U.S. Environmental
Protection
Agency

ProUCL Version 3.0 Statistical Software to Compute Upper Confidence Limits of the Unknown Population Mean

Introduction

The EPA Technical Support Center (TSC) in Las Vegas has developed ProUCL Version 3.0 software to support risk assessment and cleanup decisions at contaminated sites. Risk assessments, exposure evaluations, and cleanup decisions are often made based upon the mean concentrations of the contaminants of potential concern (COPCs). The true population mean concentrations of the COPCs at a contaminated site are often unknown, and are frequently estimated by the respective sample means based upon the data collected from the site under investigation. In order to address the uncertainties associated with the estimates of the true unknown mean concentrations of the COPCs, appropriate 95% upper confidence limits (UCLs) of the respective unknown means are frequently used in many environmental applications. The computation of an appropriate 95% UCL of practical merit depends upon the data distribution and the skewness associated with the data set under study. ProUCL can be used to compute an appropriate UCL of the unknown population mean using a discernible probability distribution (e.g., normal, lognormal, gamma) and/or a suitable non-parametric distribution-free method.

The Need for UCL Computational Software

A 95% UCL of the unknown population arithmetic mean, $:_1$*, of a COPC is often used in environmental applications to:*

- Estimate the exposure point concentration (EPC) term,
- Support risk assessment applications,
- Determine the attainment of cleanup standards,
- Estimate background level mean contaminant concentrations, or
- Compare the soil mean concentrations with site-specific soil screening levels.

In December 2002, the EPA revised the Guidance Document to Calculate the Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites (OSWER 9285.670). ProUCL, Version 3.0 consists of all parametric and non-parametric UCL computation methods as described in this revised EPA UCL Guidance Document.

ProUCL also computes the UCLs of the unknown population mean based upon the positively skewed gamma distribution, which is often better suited to model environmental data sets than the lognormal distribution. For positively skewed data sets, the default use of a lognormal distribution often results in impractically large UCLs, especially when the data sets are small. This is also illustrated in the example included in this fact sheet. In order to obtain accurate and stable UCLs of practical merit, other distributions such as a gamma distribution should be used to model positively skewed data sets. ProUCL, Version 3.0 has procedures to perform the gamma goodness-of-fit test and to compute UCLs of the population mean based upon gamma distributed data sets.

ProUCL Version 3.0 Capabilities

Performs Goodness-of-Fit Tests to Assess Normality/Lognormality of a Data Set Using:

- Informal graphical quantile-quantile (Q-Q) plot (normal probability plot) and histogram.
- Shapiro - Wilk test: to be used when the sample size is less than or equal to 50.

- Lilliefors test: to be used when the sample size is large (e.g., greater than 50).

Performs Goodness-of-Fit Test for Gamma Distribution Using:

- Informal graphical quantile-quantile (Q-Q) plot (gamma probability plot) and histogram.
- Kolmogorov-Smirnov test: available for sample sizes in the range 4-2500 (critical values computed using Monte Carlo simulations) and values of the estimated shape parameter, k in the interval [0.01, 100.0].
- Anderson-Darling test: available for sample sizes in the range 4-2500 (critical values computed using Monte Carlo simulations) and values of the estimated shape parameter, k in the interval [0.01, 100.0].

Computes the Estimates of Relevant Population Parameters:

- Computes all relevant descriptive summary statistics for raw and log-transformed data.
- Computes the maximum likelihood (ML) and minimum variance unbiased (MVU) estimates of the various population parameters such as the mean, standard deviation, quantiles, coefficient of variation, skewness, and also the MLEs of the shape parameter k and scale parameter **2** of a gamma distribution.

Computes Five Parametric UCLs:

A (1-") 100% (for all values of the confidence coefficient, (1-") in the interval [0.5, 1.0] including 0.95 except for a couple of methods) UCL of the unknown population mean, $:_1$, using five (5) parametric methods for normal, lognormal, and gamma distributions. The five parametric UCL computation methods incorporated in ProUCL are:

1. Student's-t UCL: to be used for normally (or at least approximately normally) distributed data sets. Student's-t UCL is available for all confidence coefficients, (1-") in the interval [0.5, 1.0].
2. Approximate Gamma UCL: to be used for gamma distributed data and is typically used when k hat (ML estimate of the shape parameter, k) is greater than or equal to 0.5. Approximate gamma UCL is available for all confidence coefficients (1-") in the interval [0.5, 1.0].
3. Adjusted Gamma UCL: to be used for gamma distributed data sets and should be used when k hat is greater than 0.1 and less than 0.5. Adjusted gamma UCL is available only for three confidence coefficients: 0.90, 0.95, and 0.99.
4. H-UCL based upon Land's H-statistic: to be used for lognormally distributed data sets. In ProUCL, H-UCL is available only for two confidence coefficients: 0.90 and 0.95. ProUCL can compute H-UCL for samples of size up to 2001.

