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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

calculating assessment factors based on credible limits from a Bayesian perspective, although their inferences coincided with the frequentist perspective. The idea centred on calculating the probability $\mathbb{P}[\bar{x} - k_p^* s \leqslant \mu - K_p\sigma|\mathbf{X}] = \gamma$ which is clearly the same as $\mathbb{P}[\bar{x} - k_p^* s \leqslant \psi_p(\boldsymbol{\theta})|\mathbf{X}]$ in our general notation. This probability, under distributional assumptions already discussed and with the standard Jeffreys prior distribution (Bernardo and Smith, 2000) was shown to be equivalent to $\mathbb{P}[T_{n-1,\eta} \leqslant k_p^*\sqrt{n}] = \gamma$ where $T_{n-1,\eta}$ is a random variable distributed with a non-central t-distribution with $n-1$ degrees of freedom and non-centrality parameter $\eta = K_p\sqrt{n}$. Aldenberg and Jaworska (2000) then retrieved one-sided lower (95%), median (50%) and upper (5%) under-estimate confidence/credible limits for k_p^* by setting γ to required levels (i.e. values in parenthesis). The lower 95% and upper 5% limits constitute a 90% two-sided confidence interval.

However, Aldenberg and Jaworska (2000) had indirectly determined the Bayes rules under a class of loss functions known as *generalised absolute loss* (GAL) functions, which for the problem described here, with $\text{LHC}_p \equiv \psi_p(\boldsymbol{\theta})$ and $\hat{\text{LHC}}_p \equiv \delta_p(\mathbf{X})$, can be defined as

$$L(\psi_p(\boldsymbol{\theta}), \delta_p(\mathbf{X})) = \begin{cases} C_1[\psi_p(\boldsymbol{\theta}) - \delta_p(\mathbf{X})] & \text{if } \psi_p(\boldsymbol{\theta}) \geqslant \delta_p(\mathbf{X}) \\ C_2[\delta_p(\mathbf{X}) - \psi_p(\boldsymbol{\theta})] & \text{if } \psi_p(\boldsymbol{\theta}) < \delta_p(\mathbf{X}) \end{cases} \quad (1)$$

It is clear that $C_1 > 0$ and $C_2 > 0$ represent the coefficients of cost for under- and over-estimation, respectively, moreover, when $C_1 = C_2$ we retrieve the standard absolute loss function (up to a positive scaling). In essence, the three one-sided (under-estimate) confidence limits they prescribe, what we call: (i) $\text{LHC}_p^{\text{low}}$, (ii) $\text{LHC}_p^{\text{med}}$ and (iii) $\text{LHC}_p^{\text{upp}}$, correspond to Bayes rules under GAL functions with: (i) $C_2 = 19C_1$, (ii) $C_1 = C_2$ and (iii) $C_1 = 19C_2$, respectively. A graphical interpretation of these loss functions can be viewed in Fig. 1.

The proof of our proposition is quite simple. It is known that under GAL the optimal Bayes rule is the $C_1/(C_1 + C_2)$th percentile of the posterior distribution of $\psi_p(\boldsymbol{\theta})$. In the Bayesian paradigm, we treat the data as fixed and observed, so we can equivalently define the problem as determining a Bayes rule for k_p such that the $C_1/(C_1 + C_2)$th percentile is of the form $\bar{x} - k_p s$. We can re-write this as

$$\mathbb{P}[\bar{x} - k_p s \leqslant \psi_p(\boldsymbol{\theta})] = 1 - \frac{C_1}{C_1 + C_2} \quad (2)$$

The left-hand side of Eq. (2) reduces to the same probability as Aldenberg and Jaworska (2000) reported which is $\mathbb{P}[T_{n-1,\eta} \leqslant k_p\sqrt{n}]$. The right-hand side of Eq. (2) can therefore be interpreted as playing the same role as γ which Aldenberg and Jaworska (2000) describe as being the value of the latter probability. Therefore, when $\gamma = 0.95$, which implies $C_2 = 19C_1$, we retrieve k_p^* which is the optimal decision rule for k_p that extrapolates to an optimal Bayes rule for LHC_p, what we denoted $\text{LHC}_p^{\text{low}}$. Similarly, when $\gamma = 0.5$ and 0.05 which implies $C_1 = C_2$ and $C_1 = 19C_2$, respectively, we retrieve $\text{LHC}_p^{\text{med}}$ and $\text{LHC}_p^{\text{upp}}$, respectively, also. It is clear that we simply need only consider the relative fraction C_1/C_2, and moreover, we have demonstrated the role of this proportion for purposes of inference. Effectively, if one *does* subscribe to GAL, then one can choose the value for the confidence limit in the method of Aldenberg and Jaworska (2000) in a non-arbitrary way by relating it to cost. For example, the commonly chosen 95% lower one-sided under-estimate confidence limit would be suitable if one punishes the cost of overestimation as nineteen times the cost of under-estimation.

