ATTACHMENT 3: Distribution Selection

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Section I Introduction

EPA has recently established a policy and a series of guiding principles for the use of various probabilistic risk assessment techniques. The policy states that probabilistic risk analysis techniques (including Monte-Carlo analyses) can be viable statistical tools for analyzing variability and uncertainty in risk assessments provided that adequate supporting data are available and credible assumptions are made. The policy goes on to state that when risk assessments using probabilistic techniques are submitted to the Agency for review and evaluation, a number of conditions must be satisfied: these conditions relate to the good scientific practices of transparency, reproducibility, and the use of sound methods (memo from F. Hansen, 5/15/97). One of these specific conditions of acceptance states that

> The methods used for the analysis (including all models used, all data upon which the assessment is based, and all assumptions that have a significant impact upon the results) are to be documented and easily located in the report. This documentation is to include a discussion of the degree to which the data used are representative of the population under study. Also, this documentation is to include the names of the models and software used to generate the analysis. Sufficient information is to be provided to allow the results of the analysis to be independently reproduced.

The Agency simultaneously released a series of sixteen "Guiding Principles" for the use of Monte-Carlo analysis and an Appendix dealing with the selection of appropriate input probability distributions for these analyses. The intent of the current document is to further develop these principles and guidelines for use by pesticide registrants and other interested parties by defining what we in OPP's Health Effects Division (HED) see as key criteria which a risk assessments using Monte-Carlo risk assessment techniques must adequately address. Specifically, this chapter explores the various plots, tests, techniques, and analyses which could be used to define an adequate probability distribution for use as an input parameter for a Monte-Carlo assessment submitted to HED.

Monte-Carlo Modeling Options

Once the raw input data on the exposure variable of interest is collected, a risk assessor has available a number of techniques for representing the exposure variables in a Monte Carlo analysis.

- an assessor can use the data values themselves directly in the simulation in what is termed a "trace-driven" simulation. In this technique, values from the raw input data are repeatedly selected in a random manner and used to calculated model outputs;

- an assessor can use the data to define a non-parametric empirical distribution function (EDF) where the data values themselves are used to specify a cumulative distribution and the entire *range* of values (including intermediate points) is used as model inputs. With this technique, *any* value between the minimum and maximum observed values can be selected and model input is not limited to the specific values present in the measured data.

- an assessor can attempt to fit a theoretical or parametric distribution to the data using standard statistical techniques and input parameters to the model can be selected from this fitted distribution.

There are a number of potential benefits for making distributional assumptions about exposure data (du Toit *et al*, 1986; Law and Kelton, 1991). For example,

1) Distributional assumptions permit the data to be represented compactly. A data set containing a potentially large amount of information can be summarized as a probability distribution model described by only a few parameters. Empirical distributions require that each data point be represented and can result in a data set that is cumbersome and difficult to use if the data set is large.

2) Distributional assumptions (and the exploratory data analysis which precedes them) may lead to a clearer understanding of the underlying physical mechanisms involved in generating the data and *vice-versa*.

3) Distributional assumptions permit data to be generated which are *outside* the range of historically observed data. This can be useful since many measures of performance for simulated systems depend heavily on the probability of an "extreme event" (i.e., one outside the range of the observed data) occurring. Empirical distributions, which rely solely on past data when used in the usual manner, can tend to underestimate the probability of an extreme event.

4) Distributional assumptions permit the data to be "smoothed out" which may more accurately reflect real-world values. Empirical distributions, on the other hand, may contain certain artifactual irregularities, particularly if only a small number of data values are available.

On the other hand, some authors prefer EDFs (Bratley, Fox and Schrage, 1987) arguing that the smoothing which necessarily takes place in the fitting process distorts real information. In addition, when data are limited, accurate estimation of the upper end (tail) is difficult. Unfortunately for the assessor, there is no consensus as to which method is best. Despite the above reasons supporting the use of a parametric distribution developed from distributional assumptions, the decision to seek an analytic form to represent the data is ultimately a choice which rests with the assessor. In general, the use of parametric (theoretical) distributions may be preferable to the use of empirical distributions when the data are limited, the fit of the theoretical distribution to the data is good, and there is a theoretical or mechanistic basis which supports the chosen parametric distribution. The process of selecting probability distributions and evaluating the goodness-of-fit is a process that requires judgement. Ultimately, the technique selected will be a matter of the quality and quantity of the data under evaluation and the assessor's exercise of intelligence, creativity, and honesty in assessing the variability and uncertainties inherent in the risk assessment problem.

Organization of Document

Section I of this document is this introduction to Monte-Carlo methods and a brief description of the advantages of disadvantages of parametric methods (i.e., methods which make assumptions about underlying distributions to develop theoretical distributions) and non-parametric methods (which utilize the data directly in forming an empirical distribution, thereby making no assumptions about underlying distributions).

Section II of this document focuses on parametric methods for characterizing and quantifying stochastic variability. In this section, it is explicitly assumed that the risk assessor has previously made the judgement that the data in hand are of acceptable quality and are acceptably representative of the exposure variable of interest. The discussion in this parallels the Guiding Principles section and Technical Appendix of the Agency's policy for Monte Carlo Analysis, expanding these elements to provide more technical detail. The general outline in Section II follows that developed by Law and Kelton (1991). It is organized around three fundamental activities:

(*I*) *selecting candidate theoretical distributions* to determine which general families appear to be appropriate to use on the basis of the shape, summary statistics, and simple distributional plots;

(*II*) *estimating the intrinsic parameters of the candidate distributions* to define the specific distribution; and

(*III*) *assessing the quality of the resulting fit* by examining how closely they represent the true underlying distributions for the data of interest and using various Goodness-of-Fit (GoF) tests.

Assessors have a wide variety of commercially available distribution-fitting programs, spreadsheets, and dedicated statistical packages to assist them in deciding whether or not their data can be adequately represented by a theoretical distribution function. It is expected that most assessors will make use of one or more of these programs in fitting exposure data. While these programs can save a tremendous amount of work, their use should never be reduced to a simple mechanical exercise of importing the data, running the analysis and picking the "best fitting" distribution returned by the program. Furthermore, despite their obvious utility, many of the commercial fitting-packages are limited for fitting exposure data. For example, most fitting packages currently available cannot fit singly or multiply censored data, truncated distributions, or distributional mixtures. For these data, the assessor will have to seek more selective, powerful tools.

Many times in Monte Carlo analyses, an empirical distribution function (EDF) is used to characterize a model variable if the risk assessor has determined that the data themselves provides the best representation of the exposure variable. In Section III, we define an EDF and discuss the conditions under which the use of an EDF may be preferable to a CDF. The choice of whether or not to use an EDF in an assessment employing Monte-Carlo methods is ultimately up to the risk assessor and his/her level of comfort and confidence with the data and the method. Several approaches used to implement EDFs are also discussed.

Throughout Sections II and III, each key idea will be illustrated through a case study example.

Section II Parametric Methods

Parametric methods (as opposed to the non-parametric or empirical methods discusses in Section III) rely on a mathematical description of the *distribution* of values generated by a process. This section of the document describes the three standard activities (selecting candidate distributions, estimation of parameters, and assessing goodness-of-fit) used to describe the distribution and the adequacy of this description. The general outline follows that developed by Law and Kelton (1991).

Activity I – Selecting Candidate Distributions

Activity I involves the use of prior knowledge and exploratory data analysis to make preliminary assessments of which general *families* of distributions appear to best match the input data. This evaluation is performed on the basis of the shape, summary statistics, and simple distributional and graphical plots of the input data and does not, at this stage, involve the estimation of the specific statistical parameter values associated with each of these families.

Knowledge of the various properties and parameters associated with any of the various potential distributions can aid in the selection of an appropriate distributional family. Figure 1 provides a flow chart which may be used as a guide to selecting potential distributions for further analysis based on prior knowledge of distribution characteristics. It is not intended to be all-inclusive, but does cover a range of distributions which might be commonly seen in the area of exposure and health risk assessment.