   Caution: For highly skewed data sets, H-UCL should be avoided as the H-statistic often results in unrealistically large, impractical and unusable H-UCL values. ProUCL provides warning messages and recommends the use of alternative UCLs for such highly skewed lognormally distributed data sets.

5. Chebyshev (MVUE) UCL: to be used for lognormally distributed data sets. This UCL computation method uses the MVU estimates of the standard deviation of the mean and of other parameters of a lognormal distribution. Chebyshev (MVUE) UCL is available for all confidence coefficients, (1-") in the interval [0.5, 1.0].

Computes Ten Non-parametric UCLs Based Upon Bootstrap Procedures and Chebyshev Inequality:

These UCLs can be computed for all confidence coefficients, (1-") in the interval [0.5, 1.0].

1. Central Limit Theorem (CLT) based UCL: to be used when the sample size is large.
2. Adjusted-CLT (Adjusted for skewness) UCL: to be used for skewed data sets of large sizes.

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3. Modified-t statistic (Adjusted for skewness) based UCL: may be used for mildly skewed data.
4. Chebyshev (Mean, Sd) UCL: based upon the sample mean and standard deviation, Sd.
5. Jackknife UCL for mean (same as Student's-t UCL).
6. Standard Bootstrap UCL.
7. Bootstrap-t UCL.
8. Hall's Bootstrap UCL.
9. Percentile Bootstrap UCL.
10. Bias-corrected accelerated (BCA) Bootstrap UCL.

As mentioned before, for most of the UCL computation methods, ProUCL can compute the UCLs for all confidence coefficients, (1-**"**) in the interval [0.5, 1.0]. However, since in most environmental applications (e.g., estimation of EPC), a 95% UCL of mean is used, therefore, ProUCL makes recommendations for the most appropriate 95% UCL(s) which may be used to estimate the unknown population mean concentration. The basis and theoretical justification for these recommendations can be found in the references listed in this fact sheet.

Example: An example illustrating the importance of the use of gamma distribution based UCL computation methods is discussed next. Consider a simulated positively skewed data set of size 20: 0.0086284103, 16.18078972, 7.334853523, 6.12856E-005, 1.756500498, 1.394359005, 23.41857632, 7.516539628, 0.8594623274, 39.06134332, 17.97357103, 114.885481, 9.251610362, 39.44123801, 71.64271025, 6.271065467, 0.9742964478, 0.1558884758, 0.4817911951, 0.0065875373. This data set was generated from a gamma distribution with the shape parameter, k = 0.25 and the scale parameter, **2** = 50. This can be seen from the two enclosed figures, a histogram and the associated gamma probability plot generated by ProUCL. This data set does not follow a normal or a lognormal distribution. However, using the default lognormal (as some times done in practice for positively skewed environmental data sets) distribution, one will get an unrealistically large 95% H-UCL (=498390.58) as given in the enclosed output generated by ProUCL. This in turn will lead to the use of the maximum value (=114.885) as an estimate of the EPC term – a practice often used in environmental applications. However, since the data set does follow a gamma distribution, therefore, an appropriate and more accurate estimate of the EPC term (representing the average exposure over a long period of time over an exposure area) will be obtained by using the 95% UCL (=45.067) based upon the gamma distribution as recommended in the enclosed output table generated by ProUCL, Version 3.0.

Summary

ProUCL computes parametric UCLs based upon a normal, lognormal, and a gamma distribution. ProUCL also computes UCLs using several non-parametric methods. The computation of an appropriate UCL of the unknown population mean depends upon the data distribution, therefore goodness-of-fit tests need to be performed to assess the data distribution before using one of the UCL computation methods available in ProUCL. Based upon an appropriate data distribution and the associated skewness, ProUCL provides recommendations about one or more 95% UCL computation methods that may be used to estimate the unknown mean concentration of a COPC.

