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On the application of loss functions in determining assessment factors for ecological risk

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ABSTRACT

Assessment factors have been proposed as a means to extrapolate from data on the concentrations hazardous to a small sample of species to the concentration hazardous to p% of the species in a given community (HC_p). Aldenberg and Jaworska [2000. Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicol. Environ. Saf. 46, 1–18] proposed estimators that prescribed *universal* assessment factors which made use of distributional assumptions associated with species sensitivity distributions. In this paper we maintain those assumptions but introduce loss functions which punish over- and under-estimation. Furthermore, the final loss function is parameterised such that conservatism can be asymmetrically and non-linearly controlled which enables one to better represent the reality of risk assessment scenarios. We describe the loss functions and derive Bayes rules for each. We demonstrate the method by producing a table of universal factors that are independent of the substance being assessed and which can be combined with the toxicity data in order to estimate the HC_5. Finally, through an example we illustrate the potential strength of the newly proposed estimators which rationally accounts for the costs of under- and over-estimation to choose an estimator; as opposed to arbitrarily choosing a one-sided lower confidence limit.

1. Introduction

The hazardous concentration to p% (HC_p) of a community assemblage of biological species is equivalent to the probability that a randomly selected species from this assemblage has its toxicological endpoint (typically a no observed effect concentration NOEC) violated at, or below, the HC_p. Most work focuses on the extrapolation related to inter-species variation for a given substance, and this is where we will focus also. A thorough discussion of this and related topics can be found in Posthuma et al. (2002).

It is often the case within the typical modelling assumptions that the decision rule for setting safety limits (*a.k.a.* trigger values) is equivalent to applying an assessment factor (*a.k.a.* extrapolation factor, safety factor, uncertainty factor) to some particular summary of the available toxicity data. In recent years there has been a lot of literature published on the calculation of assessment factors and ways of calculating the HC_p. This has included (and is not limited to) methods based on: confidence limits (Wagner and Løkke, 1991; Aldenberg and Slob, 1993; Aldenberg and Jaworska, 2000); bootstrapping techniques (Newman et al., 2000, 2002); Bayesian analysis with subjective knowledge (Grist et al., 2006) and without subjective knowledge (Aldenberg et al., 2002); non-parametric methods with an application of an asymmetric loss function (Chen, 2003); and calculating the mathematically expected fraction of species affected (EFSA, 2005). Furthermore, many methods have invoked species sensitivity distributions (SSDs); a model which describes the sensitivity of toxicity for different species in an ecological community. Estimating the HC_p under this modelling assumption effectively reduces to the problem of estimating the pth percentile of the SSD, which is usually assumed to be log-normal or log-logistic, where the parameters are unknown. However, these methods are often hampered by the typically small amount of toxicity data available for risk assessment.

Aldenberg and Jaworska (2000), followed up by Aldenberg et al. (2002), extensively discuss the confidence limit based method. The idea focuses on evaluating a sampling distribution of the HC_p, referred to as second order distribution fitting by Burmaster and Wilson (1996), such that uncertainty can be represented. A percentile of this second order distribution then corresponds to one's estimate at a permitted level of uncertainty. Therefore, this second order distribution admits a *class* of estimators. The HC_5 is the common benchmark safety limit reported, however, it is often

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the lower 95% one-sided confidence limit value of the HC_5 which is advocated for use as to err on the side of caution, especially in light of the typically small sample sizes. The median estimate of the HC_p is typically presented alongside the corresponding two-sided 90% confidence interval. There is, however, some post hoc justification for choosing the lower 95% estimator in EFSA (2006) who compared the estimator to community level effects from mesocosms. However, to a degree the choice of estimator is still somewhat arbitrary.

A more foundational approach to the problem is to consider loss functions; a useful tool in any statistician's toolbox as they allow one to incorporate loss on a functional level into the decision problem one faces. A loss function is in essence a measure of the *cost* for an estimator being a certain 'distance' away from the true parameter. In other words, one can specify the cost of over- and under-estimation proportional to the respective distance. Each method described above has been proposed on a different premise; no method other than Chen (2003) has proposed directly using a loss function which potentially adds great benefit to the estimation process. However, Chen (2003) proposed a method which required a minimum of 19 toxicity values (when $p=5$) which, unfortunately, is not realistically obtainable in the current risk assessment procedures, a point made clear in Luttik and Aldenberg (1997). Loss usually refers to a cost, although this may not be a financial cost, for example, the cost of losing a species in an ecological community. Choosing among the large set of potentially suitable loss functions requires reasoning, although certain loss functions are chosen as proxies for ease of calculation. Loss functions allow a risk manager in conjunction with a risk assessor to choose how 'costly' it is for an estimator to over- and under-estimate the true value. In ecotoxicological risk assessment one might argue that it is more 'expensive' to over-estimate the HC_p than under-estimate as overestimation would potentially put greater than p% of species at risk. This cost is, however, only partly financial (e.g. clean-up costs) and partly subjective (e.g. cost of losing more than p% of species). The financial costs relating to under-estimation would be in conjunction with the manufacturers R&D costs and refined risk assessments, whereas the personal subjective costs would be in relation to the possible restriction of a useful and potentially important substance. A risk assessor can decide in advance how they want to envisage cost and to what the cost relates to, for example, neglecting other dimensions of risk and focusing strictly on the cost associated with losing species from the community. The cost in the former example is almost certainly a representation of preference although it may have financial attachments.