Make Use of Prior Knowledge

The choice of input distribution should always be based on all relevant information (both qualitative and quantitative) available for a parameter. In selecting a distributional form, the risk assessor should consider the quality of the information in the database and ask a series of broad questions which might include the following:

> *Is there any mechanistic basis for choosing a distributional family? Is the shape of the distribution likely to be dictated by physical or biological properties or other mechanisms?* Ideally, the selection of candidate probability distributions should be based on consideration of the underlying physical processes or mechanisms thought to be key in giving rise to the observed variability. For example, assume that a persistent systemic pesticide is present in a lettuce plant and is not degraded or metabolized. If, due to weekly variations in sunlight, rainfall, and nutrient availability, the mass of each lettuce leaf increases each week by some random independent proportion of the mass achieved during the previous week, the distribution of residues in these lettuce plants will be lognormally distributed (Ott, 1995); in this case, the residue concentrations can be expressed as a random proportion of the quantity present in the immediately prior state. If each successive proportion is independent of the one before and many weeks pass between the initial and final states, the final residue concentration in the lettuce plant can be expressed as a <u>product</u> of random variables which gives rise naturally to a lognormal distribution. In general, if an exposure variable is the result of the <u>product</u> of a large number of other random variables, it would make sense to select a lognormal distribution for testing. As another example, the exponential distribution would be a reasonable candidate if the stochastic variable represents a process akin to inter-arrival times of events that occur at independent constant rates.
>
> *Is the variable discrete or continuous?* Can the variable only take on discrete values or is the variable continuous over some range? A discrete variable may only take one of several specific values, whereas a continuous variable may take on an infinite number of values. Examples of discrete variables would include

whether the crop is treated or not (e.g., 0 or 1), the number of times a given pesticide is applied per season, or the number of showers taken per week. Examples of continuous variable include the residue concentration of a given pesticide in a tomato, the amount of pesticide a.i. applied per acre in a season, or drinking water consumption rate.

Is the variable bounded or unbounded? If bounded, what are the bounds of the variable? What is the physical or plausible range of the variable? Is it semi-infinite (X>b)? Does it take on only positive values (X>0)?; Is it bounded by the interval [a,b]? A properly-fitted distribution should cover the range of values over which the modeled variable could theoretically extend. If a fitted distribution extends beyond the range of plausible values, then the model will produce implausible scenarios at the extreme tails of the distribution. Conversely, if a fitted distribution fails to adequately extend to cover real-world limits, the resulting model will not reflect the true nature of the potential variability.

Beta distributions are examples of bounded continuous distributions which might be considered for percent foliar dislodgeable residue (%FDR) which could vary between 0% and 100%, for example. Unbounded continuous distributions include the normal distribution: these distributions can sometimes be truncated, if necessary, to represent variables which have natural or practical physical limits (e.g., body weight). Semi-infinite continuous distributions (X>0) include the exponential distribution, the gamma distribution, the log-normal distribution, and the Weibull distribution. These distributions are all bounded on one-side (sometimes by 0) and extend to infinity and may describe variables which are censored due to limits of detection or some aspect of the experimental design. It is important to note that a correctly fitted distribution can extend *beyond* the range of observed data. This is expected since data are rarely observed at the theoretical extremes for the variable in question.

Are historical data available? Is it known that a variable of interest has been found to consistently have a certain distribution type in other data collection and distribution fitting research? Previous data may be available for similar (or even identical) situations. For example, environmental concentrations of a contaminant have sometimes to be found to be lognormally distributed. Time to complete certain tasks have been shown to follow in some cases a Weibull distribution. Human body weights have been modeled as a normal or log-normal distribution (Burmaster and Crouch, 1997). Consumption of water have been shown in some instances to be adequately represented by a log-normal distribution (see, e.g., EPA's *Exposure Factors Handbook*, the AIHC's *Exposure Factors Sourcebook*), or Roseberry and Burmaster (1997). A registrant should be aware of past modeling attempts to incorporate distributional information and may wish to incorporate this into its own assessments.

Does the sample represent a single population, or is the sample drawn from a mixture of subpopulations? Mixture models arise frequently in exposure and risk assessment. Discrete mixture distributions occur when the population of interest consists of a number of distinct subgroups, each with their own unique distribution. For example, different agricultural occupational groups may have different exposure distributions as a result of differing activities; produce grown in different regions of the country may have systematic differences in pesticide residue concentrations due to systematic differences across the U.S. in rainfall and rainfall patterns, soil types and conditions, and length of the growing season . Multi-modality provides a first strong suggestion that the observed sample is drawn from a mixture of distributions and is therefore not homogenous. As a second step, statistical tests (e.g., the non-parametric Kruskal-Wallis test) are available for assessing the homogeneity of different data sets (e.g., Florida residue data vs. California residue data) and determining whether the data sets can indeed be merged into *the* single residue distribution. Distinguishing between these different subgroups can be important for both scientific evaluations of risk and evaluations of different distributional issues. When these differences are recognized and the subgroups identified, the overall distribution can be built up from the individual distributions of the various subgroups.

Explore the Data

Exploring the data is an important step in the process of selecting plausible distributions. Exploratory data analysis can be thought of as consisting of two steps: (1) *characterizing the data through the use of summary statistics* and (2) *graphical data analysis*.

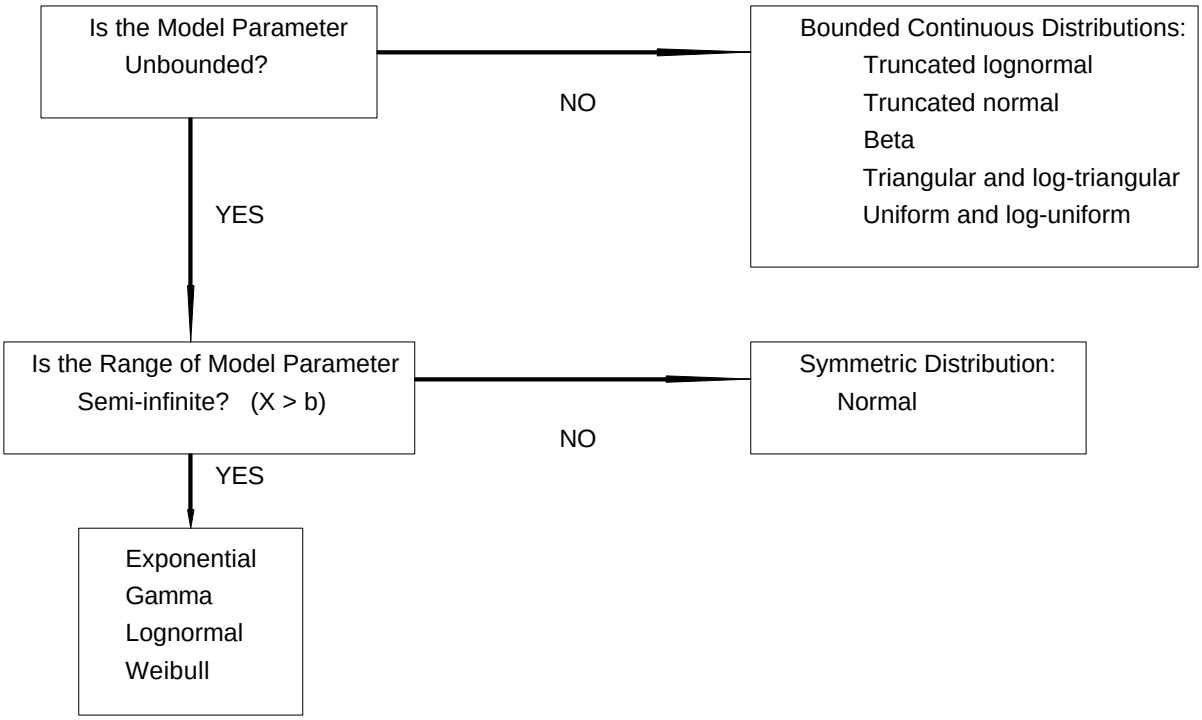
Summary Statistics. Summary statistics are useful for initially characterizing or describing the data. Common summary statistics fall into three basic groupings: (1) *measures of central tendency or location*, such as the mean or median; (2) *measures of dispersion or spread*, such as the variance; and (3) *measures of shape or skewness*.

Measures of central tendency are intended to indicate the "center" of the data and commonly include the mode, median, and mean. Other measures of location include the geometric mean and trimmed mean (Helsel and Hirsh, 1992).

Measures of spread are intended to indicate how dispersed the data are relative to some central value or specify the distance between selected observations. Common measures of spread include the range, inter-percentile ranges (e.g., inter-quartile range), standard deviation, variance, and coefficient of variation.

Measures of shape are intended to provide insights to the symmetry or asymmetry in the distribution of the data. The most frequently used measures of shape are skewness (asymmetry) and kurtosis (degree of peakedness). In some cases, these summary statistics can be used to suggest one or more appropriate distribution families for further testing as part of Activities II and III. For symmetric continuous distributions such as the normal, the mean and the median are equal. Thus, if the mean and median for any given data set are approximately equal, one might consider further analysis of the data to test the hypothesis that the distribution is normal. For exponential distributions, the coefficient of variation (defined as the standard deviation divided by the arithmetic mean, and sometimes expressed as a percent) is equal to 1 (or 100%). Therefore, if the mean and standard deviation of any given data set are numerically similar, an exponential distribution might be an appropriate distribution to hypothesize. Skewness and kurtosis values, considered together, can be used to assist in distribution selection The skewness value is a measure of the symmetry of the data, with perfectly symmetric distributions (like the normal) having a skewness value of zero. Right-skewed distributions, like the right-skewed lognormal, have positive skewness values whereas left skewed distributions have negative skewness values. Exponential distributions have a skewness value of 2. Thus, if a set of data has a coefficient of variation of approximately 1 and a skewness of approximately 2, an exponential distribution would be appropriate to consider. Many statistical and spreadsheet packages have built-in features for automatically calculating many summary statistics. Simply inspecting these output values can aid substantially in determining
candidate distributions for further analysis.

