Sampling design part 2 – interpretation

Contaminated Land Guidelines

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Cover: Prepared sample bottles and jars, sealed with EPA legal tape. Photo: EPA.

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1. Introduction

The NSW Environment Protection Authority (EPA) has prepared these guidelines to assist contaminated-land consultants, site auditors, regulators, landholders, developers, and members of the public who have an interest in the outcomes of the assessment and management of contaminated land. They will help consultants to design sampling for contaminated sites, with regard to where samples are collected, how many samples are collected, and how the data is compared to relevant criteria: they are intended to help users obtain data that is appropriately representative for the purposes of the sampling and the media being sampled, and to carry out the subsequent analysis and interpretation of the collected data.

As when following any guidance, users should justify the approaches they use, and demonstrate that they are appropriate and fit for purpose.

The guidelines are in two parts. The first part (this document) describes the application of sampling design; the second part provides guidance on interpretation of the results. This second part is not a stand-alone document and should be read in conjunction with Part 1 – Interpretation.

These Guidelines have been made in accordance with the *Contaminated Land Management Act 1997* (CLM Act). They should be read in conjunction with the CLM Act, the Contaminated Land Management Regulation 2013 (CLM Regulation), and any guidelines made or approved by the EPA under the CLM Act.

The Guidelines complement other guidelines made by the EPA, and several national guidance documents that have been approved by the EPA. Those guideline documents are listed in the reference section and are specifically referenced in the text, where appropriate.

1.1. Scope of these application guidelines

Section 2

Information on comparing sampling data to action levels. Appendix A includes a summary of common descriptive statistics, and Appendices F to L show associated procedures and worked examples.

Section 3

Summary of the main statistical distributions and information on associated data transformations and data analysis.

Section 4

Introduction of the concepts of hypothesis testing, including decision errors and methods for conducting hypothesis tests. Procedures for common methods of hypothesis testing, along with worked examples, are shown in Appendices F to L.

Section 5

Information on confidence intervals for use in estimation problems, along with the use of upper confidence limits of the mean ($UCL_{\bar{x}s}$) as another means of hypothesis testing. Appendices I to L provide procedures and worked examples for use of confidence intervals and UCLs, based on common distributions.

Section 6

Discusses trend analysis for temporal series of site contamination assessment data, including use of linear regression and the Mann–Kendall statistic.

Section 7

Includes abbreviations used and a glossary of technical terms.

Section 8

Reference list of guidance and technical documents used in this Guidance.

1.2. Environmental media

These guidelines address the sampling of soil and solid media, as these are the most common targets in the assessment of site contamination. Information is also provided for other media, including groundwater, surface water, sediments, and air. Most of the statistical procedures described in these guidelines can be applied to all of these media. General advice is provided regarding sampling for emerging contaminants, along with specific references.

This document does not specifically address biota sampling and ecotoxicity testing. For these specialty areas, see the following references:

- Australian and New Zealand Governments (ANZG) (2018) *Australian and New Zealand Guidelines for Fresh and Marine Water Quality*
- Department of Environment and Science (DES) Queensland 2018, *Monitoring and Sampling Manual: Environmental Protection (Water) Policy 2009* [sic], DES, Brisbane
- Department of Environment and Conservation (DEC) 2004, *New South Wales (NSW) Australian River Assessment System (AUSRIVAS) Sampling and Processing Manual*, DEC NSW, Sydney.

2. Comparing data results to action levels

Schedule B1 of the *National Environment Protection (Assessment of Site Contamination) Measure 1999* (NEPM 2013) discusses the application of investigation and screening levels for Tier 1 assessments for soil results.

2.1. Use of statistics in the assessment of site contamination

Statistics can be broadly categorised as either **descriptive** statistics, which describe the sample, or **inferential** statistics, which relate the sample information to characteristics of the population. In assessing site contamination, both descriptive and inferential statistics are used to characterise sites and decision areas.

Descriptive statistics are discussed further in Appendix A. See the glossary for further definitions of statistical concepts.

For inferential statistics, tests can be either **parametric** or **non-parametric**. Parametric statistical tests make assumptions about the parameters of the population distribution, whereas non-parametric tests are often described as distribution-free statistics, because they make no assumptions about the distribution; although they may make assumptions about the data.

All parametric statistical tests assume that the data are drawn from a particular probability distribution, whether the normal, log-normal, gamma, or some other known statistical model. Parametric tests generally have non-parametric counterparts, which can be used when the assumptions of the parametric test cannot be met. As non-parametric tests do not make assumptions about the distribution, they typically have lower statistical power than parametric tests (in cases where the assumptions hold). However non-parametric tests are often more accurate and more powerful than parametric tests for even modest departures from parametric test assumptions.

Two assumptions that apply to many forms of inferential statistics are, first, that the sampling data are unbiased and, second, that each member of the population has an equal chance of being included in a sample. Consequently, the data points are an independent and identically distributed sequence of observations. **Independent** means that each observation is not controlled by the value of any other observation. Independence can generally be assumed for random samples if the sample consists of less than 10% of the population. **Identically distributed** simply means that the samples have been taken from a parent population whose mean and variance is stationary over the space and time of collection.

Biased sampling can be both judgmental (also known as targeted) and arbitrary sampling, where certain observations are included or excluded because of some feature: this leads to members of the population having an unequal opportunity of being sampled. Bias can arise from a subconscious decision of the person conducting the sampling.

Basic statistical tests can be validly applied only to unbiased sample data; data from judgmental or arbitrary sampling should not be used for statistical tests. For this reason, it is recommended that data obtained using a combination of judgmental and random (probabilistic) sampling approaches is collated and considered separately, and that the formal use of statistical techniques is confined to probabilistic sample data only. This means that results from judgmental sampling – for example, validation of an excavation, or investigation of a contaminating feature such as a leaking pipeline – should be removed from a dataset before you perform statistical analysis on the remaining data.

2.2. Descriptive statistics

Terms used in statistics are referred to **statistical descriptors**. Common terms include **range**, **mean** and **percentile**.

Common statistical descriptors can be used to summarise the basic quantitative characteristics of the sampling data, allowing them to be presented in tables or illustrated graphically. Where multiple

populations or decision areas exist, it is useful to separate the data for analysis and comparison. This will generally reduce the variability of the individual datasets.

Reviewing the data numerically and graphically leads to a better understanding of the structure of the data, and also reveals patterns in distribution and relationships, and/or potential anomalies. Data should be verified and validated before it is reviewed.

The commonly used descriptive statistical terms are the sample **range**, sample measures of central tendency (**mean**, **median** and **mode**), sample **percentiles**, and sample variability (**variance**, **standard deviation** and **coefficient of variation**). A preliminary data review could include basic graphical representations of the data, such as spatial plots, box and whisker plots, frequency plots, histograms, ranked data plots, quantile–quantile (Q–Q) plots, two variable scatterplots, and temporal plots[1].

Descriptive statistics are further summarised in Appendix A, and specific procedures for determination and worked examples are included in Appendix B to Appendix D.

2.2.1. Software tool and packages

Statistical software tools and packages are available in spreadsheets, commercial software and open-access freeware. These can be used to determine both descriptive and inferential statistics. Such tools and packages are recommended – particularly freeware, as it allows easy access for checking outputs by other stakeholders including auditors and regulators, without the associated financial costs and licence restrictions associated with commercial products.

A detailed review and summary of widely available statistical software packages can be found in Appendix D of ITRC (2013). This review covers both general statistical packages for broad applications and packages specifically designed for statistical analysis of environmental data and includes both commercial and open-source freeware.

2.2.2. Data presentation

Spreadsheets and statistical software tools and packages can create sophisticated outputs to represent the sampling data and associated statistical information. For a preliminary data review, for example, they can present data in plan and cross section, both spatially and temporally, and as graphics.

As noted by DoE (1998):

> *While reporting of minima, maxima, mean, median, standard deviation, upper confidence limits etc. provides necessary information, such data may not be sufficient to characterise a site. The use of histograms or frequency distributions should also be considered to illustrate the distribution of results.*

Appendix E gives examples of the types of graphical presentations that can be easily developed.

2.3. Maximums

The maximum observed value in a dataset is important in assessing site contamination, as a site or decision area is generally considered suitable for the intended land use if the maximum observed value is below the criterion or action level. However, such a condition may be misleading. The maximum observed value of the contaminant of interest is unlikely to be the maximum value present in the population, and the relationship between the two cannot be determined in the absence of statistical analysis.

Where sampling data is highly variable, and/or based on small sample sizes, then it may not be representative of the underlying population's variability and decision errors can arise. The recommended

[1] See Sections 14.3–14.6 of Schedule B2 of the ASC NEPM (2013), USEPA (2006, G-9S) and USEPA (2006, G-9R) for further details.

approach to control decision errors is to conduct appropriate tests that allow statistical inference. Appropriate tests include hypothesis tests, such as one-sample t-tests and UCL$\bar{x}$s. Section 4 and Appendix F discuss hypothesis testing; Section 5 and Appendix I to Appendix L for skewed distributions discuss UCLs.

When comparing sample results to criteria and action levels, the sampling data also needs to meet another criterion: that no single value should exceed 250% of the relevant investigation or screening level (schedule B1, NEPM 2013).

2.4. Outliers

In statistics, **outliers** are data points that do not fall into the expected range of a defined probability distribution function. In the context of site contamination assessment however, the characteristics of a probability distribution function of a contaminant in question can be difficult to define. Complex historical site uses can result in the superposition of multiple probability distribution functions. **Hotspots** – small areas of high concentration – may also be present, with their own probability distribution function. The concept of statistical outliers, and the argument that they can be removed from the subsequent statistical analysis, do not apply in robust statistical analysis.

All data resulting from probability-based sampling must be included in the subsequent inferential statistical analysis, unless:

- it can be demonstrated with a high level of confidence that the individual data points are invalid, due to transcription errors, data coding errors, or measurement errors in the laboratory analysis

  or
- the individual data points are subsequently identified – again, with a high level of confidence – as part of a hotspot, and the hotspot is appropriately remediated or managed and thereby effectively removed from the population.

In either case, a determination is then needed as to whether further data needs to be generated through additional investigations, or if sufficient data is available to support the required decisions. These determinations should include appropriate statistical analysis of the remnant dataset.

2.5. Non-detects

As part of the assessment of site contamination, where the concentration of an analyte ranges between zero and the limits of reporting (LORs) of the laboratory method, the results are reported as less than the LORs. This is referred to as **left-censored** data. In some instances, the data below the LORs may represent another **population**, and the data, including geological logs and field notes, should be reviewed to determine if a more appropriate grouping of data is relevant. For determining mean values, mixing a large number of results below the LORs with a limited number of detected results can lead to estimation problems if simplistic methods are used.

There are various imputation methods to replace these censored values. **Direct substitution** is the easiest but least satisfactory. Generally, substitution should only be adopted where the fraction of the sample that is censored is relatively small. With substitution, a constant value is assigned to the non-detects by one of the following:

- assuming the non-detects are equal to zero
- assuming the non-detects are equal to the LORs
- assuming the non-detects are equal to some fraction of the LOR, usually one half.

The proxy value is then used as though it were the value for that measurement. However, the uncertainty associated with the substitution method increases as the proportion of non-detects in the dataset increases. Statistical determinations and inferences associated with censored data become increasingly problematic, because of errors in the estimates of parameters such as the mean, which becomes biased down. The direction and extent of the bias in variance is highly dependent on the data and substituted value.

Where non-detects below LORs exist, you should:

- always report detection limits for non-detects;
- not convert non-detects to zeros without specific justification.
- consider using non-parametric methods, if further statistical analysis is required.

Other methods of imputation – replacing data with substituted values – include **multiple imputation**, **fractional imputation** and **Bayesian modelling**. The appropriate imputation method to use depends on the size of the dataset and the proportion of measurements that is reported as non-detects. If the proportion of non-detects is high (> 50%) or the number of samples is small (n < 5), analysis may be challenging.

The method of **maximum likelihood** by first principals can be used successfully to estimate the parameters of a probability distribution even where there is censored data: for censored data points, summing is replaced by integration between limits (zero and LOR). In general, the point of maximum likelihood cannot be determined algebraically but must be solved numerically (for instance, with the hill climbing technique or Newton Rapson technique), though this is no longer an issue with access to desktop computing power.

Additionally, there are various statistical packages dealing with censored data that are suitable for laboratory measurements.

Refer to ITRC (2013) and USEPA (2015a) for further details of specific methods for managing non-detects in statistical analyses.

Importantly, Wendelberger and Campbell (1994) note that:

> *[t]he manner in which the nondetect values are handled should depend on the type of decision to be made and the magnitude and frequency of the nondetect values. If the nondetects are small in magnitude or low in frequency, the method of handling the nondetects will probably have minimal impact on the final outcome of the analysis. However, if the detection limits are close to important decision values, or if the frequency of nondetects is high, the treatment of the nondetect values can greatly influence resulting decisions.*

Whichever statistical approach is adopted, the site CSM (conceptual site model) should be re-developed in light of the proportion of the dataset samples that are non-detects. For instance, if a site has a small proportion of detections and a high proportion of non-detections, then the source of the contamination should be carefully considered when refining the CSM. An option might be to stratify the site, so that areas where there are widespread non-detections are assessed separately from areas with detections, especially if investigation levels are being exceeded.

2.6. Pseudoreplication

In site contamination assessment, the collection and analysis of duplicate and triplicate samples is conducted as part of quality assurance/quality control (QA/QC) programs. Whereas this is important in determining the data's usability, these replicate sample results must not be treated as an independent sample. Doing so is known as **pseudoreplication** because the duplicates and triplicates are not independent of the primary sample. Pseudoreplication increases the number of samples while providing another data point similar to the primary sample, resulting in bias and distortion of any statistical analysis being undertaken.

2.7. Contaminant distribution

The variation of contaminant concentrations over a site or decision area means that individual measurements cannot be used to fully describe the distribution of a contaminant. If the contaminant concentrations are plotted against their respective frequency of occurrence, the resulting curve or histogram represents the concentration distribution of that contaminant over the site or decision area.

While histograms inform the characterisation of the site or decision area, they should not be taken to represent spatial information across the site or decision area; rather, they show the range, central tendency, variation and distribution of the variables under consideration. Under the **multiple lines of**

evidence and weight of evidence approach, these parameters should be considered when interpreting the data and comparing it to the criteria or action levels.

For example, comparing the sampling results to 250% of the relevant investigation or screening level can lead to identifying apparent hotspots, with the suggestion that removal of these specific areas will make the site or decision area suitable for the proposed land use. However, closer examination of the data may show that the apparent hotspots relate to heterogeneity of the soil/fill, and that any subsequent validation would result in the identification of further 'hotspots'. In these situations, further characterisation to confirm the variability of the soil/fill may provide better information for decision making as to remediation or management. In such situations, the use of statistical tools can assist, particularly in relation to decision errors and determination of a suitable number of samples.

Schedule B1 of NEPM (2013) requires that sampling results should be checked so that the standard deviation of the variable should be less than 50% of the relevant investigation or screening level. Although 50% is an arbitrary value, it serves the purpose of warning if the variance is potentially excessive, prompting further review of the contaminant distribution.

In these cases, further segregation of the data, by depth, soil type or spatial distribution for example, may demonstrate that multiple populations are inappropriately being considered as a single population. Alternatively, the data may indeed represent a highly variable population, and further sampling is indicated.

3. Distributions, transformations and data analysis

The sampling distribution is the frequency or probability of occurrence of measured values. In the assessment of site contamination, data can be analysed using parametric (distribution based) methods, or non-parametric methods where the population is not assumed to fit a specific population distribution. Statistical software packages provide more complex calculations of UCL$\bar{x}$ using a number of parametric and non-parametric distributions, however a brief review of the predominant distributions used is warranted.

Where the sampling data has a normal (or more strictly, nearly normal), log-normal or gamma distribution, parametric methods can be applied. Where the sampling data does not have one of these distributions, non-parametric methods should be used. Non-normal datasets can have a transform applied to essentially normalise the data, which aids analysis.

3.1. Parametric methods

Population parameters are estimated from samples. Different random samples will produce different estimates of each parameter; for instance, each sample will produce a different estimate (using $\bar{x}$) of the population mean, μ. These estimates themselves have a distribution, known as the **sampling distribution**. Many common statistical methods are based on a knowledge of, or the assumed characteristics of, the sampling distributions of population parameter estimates.

3.1.1. Normal distribution

The most commonly used distribution in parametric statistics is the normal. The central limit theorem (CLT) says that the sampling distribution of the mean for **n** independent random samples approaches a normal as **n** increases. This holds for all population distributions with finite mean and variance. A key feature of the normal distribution is that the mean, median and mode are equal.

Based on the CLT, the sampling distribution of $\bar{x}$ can be approximated by a normal distribution when the sample size n is sufficiently large (> 30), irrespective of the shape of the population distribution. The larger the value of n, the better the approximation (Devore and Farnum 2005).

3.1.2. Log-normal distribution

Log transformations convert samples to natural log values, to allow the use of log-normal or exponential distributions for analysis. The log-normal is a continuous distribution in which the logarithm of a variable has a normal distribution. Thus, if the random variable x is log-normally distributed, then y = ln(x) has a normal distribution. Likewise, if y has a normal distribution, then the exponential function of y (that is, x = exp(y)) has a log-normal distribution.

In log-normal distributions, the mean, median and mode are not equal. The difference between mean and mode depends on the skewness of the population, while the median is independent of skewness.

3.1.3. Gamma distribution

The gamma distribution offers greater flexibility in terms of fitting data than the normal and log-normal distribution. Gamma distribution is a rank-order transformation wherebythe contaminant concentration data is sorted into ascending order and converted to an integer ranked list. This transform process eliminates the scale effects in contaminant concentrations that are commonly found in site contamination datasets and so reduces the effect of large differences between results in a dataset.

This distribution type is relevant to the assessment of contaminated sites due to the relationship to exponential and normal distributions. The **gamma distribution** is a two-parameter family of continuous

probability distributions. The exponential distribution and the chi-squared distribution are special cases of the gamma distribution.

Three different parametrisations for gamma distributions are in common use:

- a shape parameter k and a scale parameter θ
- a shape parameter α = k and an inverse scale parameter β = 1/θ, called a rate parameter
- a shape parameter k and a mean parameter μ = kθ = α/β.

In each of these three forms, both parameters are positive real numbers and control the shape and skewness of the distribution.

3.1.4. Parametric methods in the analysis of site contamination assessment data

When using distributions to assess site contamination data, you must take into account the limitations imposed by each distribution, as these determine how well the distribution can provide a reliable interpretation of the actual population.

Data for assessing contaminated sites is rarely normally distributed, due to the kind of processes that lead to site contamination. When the mean, median and mode are not equal, or the coefficient of variance is > 0.5, consider carefully before using the normal distribution for analysis. Similarly, be cautious when applying the log-normal distribution, as the data for assessing contaminated sites is often not truly log-normally distributed. The application of either distribution needs to the be verified by testing that the data is approximately normally distributed, or normally distributed after the log transform is applied. The distribution can be tested by using a statistical software package to construct quantile–quantile (Q–Q) plots, which graph the quantiles of the dataset against the quantiles of a specific probability distribution.

