, if the transformed data do not give noticeable benefits to the analysis, it is better to use the original data. There is no point in working with transformed data unless it adds value to the analysis.
Let \( X_1, X_2, \ldots, X_n \) represent the \( n \) data points. To apply a transformation, simply apply the transforming function to each data point. When a transformation is implemented to make the data satisfy some statistical assumption, it will need to be verified that the transformed data satisfy this assumption.

**Example: Transforming Lognormal Data**

A logarithmic transformation is particularly useful for pollution data. Pollution data are often skewed, thus the log-transformed data will tend to be symmetric. Consider the data set shown below with 15 data points. The frequency plot of this data (below) shows that the data are possibly lognormally distributed. If any analysis performed with this data assumes normality, then the data may be logarithmically transformed to achieve normality. The transformed data are shown in column 2. A frequency plot of the transformed data (below) shows that the transformed data appear to be normally distributed.

<table>
<thead>
<tr>
<th>Observed</th>
<th>Transformed</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X )</td>
<td>( \ln(X) )</td>
</tr>
<tr>
<td>0.22</td>
<td>-1.51</td>
</tr>
<tr>
<td>3.48</td>
<td>1.25</td>
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<tr>
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<tr>
<td>2.53</td>
<td>0.93</td>
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<tr>
<td>1.11</td>
<td>0.10</td>
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<td>-1.11</td>
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<td>1.64</td>
<td>0.50</td>
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<tr>
<td>1.37</td>
<td>0.31</td>
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</table>

<table>
<thead>
<tr>
<th>Observed</th>
<th>Transformed</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X )</td>
<td>( \ln(X) )</td>
</tr>
<tr>
<td>0.47</td>
<td>-0.76</td>
</tr>
<tr>
<td>0.67</td>
<td>-0.40</td>
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<td>-0.29</td>
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<td>0.80</td>
<td>-0.51</td>
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<td>0.99</td>
<td>-0.01</td>
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<tr>
<td>0.90</td>
<td>-0.11</td>
</tr>
<tr>
<td>0.28</td>
<td>-1.35</td>
</tr>
</tbody>
</table>
4.7 VALUES BELOW DETECTION LIMITS

Data generated from chemical analysis may fall below the detection limit (DL) of the analytical procedure. These measurement data are generally described as not detected, or nondetects, (rather than as zero or not present) and the appropriate limit of detection is usually reported. In cases where measurement data are described as not detected, the concentration of the chemical is unknown although it lies somewhere between zero and the detection limit. Data that includes both detected and non-detected results are called censored data in the statistical literature.

There are a variety of ways to evaluate data that include values below the detection limit. However, there are no general procedures that are applicable in all cases. Some general guidelines are presented in Table 4.7-1. Although these guidelines are usually adequate, they should be implemented cautiously.

<table>
<thead>
<tr>
<th>Percentage of Nondetects</th>
<th>Section</th>
<th>Statistical Analysis Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 15%</td>
<td>4.7.1</td>
<td>Replace nondetects with DL/2, DL, or a very small number, e.g. 0.1</td>
</tr>
<tr>
<td>15% - 50%</td>
<td>4.7.2</td>
<td>Trimmed mean, Cohen's adjustment, Winsorized mean and standard deviation.</td>
</tr>
<tr>
<td>&gt; 50% - 90%</td>
<td>4.7.3</td>
<td>Use tests for proportions (section 3.2.2)</td>
</tr>
</tbody>
</table>

Table 4.7-1. Guidelines for Analyzing Data with Nondetects

All of the suggested procedures for analyzing data with nondetects depend on the amount of data below the detection limit. For relatively small amounts below detection limit values, replacing the nondetects with a small number and proceeding with the usual analysis may be satisfactory. For moderate amounts of data below the detection limit, a more detailed adjustment is appropriate. In situations where relatively large amounts of data below the detection limit exist, one may need only to consider whether the chemical was detected as above some level or not. The interpretation of small, moderate, and large amounts of data below the DL is subjective. Table 4.7-1 provides percentages to assist the user in evaluating their particular situation. However, it should be recognized that these percentages are not hard and fast rules, but should be based on judgement.

In addition to the percentage of samples below the detection limit, sample size influences which procedures should be used to evaluate the data. For example, the case where 1 sample out of 4 is not detected should be treated differently from the case where 25 samples out of 100 are not detected. Therefore, this guidance suggests that the data analyst consult a statistician for the most appropriate way to evaluate data containing values below the detection level.