Figure 1. Selecting Continuous Theoretical Distributions



Box 1 lists data used as the case study throughout this section. The data in this Box represent a set of 25 hypothetical residue values in tomatoes. Several summary statistics for these residue data are shown in Box 2. A quick visual inspection of the data can reveal a number of important insights. Box 3 illustrates some of these insights for the sample tomato pesticide data.

BOX 1: Hypothetical Pesticide Concentrations in Tomatoes (ppm)

110.5	204.3
147.5	148.3
111.6	66.9
139.0	53.6
72.9	68.5
109.8	108.0
94.8	97.6
68.8	78.2
142.3	68.2
70.8	80.3
74.6	267.7
169.7	170.0
143.7	

Graphical Data Analysis. The risk assessor can often gain important insights by using a number of simple graphical techniques to explore the data prior to numerical analysis. The importance of this phase of visual inspection cannot be over-emphasized. A wide variety of graphical methods have been developed to aid in this exploration including frequency histograms, stem and leaf plots, dot plots, line plots for discrete distributions, box and whisker plots, and scatter plots [Tukey (1977);; du Toit et al. (1986); Morgan and Henrion, (1990)]. These graphical methods are all intended to permit visual inspection of the density function corresponding to the distribution of the data. They can assist the assessor in examining the data for skewness, behavior in the tails, rounding biases, presence of multi-modal behavior, and data outliers. Graphical methods, however, can be highly misleading in the face of considerable uncertainty due to small sample size or a high coefficient of variation.

BOX 2: Summary Statistics for Hypothetical Pesticide Concentration in Tomatoes (ppm)

Quantiles

maximum	100.0%	267.70
	99.5%	267.70
	97.5%	267.70
	90.0%	183.72
quartile	75.0%	145.60
median	50.0%	108.00
quartile	25.0%	71.86
	10.0%	67.68
	2.5%	53.60
	0.5%	53.60
minimum	0.0%	53.60

Moments

Mean	114.7056
Std Dev	51.2019
Std Error Mean	10.2404
Upper 95% Mean	135.8405
Lower 95% Mean	93.5707
N	25.0000
Sum Weights	25.0000
Sum	2867.6400
Variance	2621.6304
Skewness	1.2857
Kurtosis	1.8846
CV	44.6376

A frequency histogram is a graphical estimate of the empirical probability density function and can be compared to the fundamental shapes associated with standard analytic distributions (e.g., normal, lognormal, gamma, Weibull). Law and Kelton (1991) and Evans et al. (1993) have prepared a useful set of figures which plot many of the standard analytic distributions for a range of parameter values. Frequency histograms can be plotted on both linear and logarithmic scales and should be plotted to avoid too much jaggedness or too much smoothing (i.e., too little or too much data aggregation). If the appearance of the histogram does not change much when varying the bin width over a reasonably wide range, then the data analyst can feel confident that any observed patterns are genuine. If, on the other hand, the appearance changes in a fundamental way depending on the selected bin width, any observed patterns at a specific bin width may be an artifactual and should not be trusted. As a starting point, some authors suggest that it may be useful to select the number of bins according to $k = 1 + 3.322 \log_{10} n$ where n is the number of data points.

Line graphs apply to discrete random variables and are estimates of the probability mass function. In a line graph, the proportion of values in the sample data set equal to a particular

discrete value are plotted and compared, on the basis of shape, to the probability mass functions for discrete distributions (e.g., binomial, geometric, Poisson, negative binomial, etc.).

Box plots (Tukey box plots, box and whisker plots) can be a very effective graphic display for summarizing the distribution of a data set. Box plots provide easily explained and easily comprehended visual summaries of:

- the center of the data (median - the center line of the box)
- the spread in the data (inter-quartile range - the box length)
- the skewness (quartile skew - the relative size of the box halves)
- the range (whiskers - lines from the ends of the box to the maximum and minimum of the data or to some other selected endpoint, e.g., the 5th and 95th percentiles, etc.)

There are three basic versions of the box plot: (1) the *simple box plot*, (2) the *standard box plot*, and (3) the *truncated box plot*. In the commonly-used *standard box plot*, the whiskers extend only to the last data point within one step beyond either end of the box. A step is defined as 1.5 times the length of the box or approximately 1.5 times the inter-quartile range. Data points beyond 1.5 steps of either end of the box are plotted as individual points. When constructed in this manner, the box plot provides a rapid visual impression of the prominent features of the data. The median (or central line within the box) shows the location of the center of the data. The spread of the central 50% of the data are represented by the length of the box. And the length of the whiskers (relative to the box) show how stretched the tails of the distribution are. Individual points which extend beyond the whiskers are outside values which may be further investigated and provide clues as to the distributional form. If the distribution is symmetric (e.g., as with a normal distribution), the box will be divided into two equal halves by the median, the upper and low end whiskers will be the same length, and the number of extreme data points will be distributed equally on either end of the plot Two other kinds of box plots (simple and truncated box plots) are more fully discussed by Helsel and Hirsh (1992).

Because of the variety of box plots available, the potential for confusion exists and all box plots submitted to HED should be clearly labeled as to which values are being represented.

BOX 3: Distributional and Statistical Insights into Hypothetical Tomato Pesticide Data Set

A number of important insights on the data and its distributional form can be gained by inspecting the summary statistics commonly provided by standard statistical packages. If the distribution is normal, for example, the mean will be approximately equal to the median. From the statistics provided in Box 2, we see that the median of 108.0 is located within the 95% confidence interval of the mean (i.e., 93.6 to 135.8). We also see that the coefficient of variation of 0.446 (44.6%, as indicated in the statistical output) is less than 1, indicating that a normal distribution might be appropriate to hypothesize. Since the mean of 114.7 and standard deviation of 51.2 are not equal, an exponential distribution is unlikely to be appropriate. The skewness value of 1 (as opposed to 2) further supports the elimination of the exponential distribution as a viable candidate for further consideration.

Formal Tests for Normality and Lognormality

While examination of the summary statistics, frequency histograms, and box-and-whisker plots associated with a data set are useful exercises in exploratory data analysis, several procedures are available to formally test for normality (or lognormality when log-transformed data are used) and can be used to confirm the assumption of normality/lognormality. Such tests include Shapiro-Wilks test (for sample sizes $\leq$ 50), D'Agostino's test (for sample sizes 50), and Filliben's statistic (sample size >50), which is an extension of the Shapiro-Wilk test. The Shapiro-Wilk and D'Agostino tests are the tests of choice when testing for normality (or lognormality) and are more fully described in a number of standard texts. While the Shapiro Wilk test is one of the most powerful tests for

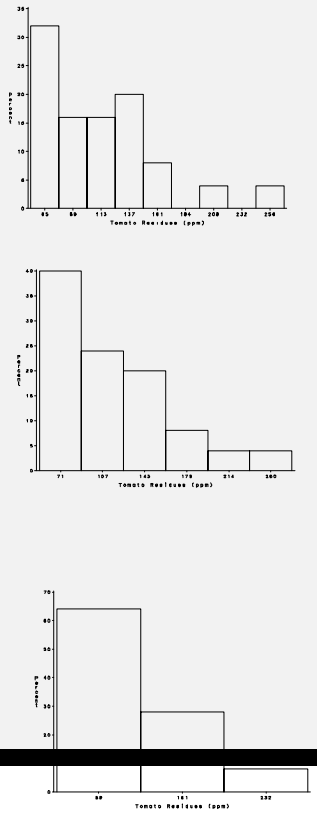
normality, it is difficult to implement by hand as it involves calculating a correlation between the quantiles of the standard normal distribution and the ordered values of the data set. It is, however, easily implemented as part of many statistical software packages. These tests (and many more) are more fully discussed in the EPA publication *Practical Methods for Data Analysis* (U.S. EPA, 1996). This EPA publication is available on-line and can be downloaded in PDF format (see References and Suggested Readings for http:// address)

It is important to remember during this activity that it is less critical for the analyst to be able to state with absolute certainty that the data are distributed in the hypothesized manner (e.g., lognormally) than it is to determine that the hypothesized distribution is "adequately representative" of the data. The basic question to be answered in the affirmative is whether the empirical distribution of the data is sufficiently well-approximated by the hypothesized distribution for the intended purpose.