It is generally recommended that skewed datasets are assessed using a gamma distribution rather than a log-normal distribution, as this produces more reliable results (EPA 2009). A log-normal transformation disguises the effect of high values that may not represent background and exaggerates the apparent standard deviation of the modelled log-normal distribution. This increases the risk of making an incorrect decision in relation the population distribution and associated statistical parameters. Therefore, for assessing skewed site contamination datasets, the gamma distribution should be used when performing parametric analysis, particularly if the sample size is less than 20 and/or contains outliers. Because of the gamma function's flexibility in accommodating a wide range of symmetric and asymmetric (skewed) distributions, it can represent log-normally distributed datasets without the risk of masking the effects of outliers.

When the site assessment data is highly skewed by extreme values or a significant number of non-detect values, it may be hard to determine an appropriate distribution for parametric analysis. In such cases non-parametric methods may give more reliable results.

3.2. Non-parametric methods

Non-parametric statistics are analysis methods that either make no assumption about the distribution of the data or the population, or, where a specific distribution is assumed, do not specify the distribution's parameters. Commonly used non-parametric methods for making inferences in the assessment of site contamination data are the **bootstrap**, **jackknife** and **Chebyshev** methods.

Compared with non-parametric methods analogous parametric methods are usually more powerful in situations where the assumptions of parametric methods hold. Where a population departs from these assumptions, the non-parametric tests can be superior.

3.2.1. Bootstrap

Bootstrapping is the practice of estimating properties of a statistical parameter by measuring those properties through randomly re-sampling the dataset with replacement data. Data points need to be independently and identically distributed. This 'new' dataset is then used to estimate the statistical parameters such as mean, median, mode, standard deviation, etc. Bootstrapping can also be used for

constructing hypothesis tests, as an alternative to statistical inference based on the assumption of a parametric model, when that assumption is in doubt.

Bootstrapping, like any non-parametric resampling method, offers a useful means of reducing the influence of extreme outliers on the overall statistical parameters of the underlying population that was sampled. However, caution is required in the use of this non-parametric method, to avoid diminishing the importance of the outliers in relation of the overall decision: where the outlier represents a hotspot, a non-parametric re-sampling method such as bootstrapping may not be appropriate. The use of this method must therefore be justified in the context of the importance of the outliers to the overall decision to be made.

3.2.2. Jackknife

Jackknifing is similar to bootstrapping, in that the method re-samples the dataset and generally produces similar results, although instead of making random replacements as in bootstrapping, the jackknifing method just randomly removes a sample in each resampling step. The re-sampled dataset can then be analysed with the same methods as those used for bootstrapping. Jackknifing is subject to the same limitations and cautions as bootstrapping.

3.2.3. Chebyshev

The Chebyshev method is a non-parametric method that does not involve resampling of the dataset but instead relies on use of the Chebyshev's inequality. This specifies that, for all distributions with finite mean and variance, no more than a certain fraction of values can be more than a certain distance from the mean. That is, no more than $1/k^2$ of the distribution's values can be more than k standard deviations away from the mean with 100% certainty.

The inequality has great utility because it can be applied to any probability distribution in which the mean and variance are defined, and so it can be applied to all practical problems. When applied to datasets for assessing site contamination, the Chebyshev method provides an option for determining statistical parameters, particularly the mean, for highly skewed datasets or ones that contain significant outliers. In most applications the Chebyshev method gives a more conservative result than the other parametric and non-parametric methods.

4. Hypothesis testing

Decision problems can be addressed as statistical hypothesis tests, which are recommended under the USEPA's DQOs (data quality objectives) process. The **null hypothesis significance testing** (NHST) framework, derived from approaches for testing data, is a method of statistical inference used to determine if a null hypothesis (H_0) should be rejected in favour of an alternative hypothesis (H_A), at a specified level of confidence. In the assessment of site contamination, H_0 is that the site or decision area is not suitable for the specified use, i.e. that the site or decision area is contaminated.

The hypothesis test is conducted on the basis that H_0 can be rejected where there is compelling evidence to the contrary, such that the findings are incompatible with H_0 being true, in which case H_A is accepted as being more likely. Alternatively, H_0 can fail to be rejected. Importantly, this does not necessarily mean that H_0 is true, but rather that there is insufficient evidence to reject the site being contaminated.

Prior to testing, an environmentally significant difference from the criterion level should be established. For H_0 to be rejected, the data must show that (with given confidence) the population parameter is at or below this level. This environmentally significant difference is greater or equal to zero to provide an environmental buffer.

The most common form of hypothesis testing is for nearly-normally distributed populations. Here estimated population means are tested using the Student's t test (t-test), which is used to test for differences in population means. This test can be carried out as:

- a **one-sample t-test**, to test whether the mean of a single population is different from a target value, such as a specified health investigation level (HIL)
- a **two-sample t-test**, to compare the means of two groups, such as site data and background data
- a **paired sample t-test**, to compare the means from the same group at different times, such as before and after remediation.

If there are non-detects, special working is required to estimate the mean and variance.

Worked examples are shown in Appendix F (a one-sample t-test) and Appendix G (a two-sample t-test). Comparable parametric methods also exist for non-normal distributions, and non-parametric methods exist for testing differences in means and/or medians in unknown distributions (see USEPA 2006, G-9S).

4.1. Sampling uncertainty and decision errors

Uncertainty in estimates is unavoidable due to a variety of factors, such as inherent variability in the characteristics of interest of the target population, the limits on the number or samples that can be collected, and the imperfect measurements that follow. Statistical methods provide quantitative tools for characterising the uncertainty in an estimate, and therefore play an important role in designing an investigation that will generate probabilistic data of a sufficient type, quality and quantity.

One can never be 'certain' about an answer derived from sampling, so the uncertainty must be specified for a statistical statement to have meaning. In statistics, uncertainty is technically referred to as **risk** or **confidence level**. The risk of incorrectly rejecting H_0 is denoted by α (alpha) and has a magnitude of between 0 and 1. The risk of incorrectly accepting H_0 is denoted by β (beta), which is also between 0 and 1. For example, if a particular statistical statement is quoted as having a 95% confidence level, ($\alpha = 0.05$), this implies that at least 95 out of I00 repeats of the sampling will correctly accept a true H_0. A power of 80% ($\beta = 0.2$) means an 80% chance of correctly rejecting a false H_0.

In the assessment of site contamination, α risk in this context is defined as the risk of deciding that the site or decision area is suitable for the proposed use when in fact it is not, and the confidence level is always equal to 1 - α. The probabilities generally used in the assessment of site contamination are $\alpha = 0.05$ and $\beta = 0.2$, or a 95% confidence level and a statistical power of 80%, although higher probabilities can be used, such as $\alpha = 0.01$ and $\beta = 0.1$, or a 99% confidence level and a statistical power of 90%.

Changing one probability inevitably changes the other. One way to obtain both a high confidence level and high statistical power is to increase the number of samples. More sophisticated sampling designs and associated analysis can also be used to increase the power. (See Section 4).

Within hypothesis testing, **decision errors** refer to the incorrect decisions that can be made about a site or decision area, based on the data collected. They arise from using data that are not sufficiently representative of the site or decision area, because of either sampling errors or measurement errors, or more commonly both. Such errors can lead to decisions that assess contaminated land as uncontaminated when it is contaminated, or that determine that remediation is required when it is not. The combination of errors from all sources is referred to as the **total study error**, and directly affects the probability of making decision errors. The statistical theory behind hypothesis testing allows the probability of making a decision error to be quantified, given the data collected and the specified level of significance.

Decision errors result from:

- **sampling errors**, which arise from using information from a sample instead of measuring the whole population
- **sampling design errors**, which arise when the sampling design does not validly capture the structure of the population. They include sampling frame selection, sampling unit definition, selection probabilities and the number of samples collected
- **measurement errors**, which arise from the variability inherent in sample collection, handling, preparation, analysis and data reduction.

Study error is managed through the correct choice of suitable sampling designs and measurement systems. Refer to Appendix H for additional information on the types of decision errors.

4.2. Use of hypothesis tests

Formal statistical methods can quantify the uncertainty associated with decisions. ITRC (2103) notes the following common decision errors that can arise in the assessment of site contamination, and hypothesis tests that can control them:

- **concluding that a site or decision area is suitable when the sample maximum is less than the criterion or action level.** This is not necessarily true. For some distributions and sample sizes, the population mean of the site or decision area may be greater than the criterion or action level, even though a particular sample maximum is less than the criterion or action level.

  This is a Type I decision error, and a one-sample hypothesis test will allow statistical inference and control of decision errors
- **concluding that a site or decision area is not suitable when the sample maximum is more than the criterion or action level.** This is not necessarily true either, as the population mean of the site or decision area may be less than the criterion or action level when the sample maximum is more than the decision criterion, depending on the nature of the distribution and the sample size.

  This is a Type II decision error, and a one-sample hypothesis test will allow statistical inference and control of decision errors. The systematic planning for the investigation should describe how maximum values will be treated – for instance, what further data analysis or investigation will be carried out if the maximum value exceeds 250% of criterion or action level
- **concluding that the failure to reject the null hypothesis 'proves' the null hypothesis (i.e. that the site is too contaminated to be acceptable).** As environmental data typically shows large random variability, the sample could by chance include a preponderance of elevated concentrations, particularly if the sample size was small and so the statistical test is of insufficient power.

  The power of the test ($1 - \beta$) should be determined and compared to the decision criteria, and/or the number of samples required to achieve the specified decision criteria determined using the combined risk value (CRV) method discussed in Part 1 of these Guidelines (i.e. not this document). If insufficient samples were collected (i.e. the test was conducted with insufficient power) further data analysis or investigation may be required
- **directly comparing the maximum value of a site or decision area with a background maximum or mean, without considering potential decision errors.** The maxima from the two datasets

should not be compared to make inferences about the means of the datasets, as decision errors are not controlled for and this can result in Type I errors. A two-sample hypothesis test is recommended to allow statistical inferences and to control decision errors.

5. Confidence intervals and upper confidence limits

A **confidence interval** is an interval used to estimate a population parameter from sample data and is composed of two parts: an interval calculated from the data and a confidence level associated with the interval. In the assessment of site contamination, the confidence interval is generally expressed as a point estimate, usually the mean, plus and minus (±) the margin of error. Because confidence intervals are expressed this way, they are determined using two-sided intervals for the t critical values.

Upper confidence limits (UCLs) are the upper component of the confidence interval and are therefore determined using the one-sided interval for the t critical values.

Hypothesis tests and confidence intervals are related, as they are determined using variations of the same formula, and often a confidence interval can be used to test a hypothesis, making it unnecessary to perform the entire hypothesis test. In assessing site contamination, a decision is generally only required as to whether the estimated population parameter exceeds the criterion or action level, and so UCLs can be used by themselves as a form of hypothesis testing.

5.1. Confidence intervals

Performance criteria are needed to estimate an unknown parameter to within a specified amount, with a given confidence level: they specify the maximum width of the confidence interval. The width of a confidence interval depends on the number of samples used to calculate the interval; the precision, or variability, of the dataset; and the specified confidence level. By placing limits on the maximum width of a confidence interval, the precision and the number of samples needed to calculate the interval can be determined. As the variability of the population being studied is generally fixed, only the confidence level and number of samples can be controlled.

For independent samples from an approximately normal distribution, or where the sample size is large ($n \geq 30$), confidence intervals for mean values are determined by using the one-sample Student's t-test. This test is reasonably robust if the population distribution deviates only moderately from normality; however, for highly skewed data sets with significant outliers, or where significant non-detects are included in the data set, other distributions or nonparametric methods should be used.

Appendix F shows how to determine confidence intervals using the one-sided Student's t-test and gives a worked example. For other distributions not discussed below, or for non-parametric methods, see USEPA (2006, G-9S).

5.2. Upper confidence limits

When assessing site contamination, the main way to determine if sites or decision areas are suitable for their proposed uses is to employ upper confidence limits (UCLs) as one-sided hypothesis tests for comparing the sample mean to the action levels or criteria. The appropriate method is determined by the population distribution, as indicated by the sampling data. The appendices give various methods, with their associated assumptions and limitations, plus worked examples:

- for normal distributions, Appendix J shows the one-sided Student's t-test method
- for log-normal distributions, Appendix K shows the Land's H-statistic method
- for skewed distributions, Appendix L shows the Chebyshev inequality method.

6. Trend analysis

Trend analyses are typically used in the assessment of site contamination to determine if a contaminant's concentrations are increasing, decreasing or remaining constant over time. The objective of a trend analysis is to determine if the changes of a contaminant concentration can be statistically correlated to time and, if so, how significant the correlation is. Two trend analysis methods are described below. These are generally applied to datasets for water or air, although they can be used when assessing remediation, such as the bioremediation of soil.

6.1. Linear regression

The calculation of a linear regression, or line of best fit, is a common way to measure the relationship between two variables. In the assessment of site contamination, a linear regression analysis is often used to assess if there is a trend between a contaminant concentration and time (for example, is the concentration of benzene in monitoring well two decreasing over time)?

Data should be presented on a time plot to determine, visually, if a trend is likely, then the Pearson Correlation Coefficient or r-value should be calculated. This is a measure of the strength of the linear relationship between the two variables. The r-value can be a value between 1 and -1, with 1 indicating a strong positive relationship between the two variables, -1 indicating a strong negative relationship, and 0 indicating no relationship at all.

While the calculation of an r-value of 0.98 may indicate a strong positive relationship between the contaminant concentration and time, it is possible that other factors are affecting this relationship. Simple linear regressions can be affected by seasonality, the distribution of the data, and the number of samples below the LORs. USEPA (2006, G-9S) states that due to these limitations, linear regressions are not recommended as a general tool for estimating and detecting trends but can be used as an informal and quick screening tool to detect if a strong linear trend is present.

6.2. Mann–Kendall

The Mann–Kendall test is used to assess trends in datasets, and being a non-parametric test, it makes no assumption regarding data distribution and is unaffected by missing data or values below the LORs.

The test compares each data point against the next data point, and a score of 1 or -1 is given for each comparison, according to whether there is an increase or decrease in concentration. (The test is not affected by the magnitude of the change.) The individual scores are tallied to provide the Mann–Kendall statistic (S): a positive S indicates an upward trend whilst a negative S indicates a downward trend. The value of S is then compared to an S-critical value. A p-value is then calculated for comparison to the adopted significance level, which determines if the null hypothesis (of no trend) is rejected or accepted.

The Mann–Kendall test is also affected by seasonality, and only data from similar months each year should be compared if this is likely to be important. Where high seasonality effects can be expected, to be able to calculate a meaningful result you need to collect data over at least four years.

The output of the Mann–Kendall test will be either 1) that the concentrations are increasing, 2) concentrations are decreasing, or 3) that there is no trend. However, following this test, a linear regression analysis can be performed to determine the strength of the trend (providing the potential limitations of the linear regression are considered). Further information on the use of the Mann–Kendall test to assess trends can be found in Gilbert (1987) USEPA (2009, G-9S) and IRTC (2013).

7. Abbreviations and glossary

7.1. Acronyms

ABC	Ambient background concentration
ANZG	Australian and New Zealand water quality guidelines
CECs	Contaminants of emerging concern
CLT	Central limit theorem
CLM	Contaminated land management
CRV	Combined risk value
CSM	Conceptual site model
CV	Coefficient of variation
DNAPLs	Dense non-aqueous phase liquids
DQIs	Data quality indicators
DQOs	Data quality objectives
DSI	Detailed site investigation
DUs	Decision units
EPA	Environment Protection Authority
HIL	Health-based investigation level
HSL	Health screening level
ISM	Incremental sampling methods
LNAPLs	Light non-aqueous phase liquids
LOR	Limits of reporting
Metals	Arsenic (As), cadmium (Cd), chromium (Cr), copper (Cu), lead (Pb), mercury (Hg), nickel (Ni) and zinc (Zn)
MoE	Margin of error
MPE	Maximum probable error
MQOs	Measurement quality objectives
NEPM	National Environmental Protection Measure
NHST	Null-hypothesis significance testing
NOW	New South Wales Office of Water
OEH	New South Wales Office of Environment and Heritage
PAHs	Polycyclic aromatic hydrocarbons
PFAS	Per- and poly-fluorinated alkyl substances
PFOS	Perfluorooctane sulfonate
PFOA	Perfluorooctanoic acid
PFHxS	Perfluorohexane sulfonate
PSH	Phase-separated hydrocarbon
PSI	Preliminary site investigation
PCoCs	Potential contaminants of concern

PID	Photoionisation detector
PTFE	Polytetrafluoroethylene
QAPP	Quality assurance project plan
QA/QC	Quality assurance/quality control
Q–Q	Quantile–quantile
RAP	Remediation action plan
RSD	Relative standard deviation
SAQP	Sampling and analysis quality plan
SOPs	Standard operating procedures
STP	Sewage treatment plant
SWL	Standing water level
TOFA	Total organic fluorine assay
TOPA	Total oxidisable precursor assay
TRHs	Total recoverable hydrocarbons, including volatile C6–C10 fractions and semi- and non-volatile C11–C40 fractions
UCLs	Upper confidence limits
$UCL_{\bar{x}}$	Upper confidence limits of means
UPSS	Underground petroleum storage system
USEPA	United States Environmental Protection Agency
UST	Underground storage tank
VOCs	Volatile organic compounds

7.2. Statistical notations

$1 - \alpha$	Confidence level
α	Type I error rate (see Glossary)
β	Type II error rate (see Glossary)
c	Criterion/action level
df	Degrees of freedom
exp	Exponential function
H_A	Alternative hypothesis
H_0	Null hypothesis
n	Number of samples or measurements in a sample (see sample definition)
θ	Scale parameter of the gamma distribution
σ	The population standard deviation, which is generally not known
σ^2	The population variance, which is generally not known
p-value	Probability value
Δ	Uppercase Greek letter delta, denoting the width of the grey region associated with hypothesis testing
s	The sample standard deviation, which is determined from the measurements taken
s^2	The sample variance, which is determined from the measurements taken

δ_0	Difference (delta) of zero
$t\alpha$	Critical value
t_0	Test statistic
μ	The population mean, which is generally not known
$UCL\bar{x}$	Upper confidence limit of mean
$\bar{x}$	The sample mean, which is determined from the measurements taken
x_i	The i^{th} measurement in the dataset

7.3. Glossary

α risk

The probability, expressed as a decimal, of making a 'type I error' when the hypothesis is tested statistically. A type I error wrongly rejects a null hypothesis when in fact the null hypothesis is true. In this document, the null hypothesis always assumes that the site is 'contaminated' and thus the α risk refers to the probability of a site being validated 'uncontaminated' when in fact it is 'contaminated'.

β risk

The probability, expressed as a decimal, of making a 'type II error' when a hypothesis is tested statistically. A type II error wrongly accepts a null hypothesis when in fact the null hypothesis is false. In this document, the null hypothesis always assumes that the site is 'contaminated' and thus the β risk refers to the probability that a site is concluded 'contaminated' when in fact the site is 'uncontaminated'.

Acceptable limit

A threshold concentration value below which the level of contamination is regarded as acceptable. An acceptable limit can either be adopted from the appropriate guidelines, or it can be derived on a site-specific basis using risk assessment. Where site remediation is involved, acceptable limits are often referred to as 'clean-up standards' or 'remediation standards'.

