UNCERTAINTY TECHNIQUES IN ENVIRONMENTAL RISK ASSESSMENT

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INTRODUCTION

How much does a chemical present a real risk to human and environment? The goal of risk assessment is to estimate the likelihood and the extent of adverse effects occurring to man, animals or ecological systems due to possible exposure(s) to substances. The assessment of whether a substance presents a risk to organisms in the environment is based on the comparison of a predicted environmental concentration (PEC) with a predicted no effect concentration to ecosystems (NOEC).

In the deterministic framework inputs are single values. In the probabilistic framework inputs are treated as random variables coming from probability distributions. The outcome is a risk distribution. A distinction ought to be made between uncertainty and inherent variability. Variability represents heterogeneity or diversity, which is not reducible through further measurement or study. Uncertainty represents ignorance about a poorly characterised phenomenon which is sometimes reducible through further measurement or study. The probabilistic risk assessment enables risk managers to see the full range of variability and uncertainty instead of being mislead into thinking that exposure, effects and eventually risk are point values.

Several techniques can be used to estimate uncertainty in a data set: bootstrapping, the maximum likelihood method (MLE) and Bayesian approaches.
Fig. 1 gives an example of the approach to construct uncertainty bands on a cumulative distribution function based on a limited data set (n = 9). The cumulative distribution function itself can be considered as a variability distribution. For each percentile or parameter of the variability distribution, a confidence interval can be calculated (i.e. an uncertainty distribution).

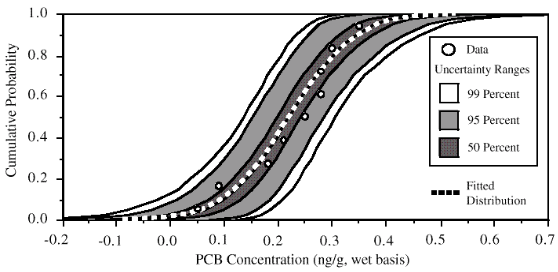

Fig. 1: example of an uncertainty band around a cumulative distribution function

The general goal of this paper is to determine which technique is most suitable and reliable for determination of these uncertainty bands. The mentioned techniques will be applied on toxicity test results (NOECs), which are used in probabilistic risk assessment. Single-species toxicity test data are combined to predict concentrations affecting only a certain percentage of species in a community. A distribution is fit to single-species data collected for many species. From this distribution of species

sensitivities, a hazardous concentration (HC_p) is identified at which a certain percentage p of all species is assumed to be affected. One can use the lower 95% tolerance limit of the estimated percentage to ensure that the specified level of protection is achieved.
In this paper, the methods will be applied on data sets found in literature. No discussion is made on the quality of these data sets or on the advantages and disadvantages of the species sensitivity distribution approach. The studied techniques have a much broader application field.

METHODS

In this section, a technical overview is given of techniques that provide estimates of confidence intervals: bootstrapping, maximum likelihood method and Bayesian approaches. At the end, an overview of the data sets used is given.

Bootstrapping: A detailed description of bootstrapping, can be found in Cullen & Frey (1999) and Davison & Hinkley (1997). Given a data set of sample size n, the general approach in bootstrap simulation is to assume a nonparametric or parametric distribution which describes the quantity of interest, to perform r replications of the original data set by randomly drawing, with replacement, n values, and then calculate r values of the statistic of interest.
In case nonparametric bootstrapping is used, samples are taken from an empirical distribution function (also called resampling) or from an empirical cumulative distribution function (using Hazen plotting system). Nonparametric or distribution-free approaches do not require assumptions regarding the probability model for the underlying population distribution. However, they also tend to yield wider estimates of confidence intervals than parametric methods do. In parametric bootstrapping, a parametric distribution (e.g. lognormal distribution) is used.