Knowledge of the various properties and parameters associated with any of the various potential distributions can aid in the selection of an appropriate distributional family. A list of selected theoretical distributions is included in Table 1 along with a brief description of some of their potential uses. As with Figure 1, it is not intended to be all-inclusive, but does cover a range of distributions which might be commonly seen in the area of exposure and health risk assessment.

BOX 4: Frequency Distribution Histograms for Hypothetical Pesticide Data

For a histogram of the pesticide residue data, the initial number of number of bins is estimated as $k = 1 + 3.322 \log_{10}(25)$ 6 The figures below show histograms for the tomato residue data for 3, 6, and 9 bins. For these data, 6 bins appear to strike a reasonable balance between too much smoothing for the 3 bin histograms and too much jaggedness apparent for the 9 bin histogram.



BOX 5: Determination of the Appropriate Distributional Family for the Hypothetical Residue Data

Box 4 suggested that a normal distribution would be appropriate to hypothesize for the hypothetical pesticide data. However, the box and whiskers plot of the actual data reveals a decidedly right-skewed distribution; in addition the Shapiro-Wilk statistic of 0.88 ($p<0.0063$) also suggests that a normal distribution is not appropriate. As indicated before (and confirmed by the shape of the histogram and box-and-whisker plot), an exponential distribution is also inappropriate for further consideration. Log-transformation of the hypothetical data produces a symmetric mound-shaped histogram and a box-and-whisker plot showing characteristics of the normal distribution (eg., a box divided into two equal halves by the median, whiskers of similar length, and an equal number of extreme data points on either end of the plot). The summary statistics further suggest that a lognormal distribution may be appropriate (mean median and a skewness value substantially closer to 0); the Shapiro-Wilk test ($W = 0.951$ with $p = 0.27$) confirms this as an appropriate distribution for further consideration and analysis as part of Activity II.

Having determined that the log-normal distribution is the distribution most appropriate for further analysis, the two subsequent activities are determining the most appropriate distribution (Activity II) and performing tests to verify that the selected distribution and its parameters adequately fit the empirical data.

Table 1 Selected Theoretical Distributions[a]

Distribution Type	Distribution Description
Discrete	
Bernoulli	The Bernoulli distribution is used to model random events when there are only two possible outcomes (e.g., success or failure, treatment or no treatment) and is used to generate other discrete random variables (e.g., binomial, geometric, and negative binomial). A Bernoulli random variable can be thought of as the outcome of an experiment that either "fails" or "succeeds" and is fully characterized by its parameter *p*, representing the probability of an event occurring.
binomial	The binomial distribution models the number of successes in *n* independent Bernoulli trials, with the with probability *p* of success in each trial. It is produced by processes that (1) can produce only one or the other or two outcomes and (2) are carried out a finite number of trials. It is fully characterized by the parameters *n*, *p*, and *x* representing the number of trials, the probability of success in each trial, and the number of successes, respectively.
discrete uniform	The discrete uniform distribution models random occurrences when there are several possible outcomes, each outcome with the same probability of occurrence. Typically used as a "first" model for a quantity that is varying among integers, but about which little is known.
geometric	The geometric distribution models the number of failures before the first success in *n* independent Bernoulli trials, each trial with an identical probability of success. It is a direct analogue of the exponential model except is limited to integers.
	.
Bounded Continuous	
beta	The beta distribution is a very flexible distribution capable of exhibiting a wide variety of shapes. It is often used to model bounded data, to model distributions for proportions or fractions, or to model time to complete some task. It can also be used as a rough model in the absence of data (see Law and Kelton, 1991). Two parameters suffice to describe this distribution (α_1, α_2)
triangular, log-triangular	The triangular distribution is often used a rough model in the absence of data when the values toward the middle of a range of possible values are more likely to occur than values near either extreme. There is no mechanistic basis for this model which is typically used to represent subjective uncertainties. If the range covers several orders of magnitude, the log-triangular distribution is sometimes used. The minimum, maximum, and most likely value suffice to describe this distribution.
uniform, log-uniform	The uniform distribution is often used in the absence of data as a crude model when the quantity is known to randomly vary between known limits but where little else is known. Its use is appropriate when we are able to identify a range of possible values, but are unable to determine which values within the range are more likely to occur than others. The minimum and maximum values suffice to describe this distribution. If the limits cover several orders of magnitude, the log-uniform is sometimes used.

Unbounded Continuous	
normal	The normal distribution models phenomena that are the result of the sum of many other random variables (by the Central Limit Theorem). In other words, if a large number of variables are added together (such that no one variable contributes a substantial amount to total variation), the result will take the shape of a normal distribution. These frequently involve small measurement errors of various types and any process whose final outcome is the result of many independently determined sums. The mean and standard deviation suffice to describe this distribution. The skewness of the normal distribution is 0 (it is symmetric) and the kurtosis is 3. As negative quantities can be generated with the normal distribution, this is in some cases theoretically inappropriate. However, as long as the coefficient of variation of less than ca. 0.2, generation of negative values is sufficiently improbable so as not to be of concern since the probability of generation of values more than five standard deviations from the mean is quite small.

Non-negative Continuous	
exponential	When events are purely random, the times between successive events are described by an exponential distribution. The exponential distribution is frequently used to describes the time between events for Poisson processes (i.e., processes for which the probability of an event per unit time interval is constant and independent of the number and timing of events which occurred in the past) or the fraction of individuals (or anything else) remaining in a system at various times after the start of an exponential decline. The mode of exponential distribution is zero and the probability of occurrence continually decreases with increased values. The skewness of an exponential distribution is two. This distribution complements the Poisson distribution which characterizes the number of occurrences per unit time and is a special case of the gamma and Weibull distributions. The exponential is less tail-heavy than the lognormal and extreme values therefore have a lower probability. It is characterized by a single parameter (β), representing the mean time between events.
gamma	The gamma distribution includes is widely used in environmental analysis to characterize pollutant concentrations as well as used in meteorological processes to characterize precipitation. It is also commonly used to represent the time to complete some task. The tail of the gamma distribution is not as tail-heavy (long) as the lognormal and it therefore ascribes a lower probability to extreme values than does the lognormal distribution . The gamma is typically describe by two parameters, a shape parameter and a scale parameter. When the shape parameter is 1, the distribution is equivalent to the exponential distribution.
lognormal	The lognormal distribution models quantities that are the product of a large number of other quantities (i.e., if one were to multiply a large number of random variables together, the result will tend toward a lognormal distribution). This distribution results when the logarithm of a random variable is described by a normal distribution . It is widely used in environmental analysis to represent positively valued data exhibiting positive skewness. Examples include concentrations of chemicals in environmental media and amounts of those media which are consumed, efficiencies of absorption, and rates of elimination of toxicants. The lognormal distribution has a heavier (longer) tail than the exponential, gamma or Weibull distributions. There are three common ways to parameterize a lognormal distribution: (1) arithmetic mean and standard deviation of the log-transformed variables; (2) geometric mean and standard deviation of the non-transformed variables; and (3) arithmetic mean and standard deviation of the non-transformed variables.
Weibull	The Weibull distribution is widely used in life data analysis, time to complete some task, and time to equipment failure. The Weibull distribution is less tail heavy than the lognormal and thus ascribes a lower probability to extreme events. It is typically described by two parameters, a scale parameter and a shape parameter. As with the gamma distribution, the distribution is equivalent to the exponential distribution when the shape parameter is 1,

The above information was obtained mainly from Hattis and Burmaster (1994), Vose (1996), Law and Kelton (1995), and Morgan and Henrion (1990)

[a]Note: Distributional plots, probability and cumulative density functions, interpretation of distributional parameters, formulae for important statistical terms (e.g., mean, standard deviation, etc.) are available from the literature (e.g., see Law and Kelton (1995), Vose (1996) and Evans et al. (1993))

Activity II – Estimation of Parameters

Once a candidate distribution family is selected (e.g., a lognormal distribution), we estimate the parameters of the candidate family in order to have a completely specified distribution for use in the simulation. Parameter estimation is generally accomplished using conventional statistical methods, the most popular of which include the method of maximum likelihood, probability plotting methods, and the method of moments. See Law and Kelton (1991), Evans et al. (1993), Gilbert (1987), and Vose (1996).

Parameter Estimation Methods

Maximum Likelihood Method. Probably the most often-used method for estimating the parameters of a distribution is the method of maximum likelihood. For some distribution families (e.g., normal, exponential, geometric), maximum likelihood estimators (MLEs) are well-defined values resulting from a straightforward algebraic calculation, but for others solving the equations is computationally intensive and special software is required.