Acceptance criteria

A statistical statement specifying how a contaminant distribution will be compared with an acceptable limit (see above definition) to determine whether a site should be evaluated as 'contaminated' or 'uncontaminated'. The concentrations of a contaminant can vary over orders of magnitude in a sampling area. All site assessments must state the appropriate acceptance criteria, as well as the appropriate acceptable limits.

Ambient air

External air environment, not including the air environment inside buildings or structures.

Arithmetic mean

The arithmetic mean is commonly referred to as the average and is used to describe the centre of the data distribution. It is obtained by summing all the values and dividing the result by the number of values.

Central tendency

The central or typical value for a probability distribution and may be considered the average value in a set of data. It is generally described by the mode, median, or, more commonly, the mean, and describes where a sample distribution is centred.

Chi-squared distribution

A type of cumulative probability distribution that varies depending on the degrees of freedom (df). It is used to test relationships between categorical variables in the same population.

Coefficient of variation (CV)

CV is the measurement of the relative homogeneity of a distribution. Low CV values, e.g. 0.5 or less, indicate fairly homogeneous contaminant distribution, while CVs with values over I–1.2 imply that the concentration distribution of a contaminant is heterogeneous and probably highly skewed to the right.

Composite sample

The bulking and thorough mixing of soil samples collected from more than one sampling location to form a single soil sample for chemical analyses.

Conceptual site model (CSM)

Provides a three-dimensional overview of the contamination at sites and their surrounds, highlighting the sources, receptors and exposure pathways between the sources and receptors.

Confidence level

The probability, expressed as a percentage, that a statistical statement is correct. Confidence level is the opposite expression of 'risk' (see definitions of α and β risks). For the purpose of this document in which a risk that needs to be regulated, the confidence level is always equal to I - α.

Contaminated

For the purpose of this document and depending on the context, 'contaminated' can have slightly different meanings. If a site or a sampling area is evaluated as 'contaminated', it means that the site or the sampling area as a whole has not met the acceptance criteria (see definition of acceptance criteria). 'Contaminated' can also be used to describe a localised area or soil that has contaminant concentrations exceeding an acceptable limit (see definition of acceptable limit). Note: depending on what the acceptance criteria are, an entire site could be considered 'uncontaminated' even though a certain percentage of the site is expected to be 'contaminated'.

Data quality objectives (DQOs)

A systematic planning process used to define the type, quantity and quality of data needed to support decisions relating to the environmental condition of a site or a specific decision area.

Decision area

A specific area or medium within a site, or offsite, about which data is being gathered so a decision can be made. For example, a decision can include part of a site, soil, a stockpile, soil gas, groundwater, surface waters or sediments.

Estimate

An estimate is a value that is inferred for a population based on data collected from a sample of units from that population. For example, the measured data from a sampling event used to calculate the sample mean ($\bar{x}$) is then used to estimate the population mean (μ).

Estimation

A technique that systematically adjusts the sample data to determine an estimated value for the population.

Geometric mean

This is similar to the **arithmetic mean** (described above), in that it is also a measure of the central tendency of the distribution of a population or sample. It is sensible to calculate geometric means only on populations or samples that contain positive values. The geometric mean is obtained by multiplying n values from the data set together, then taking the nth root of the product.

Grab samples

Samples collected from different locations that will not be composited but analysed individually.

Hotspot

A localised area where the level of contamination within that area is noticeably greater than that in surrounding areas. Note that a hotspot is only **relatively** high in contamination.

Inter well

Comparison between two groundwater monitoring wells that are separated spatially.

Intra well

Comparison of measurements over time at one groundwater monitoring well.

Maximum

The maximum observed value in a data. Important, as it generally provides a conservative estimate of the potential exposure risks. It is generally assumed that if the maximum is below the action level, then the site should be suitable for the associated land use.

Median

The middle value of the distribution. Half the data values are less than the median and half are greater.

Minimum size effect

The acceptable magnitude of the difference between the populations or groups being studied.

Mode

The value that occurs most frequently. It is determined by counting the number of times each value occurs.

Modules

A series of discrete DQOs outputs, based on logical categories, that address selected components of a site investigation. Modules can be selected for contaminant types, media, decision areas, or a workable combination of these.

Neyman–Pearson method

A method of statistical inference used to determine if a null hypothesis (H_0) should be rejected in favour of an alternative hypothesis (H_A), at a specified level of confidence.

Outlier

A data point that sits outside the expected range of the data. An outlier can have either a high or low value. Unless there is a demonstratable reason for rejecting them (such as coding error, sample contamination or equipment failure), outliers need to be retained within sample datasets.

Parameters

Numerical measures of the characteristic of interest in the population being sampled. Typical parameters are the population mean (μ), variance (σ^2) and standard deviation (σ). Parameter values are usually unknown.

Percentiles and quartiles

As their names suggest, these are descriptive values used to equally split a dataset into 100 parts. A percentile is the value that a given percentage of observations in a dataset is equal to or less than, e.g. 80% of observations in a dataset are at or below the 80th percentile, while 20% are above.

Quartiles are commonly used to break the dataset up into four equal parts, providing an indication of the distribution and variance of the data.

First quartile – the 0^{th} percentile up to (and including) the 25^{th} percentile

Second quartile – from the 25^{th} percentile up to (and including) the 50^{th} percentile

Third quartile – from the 50^{th} percentile up to (and including) the 75^{th} percentile

Fourth quartile – from the 75^{th} percentile up to (and including) the 100^{th} percentile

Population

Any large collection of objects, things or individuals with some characteristics in common, that is being studied and for which information is sought. The population under consideration must be clearly and succinctly defined to allow effective sampling design and subsequent reporting.

The population can be further defined as the **target population** and the **sampled population**, and ideally these should be the same. The target population is the set of all units that comprise the items of interest, that is the population about which a decision is required, and the sampled population is that part of the target population that is accessible and available for sampling. If the two diverge significantly, the target population should be redefined.

Probabilistic sampling

Probabilistic sampling occurs when each member of the population has a given probability (greater than zero and less than one) of being included in the sample. If the probability is the same for all population members then, and only then, will the sample be unbiased. Because inclusion in the sample is based on probability, subsequent samples won't necessarily include the same members.

Range

The range of a dataset measures the spread between the highest and lowest values in the dataset. Other measures (such as the standard deviation and the interquartile range) are required to provide an understanding of the distribution of the data.

Residual soil

The soil at a site that is not contaminated by industrial, commercial, or agricultural activities, consistent with the term 'ambient background concentration' (ABC) from the NEPM. Residual soils can include natural soils, reworked natural soils and historically imported material. Residual soils may have naturally occurring background levels of contaminants, contaminants that have been introduced from diffuse or non-point sources by general anthropogenic activity, and only low levels of contaminants attributed to industrial, commercial, or agricultural activities.

Sample

'Sample' has a number of meanings in the assessment of site contamination, including:

- as more broadly used in statistics, a representative group drawn from a population for description or measurement

- a physical amount of a material (soil, water, air, etc.) or an aliquot, taken for testing or chemical analysis
- a sampling point or sample location, being the location in plan at which a sample is collected, including description (e.g. geological logs) and field screening (e.g. PID, XRF, etc.).

Sample size

The number of samples or sampling points selected in a sampling program.

Sampling, analysis and quality plan (SAQP)

Incorporates the CSM and the DQO outputs, to provide the context and justification of the selected sampling and analysis. The methods, procedures and QC samples associated with the DQIs, including the frequency and MQOs, along with any associated contingencies, are also documented. The SAQP ensures that the data collected is representative and provides a robust basis for site assessment (NEPM 2013).

Sampling pattern

The locational pattern of sampling points within a sampling area.

Sampling point

The location at which a soil sample is collected.

Site characterisation

The assessment of the nature, level and extent of contamination. A typical site characterisation involves a preliminary site investigation (PSI), followed by a detailed site investigation (DSI), where warranted.

Site validation

The process of showing that a site is successfully remediated.

Standard deviation

Calculated by taking the square root of the variance (described below). It provides an indication of a population or sample data's typical deviation from its mean.

Statistic

Any summary number that describes the sample, such as an average or percentage. For example, the mean of a sample is described as $\bar{x}$ (x-bar) and the standard deviation as **s**. When describing the population from which the sample is drawn, a summary number is called a **parameter**.

Statistical power

The probability of correctly determining a positive result (e.g. a change or difference in the population) based on sample data.

Sub-sample

A sample that will be bulked together with other sub-samples to form a composite for chemical analyses.

Systematic planning

A planning process based on a scientific method, and which leads the project to unfold logically. Systematic planning includes established management and scientific elements. In the assessment of site

contamination, it includes the application of the **DQOs** process and development of both a **CSM** and an **SAQP**.

Variable

A characteristic, number or quantity that is the subject of the inquiry. In the assessment of site contamination, it is usually continuous numerical variables that are being assessed, for example the concentration of a contaminant in soil, soil gas or water. Discrete or discontinuous variables are at times considered, such as the number of fish in a waterbody. These are both quantitative variables in that they are derived by measurements.

Qualitative or categorical variables include ordinal or ranked variables and nominal variables. Ordinal variables are observations that take a value that can logically be ordered or ranked, such as first, second, third, whereas nominal observations take a value that cannot be organised in a logical sequence, such as presence or absence. Categorical variables are not commonly used in the assessment of site contamination and are not considered further.

Variance

The average squared distance of population or sample data points from the associated mean.

Weight of evidence/lines of evidence

‘Weight of evidence’ describes the process of collecting, analysing and evaluating a combination of different qualitative, semi-quantitative or quantitative lines of evidence to make an overall assessment of contamination.

Applying a weight-of-evidence process incorporates judgements about the quality, quantity, relevance and congruence of the data contained in the different lines of evidence (ANZG 2018).

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Appendix A: Descriptive statistics

This appendix provides a brief review of the descriptive statistics commonly used for summarising data. The following appendices show how they are used, giving specific procedures and worked examples.

Range and percentiles

The range of a dataset measures the spread between the highest and lowest observed values in the dataset. It can be expressed as an interval, such as a–b, where a is the lowest value and b is the highest, or it can be expressed as an interval width, such as b - a = c. While either approach provides an appreciation of the range of the observed values, the maximum value is of particular concern in the assessment of site contamination, and the range is generally more informative as an interval, as it shows the spread and the extremes of the data.

As the range only measures the spread between highest and lowest values, other measures – such as the **standard deviation** or the **interquartile range** (IQR) – are needed to more fully describe the data distribution.

Maximum

The maximum observed value in a dataset is important in the assessment of site contamination, as it generally provides a conservative estimate of the potential exposure risks. It is usually assumed that if the maximum is below the action level, then the site will be suitable for the associated land use. But this assumption holds true only if there is enough data, and the data is representative. If this is not the case, the maximum observed value may overestimate or underestimate the risk.

In cases where the consequences of decision error will be severe, or the number of samples seems insufficient to estimate the population mean from the sample mean, the maximum value can be used as an estimate of the population mean and termed **max test** for statistical analysis. This is often done for judgmental samples, such as with soil gas or groundwater data. Where this approach is used, it should be appropriately documented and justified.

Percentiles and quartiles

Percentiles, as suggested by the name, are descriptive values used to equally split a dataset into 100 parts. The Xth percentile in a dataset has a value greater than or equal to X% of the data – for example, the 80th percentile has a value greater than or equal to 80% of the data.

Percentiles can be used as the statistical parameter of interest, for instance for comparing to criteria or action levels. For example, ANZG (2018) states that “[f]or toxicants, it is recommended that action is triggered if the 95th percentile of the test data exceeds the guideline value”.

Quartiles are used to break up the dataset into four equal parts, providing an indication of the distribution and variance of the data. When observations are placed in ascending order by value:

- the first quartile, Q1, also called the lower quartile, is the value of the observation at or below which a quarter (25%) of observations lie, and is the 25th percentile
- the second quartile, Q2, is the median value at or below which half (50%) of observations lie, and is the 50th percentile
- the third quartile, Q3, also called the upper quartile, is the value of the observation at or below which three-quarters (75%) of the observations lie and is the 75th percentile.

The interquartile range (IQR) is used as a measure of the spread of the dataset, which also indicates its dispersion. It is the difference between the upper and lower quartiles (Q3 - Q1 = IQR) – that is, it measures the spread between the 25th and 75th percentiles. The IQR spans 50% of a dataset and eliminates the influence of outliers as it excludes the highest and lowest quarters.

Percentiles and quartiles can be used for datasets with limited observations, and for all types of data collection, as their use requires no assumptions about the underlying distribution or whether the samples

were judgmental or probabilistic. However, ANZG (2018) notes that the precision with which percentiles are estimated depends heavily on the sample size, with at least 13 samples need to estimate the 25th and 75th percentiles with an associated 95% confidence interval, and a minimum of 36 samples needed to estimate the 10th and 90th percentiles. Even larger sample sizes are required to estimate extreme percentiles, i.e. the 5th and 95th.

As the IQR does not depend on extreme values, it can be used when a dataset includes non-detects (at least where < 25% of the data is below the limits of reporting (LORs)). For datasets that are not nearly-normal, or which contain extreme values, the IQR may be more representative of the dispersion of the data than the standard deviation, can be affected by extreme observations. The IQR is therefore described as a robust estimate.

Appendix B shows how to determine quartiles.

Central tendency

Central tendency is the central or typical value for a probability distribution, and may be considered the average value in a dataset. It is generally described by the mode, median, or, most commonly, the mean, and indicates where a sample distribution is centred. While these estimates can generally be regarded as being representative or typical of the data, for small and/or highly skewed datasets they should be considered as approximations only.

Appendix C shows how to determine measures of central tendency.

Mode

The mode is the value that occurs most frequently and is determined by counting the number of times each value occurs. Since a sample mode may not exist or may not be unique (e.g. the distribution may be bimodal), it is rarely used as a measure of central tendency, although it can be useful for qualitative data such as categories.

Median

The median is the middle value of the distribution: half the data points have values greater than the median, and half have values less than it. The sample median is not influenced by extreme values and so can be used when the underlying distribution is unknown: it is commonly used to describe the centre of the distribution when non-parametric methods are employed. The median can also be used if non-detects are present, although care should be taken if there are many of them. In the event that a median is found to be non-detect while there are locations reporting values above detection levels, then consideration should be given to stratifying the site.

A number of guidelines recommend the use of median values in certain circumstances. For example:

- NEPM (2013, B2) states that when using non-parametric approaches, the median can be used to describe the centre of the distribution
- ANZG (2018) notes that for comparing test data with guideline values for physico-chemical stressors, “[a] trigger for further investigation of the test water body will be deemed to have occurred when the median concentration of a particular measurement parameter in **n** independent samples taken at the test water body exceeds the 80th percentile (or is below the 20th percentile if ‘less is worse’) of the same measurement parameter at the reference site”.

Arithmetic mean

The arithmetic mean is commonly referred to as the average and is used to describe the centre of the data distribution. The arithmetic mean is denoted as $\boldsymbol{\mu}$ (lowercase Greek letter *mu*) for the population mean or as $\bar{\mathbf{x}}$ (x-bar) for the sample mean. In the assessment of site contamination, the population mean is generally not known, so the sample mean is used as an estimate of the population mean.

Larger sample sizes tend to produce sample means that are closer to the population mean, as in theory extreme data values balance each other out. But when sample sizes are small, the arithmetic mean can

be affected by outliers, and when judgmental sampling is used, the arithmetic mean is often a biased measure of central tendency.

The mean value may be more representative of site contamination than the maximum value, by providing a better estimate of the actual contaminant concentrations that receptors would be exposed to over a period of time. However, it is important that small areas of high concentration (hotspots) are not ignored by averaging with lower values from other parts of the site or the decision area.

The arithmetic mean is calculated by dividing the sum of the sample measurements by the number of samples.

Geometric mean

The geometric mean is similar to the arithmetic mean, in that it is also a measure of the central tendency of the distribution of a population or sample. This is also described as the arithmetic mean of the logarithmic scale of a dataset, or the nth root of the product of n numbers.

Due to the log transformation involved in the calculation, the geometric mean is not as affected by outliers and is commonly used when the data is skewed or log-normally distributed. Whilst this may be beneficial in some instances, the curvature of the logarithmic function may downplay the higher values in favour of the lower ones.

Higher values are important in the assessment of site contamination. If assumptions regarding the condition of a site are based on the geometric mean, downplaying higher values may increase the chance of a Type I error. Because of this potential bias, you should not use solely geometric means (including back transformation) to compare against action levels, and if you do use them you should provide appropriate justification. Where log-transformed data are approximately normal (or at least reasonably symmetric) back transformation may be appropriate (USEPA 2009 and Viveros 1997), but for skewed datasets that are not log-normal, the geometric mean is likely to be a poor estimator of population mean (Parkhurst 1998).

Variability

An important aspect of data analysis is determining the variability of the sampling data. Calculating variability can provide an indication of how heterogenous the variables are likely to be across a decision area, and how representative the measures of central tendency are of the sampling data. The variability of data is measured by **variance**, **standard deviation** and the **coefficient of variation**.

See Appendix D for how to determine measures of variability.

Variance

Variance is the average squared distance of each data point from the sample mean. It can be affected by extreme values and by large numbers of values below the LORs.

Standard deviation

The standard deviation is calculated by taking the square root of the variance and provides an indication of the data's typical deviation from the mean. The standard deviation of a population is denoted as **σ** (Greek lowercase sigma), and for a sample by **s**. The sample standard deviation is commonly used in the site contamination assessment, as the standard deviation of the population is generally not known.

A large sample variance or standard deviation indicates that the data points are not closely clustered around the mean. Both the variance and the standard deviation are strongly influenced by the number of samples collected, and influenced by extreme values in either direction.

Coefficient of variation

The coefficient of variation (CV), or relative standard deviation (RSD), is a measurement of the relative homogeneity of a distribution. The CV is determined as the standard deviation of a distribution divided by

the mean of the distribution, i.e. CV = s/$\bar{x}$ for sample data. The RSD is determined in the same way, but expressed as a percentage, i.e. a CV of 0.5 = an RSD of 50%.

Low CV values, e.g. 0.5 or less, indicate a fairly homogeneous contaminant distribution, while CVs with values over I–1.2 imply that the concentration distribution of a contaminant is heterogeneous.

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Appendix B: Determining quartiles

Percentiles are descriptive values used to split a set of data into 100 equal parts, providing a representation of the sampling data that can be used for either normal or non-normal distributions. A percentile provides the value that a given percentage of observations in a dataset are less than or equal to (for example, 25% of observations in the dataset have values at or below the value of the 25th percentile).

Percentiles can be used in the statistical analysis of datasets that have limited observations. The dataset can also be divided by **quartiles**, which are the 25th, 50th and 75th percentiles.

Determination

To calculate percentiles, values are ordered from the lowest to the highest and assigned a rank, with the required percentile calculated using the formula shown below. While this procedure can be used for small datasets, it is commonly conducted using spreadsheets or statistical packages. Note that all percentiles of sample data are biased estimators of population percentiles.