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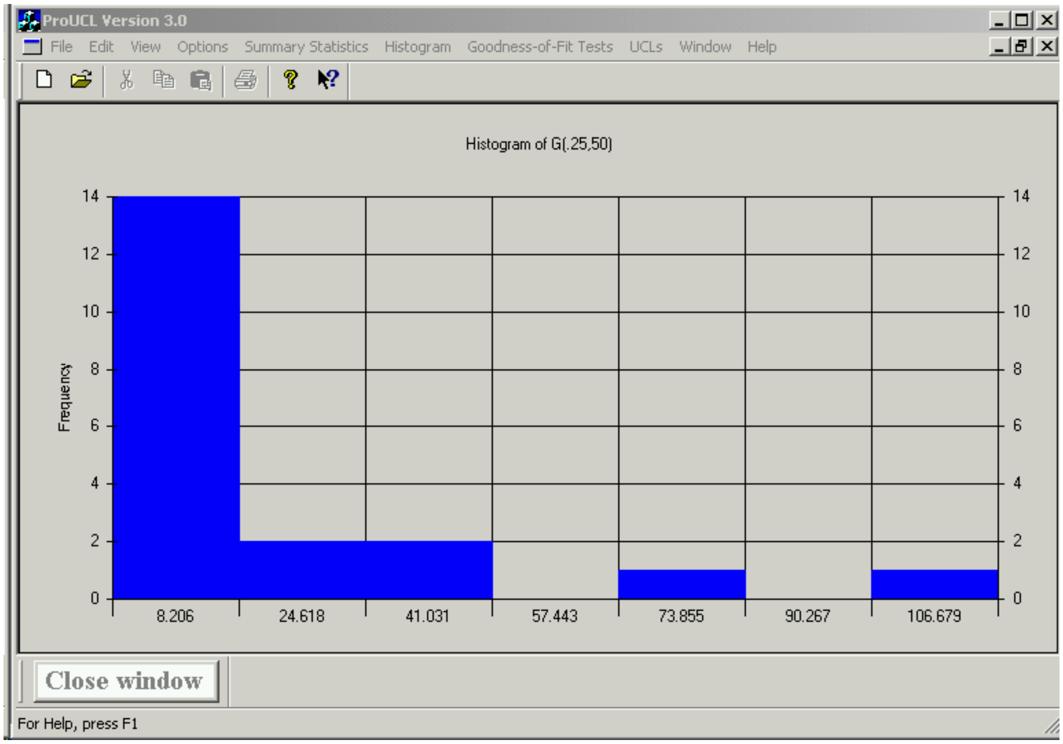
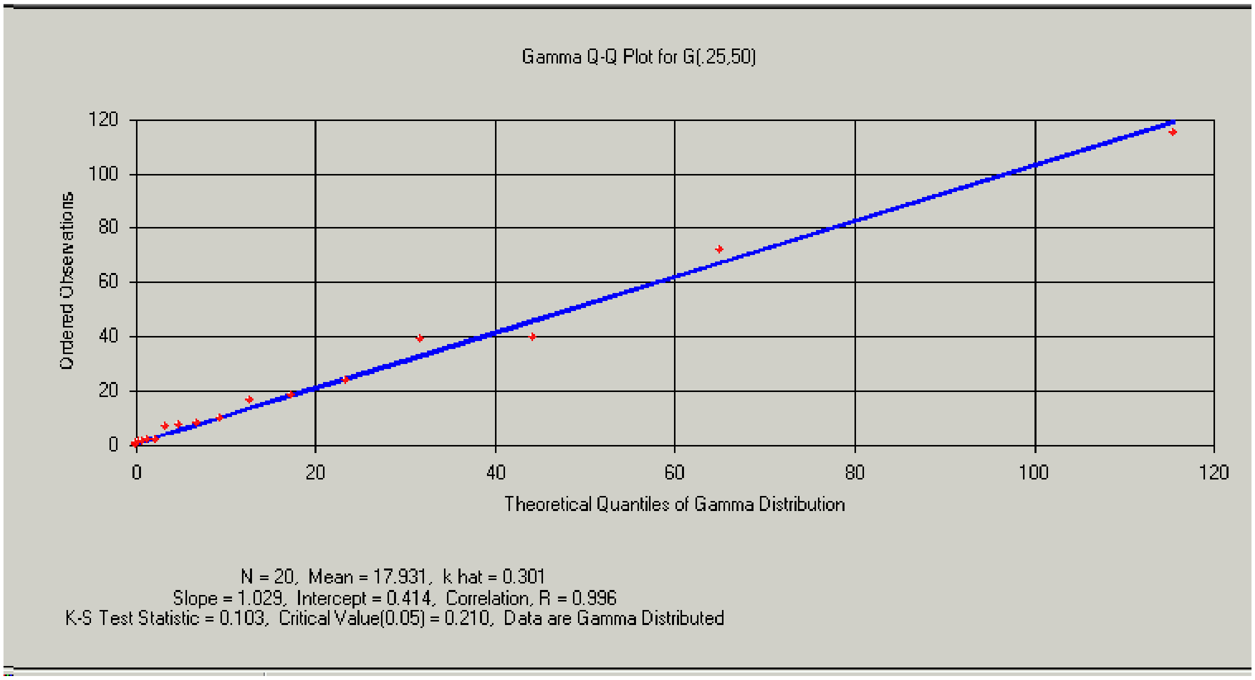