There are a number of references which derive the MLE for several common distributions (e.g, Vose (1996), Ott (1995) Evans et. al. (1993)). For the purposes of this document we will simply state that the MLE for the mean and standard deviation of a normally distributed population are simply the mean and standard deviation, respectively, of the observed sample data. For the exponential distribution, the MLE for the single parameter of the exponential distribution is the mean of the observed sample data. For the geometric distribution, the MLE for the *p* parameter is $1/(\bar{x}+1)$.

Probability Plotting Methods. Probability plotting methods, sometimes called linear least square regression methods or regression on order statistics, are based on finding probability and data scales so that the theoretical cumulative distribution function plots as a straight line. The transformed data is then plotted against the linearized CDF and ordinary linear regression is performed to estimate the parameters of the fitted distribution. This method is applicable to theoretical distributions whose CDFs are expressible as a function of one or two parameters, for example, the exponential, normal, lognormal, and Weibull distributions. The following are instructions for linearizing the CDF and estimating the parameters of the fitted distribution:

> <u>For a distribution which has been hypothesized to be normal</u>
> Construct a normal probability plot with z(p) on the abscissa (the "x" axis) vs. each x_n value on the ordinate (the "y" axis)[1]. If the normal probability plot is a straight or near-straight line, this is evidence that the distribution is normal and the data are well-modeled by a normal curve. Using ordinary least-squares regression, calculate the slope of the fitted line and its intercept. The intercept is an estimate of the arithmetic mean of the distribution while the slope is an estimate of the arithmetic standard deviation of the distribution. These values should be compared with (and comparable to) the values calculated using ML method

[1] Specialized statistical software is available to create normal probability plots. Alternatively, one can create these plots using certain spreadsheet software. For example, to create a normal probability plot using Excel or Quattro Pro, first rank the observations (r_1, r_2, r_3, ... r_n) in ascending order (from lowest to highest) and assign each observation a rank (e.g, lowest observation receives a rank of 1, the next receives a rank of two, all the way to the Nth observation which receives a rank of N). For each observation, the cumulative rank is then calculated using a plotting position formula (e.g., the Weibull plotting position formula $r_I/n+1$). This can be considered similar to a percentile value except percentile values range to 100%. Next, the normal quantile is calculated for each cumulative rank: the normal quantile is the z-score associated with each percentile and can be determined using Excel's NORMSINV function. Finally, each observation's normal quantile (or z-score) is plotted on the x-axis against each observation on the y-axis.

described above. The uncertainty in these parameter estimates can be roughly gauged by the statistical confidence interval about the intercept and slope as determined by the linear regression statistics.

<u>For a distribution which has been hypothesized to be lognormal</u>
Calculate the natural logarithms of each of the x_n values for n = 1 to N. Construct a normal probability plot with z(p) on the abscissa (the "x" axis) vs. each ln [x_n] value on the ordinate (the "y" axis) as described in the previous footnote (except than ln [x_n] is substituted for [x_n]). If the lognormal probability plot is a straight or near-straight line, this is evidence that the distribution is lognormally distributed and the data are well-modeled by a lognormal distribution. Using ordinary least-squares regression, calculate the slope of the fitted line and its intercept. The slope is an estimate of the mean of the natural logarithms of the distribution (μ) while the intercept is an estimate of the standard deviation of the logarithms (σ). These values should approximate the values for the mean and standard deviation, respectively, calculated by the following formulae:

$$\mu \quad \overline{\ln[x]} \quad \frac{\sum \ln[x_n]}{N}$$

$$\sigma \quad \sqrt{\frac{\sum (\ln[x_n] \quad \overline{\ln[x]})^2}{N \quad 1}}$$

To calculate the arithmetic mean and standard deviations from these regression values (i.e., to define the distribution in its original terms), the following formulae are used:

$$\mu \quad e^{[\mu \quad \frac{1}{2}\sigma^2]}$$

$$\sigma \quad e^{\mu}\sqrt{(e^{\sigma^2})(e^{\sigma^2} \quad 1)}$$

<u>For a distribution which has been hypothesized to be exponential</u>
First, calculate the cumulative frequency by ranking the observations from lowest to highest as described in the previous footnote. Then, for each ranked observation subtract this quantity from 1 and take the natural logarithm of this difference. Plot this value on the y-axis vs. each individual data point on the x-axis. If the plot is reasonably straight, this is evidence that the distribution is *exponentially* distributed. Using ordinary least-squares regression, calculate the slope of the fitted line <u>fixing the y-intercept of the regression line at the point (0, 1)</u>. The calculated slope of this line is the β parameter appearing in the exponential model [$f(x) = 1 - e^{-x/\beta}$] and should be compared with (and comparable to) the value calculated from the ML method for exponential distributions described above. As before, the uncertainty in this parameter estimate can be roughly gauged by the confidence interval about the slope as determined from the linear regression statistics.

For a distribution which has been hypothesized to be Weibull

The two characteristic parameters of a Weibull distribution (i.e., the scale and shape parameters) can most easily be determined by either using dedicated statistical distribution fitting software or by plotting the data on specialized commercially-available Weibull probability paper (e.g., see Craver (1996)) . In the latter case, the Weibull scale and shape parameters can be read directly from the probability plot. For a Weibull curve (with a location parameter of 0), the scale parameter is typically represented by the 63.2 %-ile.

Weibull plots can also provide information about other potential distribution families. For example, the slope of the plotted points provide additional information about the distribution family or class with slopes of 1, 3, and 5 evidence of exponential, lognormal, and normal distributions, respectively.

For a distribution which has been hypothesized to be Beta

As with the Weibull distribution, characteristic parameters of a beta distribution can most easily be determined by either using dedicated statistical distribution fitting software or by plotting the data on specialized commercially-available beta probability paper.

For a distribution which has been hypothesized to be Gamma

As with the Weibull and beta distributions, gamma parameters can most easily be estimated by using commercially-available software or gamma probability paper.

An example of these methods using the hypothetical pesticide data in shown in Box 6.

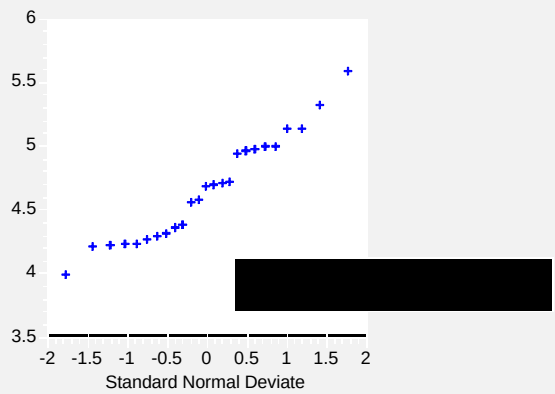
Method of Matching Moments.

The method of moments replaces each uncertain variable by its mean and variance and uses probability laws to estimate the mean and variance of the models outcome. However, the method of moments has some fairly severe limitations. For example (Vose, 1996),

- it assumes that all variables in the model are independent
- it assumes that the outcome is approximately normally distributed
- it assumes either that all variables in the model are approximately normally distributed or that the model has a very large number of uncertain variables, none of which dominates the outcome; and
- it cannot easily cope with divisions, exponents, power functions, discrete variables, etc.

BOX 6: Determination of the Appropriate Parameters for the Hypothesized Lognormal Distribution of the Pesticide Data

Having determined that a log-normal distribution is the most appropriate distribution for further analysis of the hypothetical tomato residue data, the analyst should next determine the appropriate parameters which define the distribution (i.e., the mean and standard deviation). A normal probability plot of the log-transformed values reveals a straight line with a slope of 0.4447 and an intercept of 4.65789. This intercept is an estimate of the mean of the log-transformed values (i.e., it is the ') and the slope is an estimate of the standard deviation of the log-transformed values (it is the σ')



These values are comparable to the mean and standard deviation calculated as follows:

$$\mu \quad \overline{\ln[x]} \quad \frac{\sum \ln[x_n]}{N} \quad 4.6575$$

$$\sigma \quad \sqrt{\frac{\sum (\ln[x_n] \quad \overline{\ln[x]})^2}{N \quad 1}} \quad 0.4122$$

Calculating the arithmetic mean and standard deviation from the regression values in order to define the distribution in its original terms:

$$\mu \quad e^{[\mu \quad \frac{1}{2}\sigma^2]} \quad 116.33$$

$$\sigma \quad e^{\mu}\sqrt{(e^{\sigma^2})(e^{\sigma^2} \quad 1)} \quad 55.16$$

Thus, the most appropriate distribution to hypothesize for the hypothetical tomato pesticide residue data is a lognormal distribution with these parameters.