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4.7.1 Less than 15% Nondetects - Substitution Methods

If a small proportion of the observations are not detected, these may be replaced with a small number, usually the detection limit divided by 2 (DL/2), and the usual analysis performed. As a guideline, if 15% or fewer of the values are not detected, replace them with the method detection limit divided by two and proceed with the appropriate analysis using these modified values. If simple substitution of values below the detection limit is proposed when more than 15% of the values are reported as not detected, consider using nonparametric methods or a test of proportions to analyze the data. If a more accurate method is to be considered, see Cohen's Method (section 4.7.2.1).

4.7.2 Between 15-50% Nondetects

4.7.2.1 Cohen's Method

Cohen's method provides adjusted estimates of the sample mean and standard deviation that accounts for data below the detection level. The adjusted estimates are based on the statistical technique of maximum likelihood estimation of the mean and variance so that the fact that the nondetects are below the limit of detection but may not be zero is accounted for. The adjusted mean and standard deviation can then be used in the parametric tests described in Chapter 3 (e.g., the one sample t-test of section 3.2.1.1). However, if more than 50% of the observations are not detected, Cohen's method should not be used. In addition, this method requires that the data without the nondetects be normally distributed and the detection limit is always the same. Directions for Cohen's method are contained in Box 4.7-1; an example is given in Box 4.7-2.

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**Box 4.7-1: Directions for Cohen's Method**

Let $X_1, X_2, \ldots, X_n$ represent the $n$ data points with the first $m$ values representing the data points above the detection limit (DL). Thus, there are $(n-m)$ data points are below the DL.

1. **STEP 1:** Compute the sample mean $\bar{X}_d$ from the data above the detection limit: $\bar{X}_d = \frac{1}{m} \sum_{i=1}^{m} X_i$

2. **STEP 2:** Compute the sample variance $s^2_d$ from the data above the detection limit:

$$s^2_d = \frac{\sum_{i=1}^{m} X_i^2 - \frac{1}{m} \left( \sum_{i=1}^{m} X_i \right)^2}{m-1}$$

3. **STEP 3:** Compute $h = \frac{(n-m)}{n}$ and $\gamma = \frac{s^2_d}{(\bar{X}_d - DL)^2}$

4. **STEP 4:** Use $h$ and $\gamma$ in Table A-10 of Appendix A to determine $\hat{h}$ and $\hat{\gamma}$. For example, if $h = 0.4$ and $\gamma = 0.30$, then $\hat{h} = 0.0713$. If the exact value of $h$ and $\gamma$ do not appear in the table, use double linear interpolation (Box 4.7-3) to estimate.

5. **STEP 5:** Estimate the corrected sample mean $\bar{X}$ and sample variance, $\hat{s}$, to account for the data below the detection limit, as follows:

$$\bar{X} = \bar{X}_d - \hat{\lambda}(\bar{X}_d - DL)$$

and

$$\hat{s} = s^2_d + \hat{\lambda}(\bar{X}_d - DL)^2$$
Box 4.7-2: An Example of Cohen's Method

Sulfate concentrations were measured for 24 data points. The detection limit was 1,450 mg/L and 3 of the 24 values were below the detection level. The 24 values are: 1850, 1760, <1450 (ND), 1710, 1575, 1475, 1780, 1790, 1780, <1450 (ND), 1790, 1800, <1450 (ND), 1800, 1840, 1820, 1860, 1780, 1800, 1900, 1770, 1790, 1780 mg/L. Cohen's Method will be used to adjust the sample mean for use in a t-test to determine if the mean is greater than 1600 mg/L.

STEP 1: The sample mean of the m = 22 values above the detection level is \( \bar{X}_d = 1771.9 \)

STEP 2: The sample variance of the 21 quantified values is \( s = 8593.69 \).

STEP 3: \( h = (24 - 21)/24 = 0.125 \) and \( \gamma = 8593.69/(1771.9 - 1450) = 0.083 \)

STEP 4: Table A-10 of Appendix A was used for \( h = 0.125 \) and \( \gamma = 0.083 \) to find the value of \( \lambda \). Since the table does not contain these entries exactly, double linear interpolation was used to estimate \( \lambda = 0.149839 \) (see Box 4.7-3).

STEP 5: The adjusted sample mean and variance are then estimated as follows:

\[
\bar{X} = 1771.9 - 0.149839(1771.9 - 1450) = 1723.67 \quad \text{and} \quad s^2 = 8593.69 + 0.149839(1771.9 - 1450)^2 = 24119.95
\]

Box 4.7-3: Double Linear Interpolation

The details of the double linear interpolation are provided to assist in the use of Table A-10 of Appendix A. The desired value for \( \lambda \) corresponds to \( \gamma = 0.083 \) and \( h = 0.125 \) from Box 4.7-2, Step 3. The values from Table A-10 for interpolation are:

\[
\begin{array}{ccc}
\gamma & h = 0.10 & h = 0.15 \\
0.05 & 0.11431 & 0.17925 \\
0.10 & 0.15040 & 0.18479
\end{array}
\]

