1.1 Introduction

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Welcome to ENVIRONMENTALSTATS for S-PLUS! This User's Manual provides step-by-step guidance to using this software. ENVIRONMENTALSTATS for S-PLUS is an S-PLUS module for environmental statistics. This chapter is an introduction to environmental statistics in general and ENVIRONMENTALSTATS for S-PLUS in particular, and includes information on system and user requirements, installing the software, loading and using the module, and getting technical support. The last section of the chapter is a tutorial.

1.2 What is Environmental Statistics?

Environmental statistics is simply the application of statistical methods to problems concerning the environment. Examples of activities that require the use of environmental statistics include:

- Monitoring air or water quality.
- Monitoring groundwater quality near a hazardous or solid waste site.
- Using risk assessment to determine whether a potentially contaminated area needs to be cleaned up, and, if so, how much.
- Assessing whether a previously contaminated area has been cleaned up according to some specified criterion.
- Using hydrological data to predict the occurrences of floods.

The term "environmental statistics" must also include work done in various branches of ecology, such as animal population dynamics and general ecological modeling, as well as other fields, such as geology, chemistry, epidemiology, oceanography, and atmospheric modeling. This User's Manual concentrates on statistical methods to analyze chemical concentrations and physical parameters, usually in the context of mandated environmental monitoring.

Environmental statistics is a special field of statistics. Probability and statistics deal with situations in which the outcome is not certain. They are built upon the concepts of a *population* and a *sample* from the population. *Probability* deals with predicting the characteristics of the sample, given that you know the characteristics of the population (e.g., the probability of picking an ace out of a deck of 52 well-shuffled standard playing cards). *Statistics* deals with inferring

the characteristics of the population, given information from one or more samples from the population (e.g., after 100 times of randomly choosing a card from a deck of 20 unknown playing cards and then replacing the card in the deck, no ace has appeared; therefore the deck probably does not contain any aces).

The field of environmental statistics is relatively young and employs several statistical methods that have been developed in other fields of statistics, such as sampling design, exploratory data analysis, basic estimation and hypothesis testing, quality control, multiple comparisons, survival analysis, and Monte Carlo simulation. Nonetheless, special problems have motivated innovative research, and both traditional and new journals now report on statistical methods that have been developed in the context of environmental monitoring. (See the help topic *References: Environmental Statistics—General References* for a list of general text books on environmental statistics.)

In addition, environmental legislation such as the Clean Water Act, the Clean Air Act, the Comprehensive Emergency Response, Compensation, and Liability Act (CERCLA), and the Resource and Recovery Act (RCRA) have spawned environmental regulations and agency guidance documents that mandate or suggest various statistical methods for environmental monitoring (see the help topic *References: Guidance Documents and Regulations*).

1.3 What is ENVIRONMENTALSTATS for S-PLUS?

ENVIRONMENTALSTATS for S-PLUS, created by Dr. Steven P. Millard of Probability, Statistics & Information (PSI), is a new *comprehensive* software package for environmental statistics. An add-on module to the statistical software package S-PLUS (from Insightful Corporation), it provides a set of powerful yet simple-to-use menu items and functions for performing graphical and statistical analyses of environmental data. ENVIRONMENTALSTATS for S-PLUS brings the major environmental statistical methods found in the literature and regulatory guidance documents into one statistical package, along with an extensive hypertext help system that explains *what* these methods do, *how* to use these methods, and *where* to find them in the environmental statistics literature. Also included are numerous built-in data sets from regulatory guidance documents and the environmental statistics literature. ENVIRONMENTALSTATS for S-PLUS, combined with S+SPATIALSTATS and S-PLUS for ArcView GIS, provide the environmental scientist, statistician, researcher, and technician with all the tools needed to "get the job done!"

Because ENVIRONMENTALSTATS for S-PLUS is an S-PLUS module, you automatically have access to all the features and functions of S-PLUS, including easy-to-use pull-down menus, powerful graphics, standard hypothesis tests, and the flexibility of a programming language. In addition, with ENVIRONMENTALSTATS for S-PLUS you can:

- Compute quantities associated with probability distributions (probability density functions, cumulative distribution functions, and quantiles), and generate random numbers from these distributions. (Several distributions have been added to the ones already available in S-PLUS.)
- Plot probability distributions so you can see how they change with the value of the distribution parameter(s).
- Compute several different kinds of summary statistics.
- Estimate distribution parameters and quantiles and compute confidence intervals for commonly used probability distributions.
- Perform and plot the results of goodness-of-fit tests.
- Compute optimal Box-Cox data transformations.
- Compute parametric and non-parametric prediction and tolerance intervals (including simultaneous prediction intervals).
- Perform additional hypothesis tests not already part of S-PLUS, including Chen's t-test for skewed distributions, Fisher's one-sample randomization test for location, the quantile test to detect a shift in the tail of one population relative to another, two-sample linear rank tests, the von Neumann rank test for serial correlation, and Kendall's seasonal test for trend.
- Perform power and sample size computations and create associated plots.
- Perform calibration based on a machine signal to determine decision and detection limits, and report estimated concentrations along with confidence intervals.
- Analyze singly and multiply censored (less-than-detection-limit) data with empirical cdf and Q-Q plots, parameter/quantile estimation and confidence intervals, prediction and tolerance intervals, goodness-of-fit tests, optimal Box-Cox transformations, and two-sample rank tests.
- Perform probabilistic risk assessment.
- Look up statistical methods in the environmental literature in a hypertext help system that explains the equations, links the equations to the original reference, includes abstracts of selected references, and contains a glossary of statistical and environmental terms.
- Reproduce specific examples in EPA guidance documents by using built-in data sets from these documents.