Activity III – Assessing Goodness of Fit

Activity III involves determining how well our selected (and now fully-defined) candidate distribution is in representing the true underlying distribution for our data. Having estimated the parameters of the candidate distributions, it is necessary to evaluate the "quality of the fit" and, if more than one candidate distribution was selected, to select the "best" distribution from among the candidates. A goodness of fit test (GoF test) is a statistical test in which the null hypothesis (H_o) is that the observed data are characteristic of a random variable with the hypothesized distribution function (e.g, exponential with a β parameter of 0.8). Unfortunately, there is no single, unambiguous measure of what constitutes best fit. Ultimately, the risk assessor must judge whether or not the fit is acceptable. This judgement should be based on a consideration of goodness-of-fit statistics as well as graphical comparisons of the fitted and empirical distributions, paying special attention to issues relevant to the analysis, e..g, fit in the lower or upper tails (but note that this is where the confidence intervals are widest). It is also important to consider the processes that generated the data and to look for probabilistic distribution models that arise from similar processes. Used in conjunction with the probability plots and statistical measures used in Activity I, GoF tests can, however, be powerful tools for verifying that a chosen distribution is at least reasonable.

Goodness-of-Fit Tests

Goodness-of-fit tests are formal statistical tests of the hypothesis that the set of sampled observations are an independent sample from the known or assumed distribution. The null hypothesis, H_o, is that the randomly sampled set of observations are independent, identically distributed random samples from a population with the hypothesized distribution. The GoF tests indicate whether the hypothesized distribution can be reasonably rejected as improbable. It is important to recognize that failure to reject H_o is not the same as accepting H_o as true These tests, taken alone, are not very powerful for small to moderate sample sizes (i.e., subtle but systematic disagreements between the data and the hypothesized distribution may not be detected); conversely, the tests can be too sensitive for large numbers of data points -- that is, for data sets with a large number of points, H_o will almost always be rejected.

Commonly used goodness-of-fit tests include the chi-square test, Kolmogorov-Smirnov test, and Anderson-Darling test. These are described further below.

Chi-Square Test. The chi-square test is based on the normalized difference between the square of the observed and expected frequencies and can be viewed as a comparison of the frequency histogram with the fitted probability density function or probability mass function. The chi-square test statistic is computed by dividing the entire range of the fitted distribution into k contiguous, non-overlapping intervals and counting the number of data samples falling into each interval (N_j). This count is compared to the expected number of observations in a bin. Given a sample size of n, i.e., expected number of data points in the jth bin (j = 1 to k) is np_j where $p_j = F(x_j) - F(x_{j-1})$ .The chi-square test statistic is computed as

$$\chi^2 \quad \sum_{j\ 1}^{k} \frac{(observed \quad expected)^2}{expected} \quad \sum_{j\ 1}^{k} \frac{(N_j \quad np_j)^2}{np_j}$$

The chi-square test is highly dependent on the width and number of intervals chosen. Law and Kelton recommend selecting equi-probable bin widths such that np_j 5; D'Agostino and Stephens (1986) recommend selecting k equi-probable intervals where $k = 2n^{2/5}$ For example, if one had 100 data points, one might wish to form k = 13 (equiprobability) intervals. If 13 equiprobability intervals are formed for the 100 data points, then the expected number of points in each interval (i.e., the np_j) would be calculated as follows:

$$n \times \frac{1}{k} \qquad 100 \times \frac{1}{13} \qquad 8$$

This satisifies the criteria that each bin size be chosen such that an equal number of points (in this case, 8) numbering at least five be expected in each bin. The size of each bin width is calculated by inverting the cumulative distribution function[2]. This is best illustrated by returning to our pesticide example as shown in Box 7.

Kolmogorov-Smirnov Test. The Kolmogorov-Smirnov Test is a non-parametric test based on the maximum absolute difference between the theoretical and sample (or step-wise empirical) Cumulative Distribution Functions (CDFs). Large values of this statistic indicate a poor fit while small values indicate a good fit. Critical values for the K-S statistic depend on whether or not the parameters of the distribution are known *a priori* or have to be estimated from the data. See Law and Kelton (1992) and D'Agostino and Stephens (1986).

The Kolmogorov-Smirnov test is most sensitive around the median and less sensitive in the tails and is best at detecting shifts in the empirical CDF relative to the known CDF. It is less proficient at detecting spread but is considered to be more powerful than the chi-square test.

Anderson-Darling Test. The Anderson-Darling test is designed to test goodness-of-fit in the tails of a probability density function based on a weighted-average of the squared difference between the observed and expected cumulative densities. Additional information and critical values for Anderson-Darling statistic for the all parameters known case, and for the normal , exponential, and Weibull distributions are given by Law and Kelton (1992)and D'Agostino and Stephens (1986). Because of its relative emphasis on fit in the tails, the Anderson-Darling statistic may be particularly useful to assessors as a goodness-of-fit statistic.

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[2] While these inverses can be calculated algebraically for functions with closed forms such as the exponential, use of a spreadsheet program or numerical methods may be necessary for continuous functions such as the normal, lognormal, gamma, and beta distributions. Excel© and QuatroPro© have built-in inverse functions which are called NORMSINV, LOGINV, GAMMAINV, and BETAINV, respectively, which return the value associated with any given probability. In our hypothetical pesticide example (see Box 7), the given probability is equal to 1/j for j = k down to 1, with k = 5 (i.e., 1/j = 0.2 for the first bin width, 0.4 for the second bin width, 0.6 for the third width, 0.8 for the fourth, and 1.0 for the last).

BOX 7: Equiprobability Chi-Square Test of Sample Pesticide Data

For our pesticide example, we have a total of 25 data points and desire to select *k* equi-probable intervals. We select *k* a value of 5: although the formula would yield for k a value of 7 ($k = 2(25^{2/5})=7$), we require a minimum of 5 data points per bin and thus for 25 points, 5 bins (or equiprobability intervals) are necessary. If 5 equiprobability intervals are formed for the 25 data points, then the expected number of points in each interval (i.e., the np_j) is 5 (or n x 1/k = 25 x (1/5)). With 5 bins (or intervals), the given probability is equal to 1/j for j = k down to 1 with k = 5. That is, 1/j = 0.2 for the first bin width, 0.4 for the second bin width, 0.6 for the third bin width, 0.8 for the fourth, and 1.0 for the last. The individual bin widths are calculated using Excel's LOGINV function with the assumed mean and standard deviation calculated in Activity II. The individual bin widths, observed number of points in each bin, the expected number of points in each bin, and the calculated Chi-square values are shown below:

.Calculation of Chi-Square Value for Pesticide Example Using a Lognormal (116.3, 55.2) Hypothesized Distribution

J	Interval[a]		No. Observed	No. Expected[b]	Chi-Square[c]
	Lo	Hi			
1	0	72.46	6	5	0.2
2	72.46	94.14	4	5	0.2
3	94.14	117.94	6	5	0.2
4	117.94	153.2	5	5	0
5	153.2.		4	5	0.2
TOTAL			25	25	0.8

[a] Intervals are calculated by evaluating the inverse of the hypothesized distribution at each j value. In this example, the hypothesized distribution is lognormal with an arithmetic mean of 116.3 and an arithmetic standard deviation of 55.2. Since this distribution has no closed form, the upper end of each of the 5 intervals must be evaluated with Excel (or QuatroPro) using the LOGNORMINV function with a mean (of the logs) of 4.657489 and a standard deviation (of the logs) of 0.444947 (each of which were calculated previously in Box 6).

[b] The number expected in each bin was calculated previously as n x 1/k

[c] Each chi-square value is calculated as $(\text{observed-expected})^2$ / expected. The final chi-square value is calculated as the sum of these individual chi-squared values

The degrees of freedom is given by $\nu = k - m - 1$ where k is the number of bins (or classes) and m is the number of parameters we are estimating from the data (i.e., the mean and standard deviation). From this, $\nu = 5-2-1 = 2$. The χ^2 critical value for $p = 0.1$ and 2 degrees of freedom is calculated as $\chi^2(0.9;2) = 4.6$. Since our observed χ^2 value of 0.8<4.6, , we are unable to reject the lognormal model with an arithmetic mean of 116.3 and an arithmetic standard deviation of 55.2 on the basis of this chi-squared test of fit: the Chi-square value suggests that there is no reason to conclude that our data are poorly fitted by our hypothesized lognormal distribution.