The values are ranked from lowest to highest:

$$X_{(1)}, X_{(2)}, X_{(3)}, X_{(4)} \ldots, X_{(n)}$$

The p^{th} percentile is calculated by:

$$y_p = (1 - f) \times X_i + f \times X_{(i+1)}$$

Where:

y_p	the value of the p^{th} percentile
p^{th}	the specified percentile
r	$(n - 1)p + 1$
floor(r)	calculate r and discard decimals
i	floor(r)
f	r – i
X_i	the value of the ith rank
$X_{(i + 1)}$	the value of the ith + 1 rank

The data in Table 1, below, is used for the worked examples in this and the following appendices.

Table 1 Summary of analytical results – metals in soil (mg/kg)

Sample ID or statistic	Arsenic	Chromium	Copper	Lead	Nickel	Zinc
Limits of reporting	5	2	5	5	2	5
Analytical						
Analytical sample B2-01	103	12	34	20	18	11
Analytical sample B2-02	50	21	30	7	2	10
Analytical sample D2-01	43	26	83	17	14	35
Analytical sample D2-02	9	10	29	14	5	12
Analytical sample A4-01	203	4	260	18	12	232
Analytical sample A4-02	54	5	55	17	9	41
Analytical sample C4-01	341	19	401	133	7	543
Analytical sample C4-02	34	17	46	16	10	13
Analytical sample B6-01	71	18	24	14	5	9
Analytical sample B6-02	14	6	8	17	12	5
Analytical sample D6-01	62	11	51	15	3	36
Analytical sample D6-02	6	4	18	16	24	10
Analytical sample A8-01	27	17	61	16	4	24
Analytical sample A8-02	7	10	38	20	13	10
Analytical sample C8-01	24	15	39	12	6	8
Analytical sample C8-02	13	16	17	14	19	7
Descriptive statistics						
Number of samples	16	16	16	16	16	16
Number of detects	16	16	16	16	16	16
Percentage non detects	0%	0%	0%	0%	0%	0%
Maximum	341	26	401	133	24	543
Third quartile	64.3	17.3	56.5	17.3	13.3	35.3
Median value	38.5	13.5	38.5	16.0	9.4	11.5
First quartile	13.8	9.0	27.8	14.0	5.2	9.8
Minimum	6	4	8	7	2	5
Arithmetic average	66.3	13.2	74.6	22.9	10.2	62.9
Geometric average	35.2	11.4	43.5	17.3	8.3	20.0
Mode	-	10	-	17	12	10
Variance	7,792.2	42.4	10,988.8	872.1	39.7	19,410.1
Standard deviation	88.3	6.5	104.8	29.5	6.3	139.3
Coefficient of variation (CV)	1.3	0.5	1.4	1.3	0.6	2.2
Inferential statistics						
Standard error of the mean ($SE_{\bar{x}}$)	22.1	1.6	26.2	7.4	1.6	34.8
Relative standard deviation (RSD)	133.1%	49.4%	140.5%	129.1%	61.9%	221.6%
Margin of error (MoE)	47.0	3.5	55.9	15.7	3.4	74.2

Sample ID or statistic	Arsenic	Chromium	Copper	Lead	Nickel	Zinc
Maximum probability error (MPE)	70.9%	26.3%	74.9%	68.8%	33.0%	118.1%
95% LCL$\bar{x}$ two-sided Student's t	19.3	9.7	18.7	7.1	6.8	-11.4
95% LCL$\bar{x}$ two-sided Student's t	113.4	16.7	130.5	38.6	13.5	137.1
95% LCL$\bar{x}$ one-sided Student's t	105.0	16.0	120.5	35.8	13.0	123.9
ProUCL determination	120.5	16.0	135.2	55.1	13.0	214.7
Method recommended*	Gamma	Student's t	H-UCL	Chebyshev	Student's t	Chebyshev
Criteria and number of samples						
HIL-A land use (NEPC 2013, B1)	100	100	6,000	300	400	7,400
Number of samples to be used (whole number) – CRV method	44	2	2	2	2	2
Number of samples – MPE method	15	18	16	16	14	15

Worked example

The metals data in mg/kg from Table 1 is used in this example. To determine the 25th percentile of the sampling data for arsenic (As), we proceed as follows.

The values are ordered from lowest to highest and assigned a rank:

$$X_{(1)} = 6,\ X_{(2)} = 7,\ X_{(3)} = 9,\ \mathbf{X_{(4)}} = \mathbf{13},\ \mathbf{X_{(5)}} = \mathbf{14},\ X_{(6)} = 24,\ X_{(7)} = 27,\ X_{(8)} = 34,$$

$$X_{(9)} = 43,\ X_{(10)} = 50,\ X_{(11)} = 54,\ X_{(12)} = 62,\ X_{(13)} = 71,\ X_{(14)} = 103,\ X_{(15)} = 203,\ X_{(16)} = 341$$

Bolded values are $X_{(i)}$ and $X_{(i+1)}$.

The input parameters are calculated for the 25th percentile:

$$r = (n - 1)p + 1$$

$$r = (16 - 1)\ 0.25 + 1$$

$$r = 4.75$$

$$i = 4$$

$$f = r - i$$

$$f = 0.75$$

The 25th percentile is calculated as:

$$y_{(0.25)} = (1 - f) \times X_i + f \times X_{(i+1)}$$

$$y_{(0.25)} = (1 - 0.75) \times 13 + 0.75 \times 14$$

$$y_{(0.25)} = 13.8$$

The 25th percentile of the sampling data for As is 13.8 mg/kg.

Reference

US Environmental Protection Agency (USEPA) 2009, *Statistical Analysis of Groundwater Monitoring Data at RCRA Facilities: Unified Guidance*, EPA 530/R-09-007, USEPA, Washington DC.

Appendix C: Determining measures of central tendency

The **central tendency** is a central or typical value for a probability distribution, and may be considered the average value in a set of data. Methods for calculating the **median**, the **arithmetic mean** and the **geometric mean** are shown below.

The **mode** is the value that occurs with the greatest frequency (that is, the greatest number of times): to calculate it, simply count the number of times each value occurs. As the mode does not always exist or may not be unique, it is the value of central tendency that is least commonly used, although it can be useful for describing qualitative data.

Determination

Measures of central tendency are determined as follows.

Median with an odd number of samples

$$\text{median} = X_{(n+1)/2}$$

Median with an even number of samples

$$\text{median} = \frac{1}{2}\left[X_{(n/2)} + X_{(n/2+1)}\right]$$

Arithmetic mean

$$\text{sample arithmetic mean} = \frac{(X_1 + X_2 + \ldots X_n)}{n}$$

Geometric mean

$$\text{sample geometric mean} = \sqrt[n]{(X_1 \times X_2 \times \ldots X_n)}$$

Worked example

The metals data in mg/kg from Table 1 is used in this example. To determine the measures of central tendency for the sampling data for arsenic (As), we proceed as follows.

Median

The values are ordered from lowest to highest and assigned a rank:

$$X_{(1)} = 6,\ X_{(2)} = 7,\ X_{(3)} = 9,\ X_{(4)} = 13,\ X_{(5)} = 14,\ X_{(6)} = 24,\ X_{(7)} = 27,\ \mathbf{X_{(8)}} = \mathbf{34},\ \mathbf{X_{(9)}} = \mathbf{43},$$

$$X_{(10)} = 50,\ X_{(11)} = 54,\ X_{(12)} = 62,\ X_{(13)} = 71,\ X_{(14)} = 103,\ X_{(15)} = 203,\ X_{(16)} = 341$$

Bolded values are $X_{(n/2)}$ and $X_{(n/2\ +\ 1)}$.

As n = 16, an even number, the sample median is determined as:

$$\text{sample median} = \frac{1}{2}\left[X_{(n/2)} + X_{(n/2+1)}\right]$$

$$\text{sample median} = \frac{1}{2}\left[X_{(16/2)} + X_{(16/2+1)}\right]$$

$$\text{sample median} = \frac{1}{2}\left[X_{(8)} + X_{(9)}\right]$$

$$\text{sample median} = \frac{1}{2}\left[34 + 43\right]$$

$$\text{sample median} = 38.5$$

The sample median for As is 38.5 mg/kg.

Arithmetic mean

$$\text{sample arithmetic mean} = \frac{(X_1 + X_2 + \ldots X_n)}{n}$$

$$\text{sample arithmetic mean} = \frac{(103 + 50 + \cdots 13)}{16}$$

$$\text{sample arithmetic mean} = 66.3$$

The sample arithmetic mean for As is 66.3 mg/kg.

Geometric mean

$$\text{sample geometric mean} = \sqrt[n]{(X_1 \times X_2 \times \ldots X_n)}$$

$$\text{sample geometric mean} = \sqrt[16]{(103 \times 50 \times \ldots 13)}$$

$$\text{sample geometric mean} = 35.2$$

The sample geometric mean for As is 35.2 mg/kg.

As Table 2 shows, each method provides a different result for the measure of central tendency.

Table 2 Variation in central tendency by method of calculation

Method	Result (mg/kg)
Median	38.5
Arithmetic mean	66.3
Geometric mean	35.2

For sample data that is skewed, as in this case, the median and geometric mean are similar, while the arithmetic mean is 'dragged' to the right because of the outliers in the dataset. For a nearly-normal dataset the three measures would be similar.

Choose the appropriate measure of central tendency to represent the sampling data according to the contaminant distribution and the proposed use of the selected measure.

Reference

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

Appendix D: Determining measures of variability

An important aspect of data analysis is determining the variability of the data. Calculating variability can provide an indication of how heterogenous a contaminant is likely to be across a site. The variability of the data is measured by variance, standard deviation or the coefficient of variation.

Variance, represented by $\mathbf{s^2}$, is simply the average squared distance of each data point from the sample mean, and as such can be affected by extreme values and large numbers of values below the limits of reporting (LORs). It is used to estimate the population variance $\boldsymbol{\sigma^2}$.

The **standard deviation** of a sample, represented by s, is calculated by taking the square root of the variance, and provides an indication of the population's typical deviation from the mean. The standard deviation of the population, represented by σ, is generally unknown in the assessment of site contamination, and s is therefore used as an estimate. Note that although s^2 is an unbiased estimate of σ^2, s is a **biased** estimate of σ.

The **coefficient of variation** (CV), or **relative standard deviation** (RSD), is a measurement of the relative homogeneity of a distribution. The CV is the standard deviation of a distribution divided by the mean of the distribution. The RSD is determined in the same way but expressed as a percentage.

Determination

The methods for determining the measures of variability are shown below.

Variance

$$s^2 = \frac{\Sigma(x_i - \bar{x})^2}{n - 1}$$

Standard deviation of a sample

$$s = \sqrt{\frac{\Sigma(x_i - \bar{x})^2}{n - 1}}$$

Estimate of standard deviation

Where sampling data are not available, an estimate of the standard deviation can be made by dividing the expected range by six, i.e. three standard deviations in each direction, as this should represent approximately 99.7% of a nearly-normal distribution.

$$\sigma_E = \frac{C_H - C_L}{6}$$

The relative standard deviation is determined in the same way, but expressed as a percentage, i.e. a CV of 0.5 = an RSD of 50%.

Coefficient of variation

$$CV=\frac{s}{\bar{x}}$$

Where:

s^2	variance
x_i	the value of the sample
$\bar{x}$	the arithmetic mean (see Appendix C)
n	number of samples
s	standard deviation
σ_E	estimate of population standard deviation
C_H	estimate of the highest possible value in the sampling area
C_L	estimate of the lowest possible value in the sampling area
CV	coefficient of variation
RSD	relative standard deviation

Worked example

In this example we determine the measures of variability for the sampling data for arsenic (As) in Table 1.

The values for As, shown in mg/kg, are:103, 50, 43, 9, 203, 54, 341, 34, 71, 14, 62, 6, 27, 7, 24 and 13.

The number of samples, n, is 16, and the arithmetic average of the sampling data is 66.3.

Variance

$$s^2 = \frac{\Sigma(x_i - \bar{x})^2}{n - 1}$$

$$s^2 = \frac{(103 - 66.3)^2 + (50 - 66.3)^2 \ldots (13 - 66.3)^2}{16 - 1}$$

$$s^2 = \frac{1{,}346.9 + 265.7 + \cdots 2{,}840.9}{15}$$

$$s^2 = 7{,}792.2$$

Standard deviation

$$s = \sqrt{\frac{\Sigma(x_i - \bar{x})^2}{n-1}}$$

$$s = \sqrt{7{,}792.2}$$

$$s = 88.3$$

Estimate of standard deviation

$$\sigma_E = \frac{C_H - C_L}{6}$$

$$\sigma_E = \frac{341 - 6}{6}$$

$$\sigma_E = 55.8$$

In this example, the standard deviation calculated using the sampling data is much greater than the estimate of the standard deviation. This is because the sampling data is skewed to the right and does not appear to follow a nearly-normal distribution.

This example shows that, while estimates of standard deviation can be determined when sampling data is not available, they should always be used with caution. If you calculated required sample numbers using an estimated value such as the one in this example, you would arrive at a number that was too low. Accordingly, the sampling data should be used to refine the assumptions made as part of systematic planning.

Coefficient of variation (CV)

$$CV = \frac{s}{\bar{x}}$$

$$CV = \frac{88.3}{66.3}$$

$$CV = 1.3$$

Relative standard deviation (RSD)

$$RSD = 133.1\%$$

In this example, the CV of 1.3 (equivalent to an RSD of 133.1%) shows a distribution not nearly-normal and expected to be skewed to the right. Any statistical inference should assume a log-normal or other non-normal distribution and use log-normal or non-parametric methods for analysis.

Reference

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

Appendix E: Assessing contaminant distribution

Here we show an example of the assessment of contaminant distribution, as discussed in Section 2.7, as could be done with commonly available spreadsheet and statistical software. The sampling data used in this example comes from Table 1.

Table 3 Graphical presentations of example contamination data

Figure	Description
Figure 1	Summary statistics: metals in fill (mg/kg) as box-and-whiskers plots showing minimum, first quartile, median, third quartile and maximum
Figure 2	Summary statistics: metals in fill (mg/kg) as box-and-whiskers plots showing minimum, first quartile, median, third quartile and maximum, with adjusted scale
Figure 3	Standardised summary statistics (values/criteria): metals in fill (%) as box-and-whiskers plots showing minimum, first quartile, median, third quartile and maximum
Figure 4	Standardised summary statistics (values/criteria): metals in fill (%) as box-and-whiskers plots showing minimum, first quartile, median, third quartile and maximum, with adjusted scale
Figure 5	Multiple histograms for metals in fill (mg/kg)
Figure 6	Q–Q plot for arsenic (mg/kg)
Figure 7	Q–Q plot for chromium (mg/kg)
Figure 8	Q–Q plot for copper (mg/kg)
Figure 9	Q–Q plot for lead (mg/kg)
Figure 10	Q–Q plot for nickel (mg/kg)
Figure 11	Q–Q plot for lead (mg/kg).

These outputs suggest the following regarding the sampling data:

- Figure 1 and Figure 2 – the data is generally skewed to the right in the cases of As, Cu, Pb and Zn, as a result of extreme values in the dataset. Cr and Ni look generally symmetrically distributed, suggesting a nearly-normal distribution
- Figure 3 and Figure 4 – in relation to the criteria for HIL-A residential with accessible soil, only As exceeds 50% of its criterion, with the maximum As value exceeding the criterion by 341%, i.e. > 250% of the criterion. Cu, Pb and Zn are elevated, but are below HIL-A
- Figure 5 – the histograms confirm that As, Cu, Pb and Zn are right-skewed because of extreme values. As the sample size was small (< 30), the normality of the distribution cannot be confirmed using histograms
- Figure 6 to Figure 11 – the Q–Q plots show that As, Cu, Pb and Zn are unlikely to be nearly-normally distributed, and consequently parametric methods that assume nearly-normality cannot be used for statistical inference. Instead, some form of transformation is required or another distribution type should be used.

For Cr and Ni, the Q–Q plots suggest a nearly-normal distribution, and parametric methods that assume near-normality may be appropriate for analysis.

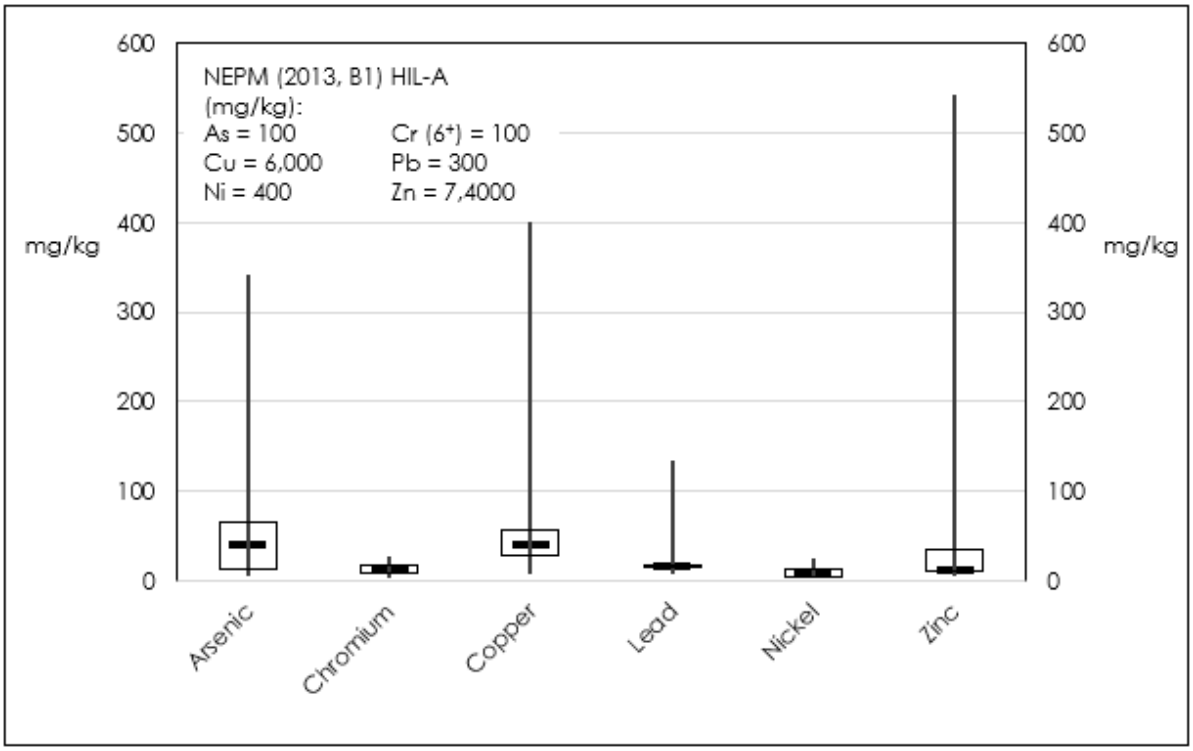

Figure 1 **Summary statistics, metals in fill (mg/kg) – minimum, first quartile, median, third quartile, maximum**