1.4 Intended Audience/Users

ENVIRONMENTALSTATS for S-PLUS and this User's Manual are intended for anyone who has to make sense of environmental data, including statisticians, environmental scientists, hydrologists, soil scientists, atmospheric scientists, geochemists, environmental engineers and consultants, hazardous and solid waste site managers, and regulatory agency analysts and enforcement officers. Some parts of ENVIRONMENTALSTATS for S-PLUS incorporate statistical meth-

ods that have appeared in the environmental literature but are not commonly found in any statistical software package. Some parts are specifically aimed at users who are required to collect and analyze environmental monitoring data in order to comply with federal and state Superfund, RCRA, CERCLA, and Subtitle D regulations for environmental monitoring at hazardous and solid waste sites. All of the functions in ENVIRONMENTALSTATS for S-PLUS, however, are useful to anyone who needs to analyze environmental data.

ENVIRONMENTALSTATS for S-PLUS is an S-PLUS module. In order to use it, you need to know how to perform basic operations in S-PLUS, such as using the pull-down menu or Command and Script Windows, reading data into S-PLUS, and creating basic data objects (e.g., data frames). See the S-PLUS documentation for more information on S-PLUS. In addition, you need to have a basic knowledge of probability and statistics. The User's Manual and the help system are not meant to be a text book in environmental statistics. See the references listed in *References: Environmental Statistics—General References* for a list of useful books and articles on this subject.

1.5 System Requirements

Because ENVIRONMENTALSTATS for S-PLUS is an S-PLUS module, it runs under every operating system that S-PLUS runs under, including Windows and UNIX. Currently only a Windows version is available. Windows users must have S-PLUS 6.0 in order to run EnvironmentalStats for S-PLUS Version 2.0. The module requires approximately 20 MB of space on your hard disk.

1.6 Installing EnvironmentalStats for S-Plus

Before you install EnvironmentalStats for S-PLUS, you should make sure you are using S-PLUS 6.0 or a later version. To determine what version of S-PLUS you are using, start S-PLUS and either choose **Help>About S-PLUS** on the menu, or type version at the S-PLUS prompt. If you are using the Professional version of S-PLUS for Windows, you should see something like the following:

```
> version
Professional Edition Version 6.0.2 Release 2 for
Microsoft Windows : 2001
```

To install ENVIRONMENTALSTATS for S-PLUS, close all Windows applications, and then simply run the Setup program included on the ENVIRONMENTALSTATS for S-PLUS distribution CD. To leave Setup before the setup is complete, select Cancel from any Setup dialog box. When you do this, Setup displays an exit dialog box that warns you that you have not completed the setup procedure.

1.7 Starting EnvironmentalStats for S-Plus

To start ENVIRONMENTALSTATS for S-PLUS, you must have already started S-PLUS. You can load the module either from the menu or from the Command Window.

- To load the module from the menu, on the S-PLUS menu bar make the following selections: File>Load Module. This brings up the Load Module dialog box. In the Module box, select envstats. For the Action buttons, select Load Module. Make sure the Attach at top of search list box is checked. Click OK.
- To load the module from the Command Window, type module(envstats) at the S-PLUS prompt.

Loading the module adds the EnvironmentalStats menu to the S-PLUS menu bar and also attaches the library of ENVIRONMENTALSTATS for S-PLUS functions to the second position in your search list (S-PLUS Professional users can type search() at the S-PLUS prompt to see the listing of directories on the search list). S-PLUS Standard and S-PLUS Professional users can access functions via the ENVIRONMENTALSTATS for S-PLUS pull-down menu. S-PLUS Professional users can access any of the functions in the ENVIRONMENTALSTATS for S-PLUS module via the command line as well.

Note: Some of the functions in ENVIRONMENTALSTATS for S-PLUS mask built-in S-PLUS functions. The masked functions are modified versions of the built-in functions and have been created to support the other functions in ENVIRONMENTALSTATS for S-PLUS, but the modifications should not affect normal use of S-PLUS. If you experience unexpected behavior of S-PLUS after attaching ENVIRONMENTALSTATS for S-PLUS, try unloading the module (see *Unloading ENVIRONMENTALSTATS for S-PLUS* below). All of the functions in ENVIRONMENTALSTATS for S-PLUS, whether they mask built-in functions or not, are described in the help system.

1.8 Getting Help

You may start the help system for ENVIRONMENTALSTATS for S-PLUS in one of five ways:

- 1. On the menu bar, select Help>Available Help>EnvironmentalStats.
- 2. On the menu bar, go to the **EnvironmentalStats** menu and select an item. A dialog box will be displayed. In the lower right-hand corner click on the **Help** button.
- 3. At the command line, type help(module="envstats").
- 4. At the command line, use the ? operator and help function just as you do in S-PLUS. For example, type ?pdfplot to call up the help file for the pdfplot function.

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 - 5. Outside of S-PLUS, select Start>Programs>S-PLUS 6.0 Professional>EnvironmentalStats, or in the S-PLUS program group doubleclick the ENVIRONMENTALSTATS icon.

In the Table of Contents, you will see the main help categories, including Pull-Down Menu, Functions, Datasets, References, and Glossary. You can access the help files for functions by category or alphabetically, and you can access data sets by source or alphabetically.

The help system for ENVIRONMENTALSTATS for S-PLUS is a separate application from the help system for S-PLUS. Words that are underlined and highlighted in color (green or blue or whatever color your help system uses for jumps) are jumps to other help windows *within* the ENVIRONMENTALSTATS for S-PLUS help system. In each help file, if a word appears under the paragraph heading SEE ALSO but is not underlined and highlighted, you must use the S-PLUS help system to look up this word.