Therefore, from a loss function perspective we have identified a class of loss functions that many authors have *indirectly* subscribed to. It is not very likely that one would ever elect to choose $\text{LHC}_p^{\text{upp}}$ from either perspective since clearly it lacks conservatism. In other words, there is unlikely to be a situation where $C_1 = 19C_2$, i.e. the associated cost of overestimation is nineteen times less relative to under-estimation. $\text{LHC}_p^{\text{med}}$ on the other hand offers a 50:50 chance of under-estimation, and so is probably not ideal either. This is also clear on the cost level as only in those few specific situations where $C_1 = C_2$ would the $\text{LHC}_p^{\text{med}}$ be of relevance. Chen (2003) and others have noted that often upper/lower confidence limits are chosen and advocated in ecotoxicological risk assessment (depending on the nature of the problem), and so it is clear that Aldenberg and Jaworska's $\text{LHC}_p^{\text{low}}$ offers the most conservatism from the three estimators they presented. Strictly speaking, the corresponding cost assumptions for using this estimator will probably not be ideal for all risk assessments where a degree of conservatism is required, in fact it may be an *over-cautious* estimator for a large number of cases. However, one thing that is clear, is that we require an asymmetric loss function which punishes overestimation more than under-estimation if we are to retrieve a truly conservative estimator.

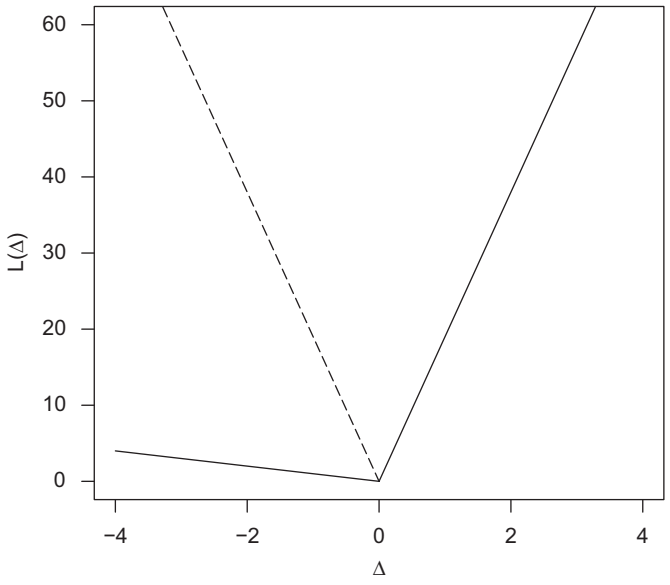

Fig. 1. A graphical representation of the generalised absolute loss function for the specification of $C_2 = 19C_1$ (lower; solid) where $\Delta \equiv \delta_p(\mathbf{X}) - \psi_p(\boldsymbol{\theta})$ is the difference between the estimated LHC_p and the true LHC_p. The union of the dashed line with the symmetric solid line represents when $C_1 = C_2$ (median). Note that without loss of generality $C_2 = 19$.

4. LINEX

In this section we discuss the concept of estimating an optimal decision for LHC_p from a completely different loss function. We first start by describing the (modified) LINEX loss function to be

$$L(\psi(\boldsymbol{\theta}), \delta_p(\mathbf{X}); \sigma) = \beta\left[\exp\left\{\alpha\frac{\delta_p(\mathbf{X}) - \psi(\boldsymbol{\theta})}{\sigma}\right\} - \alpha\left\{\frac{\delta_p(\mathbf{X}) - \psi(\boldsymbol{\theta})}{\sigma}\right\} - 1\right] \quad (3)$$

where one notices that σ is used to scale the difference between the true LHC_p and the estimator $\hat{\text{LHC}}_p$ as done by Zieliński (2005) for reasons described later on; and β is a positive constant used to scale the loss function to the correct scale of loss measurement. The LINear-EXponential (LINEX) loss function was first proposed by Varian (1975) which conveyed loss as increasing linearly on one side and exponentially on the other side. That is, not only was

the loss function asymmetric, it was not simply linearly asymmetric which as Zellner (1986) notes, was the commonly researched asymmetric class of loss functions of its time. This loss function is therefore particularly well suited to the problem of estimating the LHC_p where it is arguable that overestimation is more serious than under-estimation. GAL functions, like those discussed in Section 3, might possibly fail to adequately reflect the need for rising severity of overestimation, whereas LINEX accounts for this via a linear-exponential duality.

For suitably sized $\alpha/\sigma > 0$, $L(\cdot)$ is asymmetric about the origin with overestimation being punished more than under-estimation; in fact as $|\hat{\text{LHC}}_p - \text{LHC}_p| \to \infty$, $L(\cdot)$ approximately increases exponentially when $\hat{\text{LHC}}_p - \text{LHC}_p > 0$ and approximately linearly when $\hat{\text{LHC}}_p - \text{LHC}_p < 0$. The exponential–linearity phenomenon is reversed for $\alpha < 0$, however, we do not concern ourselves with this scenario. The fact that the cost of overestimation increases exponentially is clearly appealing when considering the scope of the problem here. Finally, via a Taylor expansion it can be seen that for small $\alpha|\hat{\text{LHC}}_p - \text{LHC}_p|/\sigma$, $L(\cdot) \approx \beta\alpha^2(\hat{\text{LHC}}_p - \text{LHC}_p)^2/2\sigma^2$. This resembles another very well-studied loss function, the squared error loss (SEL) function which is a symmetric loss function similar to standard absolute loss, except that it punishes at a quadratic rate, as opposed to a linear rate. SEL would lead to another decision rule of the form $\bar{x} - k_p^* s$, however, we do not derive this estimator here. We would, however, note that the scaling of the distance metric by σ will mean that the inferences for small α will not necessarily coincide with the inferences of the SEL.