Source: Marc Salmon, Easterly Point Environmental Pty Ltd

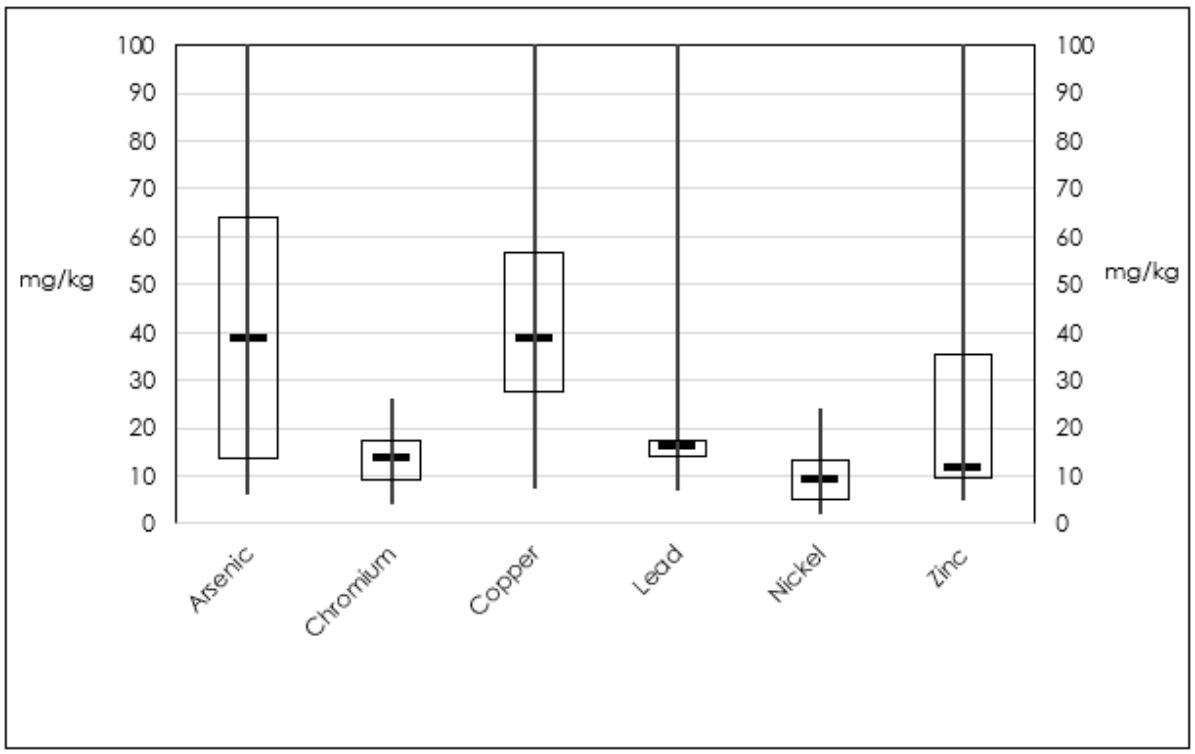

Figure 2 **Summary statistics, metals in fill (mg/kg) – minimum, first quartile, median, third quartile, maximum – scale adjusted**

Source: Marc Salmon, Easterly Point Environmental Pty Ltd

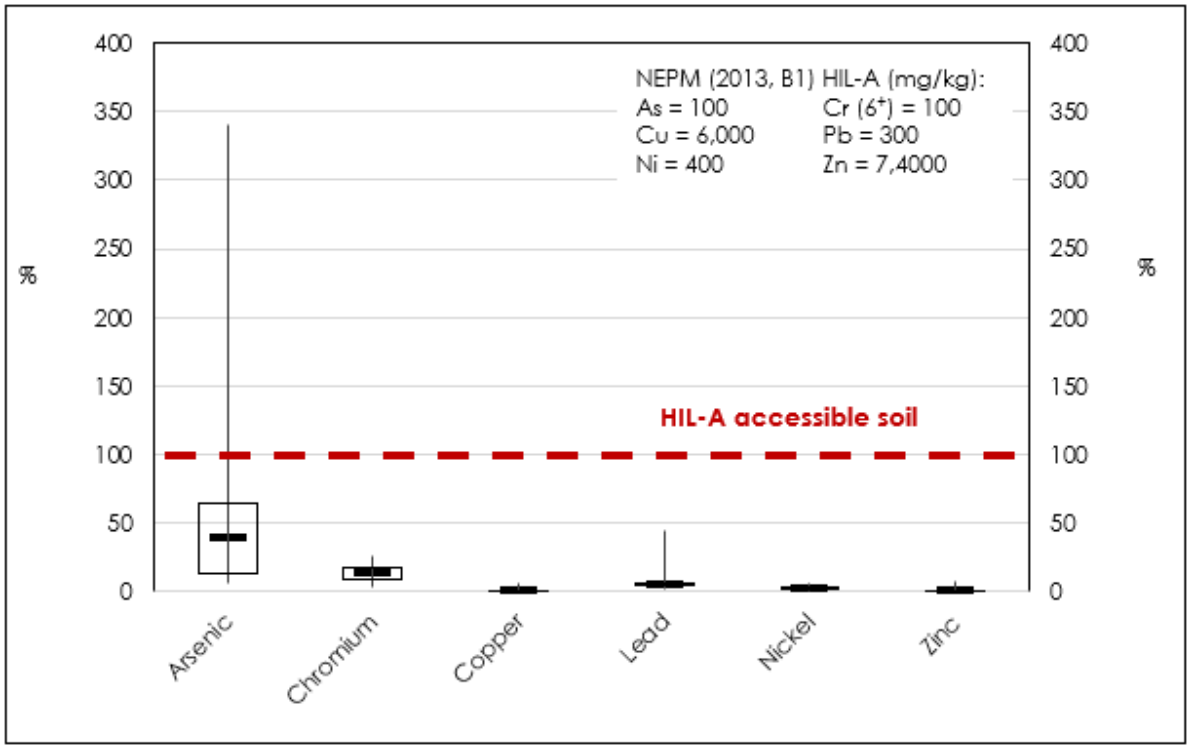

Figure 3 **Standardised summary statistics, metals in fill (%) – metals data relative to acceptance criteria**

Source: Marc Salmon, Easterly Point Environmental Pty Ltd

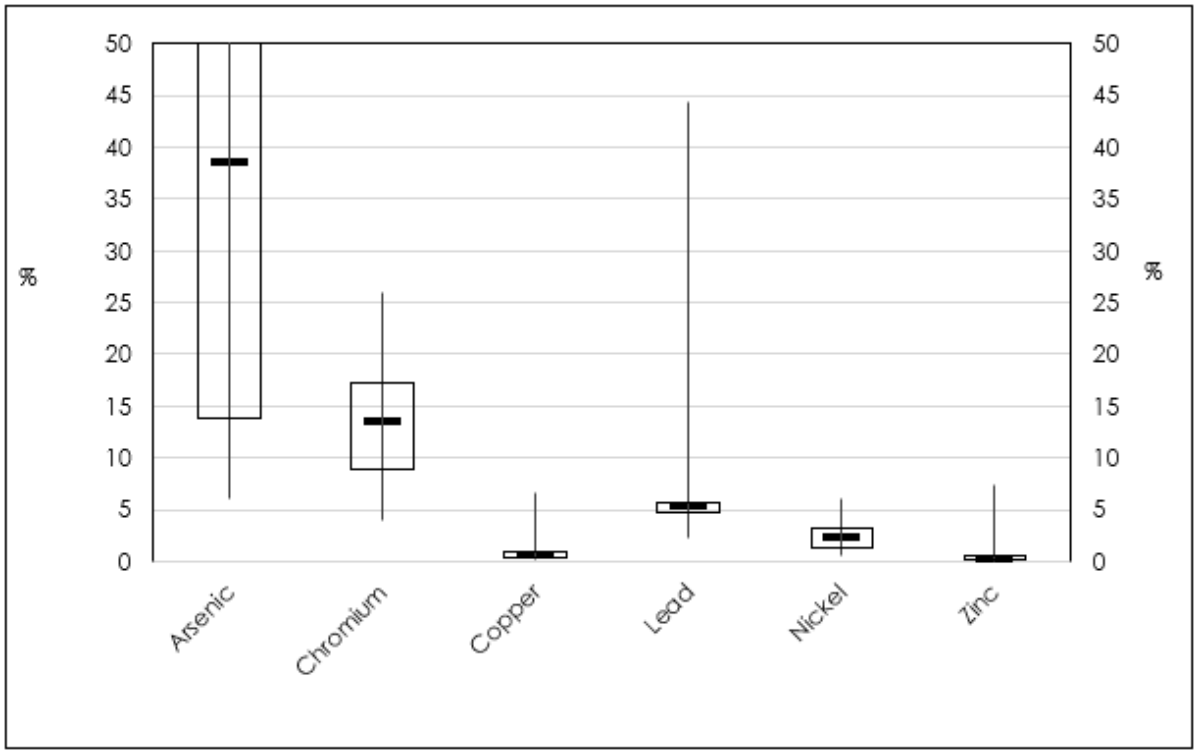

Figure 4 **Standardised summary statistics, metals in fill (%) – metals data relative to acceptance criteria – scale adjusted**

Source: Marc Salmon, Easterly Point Environmental Pty Ltd

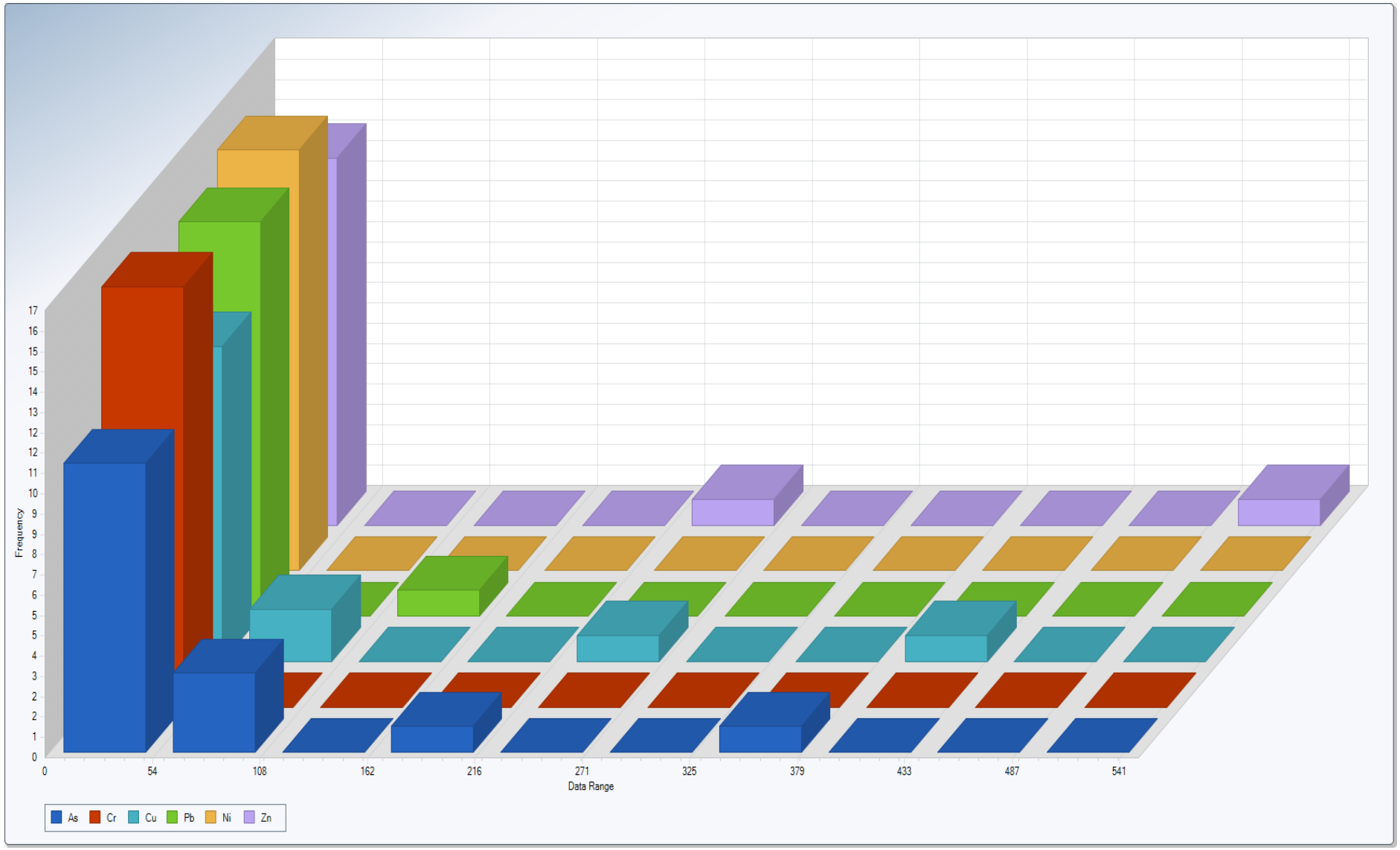

Figure 5 **Multiple histograms for metals in fill (mg/kg) – data from Table 1**

The x-axis shows concentation of the metal (in mg/kg) and the y-axis shows the number of samples.
Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

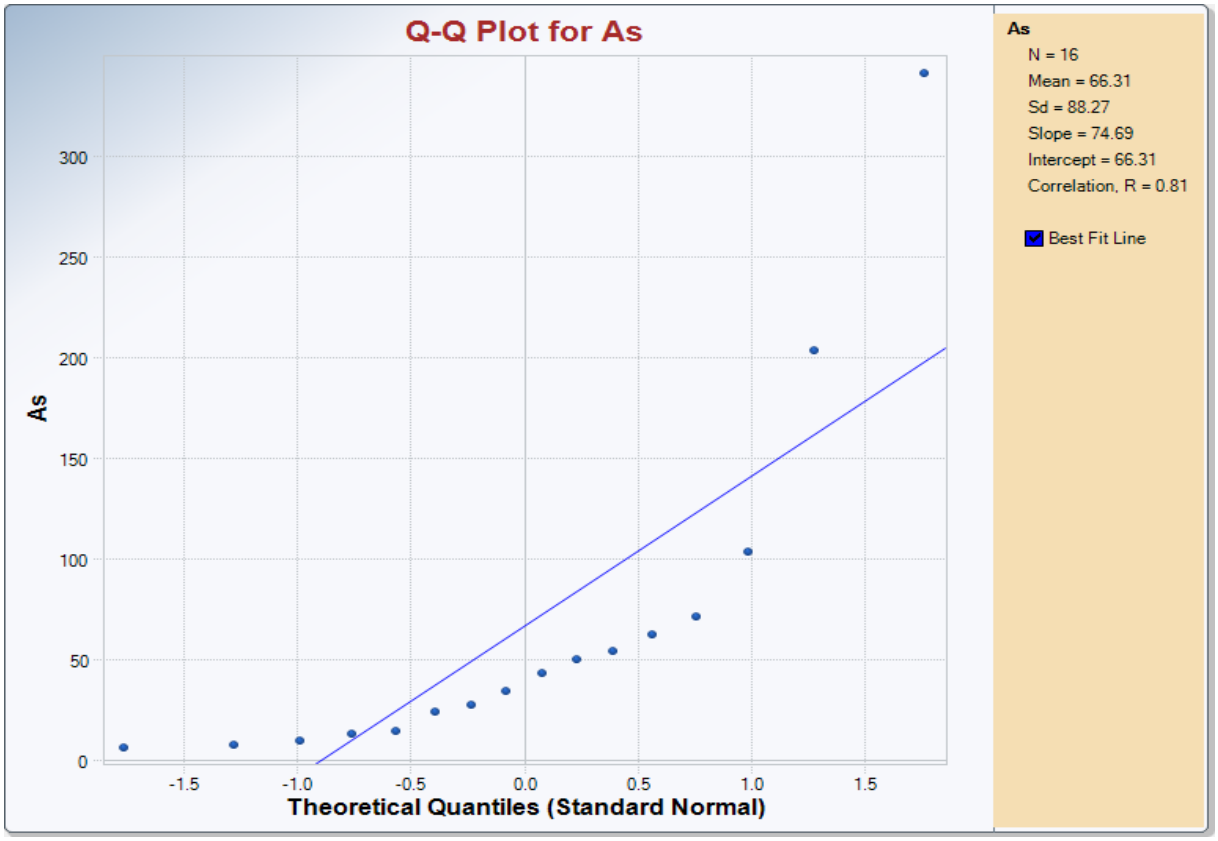

Figure 6 **Q–Q plot for arsenic (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

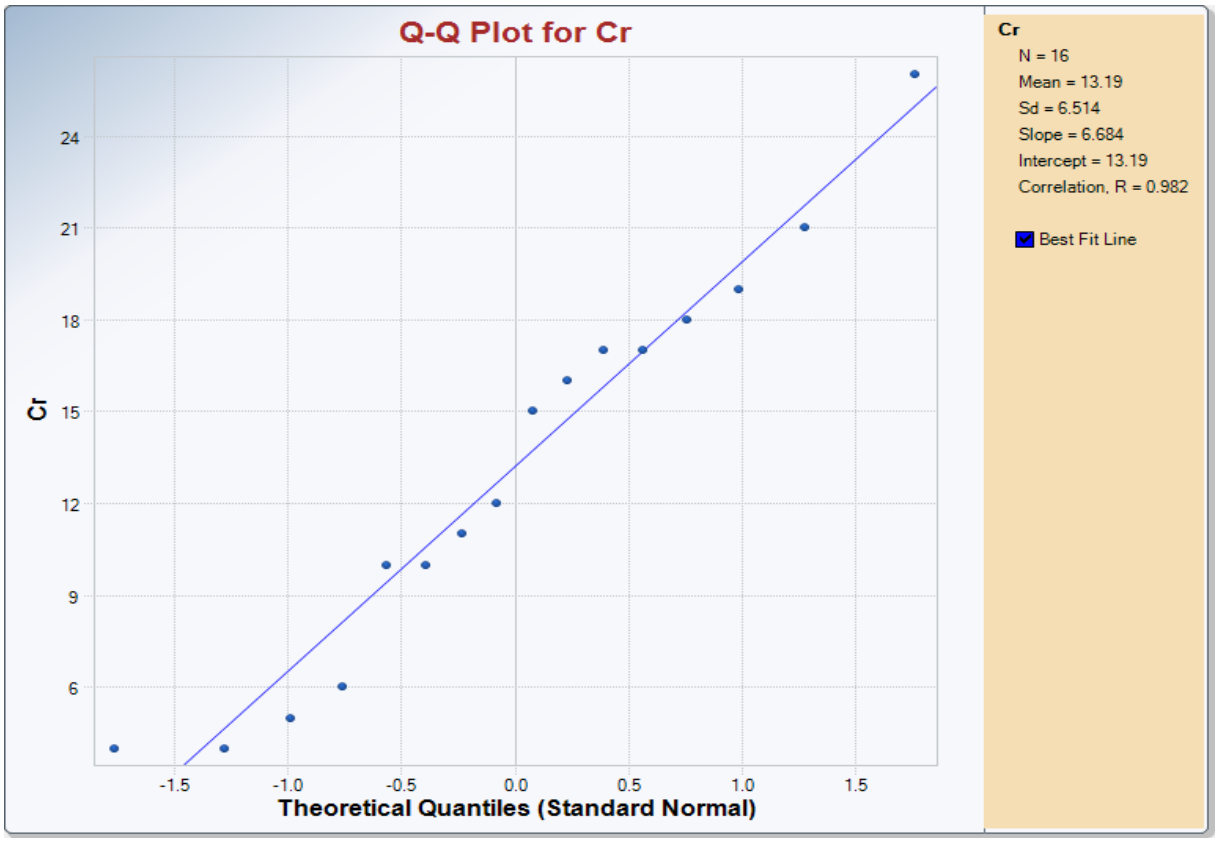

Figure 7 **Q–Q plot for chromium (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