For example, in the help system for ENVIRONMENTALSTATS for S-PLUS, in the Table of Contents choose **Functions>Functions by Category**. This will bring up the help file *EnvironmentalStats for S-PLUS Functions By Category*. Click on *Plotting Probability Distributions* and then click on pdfplot. Within that help file, under the paragraph heading SEE ALSO, you will see:

```
.Distribution.frame, Probability Distributions and Random
Numbers, cdfplot, ecdfplot, qqplot, qqplot.gestalt,
plot, plot.default, par, title.
```

You can access the help files for .Distribution.frame, Probability Distributions and Random Numbers, cdfplot, ecdfplot, qqplot, and qqplot.gestalt directly by simply clicking on these words. To look at the help file for the functions plot, plot.default, par, and title, however, you must use the S-PLUS help system.

1.9 Customizing EnvironmentalStats for S-Plus

If you plan to use ENVIRONMENTALSTATS for S-PLUS extensively, you may want to customize your S-PLUS startup routine to automatically attach the ENVIRONMENTALSTATS for S-PLUS module each time you start S-PLUS. S-PLUS Professional users can do this by adding the line module(envstats) to your .First function. If you do not have a .First function, you can create one by simply typing the following command:

> .First <- function() {module(envstats)}</pre>

If you want to automatically attach the ENVIRONMENTALSTATS for S-PLUS module each time you start S-PLUS *and* start the ENVIRONMENTALSTATS for S-PLUS help system, make sure your .First function includes the following lines:

```
module(envstats)
help(module="envstats")
```

If you are going to use ENVIRONMENTALSTATS for S-PLUS for several different projects, it is a good idea to use separate directories for each project. See the S-PLUS documentation for how to create separate "Chapters" and have S-PLUS ask you which directory you want to work in when you start S-PLUS.

1.10 Unloading EnvironmentalStats for S-Plus

To remove the ENVIRONMENTALSTATS for S-PLUS module from your S-PLUS session, S-PLUS Professional users can simply type the following command at the S-PLUS prompt:

```
> module(envstats, unload=T)
```

This command removes the ENVIRONMENTALSTATS for S-PLUS menu from the S-PLUS menu bar and the library of ENVIRONMENTALSTATS for S-PLUS functions from your search list.

1.11 A Tutorial

This section is a brief tutorial that highlights some of the major features of ENVIRONMENTALSTATS for S-PLUS. There are several ways to use this section. If you are fairly new to S-PLUS, you may want to briefly skim this section to get an idea of what you can do in ENVIRONMENTALSTATS for S-PLUS, and then come back later after you have read the other chapters of this manual. If you have used S-PLUS for a long time and have just installed ENVIRONMENTALSTATS for S-PLUS, you may want to follow this tutorial in depth right now to get acquainted with some of the features available in this S-PLUS module. Throughout this section we assume you have started S-PLUS and also loaded ENVIRONMENTALSTATS for S-PLUS.

1.11.1 The TcCB Data

The guidance document Statistical Methods for Evaluating the Attainment of Cleanup Standards, Volume 3: Reference-Based Standards for Soils and Solid Media (USEPA, 1994b, pp.6.22-6.25) contains measures of 1,2,3,4-Tetrachlorobenzene (TcCB) concentrations (ppb) from soil samples at a Reference site and a Cleanup area. There are 47 observations from the Reference site and 77 in the Cleanup area. These data are stored in the data frame epa.94b.tccb.df (see the help file Datasets: USEPA (1994b)). There is one observation coded as "ND" in this data set as presented in the guidance document. Here, we'll assume this observation is less than the smallest ob-

served value, which is 0.09 ppb. For the purposes of this tutorial, we'll set this one censored observation to the assumed detection limit of 0.09.

To look at the raw data, open the Object Explorer Window, click on the **Find Objects** button (binoculars icon), type **epa.94b.tccb.df** and click **OK**. In the Object Explorer Window, under the Object column, double-click on **epa.94b.tccb.df**. This will bring up a data sheet. Alternatively, in the Command Window, type epa.94b.tccb.df:

> epa	a.94b.tccb.	df		
	TcCB.orig	TcCB	Censored	Area
1	0.22	0.22	F	Reference
2	0.23	0.23	F	Reference
•				
124	168.64	168.64	F	Cleanup

For the remainder of this tutorial, we will assume that you have attached the data frame epa.94b.tccb.df to your search list with the following command:

> attach(epa.94b.tccb.df)

Note that if you are only going to follow the instructions for using the Menu you do not have to execute the above command.

1.11.2 Computing Summary Statistics

The summary statistics for the TcCB data are shown below.

	Cleanup	Reference
Sample Size:	77	47
# Missing:	0	0
Mean:	3.915	0.5985
Median:	0.43	0.54
10% Trimmed Mean:	0.6846	0.5728
Geometric Mean:	0.5784	0.5382
Skew:	7.717	0.9019
Kurtosis:	62.67	0.132
Min:	0.09	0.22
Max:	168.6	1.33
Range:	168.6	1.11
1st Quartile:	0.23	0.39
3rd Quartile:	1.1	0.75
Standard Deviation:	20.02	0.2836
Geometric Standard Deviation:	3.898	1.597
Interquartile Range:	0.87	0.36
Median Absolute Deviation:	0.3558	0.2669
Coefficient of Variation:	5.112	0.4739

These summary statistics indicate that the observations for the Cleanup area are extremely skewed to the right. The medians for the two areas are about the same, but the mean for the Cleanup area is much larger, indicating a few or more "outlying" observations with large values. This may be indicative of residual contamination that was missed during the cleanup process.