For Help, press F1



N = 20, Mean = 17.931, k hat = 0.301
Slope = 1.029, Intercept = 0.414, Correlation, R = 0.996
K-S Test Statistic = 0.103, Critical Value(0.05) = 0.210, Data are Gamma Distributed

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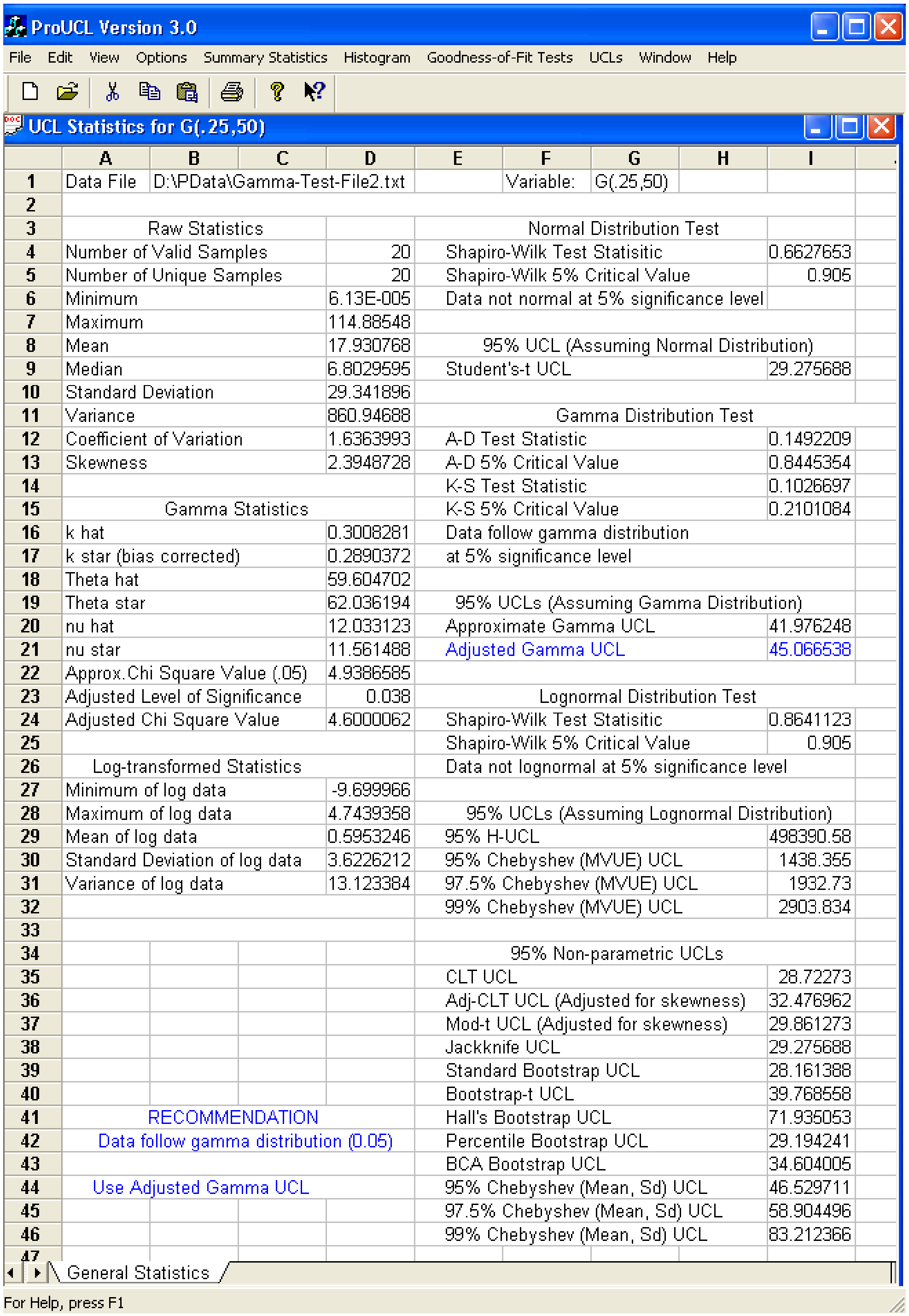