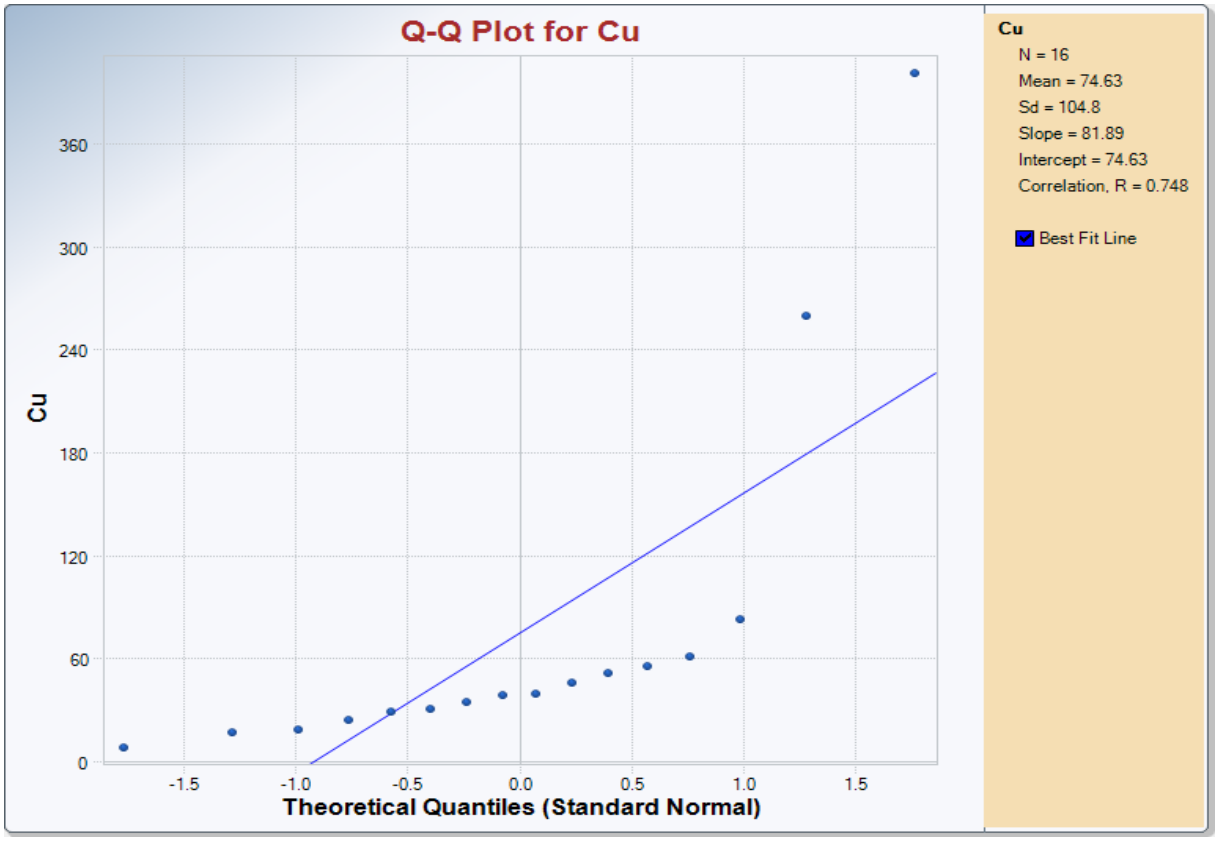

Figure 8 **Q–Q plot for copper (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

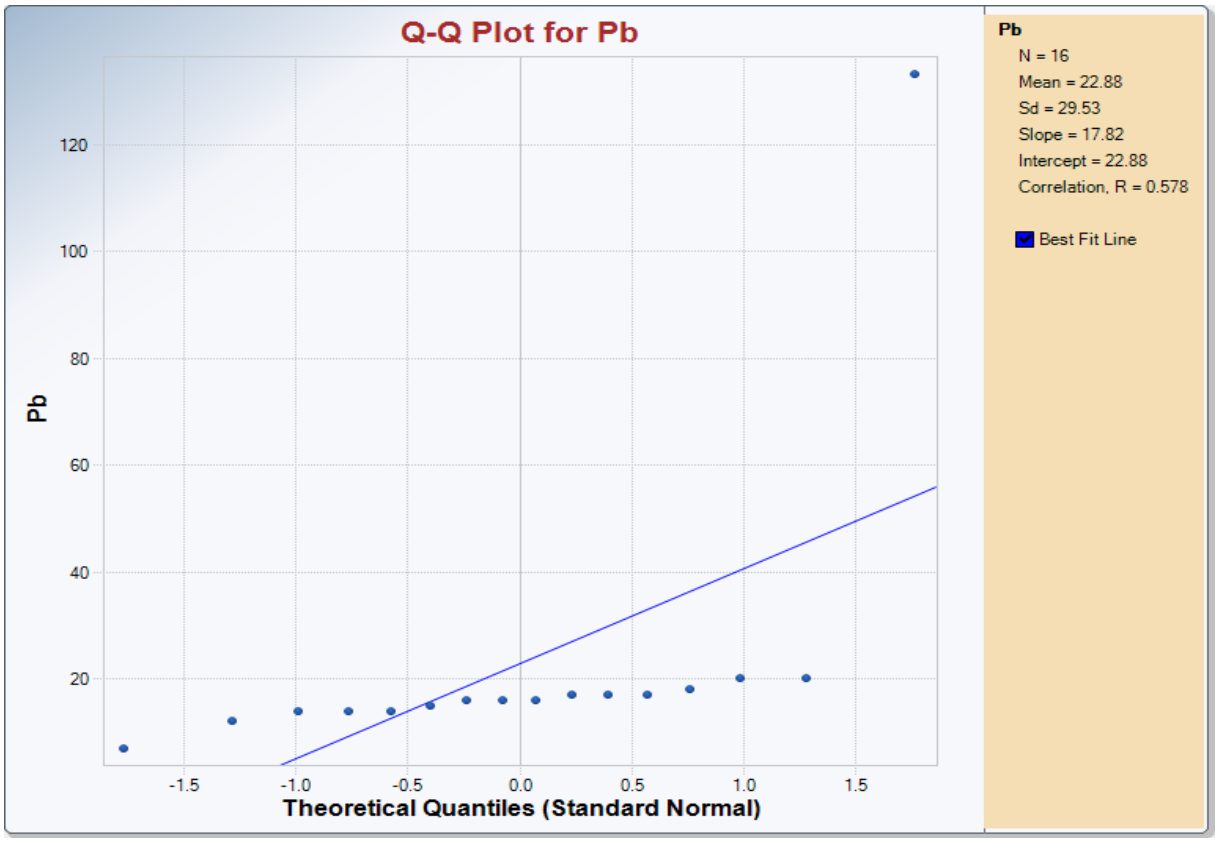

Figure 9 **Q–Q plot for lead (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

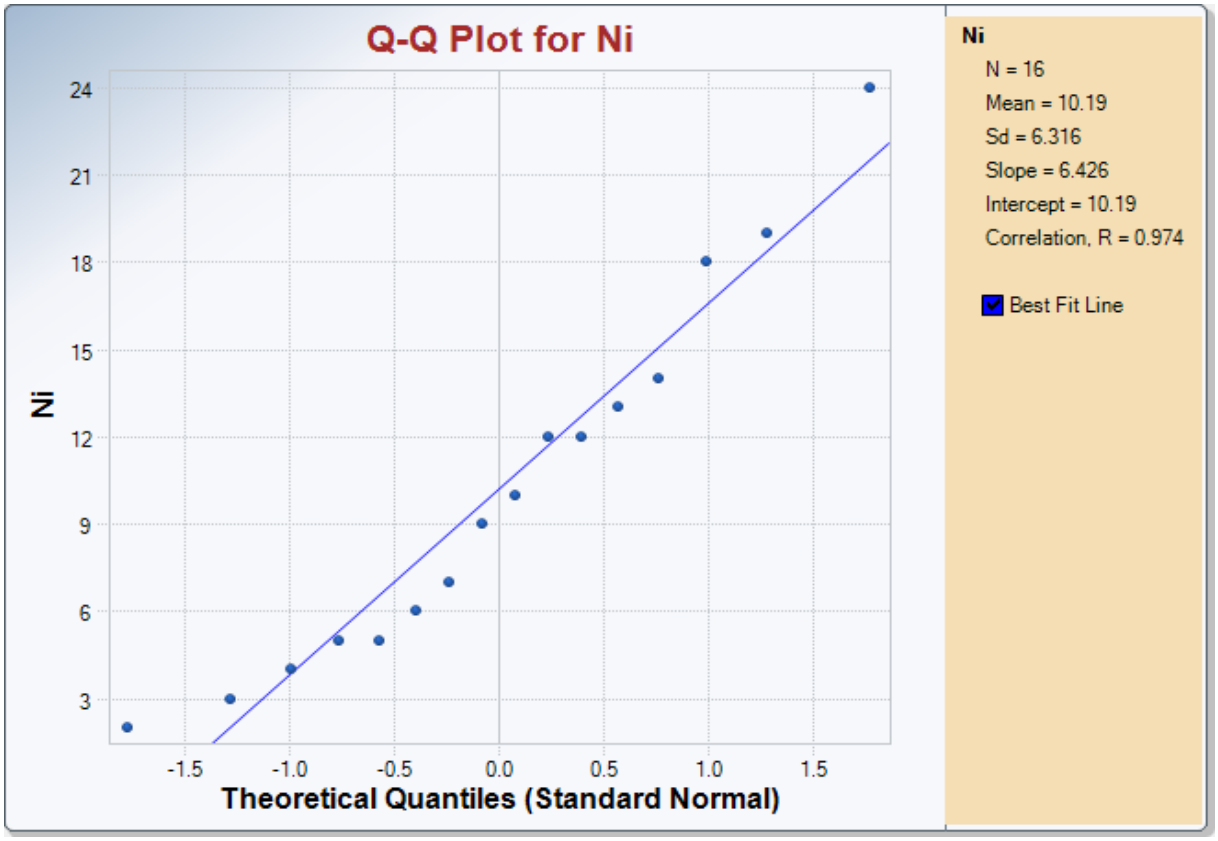

Figure 10 **Q–Q plot for nickel (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

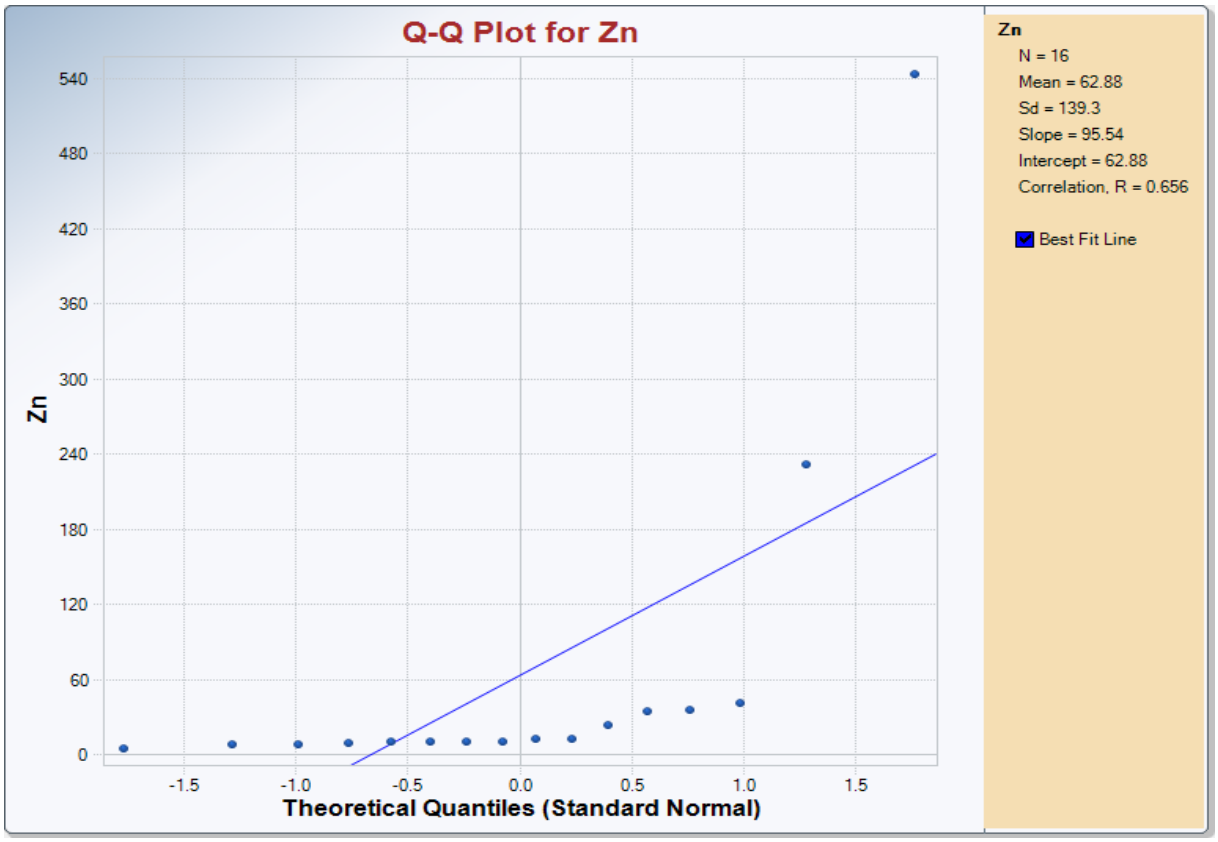

Figure 11 **Q–Q plot for zinc (mg/kg)**

Outputs from USEPA's ProUCL, created by Marc Salmon, Easterly Point Environmental Pty Ltd

Appendix F: One-sample t-test hypothesis testing

When a decision requires the comparison of a sampled population to a target value, such as a specified health investigation level (HIL), a one-sample t-test can be used. This is a parametric method, and assumes a nearly normal distribution, at least for sample sizes of < 30: it is not suitable for highly skewed datasets. See USEPA (2006, G-9S) for non-parametric methods.

Determination

Establish the null hypothesis (H_0) and alternative hypothesis (H_A). EPA policy is to always assume that the site or decision area is contaminated, so the null hypothesis is always written as:

$$H_0: \mu > \text{criterion or action level}$$

The alternative hypothesis for a one-sided test is then:

$$H_A: \mu \leq \text{criterion or action level}$$

The test statistic (t_0) is calculated using the t-score formula:

$$t_0 = \frac{\bar{x} - C}{s/\sqrt{n}}$$

Where:

μ	population mean
t_0	test statistic
$\bar{x}$	sample mean
C	criterion or action level
s	sample standard deviation
n	number of samples
$t\alpha$	critical value.

The critical value ($t\alpha$) is determined from a table of critical values of Student's t-distribution (see Table 4) or by using an appropriate software program. The confidence level ($1 - \alpha$) and the degrees of freedom ($n - 1$) are used to select $t\alpha$.

The test statistic is then compared to the critical value, and the following decisions made:

- if $t_0 < t\alpha$, then fail to reject the null hypothesis that the true population mean is greater than the criterion or action level

- if $t_0 > t\alpha$, then reject the null hypothesis that the true population mean is greater than the criterion or action level and accept the alternative hypothesis that the true population mean is less than or equal to the criterion or action level.

Whereas the signs of t_0 and $t\alpha$ are important in regard to whether an upper-tailed or lower-tailed test is being conducted, when comparing t_0 to $t\alpha$, it is the absolute values that are compared.

The probability or p-value is also determined, either approximately from a table of critical values of Student's t-distribution (see Table 4) or by using an appropriate software program. This is then compared to the selected value of alpha (α), with the following decisions made:

- if p-value > α, then fail to reject the null hypothesis that the true population mean is greater than the criterion or action level.
- if p-value < α, then reject the null hypothesis that the true population mean is greater than the criterion or action level and accept the alternative hypothesis that the true population mean is less than or equal to the criterion or action level.

  While the sign of the p-value is important in regard to whether an upper-tailed or lower-tailed test is being conducted, when comparing the p-value to α it is the absolute values that are compared.

As critical values and p-values are mathematically related, either approach will always provide the same conclusion.

Worked example

In this example we use the arsenic (As) and lead (Pb) data from Table 1 to determine whether the null hypothesis (H_0) should be rejected in favour of the alternative hypothesis (H_A). The selected criteria are the HILs for a residential land use (HILs-A), and the test is to be conducted at a confidence level of 95%, i.e. $\alpha = 0.05$.

The null hypothesis is:

$$H_0: \mu > \text{criterion}$$

The alternative hypothesis is then:

$$H_A: \mu \leq \text{criterion}.$$

The test statistic (t_0) is calculated using the t-score formula:

$$t_0 = \frac{\bar{x} - C}{s/\sqrt{n}}$$

For As, n = 16, $\bar{x}$ = 66.3, s = 88.3 and HIL-A = 100, such that:

$$t_0 = \frac{66.3 - 100}{88.3/\sqrt{16}}$$

$$t_0 = -1.53$$

For Pb, n = 16, $\bar{x}$ = 22.9, s = 29.5 and HIL-A = 300, therefore:

$$t_0 = \frac{22.9 - 300}{29.5/\sqrt{16}}$$

$$t_0 = -37.54$$

From a table of critical values of Student's t-distribution (see Table 4), at a confidence level of 95% for 15 degrees of freedom, $t\alpha = 1.75$.

Critical value

For As, as 1.53 < 1.75, i.e. $t_0 < t\alpha$, then fail to reject the null hypothesis that the true population mean is greater than the criterion.

For Pb, as 37.54 > 1.75, i.e. $t_0 > t\alpha$, then reject the null hypothesis that the true population mean is greater than the criterion and accept the alternative hypothesis that the true population mean is less than or equal to the criterion.

P-value

For As, from a table of critical values of Student's t-distribution (see Table 4), the p-value is between 0.1 and 0.05, i.e. $t\alpha$ is between 1.34 and 1.75. Using a software package, the p-value is calculated to be 0.074. As 0.074 > 0.05, i.e. the p-value > α, then fail to reject the null hypothesis that the true population mean is greater than the criterion.

For Pb, from a table of critical values of Student's t-distribution, the p-value is < 0.005, i.e. $t\alpha$ is > 2.95. Using a software package, the p-value is calculated to be 1.5×10^{-16}. As $1.5 \times 10^{-16} < 0.05$, i.e. p-value < α, then reject the null hypothesis that the true population mean is greater than the criterion and accept the alternative hypothesis that the true population mean is less than or equal to the criterion.

Critical region

In the case of As, t_0 does not fall within the critical region (the area beyond the critical value, $t\alpha$). It is therefore unlikely that the observed test statistic is more extreme than would be expected if the null hypothesis were true. Similarly, as the p-value > α, the probability of observing a p-value as extreme as 0.074 would be high, if H_0 were true. Based on both the critical value approach and the p-value approach, there is insufficient evidence at a 95% confidence level to conclude that the population mean for As < HIL-A.