Menu

To produce summary statistics for the original TcCB data using the ENVIRONMENTALSTATS pull-down menu, follow these steps.

- 1. Open the Object Explorer. If **epa.94b.tccb.df** is not visible in the Object Column, click on the **Find S-PLUS Objects** button (the binoculars icon) and in the Pattern box type **epa.94b.tccb.df**, then click **OK**.
- 2. Highlight the shortcut **epa.94b.tccb.df** in the Object column of the Object Explorer.
- 3. On the S-PLUS menu bar, make the following menu choices: **EnvironmentalStats>EDA>Summary Statistics**. This will bring up the Full Summary Statistics dialog box.
- 4. In the Data Set box, select or type **epa.94b.tccb.df** is selected. In the Variable(s) box, choose **TcCB**. In the Grouping Variables box, select **Area**.
- 5. Click **OK** or **Apply**.

Command

To produce summary statistics for the original TcCB data using the S-PLUS Command or Script Window, type this command:

> full.summary(split(TcCB, Area))

1.11.3 Looking at the TcCB Data with Histograms and Boxplots

Figure 1.1 shows the histograms for the TcCB concentrations in the Reference and Cleanup areas. Figure 1.2 shows side-by-side boxplots comparing the distribution of TcCB concentrations in the two areas. Both graphs display concentrations on the log scale. We see in these plots that most of the observations in the Cleanup area are comparable to (or even smaller than) the observations in the Reference area, but there are a few very large "outliers" in the Cleanup area.

Menu

To produce the histograms and boxplots for the log-transformed TcCB data using the S-PLUS pull-down menu, it will simplify things if we first make a new data frame called new.epa.94b.tccb.df to contain the original data and the log-transformed TcCB observations. To create the data frame new.epa.94b.tccb.df, follow these steps.

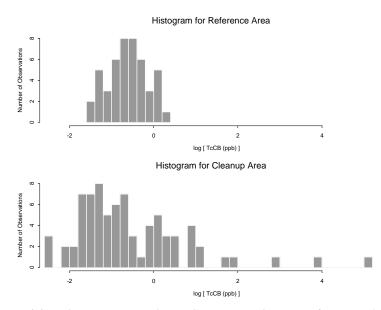
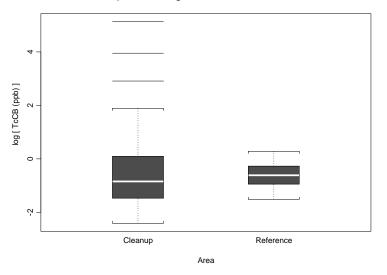


Figure 1.1. Histograms comparing TcCB concentrations at Reference and Cleanup areas.



Boxplots for Log-Transformed TcCB Data

Figure 1.2. Boxplots comparing TcCB concentrations at Reference and Cleanup areas.

- 1. Highlight the shortcut **epa.94b.tccb.df** in the Object column of the Object Explorer.
- 2. On the S-PLUS menu bar, make the following menu choices: **Data>Transform**. This will bring up the Transform dialog box.
- 3. In the Target Column box, type **log.TcCB**. In the Variable box, choose **TcCB**. In the Function box choose **log**.
- 4. Click on the **Add** button, then click **OK**. At this point, you will get a warning message telling you that you have created a new copy of the data frame epa.94b.tccb.df that masks the original copy. Close the message window. Also, the modified data frame pops up in a data window. Close the data window.
- 5. In the left-hand column of the Object Explorer, click on the **Data** folder. In the right-hand column of the Object Explorer, right-click on **epa.94b.tccb.df** and choose **Properties**. In the Name box rename this data frame to **new.epa.94b.tccb.df** and click **OK**.

To produce the histograms shown in Figure 1.1 using the S-PLUS pull-down menus or toolbars, follow these steps.

- 1. In the Object Explorer, highlight the **Data** folder in the left-hand column. In the right-hand (Object) column, left-double-click the shortcut **new.epa.94b.tccb.df**. This will bring up a data window.
- On the S-PLUS menu bar, make the following menu choices: Graph>2D Plot. This will bring up the Insert Graph dialog box. Under the Axes Type column, Linear should be highlighted. Under the Plot Type column, select Histogram and click OK. (Alternatively, left-click on the 2D Plots button, then left-click on the Histogram button.)
- 3. The Histogram/Density dialog box should appear. Under the Data Columns group, in the Data Set box, select **new.epa.94b.tccb.df**. Under the Data Columns group, in the x Columns box, choose **log.TcCB**.
- Click on the **Options** tab. Under Histogram Specs, in the Output Type box, select **Density**. For Lower Bound type −2.5. For Interval Width type 0.5.
- 5. Click **OK**. A histogram of the data for both areas is displayed in a graphsheet.
- 6. Click on the data window to bring it forward. Left click on the top of the Area column to highlight that column, then left-click in a cell of the column, then drag the column to the top of the graphsheet and drop it.

To produce the boxplots shown in Figure 1.2 using the S-PLUS pull-down menus or toolbars, follow these steps.

 On the S-PLUS menu bar, make the following menu choices: Graph>2D Plot. This will bring up the Insert Graph dialog box. Under the Axes Type column, Linear should be highlighted. Under the Plot Type column, select Boxplot and click OK. (Alternatively, left-click on the 2D Plots button, then left-click on the Box button.)