Cautions Regarding Goodness-of-Fit Tests

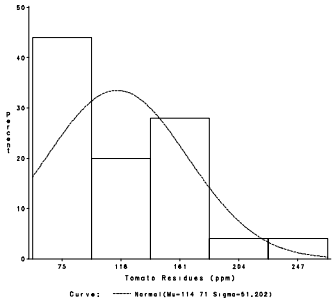
Care must be taken not to over-interpret or over-rely on the findings of goodness-of-fit tests. It is far too tempting to use the power and speed of computers to run goodness-of-fit tests against a generous list of candidate distributions, pick the distribution with the "best" goodness-of-fit statistic, and claim that the distribution that fit "best" was not rejected at some specific level of significance. This practice is statistically incorrect and should be avoided [Bratley *et al.*, 1987, page 134]. As indicated previously, Goodness-of-fit tests have notoriously low power and are generally best for rejecting poor distribution fits rather than for identifying good fits. For small to medium sample sizes, goodness-of-fit tests are not very sensitive to small (but potentially significant) differences between the observed and fitted distributions. On the other hand, for large data sets, even minute differences between the observed and fitted distributions may lead to rejection of the null hypothesis. For small to medium sample sizes, goodness-of-fit tests should best be viewed as a systematic approach to detecting gross differences.

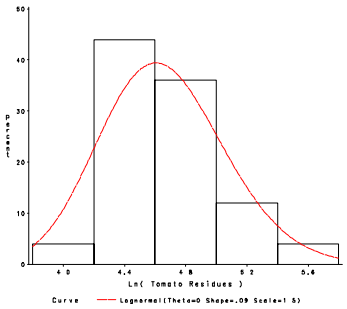
We note that there is absolutely no substitution for careful visual inspection of both the data and the theoretical distribution of the fit to the data. The human eye and brain are able to interpret and understand data anomalies far beyond the ability of any computer program or GoF tests. GOF tests may, *at best*, simply serve to confirm what the analyst has found though visual inspection. One may quite appropriately decide to retain a particular probability model despite having rejected it on the basis of GoF tests if it appears to be a good fit to the data as judged by the visual inspection of the probability plots and other comparisons.

Graphical (Heuristic) Methods for Assessing Fit

Graphical methods provide visual comparisons between the experimental data and the fitted distribution. Despite the fact that they are non-quantitative, graphical methods often can be most persuasive in supporting the selection of a particular distribution or in rejecting the fit of a distribution if one has a sufficiently large sample size. This persuasive power derives from the inherent weaknesses in numerical goodness-of-fit tests. Commonly used graphical methods for assessing goodness of fit include:

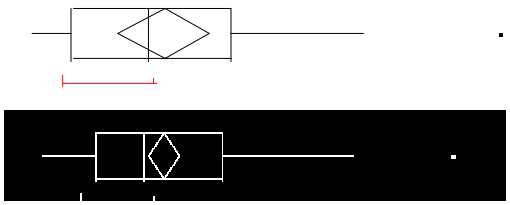
Frequency comparisons compare a histogram of the experimental data with the density function of the fitted data. Frequency comparisons must be interpreted with care since the visual comparison will depend on the number of bins used to generate the histogram of the data. Two examples of a frequency comparison are shown below for our sample pesticide data. The leftmost illustration compares the untransformed pesticide data to the normal curve while the illustration to the right compares the log-normalized pesticide residue data to the normal curve





Box plot comparisons compare a box plot of the observed data with a box plot of the fitted distribution. This is illustrated below for the sample pesticide residue data (observed) and the lognormal distribution (fitted).

Observed data



Fitted Distribution

Probability-Probability plots (P-P plots) compare the observed cumulative density function (i.e., the sample probability) with the fitted cumulative density function (i.e., the model probability). P-P plots are used to graphically evaluate how well the data fit a given (hypothesized) theoretical distribution, e.g. normal, lognormal, Weibull, etc. P-P plots tend to emphasize differences in the *middle* of the predicted and observed cumulative distributions, and are less sensitive than Q-Q plots to differences in the tails (where risk assessors are more frequently interested).

Theoretical Quantile-quantile plots (Q-Q plots) graph the *quantiles* of the specific fitted (or theorized) distribution against the *quantiles* of the actual data. To construct a theoretical Q-Q plot, one sorts the data in ascending order and calculates a cumulative frequency (as done for the normal probability plot) using the standard plotting formula (i.e., $r_I/N + 1$). At this point, the z value associated with this probability (or cumulative frequency) value is calculated and transformed to its original scale. In other words the quantile value associated with this cumulative probability from the *theoretical distribution* is calculated. This can be done with Excel or QuantroPro using their inverse cumulative probability functions (e.g., NORMINV, LOGINV, or GAMMAINV) or can sometimes be done analytically using an algebraic formula for distributions for which there is a closed form for the cumulative probability function (e.g., the exponential and Weibull distributions). [3] Finally, the actual data values are plotted against the values <u>which would have been seen</u> if the data were distributed according to the hypothesized distribution.

The theoretical Q-Q plot is used to determine how well the data set is modeled by the theorized distribution: any systematic deviations in the distribution of our sample data from the hypothesized distribution are highlighted and (ideally at least) will be readily apparent.. If the graph is linear (and there are no significant systematic deviations from linearity), this is evidence in support of the data fitting the specific hypothesized distribution. Q-Q plots tend to emphasize differences in the *tails* of the fitted and observed cumulative distributions. The *deviation* of a Q-Q plot from a straight line can provide diagnostic information about the theorized distribution. For example, if the data in the upper tail fall above the quartile line and those in the lower tail fall below it, there are too few data in the tails than would be expected in the theoretical distribution (and the theorized distribution is said to be too heavy in the tails). Conversely, if the data in the upper tail fall below the quartile line and those in the lower tail fall above it, then there are more data points in the tails than would be expected in the theorized distribution (and the theorized distribution is said to be too light in the tails). Patterns in deviations from linearity can be investigated by use of a residuals plot to detect systematic departures.

[3] The theoretical Q-Q plot for the normal (and log-transformed lognormal) distributions are essentially equivalent (except for scaling) to the normal probability plot discussed earlier and constructing Q-Q plots for the normal and lognormal distributions would therefore be of little additional value.

Section III Non-Parametric Distribution Functions

Many times in Monte Carlo analyses, a non-parametric function (or empirical distribution function (EDF)) is used to characterize a model variable. In these situations, the risk assessor has determined that the data itself provides the best representation of the exposure variable. Simply put, the risk assessor has chosen to directly use the sample values to define the distribution of the exposure variable rather than represent it by a theoretical distribution fit to the data.

D'Agostino and Stephens (p.8-9,1986) discuss the advantages of EDFs. Some of the benefits of likely interest to risk assessors include:

1. *EDFs provide complete representation of the data without any loss of information.*
2. *EDFs do not depend on any assumptions associated with parametric models.*
3. *For large samples, EDFs converge to the true distribution for all values of x.*
4. *EDFs provide direct information on the shape of the underlying distribution, e.g., skewness and bimodality; EDFs supply robust information on location and dispersion.*
5. *An EDF can be an effective indicator of peculiarities (e.g., outliers)*
6. *An EDF does not involve grouping difficulties and loss of information associated with the use of histograms*
7. *Confidence intervals are easily calculated.*
8. *EDFs can be effectively used for censored samples.*

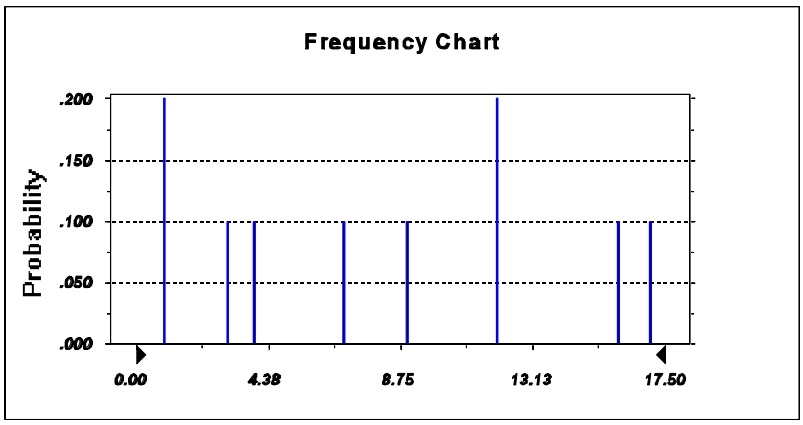
D'Agostino and Stephens also point out one of the potentially serous drawbacks to EDFs: *EDFs can be sensitive to random occurrences in the data and sole reliance on them can lead to spurious conclusions. This can be especially true if the sample size small.* In addition, we note that empirical distributions (as traditionally used) do not permit data to be generated which are *outside* the range of historically observed data and EDFs therefore tend to underestimate the probability of an extreme event.

> The choice of whether or not to use an EDF in an assessment employing Monte Carlo methods is ultimately up to the risk and his/her level of comfort and confidence with the data and the method. It must be remembered that EDFs (when used in the usual manner) rely solely on past observations and therefore preclude generation of data outside the historically-observed range. Monte-Carlo results generated from an EDF may produce tails that are too short and can therefore underestimate the probability of extreme events.

