MOSAIC_SSD: a new web-tool for the Species Sensitivity Distribution, allowing to include censored data by maximum likelihood

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Censored data are seldom taken into account in Species Sensitivity Distribution (SSD) analysis. However, they are found in virtually every dataset and sometimes represent the better part of the data. Stringent recommendations on data quality often entail discarding a lot of this meaningful data, often resulting in datasets of reduced size, which lack representativeness of any realistic community. However, it is reasonably simple to include censored data into SSD by using an extension of the standard maximum likelihood method. In this paper, we detailed this approach based on the use of the R-package fitdistrplus, dedicated to the fit of parametric probability distributions. We especially present the new web-tool MOSAIC_SSD that can fit an SSD on datasets containing any type of data, censored or not. MOSAIC_SSD predicts any Hazardous Concentration (HC) and provides in addition bootstrap confidence intervals on the predictions. Finally, we illustrate the added value of including censored data in SSD taking examples from published data.

Keywords: bootstrap, confidence interval, web interface, fitdistrplus, hazardous concentration
Introduction

The Species Sensitivity Distribution (SSD) is a central tool for risk assessment in ecotoxicology. It provides a subtle way to define hazardous concentrations for the environment compared to using arbitrary safety factors. However, the approach is still subject to heated debates regarding its optimal implementation where no consensus has been reached so far. As a result, environmental regulatory bodies often advocate country or region-specific approaches[1–5]. In studying SSD, methodological choices based on very theoretical arguments have a direct impact on legislation and significant economic and ecological outcomes. The purposes of the SSD approach are to model interspecies sensitivity variability and to provide a protective concentration for a group of species. SSD uses sensitivity data as input, such as No Effect Concentration (NEC), No Observed Effect Concentration (NOEC) or Effective Concentration for $x\%$ ($EC_x$) for a group of tested species. These can be coined Critical Effect Concentrations (CECs), which are obtained through acute or chronic toxicity bioassays. The SSD approach is based on the hypothesis that variability in species sensitivity follows a probability distribution. This distribution is extrapolated from the sample of tested species to infer a group-wide protective concentration, the Hazardous Concentration for $p\%$ of the group ($HC_p$). In general, a parametric distribution is assumed. However, assumptions about the distribution can be avoided using non-parametric methods[6].

The SSD approach has many issues[7] ranging from ecological to statistical concerns. Despite the difficulty of addressing all of them, specific aspects can be improved. Throughout the body of work mentioning SSD, there are very few occurrences of taking into account properly missing data, non-detects or censored data in general. On those rare occurrences, this is
achieved in a Bayesian framework[8], which requires a statistical expertise not accessible to untrained users. However, censored data contain crucial information and ignoring or transforming them alters the quality of the predictions based on the remaining data[9]. It is possible to deal with censored data in a more familiar frequentist framework using standard maximum likelihood methods. This also offers several advantages over common SSD approaches. In this article, we present a web-tool, MOSAIC_SSD (http://pbil.univ-lyon1.fr/software/mosaic/ssd/), to easily include censored data in a SSD analysis. MOSAIC_SSD relies on the existing R package, fitdistrplus[10].

In this paper, we first reviewed the methods to fit a distribution to data, in order to position our tool among the existing SSD approaches. Then, we explained how to take censored data into account and presented the web-tool we have designed for this purpose, MOSAIC_SSD. Finally, we illustrated the added value of including censored data in SSD using example datasets from published literature.

**Review of methods to fit an SSD**

Two steps are required to fit an SSD. The first step is to choose a distribution which seems appropriate to describe the data. Possible options include 1) a Weibull distribution[11] to emphasize the tails of the distribution, 2) a triangular distribution[11] with a finite-size support when no species are more sensitive/resilient than a certain threshold value, 3) a multimodal distribution[12,13] for an assemblage of several taxons, etc. Log-normal[14] and log-logistic[15] distributions are the customary choices[16] although an extensive list of distributions have been
applied to SSD. Alternatively, distribution-free methods can be used to avoid the subjective choice of a distribution for the data. This approach has been used for SSD in various works [6,8,17]. Among these distribution-free methods, the Kaplan-Meier estimator is a means to include censored data in SSD[8]. However, it is restricted to certain types of censored data. One difference between parametric and distribution-free methods is the following: when fitting a parametric distribution, the possibilities of shapes are restricted to a certain class of distributions and the shape is refined by adding information from the data. In a distribution-free approach, any kind of shape is allowed and the result emerge solely from the data. Therefore, distribution-free methods do not use any sort of exterior information and often require more data than parametric methods[16,17]. Consequently, when dealing with small datasets it is more reasonable to fit a parametric distribution.