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 - 2. The Boxplot dialog box should appear. The Data Set box should display **new.epa.94b.tccb.df**. In the x Columns box, choose **Area**. In the y Columns box, choose **log.TcCB**.
 - 3. Click OK.

Command

To produce the histograms shown in Figure 1.1 using the S-PLUS Command or Script Window, type these commands.

```
> par(mfrow=c(2,1))
> hist(log(TcCB[Area=="Reference"]),
    xlim=range(log(TcCB)), xlab="log [ TcCB (ppb) ]",
    ylab="Number of Observations",
    main="Histogram for Reference Area")
> hist(log(TcCB[Area=="Cleanup"]), xlim=range(log(TcCB)),
    nclass=25, xlab="log [ TcCB (ppb) ]",
    ylab="Number of Observations",
    main="Histogram for Cleanup Area")
```

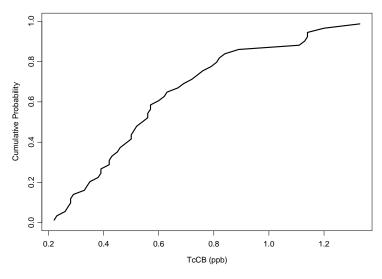
To produce the boxplots shown in Figure 1.2 using the S-PLUS Command or Script Window, type these commands:

```
> boxplot(split(log(TcCB), Area), xlab="Area",
    ylab="log [ TcCB (ppb) ]",
    main="Boxplots for Log-Transformed TcCB Data")
```

1.11.4 Quantile (Empirical CDF) Plots

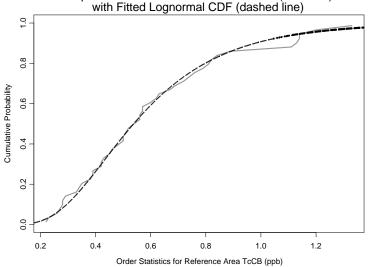
Figure 1.3 shows the quantile plot, also called the empirical cumulative distribution function (cdf) plot, for the Reference area TcCB data. You can easily pick out the median as about 0.55 ppb and the quartiles as about 0.4 ppb and 0.75 ppb (compare these numbers to the ones listed on page 8). You can also see that the quantile plot quickly rises, then pretty much levels off after about 0.8 ppb, which indicates that the data are skewed to the right (see the histogram for the Reference area data in Figure 1.1).

Figure 1.4 shows the quantile plot with a fitted lognormal distribution. We see that the lognormal distribution appears to fit these data quite well. Figure 1.5 compares the empirical cdf for the Reference area with the empirical cdf for the Cleanup area for the log-transformed TcCB data. As we saw with the histograms and boxplots, the Cleanup area has quite a few extreme values compared to the Reference area.



Quantile Plot for Reference Area TcCB Data

Figure 1.3. Quantile plot of Reference area TcCB data.



Empirical CDF for Reference Area TcCB (solid line) with Fitted Lognormal CDF (dashed line)

Figure 1.4. Empirical cdf of Reference area TcCB data compared to a lognormal cdf.

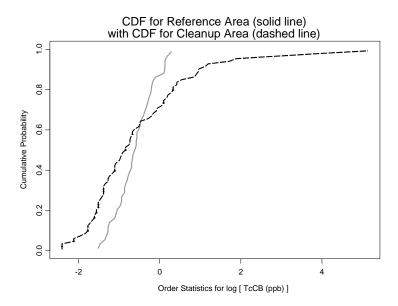


Figure 1.5. Quantile plots comparing log-transformed TcCB data at the Reference and Cleanup areas.

Menu

To produce the quantile plot of the Reference area TcCB data shown in Figure 1.3 using the ENVIRONMENTALSTATS for S-PLUS pull-down menu, follow these steps.

- 1. In the Object Explorer, highlight the **Data** folder in the left-hand column. In the right-hand (Object) column, highlight the shortcut **new.epa.94b.tccb.df** for the version of this data frame that you created earlier.
- On the S-PLUS menu bar, make the following menu choices: EnvironmentalStats>EDA>CDF Plot>Empirical CDF. This will bring up the Plot Empirical CDF dialog box.
- 3. The Data Set box should display **new.epa.94b.tccb.df**. In the Variable(s) box, choose **TcCB**. In the Subset Rows with box, type **Area==''Reference''**.
- 4. Click **OK**.

To produce the quantile plot shown in Figure 1.4 comparing the Reference area TcCB data to a lognormal distribution, follow these steps.

1. On the S-PLUS menu bar, make the following menu choices: **EnvironmentalStats>EDA>CDF Plot>Compare Two CDFs**. This will bring up the Compare Two CDFs dialog box.

- The Data Set box should display new.epa.94b.tccb.df. In the x Variable box, choose TcCB. In the Subset Rows with box, type Area=="Reference". Under the Distribution Information Group, make sure that the Estimate Parameters box is checked. In the Distribution box, select Lognormal.
- 3. Click **OK** or **Apply**.

To produce the quantile plot shown in Figure 1.5 comparing the logtransformed Reference area TcCB data to the log-transformed Cleanup area TcCB data, follow these steps.

- 1. On the S-PLUS menu bar, make the following menu choices: EnvironmentalStats>EDA>CDF Plot>Compare Two CDFs. This will bring up the Compare Two CDFs dialog box.
- For the Compare Data to choice, select Other Data. The Data Set box should display new.epa.94b.tccb.df. In the Variable 1 box, choose log.TcCB. In the Variable 2 box, choose Area. Click on the Variable 2 is a Grouping Variable box to check it.
- 3. Click **OK** or **Apply**.