Below, we discuss how an EDF is defined and present several approaches used to implement EDFs.

Discrete Representation of EDFs

Given a random sample of n observations, $X_1, X_2, \cdots, X_n$,, a discrete representation of this EDF would be represented as X = $\{X_1, X_2, \cdots, X_n,\}$. These values could be used themselves directly in the simulation in what is termed a "trace-driven" simulation. In this technique, values from the raw input data are repeatedly selected in a random manner and used to calculated model outputs. For example, given the data set X = {1,1,3,4,7,9,12,12,16,17}, a discrete representation of this data set is illustrated below:



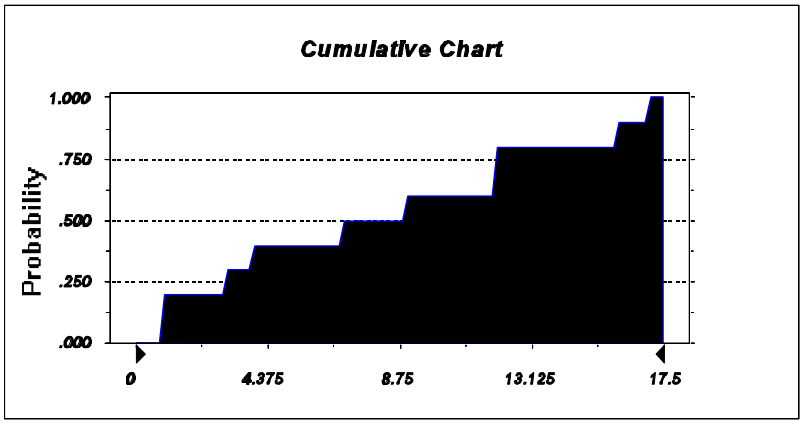
We note that with this representation no intermediate values (e.g., 2, 5, 6, 8, etc) can be generated and the simulation is limited to <u>only those values which have historically been observed and are present in the data input set.</u>

Continuous Representation of EDFs

Given a random sample of n observations, $X_1, X_2, \cdots, X_n$, sorted from smallest to largest, from a true but unknown distribution, an *empirical distribution function*, EDF, expressed on a cumulative basis may be defined as

$$prob\,(X \le x\ ) \qquad F(x\ ) \qquad \frac{number\ \ of\ \ x\ s\ \le\ x}{N}$$

For example, given the same data set X = {1,1,3,4,7,9,12,12,16,17}, the probability that X $\le$ 11 is given by F(11) = 6/10 = 0.60 since there are 6 samples with values less than or equal to 11 and there are ten samples in the entire data set. This formulation of the EDF presents some problems since all values of x^* in the range $9 < x^* \le 11$ have the same probability (called *constant interpolation*), i.e., prob ($X \le 10$) = 6/10, prob ($X \le 10.5$) = 6/10, prob ($X \le 11.5$) = 6/10, and so on. Defined this way, the EDF is a step function with abrupt jumps at the sample values as illustrated below:



The EDF is then expressed as

$$F_n(x) \quad \begin{cases} 0 & x < x[1] \\ \dfrac{k}{n} & x[k\ \ 1] < x \le x[k] \qquad for\ \ k \quad 1,2, \quad ,n \\ 1 & x > x[n] \end{cases}$$

where x[0] is set to zero. As with the discrete representation, values below the sample minimum and beyond the sample maximum cannot be generated. However, unlike the discrete representation, <u>any</u> value between the maximum and minimum can be generated.

Linear Interpolation of Continuous EDFs. It may be unsettling to define the EDF as a step function with abrupt jumps at certain values and so interpolation is often used to estimate the probabilities of values in between sample values. Generally , for values between observations, i.e., $X_{k-1} \le x < X_k$, linear interpolation is used, although higher order interpolation is sometimes used. The EDF for linear interpolation between sample values is simply

$$F_n(x) \quad \begin{cases} 0 & x < x[1] \\ \dfrac{k}{n} \quad \dfrac{x - x[k]}{n(x[k] - x[k-1])} & x[k-1] < x \le x[k] \qquad for \quad k \ \ 1,2, \quad n \\ 1 & x > x[n] \end{cases}$$

Extended EDF. The linearly interpolated EDF cannot produce values beyond the values in the data sample. This may be an unreasonable restriction in many cases. For example, the probability that a previously observed largest value in a sample based on n observations will be exceeded in a sample of N future observations may be estimated using the relationship $prob = 1 - n/(N + n)$. If the next sample size is the same as the original sample size, there is a 50% likelihood that the new sample will have a largest value greater than the original sample's largest value. Restricting the EDF to the smallest and largest sample values may produce distributional tails that are too short.

In order to get around this problem, one may extend the EDF to include plausible minimum and maximum values. The extended EDF expands the linearly interpolated EDF by including a user-defined absolute minimum, x_{min}, and absolute maximum, x_{max}, which are beyond the data sample.

$$F_n(x) \quad \begin{array}{ll} 0 & x < x[0] \\ \dfrac{k}{n \quad 1} \quad \dfrac{x - x[k]}{(n \quad 1)\,(x[k] - x[k-1])} & x[k-1] < x \le x[k] \quad for \quad k \quad 1,2, \quad n \quad 1 \\ 1 & x > x[n \quad 1] \end{array}$$

where $x[0] = x_{min}$ and $x[n+1] = x_{max}$.

References and Suggested Readings

American Industrial Health Council, *Exposure Factors Sourcebook*, May, 1984.

P. Bratley, B. L. Fox, L. E. Schrage, *A Guide to Simulation*, Springer-Verlag, New York (1987).

D.E. Burmaster and E.A.C. Crouch, "Lognormal Distributions for Body Weight as a Function of Age for Males and Females in the United States 1976-1980. Risk Analysis, **1**, 499-505 (1997)

J.S. Craver, *Graph Paper From Your Computer or Copier*, Fisher Books. 3rd. Ed., (1996)

R.B. D'Agostino and M.B. Stevens, Goodness of Fit Techniques, Marcel Deker (1986)

Decisioneering, Inc. (1996) Crystal Ball Version 4.0 User Manual, pages 269-275.

M. Evans, N. Hastings, and B. Peacock, *Statistical Distributions*, John Wiley & Sons, New York (1993).

R. O. Gilbert, *Statistical Methods for Environmental Pollution Monitoring*, Van Nostrand Reinhold, New York (1987).

L. C. Hamilton, *Regression with Graphics - A Second Course in Applied Statistics*, Duxberry Press, Belmont, CA (1992).

D. Hattis and D.E. Burmaster, "Assessment of Variability and Uncertainty Distributions for Practical Risk Analysis", **14**, 713-730 (1994),

D. R. Helsel and R. M. Hirsh, *Statistical Methods in Water Resources*, Elsevier, New York (1992).

A. M. Law and W. D. Kelton, *Simulation Modeling and Analysis*, Chapter 6, 325-419 (especially 356-404), McGraw-Hill, New York (1991).

J. Lipton, W. D. Shaw, J. Holmes, and A. Patterson, "Short Communication: Selecting Input Distributions for Use in Monte Carlo Simulations", Regulatory *Toxicology and Pharmacology*, **21**, 192-198 (1995).

M.G. Morgan and M. Henrion. *Uncertainty: A Guide to Dealing With Uncertainty in Quantitative Risk and Policy Analysis*. Cambridge University Press (1990)

W. Nelson, Applied Life Data Analysis, John Wiley & Sons, New York (1982).

Wayne R. Ott, *Environmental Statistics and Data Analysis*, Lewis Publishers (1995).

Palisades. *@RISK Users Manual*

A.M. Roseberry and D.E. Burmaster, "Lognormal Distributions for Water Intake by Children and Adults," Risk Analysis **12**, 99-104 (1992).

S. H. C. du Toit, A. G. W. Steyn, R.H. Stumpf, *Graphical Exploratory Data Analysis*, Springer-Verlag, New York (1986).

M. B. Wilk and R. Gnanadesikan, “Probability plotting methods for the analysis of data”, *Biometrika*, **55**(1), 1-17, (1968).

U.S. EPA, *Guidance for Data Quality Assessment: Practical Methods of Data Analysis* EPA QA/G-9, EPA/600.R-96/084, July, 1996. Available on-line at http://Earth2.epa.gov/ncerqa/qa/docs/epaqag9.PDF

U.S. EPA *Exposure Factors Handbook* August, 1996. DRAFT. EPA/600/P-95-002a,b,c

D. Vose, *Quantitative Risk Assessment: A Guide to Monte-Carlo Simulation Modeling*. John Wiley and Sons (1996)