Each parametric distribution is determined by a set of parameters, so the second step is to estimate them. Parameter estimation is performed by optimizing a chosen criterion: the likelihood or some goodness-of-fit distance. The likelihood function gives the probability of observing the data given the parameters. Maximizing the likelihood implies selecting the parameters for which the probability of observing the data is highest. Maximum likelihood is by far the most standard approach to distribution fitting and more generally to model fitting. It is backed with a consequent body of theoretical work ensuring many interesting asymptotic properties[18]: the maximum likelihood estimate converges to the true value of the parameters (consistency), it is the fastest estimate to converge (efficiency), the difference with the true value is normally distributed (normality), which provides confidence intervals on the parameters. This approach is used by the Australian software Burrlioz[19], for instance, which fits a Burr III
distribution to the toxicity data. Moreover, a natural extension of the likelihood function makes it possible to take into account censored data[20].

Another popular method to determine the distribution parameters that best describe the data is the least-square regression on the empirical Cumulative Distribution Function (CDF), which minimizes the sum of the squared vertical distances between the CDF and the data. It is also known as the Cramer-Von Mises distance[21]. This approach is adopted by the software CADDIS_SSD[22], from US EPA, which performs a least-square regression on the CDF with a log-probit function. The software SSD MASTER[23] uses the same method, but tries several other distributions: normal, logistic, Gompertz and Fisher-Tippett. However, regression on the CDF is not an easy method to include censored data, because constructing the CDF implies sorting the data, which is not trivial with censored data. In addition, there is no unique way to build a CDF. Several possible plotting positions[1,24] all have desirable properties, but none of them represent the data more faithfully than any other. Therefore, the resulting SSD and its predictions depend on purely arbitrary decisions regarding the plotting positions, a fact that undermines its scientific credibility.

A third common approach to determine the distribution parameters is to match the moments of the empirical distribution with those of the model. This is numerically easy when there is an analytical formula for the determination of the parameters. Moment matching is equivalent to maximum likelihood for the distributions of the exponential family, such as the normal, exponential, gamma distributions, but not for the logistic distribution. ETX[25] is a free software which uses the moment matching method[14,15]. It fits a log-normal and a log-logistic distribution by moment matching and computes confidence intervals. Moment matching is
sensitive to outliers and can give unrealistic results[26]. However, it can be useful when the maximum likelihood computation is intractable[26]. However, moment determination with censored data is not trivial. Therefore, this method cannot be straightforwardly extended to include censored data.

This brief review of the classical SSD approaches shows that several methodological choices must be made in order to fit an SSD: whether or not to use a non-parametric method, selection of the distribution and of the parameter estimation method. Apart from maximum likelihood, there is no straightforward approach for a non-expert in statistics to make use of all types of censored data. Indeed, all of the available turn-key software for SSD fitting require the use of non-censored data. Yet, there is a possibility to use the R-package \textit{fitdistrplus}[10] to fit censored data using maximum likelihood, with the following scheme.

**Maximum likelihood for censored data**

Maximum likelihood provides a single framework to cope with both censored and non-censored data. Censored data is a general name given to data which are not in the form of fixed values but belong to an interval, bounded or not. Censored sensitivity data occur when it is not possible to determine a CEC for a given species. Possible reasons are 1) that the highest concentration tested does not have any noticeable effect, 2) that only a tiny amount of contaminant already stamps out all the individuals, 3) that the measurement is simply too imprecise to be reasonably described by a single value instead of an interval. In such cases, it is only possible to give a \textit{lower} bound, a \textit{higher} bound or an \textit{interval} to the CEC. Such data are called \textit{right-censored}, \textit{left-censored} or \textit{interval-censored}, respectively. Censored data can also
occur when there are multiple values for the sensitivity of one species to a given toxicant. When
the quality of the data seem equivalent, ECHA's advice[5] are to use the geometric mean as a
replacement for the different values. It might be more cautious to use these multiple values to
define an interval containing the sensitivity of that species. Censored data are very different from
doubtful or questionable data, obtained from failed experiments. They are produced using a valid
experimental procedure and they contain information as valid as non-censored data. Censorship
is very common, especially for rare species where there are scant data available and for which no
standard test procedure exists. There is a downside in discarding censored data, as they could
represent the better part of an extended dataset. For instance, in the work by Dowse et al.[8],
discarding censored data entails a division of the number of tested species by a factor 8.

In spite of their ubiquity, censored data appear to be very much ignored in ecotoxicology.