	A	B	C	D	E	F	G	H	I
1	Data File	D:\PData\Gamma-Test-File2.txt				Variable:	G(.25,50)		
2									
3	Raw Statistics				Normal Distribution Test				
4	Number of Valid Samples			20	Shapiro-Wilk Test Statisitic				0.6627653
5	Number of Unique Samples			20	Shapiro-Wilk 5% Critical Value				0.905
6	Minimum			6.13E-005	Data not normal at 5% significance level				
7	Maximum			114.88548					
8	Mean			17.930768	95% UCL (Assuming Normal Distribution)				
9	Median			6.8029595	Student's-t UCL				29.275688
10	Standard Deviation			29.341896					
11	Variance			860.94688	Gamma Distribution Test				
12	Coefficient of Variation			1.6363993	A-D Test Statistic				0.1492209
13	Skewness			2.3948728	A-D 5% Critical Value				0.8445354
14					K-S Test Statistic				0.1026697
15	Gamma Statistics				K-S 5% Critical Value				0.2101084
16	k hat			0.3008281	Data follow gamma distribution				
17	k star (bias corrected)			0.2890372	at 5% significance level				
18	Theta hat			59.604702					
19	Theta star			62.036194	95% UCLs (Assuming Gamma Distribution)				
20	nu hat			12.033123	Approximate Gamma UCL				41.976248
21	nu star			11.561488	Adjusted Gamma UCL				45.066538
22	Approx.Chi Square Value (.05)			4.9386585					
23	Adjusted Level of Significance			0.038	Lognormal Distribution Test				
24	Adjusted Chi Square Value			4.6000062	Shapiro-Wilk Test Statisitic				0.8641123
25					Shapiro-Wilk 5% Critical Value				0.905
26	Log-transformed Statistics				Data not lognormal at 5% significance level				
27	Minimum of log data			-9.699966					
28	Maximum of log data			4.7439358	95% UCLs (Assuming Lognormal Distribution)				
29	Mean of log data			0.5953246	95% H-UCL				498390.58
30	Standard Deviation of log data			3.6226212	95% Chebyshev (MVUE) UCL				1438.355
31	Variance of log data			13.123384	97.5% Chebyshev (MVUE) UCL				1932.73
32					99% Chebyshev (MVUE) UCL				2903.834
33									
34					95% Non-parametric UCLs				
35					CLT UCL				28.72273
36					Adj-CLT UCL (Adjusted for skewness)				32.476962
37					Mod-t UCL (Adjusted for skewness)				29.861273
38					Jackknife UCL				29.275688
39					Standard Bootstrap UCL				28.161388
40					Bootstrap-t UCL				39.768558
41	RECOMMENDATION				Hall's Bootstrap UCL				71.935053
42	Data follow gamma distribution (0.05)				Percentile Bootstrap UCL				29.194241
43					BCA Bootstrap UCL				34.604005
44	Use Adjusted Gamma UCL				95% Chebyshev (Mean, Sd) UCL				46.529711
45					97.5% Chebyshev (Mean, Sd) UCL				58.904496
46					99% Chebyshev (Mean, Sd) UCL				83.212366
47									

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Computer Requirements to Operate ProUCL

Installation of ProUCL Version 3.0 requires a microprocessor speed of at least 200MHz, 12 MB of hard drive space, 48 MB of memory (RAM), and Windows 98 (or newer) operating system. ProUCL is compatible with Windows NT-4, Windows 2000, Windows XP, and Windows ME.

Installation

ProUCL can be downloaded from the TSC website at www.epa.gov/nerlesd1/tsc/tsc.htm. The website contains download and usage instructions.

Find More Information About ProUCL

The TSC website at www.epa.gov/nerlesd1/tsc/tsc.htm provides additional information. EPA technical issue papers used in the development of ProUCL are also available at the TSC website. For additional information, contact:

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Phone: 702-798-2270

The website containing information on the 2002 EPA guidance for calculating the 95% UCLs is: www.epa.gov/superfund/programs/risk/ragsa/ucl.pdf.

References

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Notice

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