There are 0.05 units between 0.10 and 0.15 on the h-scale and 0.025 units between 0.10 and 0.125. Therefore, the value of interest lies (0.025/0.05)100% = 50% of the distance along the interval between 0.10 and 0.15. To linearly interpolate between tabulated values on the h axis for \( \gamma = 0.05 \), the range between the values must be calculated, 0.17925 - 0.11431 = 0.06494; the value that is 50% of the distance along the range must be computed, 0.06494 x 0.50 = 0.03247; and then that value must be added to the lower point on the tabulated values, 0.11431 + 0.03247 = 0.14678. Similarly for \( \gamma = 0.10 \), 0.18479 - 0.11804 = 0.06675, 0.06675 x 0.50 = 0.033375, and 0.11804 + 0.033375 = 0.151415.

On the \( \gamma \)-axis there are 0.033 units between 0.05 and 0.083 and there are 0.05 units between 0.05 and 0.10. The value of interest (0.083) lies (0.033/0.05 x 100) = 66% of the distance along the interval between 0.05 and 0.10, so 0.151415 - 0.14678 = 0.004635, 0.04635 x 0.66 = 0.003059. Therefore,

\[
\lambda = 0.14678 + 0.003059 = 0.149839.
\]
4.7.2.2 Trimmed Mean

Trimming discards the data in the tails of a data set in order to develop an unbiased estimate of the population mean. For environmental data, nondetects usually occur in the left tail of the data so trimming the data can be used to adjust the data set to account for nondetects when estimating a mean. Developing a 100p% trimmed mean involves trimming p% of the data in both the lower and the upper tail. Note that p must be between 0 and .5 since p represents the portion deleted in both the upper and the lower tail. After np of the largest values and np of the smallest values are trimmed, there are n(1-2p) data values remaining. Therefore, the proportion trimmed is dependent on the total sample size (n) since a reasonable amount of samples must remain for analysis. For approximately symmetric distributions, a 25% trimmed mean (the midmean) is a good estimator of the population mean. However, environmental data are often skewed (non-symmetric) and in these cases a 15% trimmed mean performance may be a good estimator of the population mean. It is also possible to trim the data only to replace nondetects. For example, if 3% of the data are below the detection limit, a 3% trimmed mean could be used to estimate the population mean. Directions for developing a trimmed mean are contained in Box 4.7-4 and an example is given in Box 4.7-5. A trimmed variance is rarely calculated and is of limited use.

**Box 4.7-4: Directions for Developing a Trimmed Mean**

Let \( X_1, X_2, \ldots, X_n \) represent the n data points. To develop a 100p% trimmed mean (0 < p < 0.5):

**STEP 1:** Let \( t \) represent the integer part of the product np. For example, if \( p = .25 \) and \( n = 17 \), then \( np = (.25)(17) = 4.25 \), so \( t = 4 \).

**STEP 2:** Delete the \( t \) smallest values of the data set and the \( t \) largest values of the data set.

**STEP 3:** Compute the arithmetic mean of the remaining \( n - 2t \) values:

\[
\bar{X} = \frac{1}{n-2t} \sum_{i=1}^{n-2t} X_i
\]

This value is the estimate of the population mean.

**Box 4.7-5: An Example of the Trimmed Mean**

Sulfate concentrations were measured for 24 data points. The detection limit was 1,450 mg/L and 3 of the 24 values were below this limit. The 24 values listed in order from smallest to largest are: 1,450 (ND), 1,450 (ND), 1,475, 1,575, 1,710, 1,760, 1,770, 1,780, 1,780, 1,790, 1,790, 1,800, 1,800, 1,820, 1,840, 1,850, 1,860, 1,900 mg/L. A 15% trimmed mean will be used to develop an estimate of the population mean that accounts for the 3 nondetects.

**STEP 1:** Since \( np = (24)(.15) = 3.6 \), \( t = 3 \).

**STEP 2:** The 3 smallest values of the data set and the 3 largest values of the data set were deleted. The new data set is: 1,475, 1,575, 1,710, 1,760, 1,770, 1,780, 1,780, 1,790, 1,790, 1,790, 1,800, 1,800, 1,800, 1,820, 1,840, 1,850, 1,860, 1,900 mg/L.