Bayesian approach: The Bayesian statistical method reverses the role of sample and model: the sample is fixed and unique, and the model itself is uncertain. This statistical viewpoint corresponds better to the practical situation the individual researcher is facing: there is only one sample and there are doubts what model to use, or, if the model is chosen, what values the parameters will take. The uncertainty of the model is modelled by assuming that the parameters of the model are distributed. More details are found in Aldenberg & Jaworska (2000).

Maximum likelihood estimation (MLE): The general idea is to choose an estimator for the parameter(s) in a distribution so as to maximise a function of the sample observations.

Data sets: Four different data sets were considered. Data Set 1, a synthetic data set, contains 20 positive values drawn randomly from a known lognormal distribution ($\exp[N(\mu,\sigma)]$ with $\mu = 2$ and $\sigma = 1$). The arithmetic mean of the parent distribution equals $\exp[\mu + 0.5\sigma^2] = 12.2$, approximately, and the arithmetic mean of the considered sample of 20 values equals 14, exactly.
Data Set 2, 3 and 4 consist of toxicity database of respectively Cd (Cadmium), Cu (Copper) and LAS (Linear Alkylbenzosulfonate, a chemical used in detergents). The data sets can be found in Versteeg et al. (1999).

RESULTS AND DISCUSSION

Two-dimensional analysis of variability and uncertainty was performed. It can be used to produce a point estimate, if so desired by an analyst or decision-maker.

Results are shown in Figures 2 and 3. The following remarks can be made:

- There is a distinct difference in shape between the parametric and non-parametric distributions. The parametric uncertainty band is much smoother than the non-parametric one.
- The results illustrate that, for a positively skewed quantity, the uncertainty in the distribution becomes largest at the upper tail.

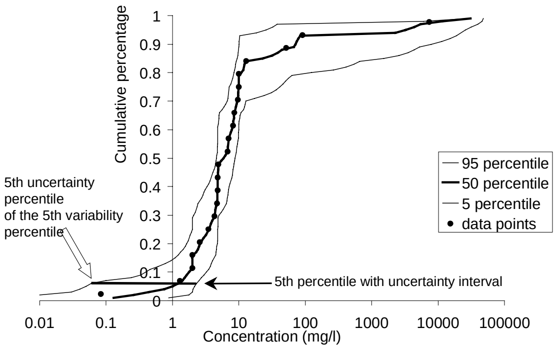

Fig. 2: Non-parametric bootstrapping (Emp CDF) for the Cd data set

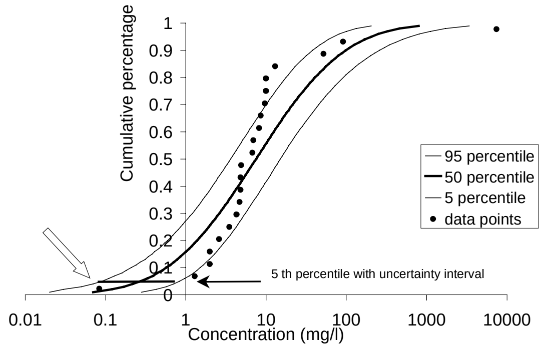

Fig. 3: Parametric bootstrapping (lognormal distribution) for the Cd data set

In order to select a point estimate, it is necessary to specify both the percentile of the population of interest, which reflects variability, and the desired confidence level or probability band, which reflects uncertainty. For example, one point estimate would be the 5th-percentile of uncertainty for the 5th-percentile of variability (indicated by arrow on Figures 2 and 3).

First, the hypothetical lognormal data set 1 was studied. Fig. 4 represents the 90% uncertainty intervals of the 5th-percentile obtained with all methods tested on the 20 data points of the hypothetical lognormal distribution.