In Section 2 we define notation, definitions and formalise the problem. In Section 3 we place a new perspective on a well-reported method for estimation of hazardous concentrations. Motivated by the latter, in Section 4 we propose a different loss function for the application of estimating hazardous concentrations and derive its optimal form as well propose a strategy for refining its elicitation in Section 7. In light of discovering that all estimators discussed within this paper are of the same form, we provide a look-up table of assessment shift-factors in Section 5 and compare them in an example in Sections 6 and 7.3. A discussion is made and conclusions drawn in Sections 8 and 9, respectively.

2. The problem and notation

We assume we have observed n $\log_{10}$-toxicity data values which are all of the same endpoint $x_1, x_2, \ldots, x_n$ (e.g. LC50, NOECs) for a substance under current assessment such that each x_i is independently identically distributed (*i.i.d.*) normal with unknown mean μ and unknown standard deviation σ. Let $\mathbf{X}$ be a vector of the log-toxicity data; $\bar{x}$ be the mean and s^2 be the unbiased sample variance of the log-toxicity data; and for convenience, define $\boldsymbol{\theta}=(\mu,\sigma^2)$. Let LHC_p be the log (base 10) of the true HC_p, and $\hat{\mathrm{LHC}}_p$ be the log (base 10) of the estimated HC_p. It is simple to see, from Aldenberg and Jaworska (2000) for example, that if μ and σ^2 were known with certainty, i.e. non-random, then one has $\mathrm{LHC}_p \equiv \psi_p(\boldsymbol{\theta}) = \mu - K_p\sigma$, where K_p is the $(100-p)$th percentile of the normal distribution, e.g. $K_5 = 1.6445$.

A loss function is defined to be a function that measures the *cost* or *regret* associated with a particular event. Although 'cost' is usually perceived as monetary, this need not be the case, and instead loss can be thought of as, say, mortality. We define loss functions here to be of the form $L(\hat{\mathrm{LHC}}_p, \mathrm{LHC}_p)$ so that we consider the cost associated with either over- or under-estimating the true LHC_p.

The method which we apply to determine an optimal decision is by determining the *Bayes rule* which is defined to be the decision rule that minimises the posterior expected loss. In other words, if we define our decision rule to be $\delta_p(\mathbf{X})$, then our optimal Bayes rule is defined to be

$$\delta_p(\mathbf{X})^* = \underset{\delta_p(\mathbf{X})}{\operatorname{argmin}}\, \mathbb{E}^{\boldsymbol{\theta}|\mathbf{X}} L(\delta_p(\mathbf{X}), \psi_p(\boldsymbol{\theta}))$$

where the expectation is taken with respect to the posterior distribution of $\boldsymbol{\theta}$, i.e. $\mathbb{P}[\boldsymbol{\theta}|\mathbf{X}]$, which is denoted as $\boldsymbol{\theta}|\mathbf{X}$ in the above equation; and the minimisation is carried out with respect to all possible decision rules $\delta_p(\mathbf{X})$.

There do exist other forms of risk measurement. However, by a very well-known theorem of Wald (1950), any *admissible* decision rule is a Bayes rule with respect to some prior distribution (possibly an improper prior distribution), whereby *admissibility* is defined to mean that no other decision rule *dominates* it in terms of risk. It is therefore argued by many, for example, Bernardo and Smith (2000) that it is pointless to work in decision theory outside the Bayesian framework.

The problem we explore is how to estimate a suitably conservative value of the LHC_p for a given dataset. In the case of many reports such as Aldenberg and Jaworska (2000) and EFSA (2005), this problem has reduced to determining an *assessment shift-factor*, denoted k_p^* here, which acts on the data through the form $\bar{x} - k_p^* s$ to yield an estimate of the LHC_p for the prescribed risk measure. This is the typical envisagement of this particular type of decision rule since on the original scale it amounts to dividing the geometric mean of the toxicity data by the geometric standard deviation times some assessment factor. Furthermore, the form is such that like previous studies, the assessment shift-factors are *universal* in the sense that they do not depend on the data itself. Not surprisingly, in our derivation the optimal decision rules will also reduce to this form. We do, however, note that not all Bayes rules will lead to estimators of this form. Prior distributional choice will clearly affect the form, as well as other, perhaps less practical, loss functions.

Another related problem is that of estimating the potentially affected fraction of species at risk for a given environmental concentration. Aldenberg and Jaworska (2000) discussed this problem from a sampling distribution perspective. It is justifiable to utilise loss functions for the related problem, which we expect to have implications on the current techniques employed, however, this is not something we explore in this paper.

3. A common decision rule

Aldenberg and Jaworska (2000), who had extended ideas from the likes of Wagner and Løkke (1991), presented a method for