It is apparent that LINEX offers a free parameter with which one can non-linearly tweak asymmetric conservatism as one may wish, thus giving another point in its favour. To understand the role of $\alpha > 0$, we have plotted the standard LINEX loss function over a few values of interest, see Fig. 2. It is worth recalling that we can multiply a loss function by an arbitrary positive constant so that without loss of generality we still determine the same decision rule. Therefore, when considering Fig. 2 one might scale the loss functions accordingly.

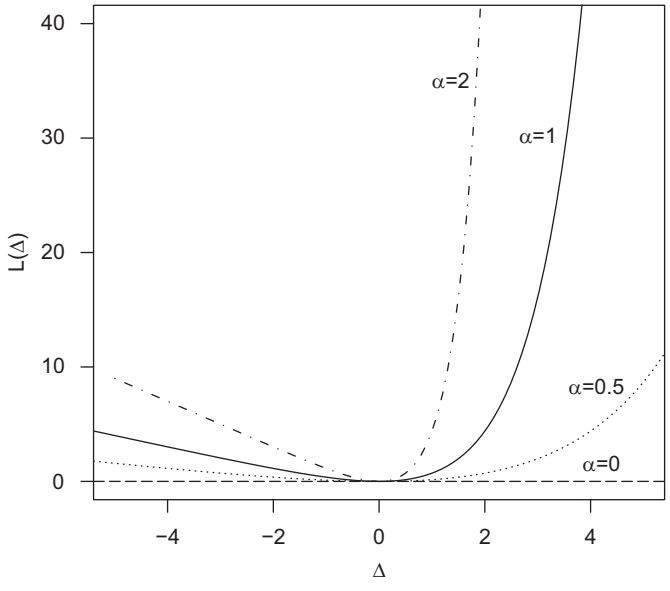

Fig. 2. Figure of the standard LINEX loss function $L(\Delta) = \beta[e^{\alpha\Delta} - \alpha\Delta - 1]$ where $\Delta = \delta_p(\mathbf{X}) - \psi_p(\boldsymbol{\theta})$; Δ is the standard distance between the estimated LHC_p and the true LHC_p. Without loss of generality we have chosen $\beta = 1$ for all plotted loss functions. It is clear that as α as increases then overestimation becomes very 'expensive'. We have ignored the metric-scaling by σ in this case as the figure is for illustrative purposes only. Solid: $\alpha = 1$, dashed: $\alpha = 0$, dotted: $\alpha = \frac{1}{2}$, dot-dash: $\alpha = 2$.

In Appendix A we prove that the optimal Bayes rule for estimating the LHC_p is of the form $\bar{x} - k_p^* s$ where k_p^* is the *unique* solution to

$$\int_0^\infty t^{(n-2)/2} \exp\left\{-\alpha k_p^* \sqrt{t} - \left(\frac{n-1}{2}\right)t\right\} \mathrm{d}t = \Gamma\left(\frac{n}{2}\right)\left[\frac{n-1}{2}\right]^{-n/2} \exp\left\{-\alpha\left[K_p + \frac{\alpha}{2n}\right]\right\} \quad (4)$$

It is obvious that we cannot explicitly write down a formula to calculate k_p^* in this instance, however, there are two possible ways to proceed. The first is to identify the connection of the left-hand side of Eq. (4) to that of a particular solution of the parabolic cylinder function from which look-up tables and general mathematics software can be used, see for instance Zieliński (2005). The second way, the direction which we take, is to use numerical integration and solve for the singular root. As this was particularly computationally efficient, a strict control on the accuracy was maintained.

5. Look-up table for $p = 5$

In Table 1 we present a selection of assessment shift-factors k_5 to estimate the LHC_5 based on Bayes rules under the LINEX loss function for a variety of values for α, as well as the lower, median and upper assessment shift-factors determined by Aldenberg and Jaworska (2000). A copy of the code for use with R (R Development Core Team (2006)) can be obtained by contacting the author.

6. Example

We consider a frequently used data set which was discussed in Aldenberg and Jaworska (2000) but originated from Van Straalen and Denneman (1989). The data are that of NOEC toxicity values for soil organisms tested with Cadmium. The data and summary statistics are described in Table 2.