- The maximum likelihood method and the Bayesian approach lead to the same solutions, as Aldenberg & Jaworska (2000) already concluded.
- The median 5th-percentiles of all methods are close to each other and always lower than the real 5th-percentile.
- The real 5th-percentile lies within the 90%-uncertainty intervals of all methods. This is to be expected, as data set 1 is lognormally distributed.
- Non-parametric bootstrapping results in wider confidence limits than the other techniques. The parametric bootstrap also has wider confidence bands than the parametric MLE and Bayesian analysis.
- The parametric bootstrap showed a behaviour similar to the MLE and Bayesian analysis, although with wider confidence bands. Because MLE and Bayesian

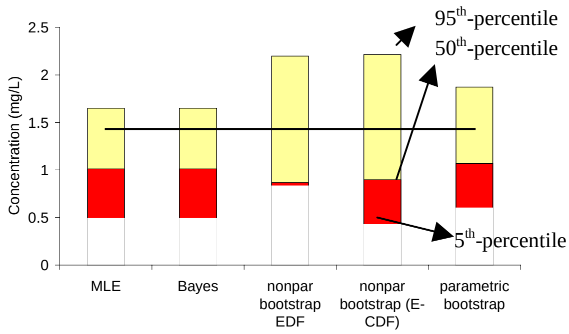

Fig. 4: 90% uncertainty intervals of the 5th-percentile for all methods for the hypothetical lognormal data set (thick line = real 5th-percentile)

analysis are easier to use and not so computationally intensive, they should be preferred over the parametric bootstrap.

Then, two actual toxicity data sets (LAS - data set 4 and Cu - data set 3) were studied. The following conclusions can be made (see Fig. 5 and Fig. 6):

- For LAS, a possible median 5th-percentile could be identified that could be situated within the 90%-uncertainty bands of all methods. Fig. 5 shows large similarities to Fig. 4. For Cu, no possible variability 5th-percentile could be identified that would lie within the 90%-uncertainty bands of all methods.
- For LAS, a factor of 2.4 and for Cu, a factor of almost 5 was found between the estimated median 5th-percentiles of the various methods. However, given the fact that other, larger uncertainties exist in using the species sensitivity distribution approach (e.g. the uncertainty of lab to field extrapolations) the applied method is not a major issue.
- The nonparametric resampling bootstrap showed it was too arbitrarily and inaccurate.

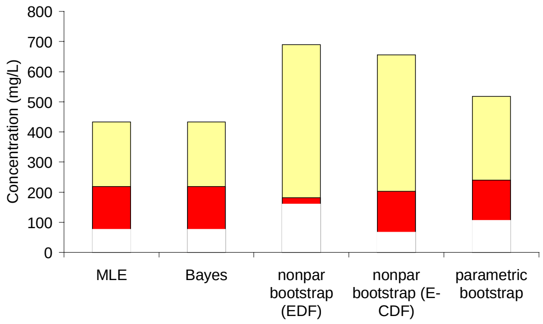

Fig. 5: 90% uncertainty intervals of the 5th-percentile following various methods for 17 data points of the LAS data set

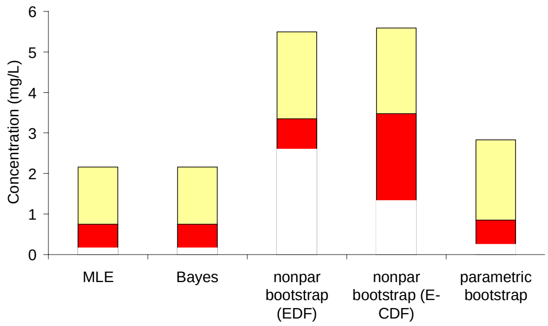

Fig 6: 90% uncertainty intervals of the 5th-percentile following various methods for 20 data points of the Cu data set

CONCLUSIONS

In probabilistic risk assessment, risk managers can see the full range of variability and uncertainty instead of being mislead into thinking that exposure, effects and eventually risk are point values. Several techniques can be used to estimate uncertainty in a data set: bootstrapping, the maximum likelihood method (MLE) and Bayesian approaches. All methods give similar uncertainty estimates, considering the fact that other, larger uncertainties exist in the risk assessment process.

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