In the case of Pb, t_0 falls within the critical region, and it is likely that the observed test statistic is more extreme than would be expected if the null hypothesis were true. And, as the p-value < α, the probability of observing a p-value as extreme as 1.5×10^{-16} would be low, if H_0 were true. Based on both the critical value approach and the p-value approach, there is sufficient evidence at a 95% confidence level to reject the null hypothesis and to accept the alternative hypothesis that the population mean for Pb < HIL-A.

Reference

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

Table 4 Critical values of the Student's t-distribution

Degrees of freedom	Significance level for one-sided interval (α), e.g. confidence limits	15%	10%	5%	2.5%	1%	0.5%
	Confidence level for one-sided interval ($t_{1-\alpha}$), e.g. confidence limits	85%	90%	95%	97.5%	99%	99.5%
	Significance level for two-sided interval ($\alpha/2$), e.g. confidence intervals	30%	20%	10%	5%	2%	1%
	Confidence level for two-sided interval ($t_{1-\alpha/2}$), e.g. confidence intervals	70%	80%	90%	95%	98%	99%
1		1.963	3.078	6.314	12.706	31.821	63.657
2		1.386	1.886	2.920	4.303	6.965	9.925
3		1.250	1.638	2.353	3.182	4.541	5.841
4		1.190	1.533	2.132	2.776	3.747	4.604
5		1.156	1.476	2.015	2.571	3.365	4.032
6		1.134	1.440	1.943	2.447	3.143	3.707
7		1.119	1.415	1.895	2.365	2.998	3.499
8		1.108	1.397	1.860	2.306	2.896	3.355
9		1.100	1.383	1.833	2.262	2.821	3.250
10		1.093	1.372	1.812	2.228	2.764	3.169
11		1.088	1.363	1.796	2.201	2.718	3.106
12		1.083	1.356	1.782	2.179	2.681	3.055
13		1.079	1.350	1.771	2.160	2.650	3.012
14		1.076	1.345	1.761	2.145	2.624	2.977
15		1.074	1.341	1.753	2.131	2.602	2.947
16		1.071	1.337	1.746	2.120	2.583	2.921
17		1.069	1.333	1.740	2.110	2.567	2.898
18		1.067	1.330	1.734	2.101	2.552	2.878
19		1.066	1.328	1.729	2.093	2.539	2.861
20		1.064	1.325	1.725	2.086	2.528	2.845
21		1.063	1.323	1.721	2.080	2.518	2.831
22		1.061	1.321	1.717	2.074	2.508	2.819
23		1.060	1.319	1.714	2.069	2.500	2.807
24		1.059	1.318	1.711	2.064	2.492	2.797
25		1.058	1.316	1.708	2.060	2.485	2.787
26		1.058	1.315	1.706	2.056	2.479	2.779
27		1.057	1.314	1.703	2.052	2.473	2.771
28		1.056	1.313	1.701	2.048	2.467	2.763
29		1.055	1.311	1.699	2.045	2.462	2.756

Degrees of freedom	Significance level for one-sided interval (α), e.g. confidence limits	15%	10%	5%	2.5%	1%	0.5%
	Confidence level for one-sided interval ($t_{1-\alpha}$), e.g. confidence limits	85%	90%	95%	97.5%	99%	99.5%
	Significance level for two-sided interval ($\alpha/2$), e.g. confidence intervals	30%	20%	10%	5%	2%	1%
	Confidence level for two-sided interval ($t_{1-\alpha/2}$), e.g. confidence intervals	70%	80%	90%	95%	98%	99%
30		1.055	1.310	1.697	2.042	2.457	2.750
40		1.050	1.303	1.684	2.021	2.423	2.704
60		1.046	1.296	1.671	2.000	2.390	2.660
120		1.041	1.289	1.658	1.980	2.358	2.617
∞		1.036	1.282	1.645	1.960	2.326	2.576

Modified from USEPA 2006, G-9S.

Appendix G: Two-sample t-test hypothesis testing

A decision may require two independent populations to be compared – for example, a potentially contaminated area and a background area, or concentration levels from up-gradient monitoring wells and downgradient monitoring wells. In such cases a two-sample t-test can be used.

This is a parametric method, so the assumption of normality should be checked; see USEPA (2006, G-9S) for non-parametric methods, if those are required. Two-sample t-tests can also be used for paired populations, such as concentrations before and after remediation; again, see USEPA (2006, G-9S) for parametric and non-parametric methods for paired data.

The method used for conducting a two-sample t-test varies depending on whether the variances (s^2) of the two samples are equal or unequal. For environmental data, the variances are generally unequal, and this method is used in the following determination.

Determination

Establish the null hypothesis (H_0) and alternative hypothesis (H_A). As the objective is to compare two populations, the null hypothesis is set to be that the two populations are equal:

$$H_0: \mu_1 - \mu_2 = \delta_0$$

The alternative hypothesis for a one-sided test is then:

$$H_A: \mu_1 - \mu_2 > \delta_0$$

To calculate the test statistics (t_0) for unequal variance, it is first necessary to determine the degrees of freedom (df) using the Welch–Satterthwaite equation:

$$df = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\frac{(s_1^2)^2}{n_1^2(n_1\text{-}1)} + \frac{(s_2^2)^2}{n_2^2(n_2\text{-}1)}}$$

The test statistic, t_0, is then calculated using the Welch's t-test formula, which a modification of the Student's t-test formula:

$$t_0 = \frac{(\bar{x}_1 - \bar{x}_2) - \delta_0}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

Where:

μ_1 population 1

μ_2 population 2

df degrees of freedom

s_1^2 sample variance from population 1

s_2^2 sample variance from population 2

n_1 number of samples from population 1

n_2 number of samples from population 2

t_0 test statistic

$t\alpha$ critical value

$\bar{x}_1$ sample mean from population 1

$\bar{x}_2$ sample mean from population 2

δ_0 difference (delta) of zero

Critical value

The critical value ($t\alpha$) is determined from a table of critical values of Student's t-distribution (see Table 4) or using an appropriate software program. The confidence level ($1 - \alpha$) and the degrees of freedom are used to select $t\alpha$.

The test statistic is then compared to the critical value, and the following decisions made:

- if $t_0 < t\alpha$, then fail to reject the null hypothesis that the difference between the population means is zero
- if $t_0 > t\alpha$, then reject the null hypothesis that the difference between the population means is zero and accept the alternative hypothesis that the mean of population 1 is greater than the mean of population 2.

While the signs of t_0 and $t\alpha$ are important in regard to whether an upper-tailed or lower-tailed test is being conducted, when comparing t_0 to $t\alpha$ it is the absolute values that are compared.

p-value

The probability or p-value is also determined, either approximately from a table of critical values of Student's t-distribution (see Table 4) or using an appropriate software program. The p-value is then compared to the selected value of alpha (α) and the following decisions made:

- if p-value > α, then fail to reject the null hypothesis that the difference between the population means is zero
- if p-value < α, then reject the null hypothesis that the difference between the population means is zero and accept the alternative hypothesis that the mean of population 1 is greater than the mean of population 2.

While the sign of the p-value is important in regard to whether an upper-tailed or lower-tailed test is being conducted, when comparing the p-value to α it is the absolute values that are compared.

As critical values and p-values are mathematically related, either approach will always provide the same conclusion.

Worked example

In this example we use the arsenic (As) data from Table 1 to determine whether the contamination is limited only to the surficial soils (population 1), and therefore if the deeper soils (population 2) can be

considered separately. The descriptive statistics for the two datasets, and the original combined dataset for comparison, are shown in Table 5.

Table 5 **Arsenic summary statistics by population (mg/kg) – simulated data from Table 1**

Statistic	Surface population 1	Depth population 2	Combined
Maximum	341	54	341
Mean	109.3	23.4	66.3
Medium	66.5	13.5	38.5
Minimum	24	6	6
Variance	12,093.4	390.3	7,792.2
Standard deviation	110.0	19.8	88.3

The test is to be conducted at a confidence level of 95%, i.e. $\alpha = 0.05$.

The null hypothesis is:

$$H_0: \mu_1 - \mu_2 = \delta_0$$

The alternative hypothesis for a one-sided test is then:

$$H_A: \mu_1 - \mu_2 > \delta_0$$

The degrees of freedom is first calculated using the Welch–Satterthwaite equation:

$$df = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\frac{(s_1^2)^2}{n_1^2(n_1 - 1)} + \frac{(s_2^2)^2}{n_2^2(n_2 - 1)}}$$

$$df = \frac{\left(\frac{12{,}093.4}{8} + \frac{390.3}{8}\right)^2}{\frac{(12{,}093.4)^2}{8^2(8 - 1)} + \frac{(390.3)^2}{8^2(8 - 1)}}$$

$$df = \frac{1{,}560.5^{\,2}}{3.3 \times 10^5 + 340}$$

$$df = 7.45$$

Rounded down to the next integer, the degrees of freedom is seven (7). A conservative approach is to estimate the degrees of freedom by using the smaller of $n_1 - 1$ or $n_2 - 1$: in this case, that number is also seven.

The test statistic, t_0, is then calculated using Welch's t-test formula:

$$t_0 = \frac{(\bar{x}_1 - \bar{x}_2) - \delta_0}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

$$t_0 = \frac{(109.3 - 23.4) - 0}{\sqrt{\left(\frac{12{,}093.4}{8}\right) + \frac{390.3}{8}}}$$

$$t_0 = 2.174$$

Critical value

From a table of critical values of Student's t-distribution (see Table 4), at a confidence level of 95% for seven degrees of freedom, $t\alpha = 1.895$.

As 2.174 > 1.895, i.e. $t_0 > t\alpha$, then the null hypothesis that the population means are equal is rejected, and the alternative hypothesis H_A (that the mean of population 1 is greater than the mean of population 2) is accepted, i.e. $\mu_1 - \mu_2 > \delta_0$.

p-value

From a table of critical values of Student's t-distribution, the p-value is between 0.025 and 0.05, i.e. $t\alpha$ is between 2.365 and 1.895. Using a software package, the p-value is calculated to be 0.033.
As 0.033 < 0.05, i.e. the p-value < α, then the null hypothesis H_0 (that the population means are equal) is rejected, and the alternative hypothesis H_A (that the mean of population 1 is greater than the mean of population 2) is accepted, i.e. $\mu_1 - \mu_2 > \delta_0$.

Critical region

As t_0 falls within the critical region, it is likely that the observed test statistic is more extreme than would be expected if the null hypothesis were true. And, as the p-value < α, the probability of observing a p-value as extreme as 0.033 would be low, if H_0 were true. Both the critical-value approach and the p-value approach give sufficient evidence at a 95% confidence level to reject the null hypothesis and to accept the alternative hypothesis that the mean of population 1 is greater than the mean of population 2.

Based on review of the summary data, relative to a HIL-A of 100 mg/kg, and the results of the two-sample t-test, it appears that significant impacts relate to the surficial soils rather than the deeper soils. Accordingly, for the design of further investigations and consideration of remedial options, the surficial soils and deeper soils should be considered as separate decision areas. The actual depths which these two populations encompass will need to be determined by further investigations.

Reference

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

Appendix H: Decision errors

Statistical hypothesis testing using a null hypothesis significance testing (NHST) framework – the testing of the null hypothesis (H_0) against an alternative hypothesis (H_A) – can lead to the following four outcomes:

- accepting H_0 when H_0 is true – this is a correct decision for the confidence level of the test ($1 - \alpha$), e.g. $\alpha = 0.05$ and confidence level = 95%
- rejecting H_0 when H_0 is true – this is a Type I or α decision error and results in the false rejection of H_0
- accepting H_0 when H_0 is false – this is a Type II or β decision error and results in the false acceptance of H_0
- rejecting H_0 when H_0 is false – this is a correct decision. The power of the test is ($1 - \beta$), e.g. $\beta = 0.20$ and power = 80%.

These outcomes are summarised in Table 6.

Table 6 Decision errors in hypothesis testing

Decision made	Actual condition – H_0 is true	Actual condition – H_0 is false (H_A is true)
Accept H_0 (fail to reject H_0)	Correct decision $1 - \alpha$ = confidence level	Decision error (Type II error) **False acceptance**
Reject H_0 (accept H_A)	Decision error (Type 1 error) **False rejection**	Correct decision $1 - \beta$ = power of test

In the context of the assessment of site contamination, the null hypothesis is that the site or decision area is contaminated. Decision errors are therefore generally defined as follows:

- the site or decision area is considered not to be contaminated when it actually is – a Type I error. Type I errors can lead to unacceptable risks to human health and/or the environment, and the regulatory framework is established to preferentially protect against Type I errors
- the site or decision area is considered to be contaminated when it actually is not – a Type II error. Type II errors can lead to sites or decision areas being remediated unnecessarily, or land being used for a less-sensitive land use, or unwarranted restrictions on the surrounding environment (such as water-use restrictions or fishing bans).

Appendix I: 95% confidence intervals

Confidence intervals can be used as an indicator of uncertainty around a point estimate, in this case the mean. By choosing a method for expressing uncertainty, a performance metric that quantifies uncertainty can be specified, allowing limits to be established against which the quantity and quantity of the data can be compared (USEPA 2006, G-4).

A method for determining the 95% confidence interval (CI) of the mean for a nearly-normal distribution is shown, using the Student's t formula. For mildly skewed datasets, the Student's t-statistic should be used, but for moderate to highly skewed datasets, the confidence interval based on the t-statistic can fail to cover the population mean, especially for small sample sizes (USEPA 2006, G-9S). It is therefore important to test the data for normality. This is most easily done by constructing normal Q–Q plots, using appropriate statistical software packages. For other distributions or non-parametric methods, refer to USEPA (2006, G-9S).

Determination

The test statistic is calculated using the one-sided Student's t-UCL formula:

$$95\%\ \text{confidence interval} = [0, \bar{x} + t_{\alpha/2,\, n-1}\ \frac{s}{\sqrt{n}}]$$

Where:

$\bar{x}$	sample mean
$t_{\alpha/n-1}$	critical value
s	sample standard deviation
n	number of samples
$s/\sqrt{n}$	standard error of the mean ($SE\bar{x}$).

The standard error of the mean ($SE\bar{x}$) describes the variability in the sampling distribution (i.e. the distribution of means from multiple sampling events of the same population), not the variability in the underlying population. One of the key features of the $SE\bar{x}$ is that it decreases as the sample size increases (Devore and Farnum, 2005).

The $SE\bar{x}$ multiplied by the critical value gives the margin of error (MoE), which can be defined as the radius, or half the width, of a confidence interval for a particular statistic at a specified confidence level (in the equation above, at a 95% confidence level). The MoE also decreases as the number of samples increases.

The critical value is determined from a table of critical values of Student's t-distribution (Table 4 in Appendix F) or using an appropriate statistical software package. The confidence level ($1 - \alpha$) and the degrees of freedom ($n - 1$) are used to select $t_{\alpha/2,n-1}$ for a two-sided interval.

Worked example

In this example we use the metals data from Table 1 to determine the 95% confidence interval for chromium (Cr) for surface fill ($n = 8$) and all fill ($n = 16$), at a confidence level of 95% ($\alpha = 0.05$).

The 95% confidence interval is calculated using the Student's t-UCL formula:

$$95\%\ \text{confidence interval} = [0, \bar{x} + t_{\alpha,\, n-1}\ \frac{s}{\sqrt{n}}]$$

Surface fill

The critical value is selected for a two-sided interval from a table of critical values of Student's t-distribution (Table 4 in Appendix F). At seven (7) degrees of freedom the critical value is 2.365.

For surface fill, $\bar{x} = 15.3$, $s = 6.5$ and $n = 8$:

$$95\%\ \text{confidence interval} = 15.3 \pm 2.365 * \frac{6.5}{\sqrt{8}}$$

$$95\%\ \text{confidence interval} = 15.3 \pm 5.4$$

$$95\%\ \text{confidence interval} = 9.8 \text{ to } 20.7\ \text{mg/kg}$$

All fill

The critical value is selected for a two-sided interval from a table of critical values of Student's t-distribution (Table 4 in Appendix F). At 15 degrees of freedom the critical value is 2.131.

For surface fill, $\bar{x} = 13.2$, $s = 6.5$ and $n = 16$:

$$95\%\ \text{confidence interval} = 15.3 \pm 2.131 * \frac{6.5}{\sqrt{16}}$$

$$95\%\ \text{confidence interval} = 15.3 \pm 3.5$$

$$95\%\ \text{confidence interval} = 9.7 \text{ to } 16.7\ \text{mg/kg}$$

Based on similar datasets, the greater number of samples used in the analysis for all fill samples (16) results in a smaller MoE, and therefore a narrower confidence interval, than does the smaller number of samples used in analysing the surficial fill (8 samples). Figure 12 illustrates this for both Cr and nickel (Ni); Table 7 and Table 8 show the associated summary statistics.

The maximum probable error (MPE), which is a relative measure based on the MoE divided by the mean ($MPE = MoE/\bar{x}$), can be used to specify the required statistical precision for data collection. For example, for Ni, Table 7 and Table 8 show that the MPE for eight (8) samples is 52.6%, while 16 samples are required to achieve an MPE of 33.0%.

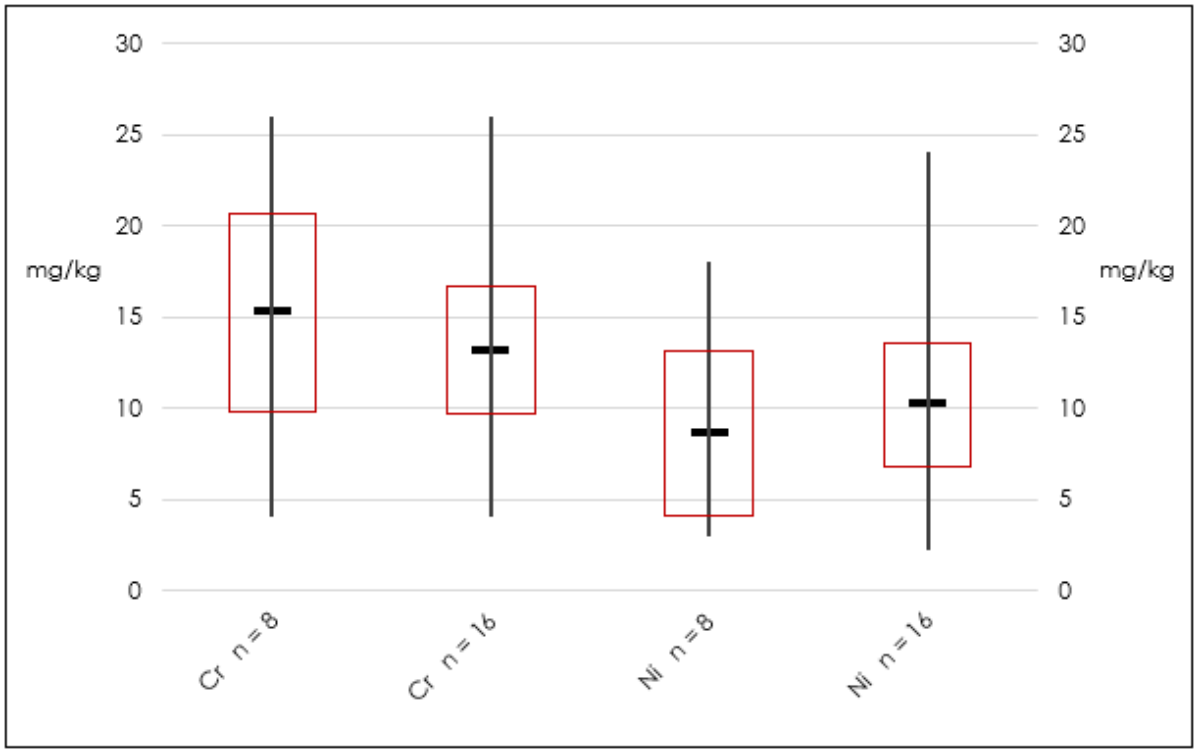

Figure 12 **Summary statistics for Cr and Ni data with variable n (mg/kg) – minimum, 95% LCL, mean, 95% UCL, maximum**

Source: Marc Salmon, Easterly Point Environmental Pty Ltd

Table 7 **Summary statistics for Cr and Ni data (mg/kg) – surface locations**

Surface data	Chromium	Nickel
Number of samples	8	8
Sample mean	15.3	8.6
Standard deviation	6.5	5.4
Standard error of the mean (SE$\bar{x}$)	2.3	1.9
Relative standard deviation (RSD)	42.6%	62.9%
Margin of error (MoE)	5.4	4.5
Maximum probable error (MPE)	35.6%	52.6%

Table 8 **Summary statistics for Cr and Ni data (mg/kg) – all locations**

All data	Chromium	Nickel
Number of samples	16	16
Sample mean	13.2	10.2
Standard deviation	6.5	6.3
Standard error of the mean (SE$\bar{x}$)	1.6	1.6
Relative standard deviation (RSD)	49.4%	61.9%
Margin of error (MoE)	3.5	3.4
Maximum probable error (MPE)	26.3%	33.0%

References

Devore J & Farnum N 2005, *Applied Statistics for Engineers and Scientists*, 2nd Edition, Brooks/Cole, Cengage Learning, Belmont CA.