Aldenberg and Jaworska (2000) determined a median estimate of k_5 to be $k_5^* = 1.7318$ with a corresponding 90% confidence/credible interval $(3.3995, 0.9204)$. This results in a median

Table 1
Table of values for k_5 based on a variety methods for n ranging between 3 and 20

n	$k^*_{AJ_{\text{low}}}$	$k^*_{AJ_{\text{med}}}$	$k^*_{AJ_{\text{upp}}}$	$k^*_{\alpha=0.5}$	$k^*_{\alpha=1}$	$k^*_{\alpha=3}$	$k^*_{\alpha=5}$
3	7.6559	1.9384	0.6391	1.6616	1.9266	4.6118	20.5499
4	5.1439	1.8295	0.7433	1.6682	1.8527	3.2254	7.7438
5	4.2027	1.7793	0.8178	1.6678	1.8089	2.7031	4.8538
6	3.7077	1.7505	0.8748	1.6662	1.7802	2.4368	3.7399
7	3.3995	1.7318	0.9204	1.6643	1.7600	2.2767	3.1794
8	3.1873	1.7187	0.9580	1.6627	1.7450	2.1702	2.8494
9	3.0312	1.7091	0.9899	1.6612	1.7334	2.0944	2.6340
10	2.9110	1.7016	1.0173	1.6599	1.7243	2.0376	2.4832
11	2.8150	1.6958	1.0413	1.6588	1.7168	1.9936	2.3719
12	2.7363	1.6910	1.0625	1.6578	1.7106	1.9585	2.2866
13	2.6705	1.6870	1.0814	1.6570	1.7054	1.9298	2.2191
14	2.6144	1.6837	1.0985	1.6562	1.7010	1.9059	2.1645
15	2.5660	1.6808	1.1140	1.6555	1.6972	1.8857	2.1193
16	2.5237	1.6784	1.1281	1.6549	1.6938	1.8684	2.0814
17	2.4863	1.6762	1.1411	1.6544	1.6909	1.8534	2.0490
18	2.4529	1.6743	1.1531	1.6539	1.6883	1.8403	2.0212
19	2.4230	1.6727	1.1642	1.6535	1.6859	1.8288	1.9969
20	2.3960	1.6712	1.1746	1.6531	1.6838	1.8185	1.9756

$k^*_{AJ_{\text{low}}}$, $k^*_{AJ_{\text{med}}}$ and $k^*_{AJ_{\text{upp}}}$ correspond to the 95% lower, 50% median and 5% upper confidence limits based on the methods of Aldenberg and Jaworska (2000). k^*_α correspond to the optimal Bayes rule under the LINEX loss function which are unique solutions given by Eq. (4); for $\alpha = 0.5, 1, 3$ and 5.

Table 2
NOEC values for toxicity of Cadmium (μg Cd/g) of seven soil organisms

Species	NOEC (μg Cd/mg)	Log_{10} NOEC
1	0.97	−0.01323
2	3.33	0.52244
3	3.63	0.55991
4	13.50	1.13033
5	13.80	1.13988
6	18.70	1.27184
7	154.00	2.18752
$\bar{x}$		0.97124
s		0.70276

estimate of the HC_5 to be $10^{0.97124-1.7318\times0.70276}$ which equals 0.568 μg Cd/mg with a 90% confidence/credible interval (0.038, 2.112).

Under LINEX loss, $k_5^* = 1.6643, 1.7600, 2.2767$ and 3.1794 for $\alpha = 0.5, 1, 3$ and 5, respectively. This would give estimates for the HC_5 to be 0.633, 0.542, 0.235 and 0.0545 μg Cd/mg, respectively. When $\alpha = 1$ we notice that we retrieve a more conservative estimate than that of the Aldenberg and Jaworska (2000) median estimator; and by time we reach $\alpha = 5$ it becomes clear that we are encroaching on lower-confidence limit boundaries as given by Aldenberg and Jaworska (2000). Choosing α sensibly so that one can err on the side of caution whilst not over punishing overestimation is a decision for risk assessors to make, as is choice of p. We do not attempt to justify a particular value nor give vindication to the possible options presented above since selection depends on the situation and cost–benefit portfolio; we simply illustrate the explicit effect of α. However, we will next aim to describe ways in which one *might* elicit suitable value(s) for α.

7. On the choice of α for LINEX

We have prescribed a loss function [LINEX] which fits in neatly to the ecotoxicological field of risk assessment as it offers a controllable asymmetrical conservatism parameter. However, choice of this parameter is clearly a difficult task for the risk assessor as is their choice of what percentile to choose, p, since this is unfamiliar territory.

7.1. Development

We start by recalling that the role of $\beta > 0$ in Eq. (3) does not alter inferences and is only chosen to multiply loss to a more suitable scale. We will therefore take $\beta = 1$ for the remainder of the discussion.