Command

To produce the quantile plot of the Reference area TcCB data shown in Figure 1.3, type the following command.

```
> ecdfplot(TcCB[Area=="Reference"], xlab="TcCB (ppb)",
main="Quantile Plot for Reference Area TcCB Data")
```

To produce the quantile plot shown in Figure 1.4 comparing the Reference area TcCB data to a lognormal distribution, type the following command.

```
> cdf.compare(TcCB[Area=="Reference"], dist="lnorm",
    xlab="Order Statistics for Reference Area TcCB
    (ppb)", main=paste("Empirical CDF for ",
    "Reference Area TcCB (solid line)\n",
    "with Fitted Lognormal CDF (dashed line)", sep=""))
```

To produce the quantile plot shown in Figure 1.5 comparing the log-transformed Reference area TcCB data to the log-transformed Cleanup area TcCB data, type the following command.

```
> cdf.compare(log(TcCB[Area=="Reference"]),
    log(TcCB[Area=="Cleanup"]),
    xlab="Order Statistics for log [ TcCB (ppb) ]",
    main=paste("CDF for Reference Area (solid line)",
        "with CDF for Cleanup Area (dashed line)",
        sep="\n"))
```

1.11.5 Assessing Goodness-of-Fit with Quantile-Quantile Plots

Figure 1.6 displays the normal Q-Q plot for the log-transformed Reference area TcCB data (i.e., we are assuming these data come from a lognormal distribution), along with a fitted least squares line. Figure 1.7 displays the corresponding Tukey mean-difference Q-Q plot. As we saw with the quantile plot, the log-normal model appears to be a fairly good fit to these data.

Menu

To create the normal Q-Q plot for the log-transformed Reference area data shown in Figure 1.6, follow these steps.

- 1. In the Object Explorer, highlight the **Data** folder in the left-hand column. In the right-hand (Object) column, highlight the shortcut **epa.94b.tccb.df**.
- 2. On the S-PLUS menu bar, make the following menu choices: **EnvironmentalStats>EDA>Q-Q Plot>Q-Q Plot**. This will bring up the Q-Q Plot dialog box.
- The Data Set box should display epa.94b.tccb.df. In the x Variable box, choose TcCB. In the Subset Rows with box, type Area=="Reference". In the Distribution box, make sure Lognormal is selected.
- 4. Click on the **Plotting** tab. Click on the **Add a Line** box to select this option.
- 5. Click **OK** or **Apply**.

To create the Tukey mean-difference Q-Q plot for the Reference area TcCB data fitted to a normal distribution shown in Figure 1.7, follow the same steps as above, but in Step 3 also check the **Estimate Parameters** box, and in Step 4 under Plot Type select **Tukey M-D**.

Command

To produce the Q-Q plot of the Reference area TcCB data fitted to a lognormal distribution shown in Figure 1.6, type the following command.

```
> qqplot(TcCB[Area=="Reference"], dist="lnorm",
    add.line=T, ylab="Quantiles of log [ TcCB (ppb) ]",
    main=paste("Normal Q-Q Plot for",
    "Log-Transformed Reference Area TcCB Data"))
```

To create the Tukey mean-difference Q-Q plot for the Reference area data fitted to a lognormal distribution shown in Figure 1.7, type the following command.

```
> qqplot(TcCB[Area=="Reference"], dist="lnorm",
    plot.type="Tukey", estimate.params=T, add.line=T,
    main=paste("Tukey Mean-Difference Q-Q Plot for",
```

```
"\nReference Area TcCB Fitted to ",
"Lognormal Distribution", sep=""))
```

Normal Q-Q Plot for Log-Transformed Reference Area TcCB Data

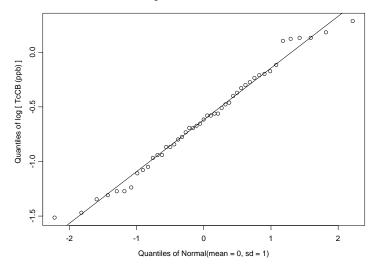


Figure 1.6. Normal Q-Q plot for the log-transformed Reference area TcCB data.

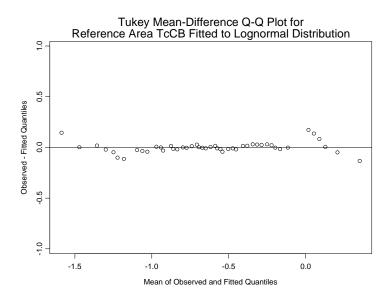


Figure 1.7. Tukey mean-difference Q-Q plot for the Reference area TcCB data fitted to a lognormal distribution.

1.11.6 Estimating Distribution Parameters

In ENVIRONMENTALSTATS for S-PLUS you can estimate parameters for several parametric distributions. For example, for the lognormal distribution, you can estimate the mean and standard deviation based on the log-transformed data, or you can estimate the mean and coefficient of variation based on the original data. For either parameterization, you can compute a confidence interval for the mean. Here are the results for the log-transformed Reference area TcCB data:

Results of Distribution Parameter Estimation

Assumed Distribution:	Lognormal
Estimated Parameter(s):	meanlog = -0.6195712 sdlog = 0.467953
Estimation Method:	mvue
Data:	TcCB[Area=="Reference"]
Sample Size:	47
Confidence Interval for:	meanlog
Confidence Interval Method:	Exact
Confidence Interval Type:	two-sided
Confidence Level:	95%
Confidence Interval:	LCL = -0.7569673 UCL = -0.4821751

and here are the results for the original Reference area TcCB data:

Results of Distribution Parameter Estimation

Assumed Distribution:	Lognormal
Estimated Parameter(s):	mean = 0.5989072 cv = 0.4899539
Estimation Method:	mvue
Data:	TcCB[Area=="Reference"
Sample Size:	47
Confidence Interval for:	mean

]

Confidence In	terval Method:	Land
Confidence In	terval Type:	two-sided
Confidence Le	vel:	95%
Confidence In	terval:	LCL = 0.5243786 UCL = 0.7016992

Menu

To compute the estimated mean and standard deviation for the log-transformed Reference area TcCB data, follow these steps.