US Environmental Protection Agency (USEPA) 2006, *Guidance on Systematic Planning Using the Data Quality Objectives Process (QA/G-4)*, EPA/240/B-06/001, USEPA, Washington DC.

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

Appendix J: 95% UCL$\bar{x}$ for normal distributions

Here we show a method for determining the 95% upper confidence limit of the mean (UCL$\bar{x}$) for a nearly-normal distribution, using the Student's t formula.

For mildly skewed datasets, the Student's t-statistic should be used, but for moderate to highly skewed datasets, the 95% UCL$\bar{x}$ based on the t-statistic may not cover the population mean, especially for small sample sizes. It is therefore important to test the data for normality. This is most easily done by constructing normal Q–Q plots, using appropriate statistical software packages.

Determination

The test statistic is calculated using the one-sided Student's t-UCL formula:

$$95\%\ \mathrm{UCL}\bar{x} = \bar{x} + t_{\alpha,n-1}\frac{s}{\sqrt{n}}$$

Where:

95% UCL$\bar{x}$	test statistic
$\bar{x}$	sample mean
$t_{\alpha,n-1}$	critical value
s	sample standard deviation
n	number of samples

The critical value is determined from a table of critical values of Student's t-distribution (Table 4 in Appendix F), or using an appropriate statistical software package. The confidence level ($1 - \alpha$) and the degrees of freedom ($n - 1$) are used to select $t_{\alpha,n-1}$.

Worked example

Here we use the metals data from Table 1 to determine the 95% UCL$\bar{x}$ for arsenic (As) and chromium (Cr) at a confidence level of 95% ($\alpha = 0.05$), at 15 degrees of freedom ($16 - 1 = 15$).

The 95% UCL$\bar{x}$ is calculated using the Student's t-UCL formula:

$$95\%\ \mathrm{UCL}\bar{x} = \bar{x} + t_{\alpha,n-1}\frac{s}{\sqrt{n}}$$

The critical value is selected from a table of critical values of Student's t-distribution (Table 4 in Appendix F). In this instance it is 1.753.

Arsenic

For As, $\bar{x} = 66.3$, $s = 88.3$ and $n = 16$:

$$95\%\ \text{UCL}_{\bar{x}} = 66.3 + 1.753\ \frac{88.3}{\sqrt{16}}$$

$$95\%\ \text{UCL}_{\bar{x}} = 66.3 + 38.7$$

$$95\%\ \text{UCL}_{\bar{x}} = 105.0$$

Chromium

For Cr, $\bar{x} = 13.2$, $s = 6.5$ and $n = 16$:

$$95\%\ \text{UCL}_{\bar{x}} = 13.2 + 1.753\ \frac{6.5}{\sqrt{16}}$$

$$95\%\ \text{UCL}_{\bar{x}} = 13.2 + 2.85$$

$$95\%\ \text{UCL}_{\bar{x}} = 16.05$$

The coefficient of variation (CV) for As is 1.3, suggesting a distribution that is not nearly-normal: this is confirmed by the Q–Q plot for As (Figure 6 in Appendix E). Figure 1, Figure 2 and Figure 5 show that the dataset is skewed to the right, indicating that it can't be appropriately analysed with a Student's t-distribution. Running the data through a statistical software package gives the same conclusion: the software recommends the use of a gamma distribution and calculates a 95% $\text{UCL}_{\bar{x}}$ of 120.5 mg/kg.

The CV for Cr is 0.5, suggesting a distribution that is nearly-normal: this is confirmed by the distribution shown in Figure 1 and Figure 2 and the Q–Q plot for Cr in Figure 7. Cr appears to be normally and symmetrically distributed, and therefore the calculated value is likely to be an accurate estimate of the 95% $\text{UCL}_{\bar{x}}$. A statistical software package confirmed this: it recommended use of a Student's t-distribution and calculated a 95% UCL for the mean of 16.04 mg/kg.

Based on use of the Student's t-UCL formula to calculate these 95% $\text{UCL}_{\bar{x}}$, there is a 95% probability that the mean concentration of Cr will not exceed 16.05 mg/kg. The As dataset needs to be analysed further by another method.

References

US Environmental Protection Agency (USEPA) 2002, *Calculating Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites*, OSWER 9285.6-10, USEPA, Washington DC.

US Environmental Protection Agency (USEPA) 2006, *Data Quality Assessment: Statistical Methods for Practitioners (QA/G-9S)*, EPA/240/B-06/003, USEPA, Washington DC.

US Environmental Protection Agency (USEPA) 2015, *ProUCL Version 5.1.002: Technical Guide: Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations*, EPA/600/R-07/041, USEPA, Washington DC.

Appendix K: 95% UCL$\bar{x}$ for log-normal distributions

Here we show a method for determining the 95% upper confidence limit of the mean (UCL$\bar{x}$) for a log-normal distribution, using the Land's H-statistic.

This method assumes log-normality, and it is very important to test this assumption. The easiest way to do this is to construct log-normal Q–Q plots using an appropriate statistical software package.

Determination

The test statistic is calculated using the one-sided Land's H-statistic:

$$95\%\ \text{H-UCL}\bar{x} = \exp\left(\bar{y} + \frac{s_y^2}{2} + \frac{s_y H_{1-\alpha}}{\sqrt{n-1}}\right)$$

Where:

95% H-UCL$\bar{x}$	test statistic
exp	exponential function, i.e. 2.7183 to the power of the value inside the brackets
$\bar{x}$	mean of the log-transformed sample measurements
s_y^2	variance of the log-transformed sample measurements
s_y	standard deviation of the log-transformed sample measurements
$H_{1-\alpha}$	H-statistic critical value, at the stated confidence level ($1 - \alpha$), which depends on the values of s_y and n
n	number of samples

The sample data is transformed using the natural logarithm, i.e. a logarithm to the base **e** (2.7183), such that $y_i = \ln x_i$, and the descriptive statistics $\bar{y}$, s_y^2 and s_y are determined from the transformed data.

The value of $H_{1-\alpha}$ is selected from Table 9 for a 95% confidence level, based on the values for s_y and n. For other confidence levels, refer to USEPA (2006, G-9S), and for values of s_y and n not listed in Table 9, use interpolation.

Worked example

Here we use the metals data from Table 1 to determine the 95% H-UCL$\bar{x}$ for arsenic (As) and copper (Cu) at a confidence level of 95% ($\alpha = 0.05$).

Arsenic

The sample data is transformed using the natural logarithm, and for As, $\bar{y} = 3.561$, $s_y^2 = 1.347$, $s_y = 1.160$ and $n = 16$.

The value of H is selected from Table 9. Based on s_y and n, H is between 2.564 and 3.163. By interpolation, $H = 2.958$.

The test statistic is calculated from:

$$95\%\ \text{H-UCL}\bar{x} = \exp\left(\bar{y} + \frac{s_y^2}{2} + \frac{s_y H_{1-\alpha}}{\sqrt{n-1}}\right)$$

$$95\%\ \text{H-UCL}\bar{x} = \exp\left(3.561 + \frac{1.347}{2} + \frac{1.160 * 2.958}{\sqrt{16-1}}\right)$$

$$95\%\ \text{H-UCL}\bar{x} = \exp(5.120)$$

$$95\%\ \text{H-UCL}\bar{x} = 167.4$$

The coefficient of variation (CV) for As is 1.3, suggesting a distribution that is not nearly-normal: this is confirmed by the Q–Q plot for As (Figure 6 in Appendix E). Figure 1, Figure 2 and Figure 5 show that the dataset is skewed to the right. While this suggests that an H-UCL$\bar{x}$ may be appropriate, when a statistical software package was used to generate a range of distributions for calculating the 95% UCL$\bar{x}$, it recommended a gamma distribution.

Although the As data appear log-normal, the Land's H-statistic is sensitive to deviations from log-normality, and produces very high values for large variance or skewness, or where n is small (< 30) (USEPA 2002). Accordingly, USEPA (2015) recommends that positively skewed datasets should first be tested for a gamma distribution. If the dataset follows a gamma distribution, the UCL$\bar{x}$ should then be computed using a gamma distribution.

Assuming a gamma distribution for the As data, the software package determined a 95% UCL$\bar{x}$ of 120.5 mg/kg – markedly different from the 95% H-UCL$\bar{x}$ of 167.4 mg/kg. As both exceed the HIL-A for As of 100 mg/kg, further data analysis or investigations would be recommended.

Copper

The sample data is transformed using the natural logarithm, and for Cu, $\bar{y} = 3.773$, $s_y^2 = 0.950$, $s_y = 0.974$ and $n = 16$.

The value of H is selected from Table 9. Based on s_y and n, H is between 2.432 and 2.744. By interpolation, H = 2.619.

The test statistic is calculated from:

$$95\%\ \text{H-UCL}\bar{x} = \exp\left(\bar{y} + \frac{s_y^2}{2} + \frac{s_y H_{1-\alpha}}{\sqrt{n-1}}\right)$$

$$95\%\ \text{H-UCL}\bar{x} = \exp\left(3.773 + \frac{0.950}{2} + \frac{0.974 * 2.619}{\sqrt{16-1}}\right)$$

$$95\%\ \text{H-UCL}\bar{x} = \exp(4.907)$$

$$95\%\ \text{H-UCL}\bar{x} = 135.2$$

The CV for Cu is 1.4, suggesting a distribution that is not nearly-normal. This is confirmed by the Q–Q plot for Cu in Figure 8. Figure 1 and Figure 5 show that the dataset is skewed to the right, suggesting that an H-UCL$\bar{x}$ may be appropriate. This was confirmed by using a statistical software package to generate a range of distributions for calculating the 95% UCL$\bar{x}$. In both cases the 95% UCL$\bar{x}$ was 135.2 mg/kg.

Table 9 Values of H for one-sided 95% confidence level for computing H-UCL on a log-normal mean

S_y	n = 3	n = 5	n = 7	n = 10	n = 12	n = 15	n = 21	n = 31	n = 51	n = 101
0.10	2.750	2.035	1.886	1.802	1.775	1.749	1.722	1.701	1.684	1.670
0.20	3.295	2.198	1.992	1.881	1.843	1.809	1.771	1.742	1.718	1.697
0.30	4.109	2.402	2.125	1.977	1.927	1.882	1.833	1.793	1.761	1.733
0.40	5.220	2.651	2.282	2.089	2.026	1.968	1.905	1.856	1.813	1.777
0.50	6.495	2.947	2.465	2.220	2.141	2.068	1.989	1.928	1.876	1.830
0.60	7.807	3.287	2.673	2.368	2.271	2.181	2.085	2.010	1.946	1.891
0.70	9.120	3.662	2.904	2.532	2.414	2.306	2.191	2.102	2.025	1.960
0.80	10.43	4.062	3.155	2.710	2.570	2.443	2.307	2.202	2.112	2.035
0.90	11.74	4.478	3.420	2.902	2.738	2.589	2.432	2.310	2.206	2.117
1.00	13.05	4.905	3.698	3.103	2.915	2.744	2.564	2.423	2.306	2.205
1.25	16.33	6.001	4.426	3.639	3.389	3.163	2.923	2.737	2.580	2.447
1.50	19.60	7.120	5.184	4.207	3.896	3.612	3.311	3.077	2.881	2.713
1.75	22.87	8.250	5.960	4.795	4.422	4.081	3.719	3.437	3.200	2.997
2.00	26.14	9.387	6.747	5.396	4.962	4.564	4.141	3.812	3.533	3.295
2.50	32.69	11.67	8.339	6.621	6.067	5.557	5.013	4.588	4.228	3.920
3.00	39.23	13.97	9.945	7.864	7.191	6.570	5.907	5.388	4.947	4.569
3.50	45.77	16.27	11.56	9.118	8.326	7.596	6.815	6.201	5.681	5.233
4.00	52.31	18.58	13.18	10.38	9.469	8.630	7.731	7.024	6.424	5.908
4.50	58.85	20.88	14.80	11.64	10.62	9.669	8.652	7.854	7.174	6.590
5.00	65.39	23.19	16.43	12.91	11.77	10.71	9.579	8.688	7.929	7.277
6.00	78.47	27.81	19.68	15.45	14.08	12.81	11.44	10.36	9.449	8.661
7.00	91.55	32.43	22.94	18.00	16.39	14.90	13.31	12.05	10.98	10.05
8.00	104.6	37.06	26.20	20.55	18.71	17.01	15.18	13.74	12.51	11.45
9.00	117.7	41.68	29.46	23.10	21.03	19.11	17.05	15.43	14.05	12.85
10.00	130.8	46.31	32.73	25.66	23.35	21.22	18.93	17.13	15.59	14.26

From Gilbert (1987)

For values of s_y and n not listed, use interpolation.

For other confidence levels, refer to USEPA (2006, G-9S).

References

Gilbert RO 1987, *Statistical Methods for Environmental Pollution Monitoring*, John Wiley & Sons, Inc., Brisbane.

US Environmental Protection Agency (USEPA) 2002, *Calculating Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites*, OSWER 9285.6-10, USEPA, Washington DC.

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US Environmental Protection Agency (USEPA) 2015, *ProUCL Version 5.1.002: Technical Guide: Statistical Software for Environmental Applications for Data Sets with and without Nondetect Observations*, EPA/600/R-07/041, USEPA, Washington DC.

Appendix L: 95% UCL$\bar{x}$ for skewed distributions

Here we give a method for determining the 95% upper confidence limit of the mean (UCL$\bar{x}$) when the distribution cannot be identified. It is based on the non-parametric Chebyshev inequality formula.

The Chebyshev inequality formula makes no assumptions about distribution. For moderately skewed datasets it yields conservative but realistic values for UCL$\bar{x}$. But for highly skewed datasets it can substantially underestimate the UCL$\bar{x}$, especially for small sample sizes, because it assumes that the standard deviation of the underlying distribution is known. In such cases you can use higher confidence limits (USEPA 2015): statistical software packages will usually recommend these.

Determination

For unknown distributions, the test statistic is calculated using the one-sided Chebyshev inequality formula:

$$95\%\ UCL\bar{x} = \bar{x} + k_{(1-\alpha)} \frac{s}{\sqrt{n}}$$

Where:

95% UCL$\bar{x}$	test statistic
$\bar{x}$	sample mean
$k_{(1-\alpha)}$	critical value
s	sample standard deviation
n	number of samples

The critical value, k, which is based on the one-sided Chebyshev inequality, is selected from Table 10. It is determined as:

$$k = \sqrt{\frac{1}{\alpha} - 1}$$

Table 10 Critical values based on the Chebyshev Theorem

Confidence level %	alpha (α)	k
99	0.01	9.95
95	0.05	4.36
90	0.10	3.00
85	0.15	2.38
80	0.20	2.00
75	0.25	1.73

Adapted from CL:AIRE (2008).

Worked example

Here we use the metals data from Table 1 to determine the 95% UCL of the mean for arsenic (As) and zinc (Zn), at a confidence level of 95% (α = 0.05).

The test statistic is calculated using the Chebyshev inequality formula:

$$95\%\ UCL_{\bar{x}} = \bar{x} + k_{(1-\alpha)} \frac{s}{\sqrt{n}}$$

The critical value is selected from Table 10. For $\alpha = 0.05$, $k_{(1-\alpha)} = 4.36$.

Arsenic

For As, $\bar{x} = 66.3$, $s = 88.3$ and $n = 16$:

$$95\%\ UCL_{\bar{x}} = 66.3 + 4.36 \frac{88.3}{\sqrt{16}}$$

$$95\%\ UCL_{\bar{x}} = 66.3 + 96.2$$

$$95\%\ UCL_{\bar{x}} = 162.5$$

Zinc

For Zn, with $\bar{x} = 62.9$, $s = 139.3$ and $n = 16$:

$$95\%\ UCL_{\bar{x}} = 62.9 + 4.36 \frac{139.3}{\sqrt{16}}$$

$$95\%\ UCL_{\bar{x}} = 62.9 + 151.9$$

$$95\%\ UCL_{\bar{x}} = 214.7$$

Table 1 shows that the coefficient of variation (CV) for As is 1.3, suggesting a distribution that is not nearly-normal. This is confirmed by the Q–Q plot for As in Figure 6. Figure 1 and Figure 2, and the histogram in Figure 5, show that the dataset is skewed to the right, implying that a Student's t-distribution is not appropriate for this dataset. A statistical software package confirmed this, and also determined that the Chebyshev inequality method produced an overly conservative $UCL_{\bar{x}}$ for this dataset. The package recommended the use of a gamma distribution; this led to a calculated value for the 95% $UCL_{\bar{x}}$ of 120.5 mg/kg.

The dataset for Zn has a CV of 2.2 and is highly skewed to the right, as can be seen from Figure 1 and Figure 2, the Q–Q plot for Zn in Figure 11, and the histogram in Figure 5. The skewness suggests that a Student's t-distribution is not appropriate for this dataset. A statistical software package confirmed this, also finding that the dataset does not follow a discernible distribution. The package therefore recommended the use of the Chebyshev inequality method, which calculated a 95% $UCL_{\bar{x}}$ of 214.7 mg/kg.

References

Contaminated Land: Applications in Real Environments (CL:AIRE) 2008, *Guidance on Comparing Soil Contamination Data with a Critical Concentration*, The Chartered Institute of Environmental Health and CL:AIRE, London.

US Environmental Protection Agency (USEPA) 2002, *Calculating Upper Confidence Limits for Exposure Point Concentrations at Hazardous Waste Sites*, OSWER 9285.6-10, USEPA, Washington DC.

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