We must now address the fact that the LINEX loss function was modified so that the difference in the LHC_p and $\text{L}\hat{\text{H}}\text{C}_p$ was scaled by the inter-species variation in sensitivity, i.e. we considered $(\text{L}\hat{\text{H}}\text{C}_p - \text{LHC}_p)/\sigma$. The ramifications of this are that α can be chosen, say, for a particular ecological community, and would not need to be re-considered on the premise of substance effects for each substance assessed other than for the differences in cost/benefits attainable; thus, we have a re-usable loss function. Zieliński (2005) describes this difference as measure of *discrepancy*. This might at first seem a difficult concept to grasp, but consider the idea of punishing the overestimation of the HC_p by, say 100, when α is fixed. Then, if the standard deviation of the foundational distribution was, say, double for another substance with similar cost portfolios, then surely punishment should not be as harsh because, *a priori*, variability is higher for the latter substance. However, scaling the difference by the standard deviation of the SSD enables the difference to be thought of on a 'standardised' scale. Therefore, in essence, the scaling ensures that the loss is dependent only on the actual percentage of species which are more sensitive than $\hat{\text{H}}\text{C}_p$.

This argument is more pertinent for the consideration of LINEX loss as opposed to GAL. To demonstrate this we consider the situation of not scaling. Let L_L be a *standard* LINEX loss function, i.e. where we do not scale the amount of overestimation $\Delta = \text{L}\hat{\text{H}}\text{C}_p - \text{LHC}_p$. Also, let L_G be a GAL function. Then, considering the loss of under-estimation to overestimation, i.e.

$$\frac{L_L(-\Delta)}{L_L(\Delta)} = \frac{e^{-\alpha\Delta} + \alpha\Delta - 1}{e^{\alpha\Delta} - \alpha\Delta - 1}$$
$$\frac{L_G(-\Delta)}{L_G(\Delta)} = \frac{C_1}{C_2}$$

with $\Delta > 0$, we notice that under GAL this proportion is *independent* of Δ whereas, in general, under LINEX that is not the case. The implication of this is that while the choice of α should reflect the cost–benefit portfolio of the current assessment, it must also take into account the variability of the SSD since overestimation is much more serious for certain assessments than it is for others. This clearly is an undesirable property since it would require the risk assessor to know the SSD in advance of selecting α. Therefore, if we instead elect to advocate modified LINEX loss, the risk assessor could choose α by considering the metric of under- and over-estimation on a scale which is independent of the unknown SSD.

Now, define the *discrepancy factor* to be $t = (\text{L}\hat{\text{H}}\text{C}_p - \text{LHC}_p)/\sigma$. Then clearly $\hat{\text{H}}\text{C}_5 = \text{HC}_5 \times 10^{t\sigma}$ where, of course, $\sigma > 0$. We need to consider a starting point for elicitation, and we feel that possibly a good place would be to consider $t = 2$. This corresponds to the case where we overestimate by 100 on the 'standardised' scale; equivalent to overestimating by 100^{σ} on the standard scale, where σ is the (unknown) standard deviation of the SSD (on the log-scale). Suppose we now told you that this would cost \$100 (the dollar sign simply indicates some unit of cost), where of course here the 'cost' is arbitrarily chosen to be that of cost–benefit for applying the substance independent of the underlying variability of the sensitivity distribution. Furthermore, the cost is *not* necessarily financial. The question we would then ask would be: if $t = -2$, i.e. you underestimate by 100 (on the standardised scale) what *relative* cost would you associate with this situation? In other words, what percentage of \$100 would you feel is an adequate representation of this cost given the cost of the overestimation case? Notice, we could equally as well approach this problem from the opposite direction by stating a base line for the case $t = -2$ and asking the risk assessor how much 'worse' would the $t = 2$ case be.

Therefore, if the data was representative of a particular community and underestimating by 100 (again, standardised) costs \$100 m, where $m \in (0, 1)$ represents the proportion of the original cost for overestimation (\$100) associated with the corresponding under-estimation, then solving the equation

$$m = \frac{e^{-2\alpha} + 2\alpha - 1}{e^{2\alpha} - 2\alpha - 1} \tag{5}$$

for α will yield an elicitated value for α. Eq. (5) will typically be solved numerically, possibly with a standard spreadsheet application.

7.2. The risk assessment procedure

To summarise the recipe for estimating the HC_p relative to the modified LINEX loss function, we concisely detail the steps to our proposal here.

(1) *Determining* α:
   (a) Assign a percentage, *independent* of the SSD, of the cost for underestimation relative to the cost associated with overestimating by 100. Recall that this is equivalent to assigning a cost to underestimating by 2σ on the log-scale (where σ is the unknown standard deviation of the SSD on the log-scale) given that overestimating by 2σ costs \$100. Set this fraction as m.
   (b) Solve Eq. (5) for α.
(2) *Determining* $\hat{\mathrm{HC}}_p$:
   (a) Given sample size n, percentile p and α; using suitable optimisation software solve Eq. (4) for k_p^*.
   (b) $\hat{\mathrm{LHC}}_p = \bar{x} - k_p^* s$.
   (c) $\hat{\mathrm{HC}}_p = 10^{\hat{\mathrm{LHC}}_p}$.