- 1. On the S-PLUS menu bar, make the following menu choices: **EnvironmentalStats>Estimation>Parameters**. This will bring up the Estimate Distribution Parameters dialog box.
- For Data to Use, make sure the Pre-Defined Data button is selected. In the Data Set box, select or type epa.94b.tccb.df. In the Variable box, select TcCB. In the Subset Rows with box, type Area=="Reference".
- 3. In the Distribution/Estimation section, in the Distribution box select **Lognormal**, and for Estimation Method select **mvue**.
- 4. Under the Confidence Interval section, **check** the Confidence Interval box. In the CI Type box, select **two-sided**. In the CI Method box, select **exact**. In the Confidence Level (%) box, select **95**.
- 5. Click **OK** or **Apply**.

To compute the estimated mean and coefficient of variation for the original Reference area TcCB data, follow the same steps above, but in Step 3 for Distribution select **Lognormal** (Alternative) and in Step 4 for CI Method select land.

Command

To compute the estimated mean and standard deviation for the log-transformed Reference area TcCB data, type this command:

> elnorm(TcCB[Area=="Reference"], ci=T)

To compute the estimated mean and coefficient of variation for the original Reference area TcCB data, type this command:

```
> elnorm.alt(TcCB[Area=="Reference"], ci=T)
```

1.11.7 Testing for Goodness of Fit

ENVIRONMENTALSTATS for S-PLUS contains several new or modified S-PLUS menu items and functions for testing goodness of fit. Here we will use the Shapiro-Wilk test to test the adequacy of a lognormal model for the Reference area TcCB data.

Results of Good	ness-of-Fit Test	
Test Method:		Shapiro-Wilk GOF
Hypothesized Di	stribution:	Lognormal
Estimated Param	eter(s):	meanlog = -0.6195712 sdlog = 0.467953
Estimation Meth	od:	mvue
Data:		TcCB.ref
Sample Size:		47
Test Statistic:		W = 0.9789915
Test Statistic	Parameter:	n = 47
P-value:		0.5512532
Alternative Hyp	othesis:	True cdf does not equal Lognormal Distribution.

ENVIRONMENTALSTATS for S-PLUS also contains a plotting method for the results of goodness-of-fit tests, as well as a function or menu choice to produce four summary plots on one page, as shown in Figure 1.8.

Menu

To perform the Shapiro-Wilk goodness-of-fit test for lognormality on the Reference area TcCB data and produce a summary plot of the results, follow these steps.

- On the S-PLUS menu bar, make the following menu choices: EnvironmentalStats>Hypothesis Tests>GOF Tests>One Sample>Shapiro-Wilk. This will bring up the Shapiro-Wilk GOF Test dialog box.
- For Data to Use, select Pre-Defined Data. For Data Set make sure epa.94b.tccb.df is selected, for Variable select TcCB, and in the Subset Rows with box type Area=="Reference". In the Distribution box select Lognormal.
- 3. Click on the **Plotting** tab. Under Plotting Information, in the Significant Digits box select **3**, then click **OK** or **Apply**.

Command

To perform the Shapiro-Wilk goodness-of-fit test for lognormality on the Reference area TcCB data, type these commands.

```
> TcCB.ref <- TcCB[Area=="Reference"]
> sw.list <- sw.gof(TcCB.ref, dist="lnorm")
> sw.list
```

To produce a summary plot of the results, type this command.

> plot.gof.summary(sw.list, digits=3)

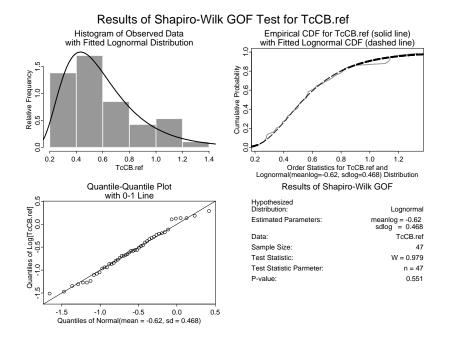


Figure 1.8. Summary plots of Shapiro-Wilk goodness-of-fit test for Reference area TcCB data.

1.11.8 Estimating Quantiles and Computing Confidence Limits

ENVIRONMENTALSTATS for S-PLUS contains a menu item and functions for estimating quantiles and optionally constructing confidence limits for the quantiles. Here we will estimate the 90th percentile of the distribution of the Reference area TcCB, assuming the true distribution is a lognormal distribution, and compute a 95% confidence interval for this 90th percentile.

Menu

To estimate the 90th percentile and compute a two-sided 95% confidence interval for this percentile, follow these steps.