**STEP 3:** Compute the arithmetic mean of the remaining \( n-2t \) values:

\[
\bar{X} = \frac{1}{24-(2)(3)}(1475 + \ldots + 1840) = 1755.56
\]

Therefore, the 15% trimmed mean is 1755.56 mg/L, which is an estimate of the population mean.
4.7.2.3 Winsorized Mean and Standard Deviation

Winsorizing replaces data in the tails of a data set with the next most extreme data value. For environmental data, nondetects usually occur in the left tail of the data. Therefore, winsorizing can be used to adjust the data set to account for nondetects. The mean and standard deviation can then be computed on the new data set. Directions for winsorizing data (and revising the sample size) are contained in Box 4.7-6 and an example is given in Box 4.7-7.

**Box 4.7-6: Directions for Developing a Winsorized Mean and Standard Deviation**

Let $X_1, X_2, \ldots, X_n$ represent the $n$ data points and $m$ represent the number of data points above the detection limit (DL), and hence $n-m$ below the DL.

**STEP 1:** List the data in order from smallest to largest, including nondetects. Label these points $X_{(1)}, X_{(2)}, \ldots, X_{(n)}$ (so that $X_{(1)}$ is the smallest, $X_{(2)}$ is the second smallest, and $X_{(n)}$ is the largest).

**STEP 2:** Replace the $n-m$ nondetects with $X_{(m+1)}$ and replace the $n-m$ largest values with $X_{(n-m)}$.

**STEP 3:** Using the revised data set, compute the sample mean $\bar{X}$, and the sample standard deviation, $s$:

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

and

$$s = \sqrt{\frac{\left(\sum_{i=1}^{n} X_i^2\right) - n \bar{X}^2}{n-1}}$$

**STEP 4:** The Winsorized mean $\bar{X}_w$ is equal to $\bar{X}$. The Winsorized standard deviation is $s_w = \frac{s(n-1)}{(2m-n-1)}$.

**Box 4.7-7: An Example of a Winsorized Mean and Standard Deviation**

Sulfate concentrations were measured for 24 data points. The detection limit was 1,450 mg/L and 3 of the 24 values were below the detection level. The 24 values listed in order from smallest to largest are: < 1450 (ND), < 1450 (ND), < 1450 (ND), 1475, 1575, 1710, 1760, 1760, 1760, 1780, 1780, 1780, 1790, 1790, 1790, 1800, 1800, 1800, 1820, 1840, 1840, 1840, 1840, 1840 mg/L.

**STEP 1:** The data above are already listed from smallest to largest. There are $n=24$ samples, 21 above DL, and $n-m=3$ nondetects.

**STEP 2:** The 3 nondetects were replaced with $X_{(1)}$ and the 3 largest values were replaced with $X_{(n-3)}$. The resulting data set is: 1475, 1475, 1475, 1475, 1575, 1710, 1760, 1760, 1760, 1770, 1780, 1780, 1780, 1780, 1780, 1780, 1790, 1790, 1790, 1800, 1800, 1800, 1800, 1800, 1820, 1840, 1840, 1840, 1840 mg/L.

**STEP 3:** For the new data set, $\bar{X} = 1731$ mg/L and $s = 128.52$ mg/L.

**STEP 4:** The Winsorized mean $\bar{X}_w = 1731$ mg/L. The Winsorized sample standard deviation is:

$$s_w = \frac{128.52(24 - 1)}{2(21) - 24 - 1} = 173.88$$
4.7.3 Greater than 50% Nondetects - Test of Proportions

If more than 50% of the data are below the detection limit but at least 10% of the observations are quantified, tests of proportions may be used to test hypotheses using the data. Thus, if the parameter of interest is a mean, consider switching the parameter of interest to some percentile greater than the percent of data below the detection limit. For example, if 67% of the data are below the DL, consider switching the parameter of interest to the 75\textsuperscript{th} percentile. Then the method described in 3.2.2 can be applied to test the hypothesis concerning the 75\textsuperscript{th} percentile. It is important to note that the tests of proportions may not be applicable for composite samples. In this case, the data analyst should consult a statistician before proceeding with analysis.

If very few quantified values are found, a method based on the Poisson distribution may be used as an alternative approach. However, with a large proportion of nondetects in the data, the data analyst should consult with a statistician before proceeding with analysis.
### TABLE A-10: VALUES OF THE PARAMETER $\hat{\sigma}$ FOR COHEN'S ESTIMATES ADJUSTING FOR NONDETECTED VALUES

<table>
<thead>
<tr>
<th>$v$</th>
<th>.01</th>
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<th>.03</th>
<th>.04</th>
<th>.05</th>
<th>.06</th>
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<th>.09</th>
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### Table Entry Details

- Values are rounded to three decimal places.
- The table shows the parameter $\hat{\sigma}$ for various values of $v$ and $h$.
- Each row represents a different $v$ value, with columns for $h$ values ranging from 0.25 to 0.90 in increments of 0.05.
- The data is extracted from the EPA QA/G-9 QA00 Version A-18, Final July 2000.