7.3. Example revisited

Say a risk assessor considers that m should be set to 0.05 on the basis that the *relative* cost of underestimation should be 5% of the cost corresponding to overestimation in the case where the discrepancy factor is measured as ± 2. This would lead them to choose $\alpha^* = 2.13$. Alternatively, the scenario might be such that they believe the cost–benefit portfolio of the ecological community for application with this substance warrants $m = 0.10$. Then they would choose $\alpha^* = 1.67$. Finally, the scenario faced by the risk assessor might be such that the ecological community is extremely valuable but they believe that the advocacy by some of using a lower-confidence (95%) limit as prescribed by Aldenberg and Jaworska (2000) is too over-cautious and opaque in meaning. Moreover, they want to perform a 'quick' initial risk assessment using this method. Therefore, the risk assessor might choose $m = 0.001$, i.e. 0.1% relative cost, which translates to $\alpha^* = 4.49$. Overall, the risk assessor has given one possible description of a loss function for each of the three scenarios that they feel is adequate, which in turn gives $k^* = 2.02, 1.91$ and 2.89, and finally, translates to estimates of the HC_5 being 0.3562, 0.4256 and 0.0871 μg Cd/mg, respectively.

The starting point of $t = 2$ was a suggested point, although $t = 1$ or 3 or any other value may be more suitable for elicitation; it is quite frankly a decision that should be made by the risk manager via discussion with the risk assessor. Furthermore, one must remember that the loss function is constrained by its parametric form, and therefore eliciting α at $t = t_1$ may not completely reflect desired loss at $t = t_2$; room for accommodation must therefore be allowed. By virtue of the linear–exponential duality, at $t = 1$ the risk assessor has, for the three different scenarios, assigned relative (to \$100) costs of \$8.06, \$11.06 and \$1.05, respectively; however, let us not forget that this situation is tremendously less grave than the case $t = 2$. The associated percentages of these costs to that of $t = -1$ are 24%, 32% and 4%, respectively. Therefore one may wish to try a range of starting bases to determine a suitable value (or interval) for α by trading-off different start points. We have plotted a contour plot in Fig. 3 detailing how relative underestimation to overestimation costs depend on α and discrepancy factor t.

7.4. Generality

Considering whether the risk assessor would want to adjust his value for α whilst he adjusted his choice for p is not clear. If the risk assessor first chose $p = 5$ and selected $\alpha = \alpha_1$, then later decided he was now more interested in $p = 10$; should he change his value for α to $\alpha_2 > \alpha_1$? By increasing p we increase the potential affected fraction of species, and so one may argue that choosing $\alpha = \alpha_2$ is more pertinent as it acknowledges that more species are at risk. However, going from $p = 5$ to 10 implies that the risk assessor is setting the acceptability level irrespective of estimation uncertainty; thus, we can assume this is a starting base. So without loss of generality, it can be argued α should reflect the level of conservatism required independent of the choice of p, although, it is clearly obvious that k_p^* is a function of p.

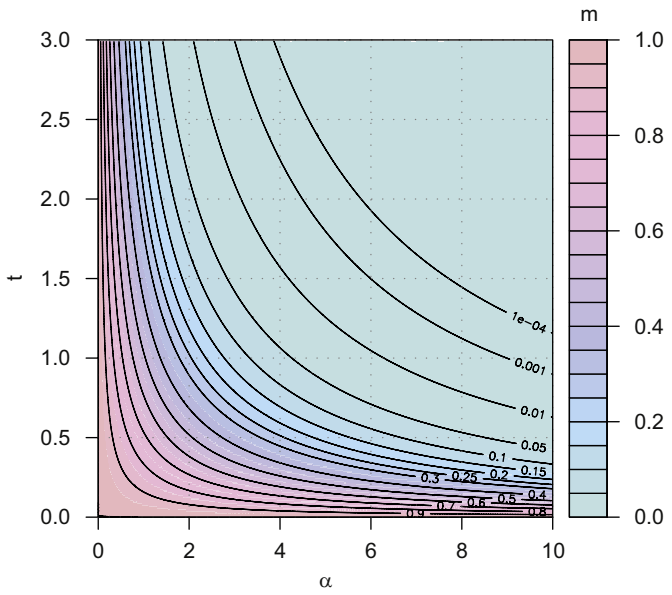

Fig. 3. A contour plot showing the relation of α (x-axis), t (y-axis) and m (contours). The graph is representative on the 'standardised' scale, hence independent of substance variation, i.e. t is the discrepancy factor. Contour lines for specific cases have been overlaid including the cases $m = 0.001, 0.05$ and 0.1 for the examples discussed in Section 7.3. The m-scale (contour labels) can be viewed as percentages by multiplying m by 100, e.g. $m = 0.05$ implies that the cost of underestimating is only 5% relative to the cost of overestimating by a particular value t on the 'standardised' scale.

If different groups of organisms do not fit together in a single SSD then it may be more appropriate to consider treating the groups separately and thus fit separate SSDs (Solomon and Takacs, 2002). In such cases, risk assessor/managers would need to consider using different values of α for each SSD, to reflect the potentially differing cost–benefit portfolios per group of organisms (e.g. differing ecological role or importance). Should data from multiple groups of organisms be deemed concurrent with a single underlying SSD, then either a single or multiple values of α could be used, depending on whether the cost–benefit portfolios differed between groups.