- 22 1. Getting Started
 - 1. On the S-PLUS menu bar, make the following menu choices: **EnvironmentalStats>Estimation>Quantiles**. This will bring up the Estimate Distribution Quantiles dialog box.
 - For Data to Use, make sure the Pre-Defined Data button is selected. In the Data Set box, select epa.94b.tccb.df. In the Variable box, select TcCB. In the Subset Rows with box, type Area=="Reference".
 - 3. In the Quantile(s) box, select **0.90**.
 - 4. Under the Distribution/Estimation group, for Type, select the **Parametric** button. In the Distribution box, select **Lognormal**. For Estimation Method, select **qmle**.
 - 5. Under the Confidence Interval group, make sure the Confidence Interval box is **checked**. For CI Type, select **two-sided**. For CI Method, select **exact**. For Confidence Level (%), select **95**.
 - 6. Click **OK** or **Apply**.

Command

To estimate the 90th percentile and compute a two-sided 95% confidence interval for this percentile, type this command.

```
> eqlnorm(TcCB[Area=="Reference"], p=0.9, ci=T)
```

Results of Distribution Parameter Estimation

Assumed Distribution:	Lognormal
Estimated Parameter(s):	meanlog = -0.6195712 sdlog = 0.467953
Estimation Method:	mvue
Estimated Quantile(s):	90'th %ile = 0.9803307
Quantile Estimation Method:	qmle
Data:	TcCB[Area=="Reference"]
Sample Size:	47
Confidence Interval for:	90'th %ile
Confidence Interval Method:	Exact
Confidence Interval Type:	two-sided
Confidence Level:	95%
Confidence Interval:	LCL = 0.8358791 UCL = 1.215498

1.11.9 Comparing Two Distributions Using Nonparametric Tests

ENVIRONMENTALSTATS for S-PLUS contains menu items and functions for performing general two-sample linear rank tests (to test for a shift in location) and a special quantile test that tests for a shift in the tail of one of the distributions. In this example we will compare the Reference and Cleanup area TcCB data. Here are the results for the Wilcoxon rank sum test.

Results of Hypothesis Test		
Null Hypothesis:	Fy(t) = Fx(t)	
Alternative Hypothesis:	Fy(t) > Fx(t) for at least one t	
Test Name:	Two-Sample Linear Rank Test: Wilcoxon Rank Sum Test Based on Normal Approximation	
Data:	x = TcCB[Area == "Cleanup"] y = TcCB[Area == "Reference"]	
Sample Sizes:	nx = 77 ny = 47	
Test Statistic:	z = -1.171872	
P-value:	0.8793758	

and here are the results for the quantile test

Results of Hypothesis Test	-
Null Hypothesis:	e = 0
Alternative Hypothesis:	<pre>Tail of Fx Shifted to Right of Tail of Fy. 0 < e <= 1, where Fx(t) = (1-e)*Fy(t) + e*Fz(t), Fz(t) <= Fy(t) for all t, and Fy != Fz</pre>
Test Name:	Quantile Test
Data:	x = TcCB[Area=="Cleanup"] y = TcCB[Area=="Reference"]
Sample Sizes:	nx = 77 ny = 47

```
Test Statistics:

k (# x obs of r largest) = 9

r = 9

Test Statistic Parameters:

m = 77

n = 47

quantile.ub = 0.928

P-value:

0.01136926
```

Note that the Wilcoxon rank sum test is not significant at the 0.10 level (p=0.88), while the quantile test is significant at the 0.011 level. The quantile test picked up the portion of large outlying values in the Cleanup area data.

Menu

To perform the Wilcoxon rank sum test, follow these steps.

- On the S-PLUS menu bar, make the following menu choices: EnvironmentalStats>Hypothesis Tests>Compare Samples>Two Samples>Linear Rank Test. This will bring up the Two-Sample Linear Rank Test dialog box.
- 2. For Data Set, select **epa.94b.tccb.df**. For Variable 1 select **TcCB**, for Variable 2 select **Area**, and **check** the box that says Variable 2 is a Grouping Variable.
- 3. For Test select **Wilcoxon**, and for Shift Type select **Location**. Under Alternative Hypothesis select **greater**, then click **OK** or **Apply**.

To perform the quantile test, follow these steps.

- On the S-PLUS menu bar, make the following menu choices: EnvironmentalStats>Hypothesis Tests>Compare Samples>Two Samples>Quantile Test. This will bring up the Two-Sample Quantile Test dialog box.
- 2. For Data Set, select **epa.94b.tccb.df**. For Variable 1 select **TcCB**, for Variable 2 select **Area**, and **check** the box that says Variable 2 is a Grouping Variable.
- 3. Under Alternative Hypothesis select greater. For Specify Target select Rank, and for Target Rank type 9, then click OK or Apply.

Command

To perform the Wilcoxon rank sum test, type this command

```
> wilcox.test(TcCB[Area=="Cleanup"],
        TcCB[Area=="Reference"], alternative="greater")
```

or this command

Note that by default the S-PLUS function wilcox.test computes the "corrected" z-statistic while the ENVIRONMENTALSTATS for S-PLUS function two.sample.linear.rank.test computes the "uncorrected" z-statistic.

To perform the quantile test, type this command.

```
> quantile.test(TcCB[Area=="Cleanup"],
    TcCB[Area=="Reference"], alternative="greater",
    target.r=9)
```

1.12 Summary

- Environmental statistics is the application of statistics to environmental ٠ problems.
- ENVIRONMENTALSTATS for S-PLUS is an S-PLUS module for environ-• mental statistics. It includes several menu items and functions for creating graphs and performing statistical analyses that are commonly used in environmental statistics.
- To use ENVIRONMENTALSTATS for S-PLUS you should be familiar with • the basic operation of S-PLUS and have an elementary knowledge of probability and statistics.
- ENVIRONMENTALSTATS for S-PLUS has an extensive help system that includes basic explanations in English, as well as equations and references.