8. Discussion

Loss functions have long been a practical tool in statistical decision theory, yet they have not truly been exploited in the vast field of ecotoxicology. We have presented two reasonably interpretable loss functions and shown ways in which an estimator for the true HC_p can be derived such that a degree of conservatism can be selected. Moreover, we have demonstrated that estimators proposed by Aldenberg and Jaworska (2000), which extended research from Wagner and Løkke (1991), are in fact optimal estimators based on three different loss functions all belonging to the same class. It is clearly debatable as to whether these loss functions are the best choice for the application.

In the final example the degree of conservatism was asymmetrically controllable as well as featuring exponential–linear duality, a very appealing feature from the risk assessor's perspective. The inclusion of suitable loss functions such as LINEX

allows one to estimate on the side of caution without feeling necessitated to be over cautious and apply lower/upper confidence limits. Moreover, we have demonstrated an entirely sound and appropriate way of visualising the assessment factors applied within the field of environmental protection. Although this method only incorporated the risk associated with respect to inter-species variation, it clearly offers a useful introduction into the application of loss functions. We have therefore demonstrated that there exists a potentially more fundamental perspective on the development of assessment factors associated with inter-species variation, especially for lower-tier risk assessments when the other dimensions of risk and uncertainty can be effectively represented in other ways. For example, some first tier risk assessments combine this with exposure by dividing an estimate of the 90th percentile of the exposure distribution by the estimated HC_p.

Like Wagner and Løkke (1991) and Aldenberg and Jaworska (2000) we assume the toxicity data to be log-normal. Suitability of this distribution choice is discussed in these papers as well as many others; however, we will not focus on this here. We do however believe that should the data be suitable (i.e. suitable endpoint, well-defined ecological community, etc.) for making the parametric assumptions then the application of loss functions such as LINEX enables estimation in the face of uncertainty to be more reflective of prior concerns.

We have demonstrated the potential of loss functions by applying them to the estimation of the HC_p, and is therefore directly relevant to first-tier risk assessments and environmental quality standard-setting contexts, where the HC_p is used as a proxy for ecological protection. In higher tier risk assessments other measures of risk may be used, e.g. estimates of the proportion of species affected based on combining an SSD and exposure distribution (Aldenberg et al., 2002), or estimates of the frequency of community impacts obtained by comparing effect levels from mesocosm experiments with exposure distributions (Solomon and Takacs, 2002). Loss functions could also be applied to these estimates of risk, to allow risk assessors and managers to take appropriate account of the relative costs of over- or under-estimating risk.

This paper has also demonstrated that use of a lower confidence limit, as estimated for the HC_p by the method of Aldenberg and Jaworska (2000), is equivalent to a particular Bayes rule under a GAL loss function, *qua* the standard applied prior distribution. This insight opens up an objective approach for the choice of which confidence limit to use, showing that it should reflect the relative costs of over- and under-estimating risk rather than simply adopting the conventional 95% limit. Equally importantly, this paper has shown that other forms of loss function could be considered and introduced LINEX as one alternative. The LINEX loss function is unfamiliar and more complex to implement than GAL but this will be justified if it reflects better the relative costs of over- and under-estimating risk. Both are asymmetric and therefore able to reflect differential costs for over- and under-estimation, but in different ways, as can be seen by comparing Figs. 1 and 2. GAL is more appropriate if costs increase linearly with the degree of over- or under-estimation but LINEX is more appropriate if costs increase exponentially for overestimation.

Maltby et al. (2005) and Van den Brink et al. (2006) have used a different approach to guide the choice of confidence limit for the HC_p, by comparing it with data on effects on aquatic communities in mesocosm studies. It would be possible to repeat these comparisons for LINEX estimates of the HC_p, taking different values of α. However, from a decision-theoretic perspective it would be more appropriate to apply loss functions to estimating the community effect itself, since this is a more direct representation of the risk management objective. This could be done by modelling the relationship between standard toxicity tests and effects in mesocosms, similar to the regression analysis shown in Fig. 9 of EFSA (2006), but applying a suitable loss function to take account of the relative costs of under- and over-estimating effects at the community level. This would be a logical extension of the loss function approaches proposed in this paper.

9. Conclusions

The interpretation of risk for purposes of probabilistic risk assessment have been made clear from a loss function perspective. The assessment factors proposed by Aldenberg and Jaworska (2000) have been shown to be optimal Bayes rules under GAL functions. Moreover, the level of certainty for these estimators has been identified as being related to the relative slope of the loss function for over- and under-estimation. A modified LINEX loss function was proposed and discussed which punishes over- and under-estimation in a non-linear approach. We therefore propose that more research is performed in identifying suitable loss functions for the purpose of estimating the HC_p and other areas of environmental probabilistic risk assessment, especially measures of impact rather than toxicity alone.

Protection of human subjects and animal welfare

We can formally assure the editor that no studies involving humans or experimental animals were conducted for this research. All the data used have been described in other journals and books.

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Appendix A. Derivation of the Bayes rule under LINEX loss

With the standard Jeffreys prior $p(\mu,\sigma^2)\propto\sigma^{-2}$ for $\sigma^2>0, \mu\in\mathbb{R}$, we can determine the posterior distribution of μ and σ^2 to be $p(\mu,\sigma^2|\mathbf{X})=p(\mu|\sigma^2;\mathbf{X})p(\sigma^2|\mathbf{X})$ such that

$$\mu|\sigma^2;\mathbf{X}\sim N(\bar{x},\sigma^2/n)$$
$$\sigma^2|\mathbf{X}\sim\mathcal{IG}((n-1)/2,(n-1)s^2/2)$$

Whilst we have chosen to parameterise the posterior distribution of σ^2 as an Inverse-Gamma distribution, Aldenberg and Jaworska (2000) used an equivalent form, the Inverse-Chi distribution for $p(\sigma|\mathbf{X})$. We also note that the second parameter of the Inverse-Gamma distribution is a scale parameter and not a rate parameter. We next look for a Bayes rule $\delta_p^*(\mathbf{X})$ which we denote δ^* such that the Bayes posterior expected loss is minimised with respect to this rule. The posterior expected loss, with δ shorthand for $\delta_p(\mathbf{X})$, is defined to be

$$\mathbb{E}^{\theta|\mathbf{X}}\beta\left[\exp\left\{\alpha\frac{(\delta-\mu+K_p\sigma)}{\sigma}\right\}-\alpha\frac{(\delta-\mu+K_p\sigma)}{\sigma}-1\right]$$

The first of two important calculations required is

$$\mathbb{E}^{\theta|\mathbf{X}}\left[\frac{\mu}{\sigma}\right]=\mathbb{E}^{\sigma^2|\mathbf{X}}\{\mathbb{E}^{\mu|\sigma^2,\mathbf{X}}[\mu\sigma^{-1}|\sigma^2]\}$$
$$=\bar{x}\frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n-1}{2}\right)}\left[\frac{n-1}{2}s^2\right]^{-1/2}$$

from which we deduce that

$$\mathbb{E}^{\theta|\mathbf{x}}\left[\frac{(\delta-\mu+K_p\sigma)}{\sigma}\right] = \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n-1}{2}\right)}\left[\frac{n-1}{2}s^2\right]^{-1/2}[\delta-\bar{x}]+K_p$$

The second important calculation is

$$\mathbb{E}^{\theta|\mathbf{x}}\left[\exp\left\{\alpha\frac{(\delta-\mu+K_p\sigma)}{\sigma}\right\}\right] = \exp\left\{\alpha K_p+\frac{\alpha^2}{2n}\right\}\frac{\left[\frac{n-1}{2}\right]^{(n-1)/2}}{\Gamma\left(\frac{n-1}{2}\right)} \times\int_0^\infty t^{(n-3)/2}\exp\left\{-\left(\frac{n-1}{2}\right)t+\alpha s^{-1}t^{1/2}(\delta-\bar{x})\right\}\mathrm{d}t$$

This combined with the first result implies that the posterior expected loss can be re-written as

$$\beta\exp\left\{\alpha K_p+\frac{\alpha^2}{2n}\right\}\frac{\left[\frac{n-1}{2}\right]^{(n-1)/2}}{\Gamma\left(\frac{n-1}{2}\right)} \times\int_0^\infty t^{(n-3)/2}\exp\left\{-\left(\frac{n-1}{2}\right)t+\alpha\sqrt{t}\frac{(\delta-\bar{x})}{s}\right\}\mathrm{d}t - \beta\alpha\left[\frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n-1}{2}\right)}\left[\frac{n-1}{2}s^2\right]^{-1/2}(\delta-\bar{x})+K_p\right]-\beta$$

A Bayes rule δ^* is determined by minimising the above with respect to δ and solving for its root. This is equivalent to solving

$$\int_0^\infty t^{(n-2)/2}\exp\left\{\alpha\sqrt{t}\frac{(\delta-\bar{x})}{s}-\left(\frac{n-1}{2}\right)t\right\}\mathrm{d}t = \Gamma\left(\frac{n}{2}\right)\left[\frac{n-1}{2}\right]^{-n/2}\exp\left\{-\alpha\left[K_p+\frac{\alpha}{2n}\right]\right\} \quad (A.1)$$

for δ.

However, notice that δ only appears in the form $(\delta-\bar{x})/s$ within the left-hand side of Eq. (A.1), which implies that the right-hand side is independent of the toxicity data and dependent on n and p only. Moreover, this implies that in general, $(\delta-\bar{x})/s$ is a constant. Let us call such a value $-k_p^*$ from which we deduce k_p^* is our assessment shift factor since $\delta^*=\bar{x}-k_p^*s$ and δ^* is a Bayes rule/action for estimating the LHC_p. We omit proof of uniqueness but note that it is reasonably easy to show.

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