To our knowledge, there is no example of SSD including all types of censored data in a
frequentist framework. It is possible in a Bayesian framework[24,27,28], but fitting a Bayesian
model requires a certain statistical expertise. Censored data are typically either discarded or
substituted with arbitrary values, which is a bias-prone approach in general[9]. However, there is
a simple method to include censored data in a frequentist framework. Parameter estimation of a
distribution on any type of censored data can be performed using a natural extension of the
maximum likelihood method[29]. Let $x_i$ be $N$ sensitivity data following distribution $f$ of
parameter $\theta$. The likelihood function for non-censored data writes as follows:

$$L(\theta) = \prod_{i=1}^{N} f(x_i|\theta)$$

(1)

This likelihood function can be extended to censored data. Let $x_i$ be the $N_{nc}$ non-censored data,
the $N_{lc}$ upper bounds for left-censored data, $x_{k}^{low}$ the $N_{rc}$ lower bounds for right-censored data and $(x_{l}^{low}, x_{l}^{up})$ the $N_{ic}$ pairs of bounds for interval-censored data. Then, the previous likelihood function is now extended to:

$$L(\theta) = \prod_{i=1}^{N_{nc}} f(x_{i} | \theta) \times \prod_{j=1}^{N_{lc}} \left( F(x_{j}^{up} | \theta) \right) \times \prod_{k=1}^{N_{rc}} \left( 1 - F(x_{k}^{low} | \theta) \right) \times \prod_{l=1}^{N_{ic}} \left( F(x_{l}^{up} | \theta) - F(x_{l}^{low} | \theta) \right)$$

where $F$ is the cumulative distribution function of distribution $f$.

We see that the likelihood function for censored data (eq. 2) writes as a product of four terms, the first being the likelihood for non-censored data (eq. 1) and the next three corresponding to the left-censored data, right-censored data and interval-censored data respectively.

**MOSAIC_SSD**

It is possible to use the method described in the previous section using the R-package `fitdistrplus[10]`. R-packages `survival[30]` and `NADA[31]` offer the same possibility. However, they require a certain fluency in the R programming language, preventing the widespread use of censored data in ecotoxicology. Minitab[32] is a commercial software with a graphical user interface which fits multiple distributions to censored data rather easily, but there does not seem to be any open-source alternative.

Moreover, `fitdistrplus` and these other packages and software are not specifically designed for SSD and their versatility in the choice of distributions and fitting methods might discourage inexperienced users. Thus, we developed a web-interface, MOSAIC_SSD (http://pbil.univ-lyon1.fr/software/mosaic/ssd/), which is a wrap up of `fitdistrplus` into a SSD-dedicated online tool. MOSAIC_SSD enables anyone to perform a simple, yet statistically sound SSD analysis.
including censored data without worrying about the conceptually difficult underlying statistical questions. The web interface is easily accessible via any browser and simple to use: given an input dataset, it sends the calculation to a server then hands in the result. The input dataset is a text file uploaded by the user with a straightforward encoding. A non-censored dataset is given in one column. A censored dataset is given as two columns: a "NA" in the right – resp. left – column and a number on the left – resp. right – denotes a right – resp. left – censored data. Two differing numbers denote an interval-censored data and two identical numbers a non-censored data.

Few options are offered to keep the tool more user-friendly. The user can choose one or two among the log-normal and log-logistic distributions. These two distributions are the most widely used[16], and parameter estimation appears robust enough to accommodate for most datasets, as they contain only two parameters. In order to select which distribution describes the data best, the first step is to perform a qualitative assessment by looking at the representative curves. The value of the likelihood function for each model can then be used as a further decision criterion. The log-logistic distribution has heavier tails than the log-normal and is therefore more conservative in the determination of the $HC_6[15]$.

The second choice left to the user is to decide whether to compute the bootstrap 95% confidence intervals. The calculation runs slightly longer with the bootstrap but it yields confidence intervals on the parameters of the distribution and on several computed $HC_p (p = 5, 10, 20, 50)$. The bootstrap procedure is not guaranteed to converge, the number of iterations required being strongly dependent on the dataset. Therefore, an automatic check of bootstrap convergence is implemented. The procedure is run several times in parallel, comparing
the magnitude of the results fluctuations to the span of the confidence interval. This comparison

determines whether the bootstrap has converged. In the case were the bootstrap procedure fails to

converge, additional computations are launched. If the bootstrap finally converges, or if the

process has reached the time limit, the user is advised whether the confidence intervals are

reliable. Calculating the confidence intervals using a bootstrap method has the advantage of

using a unified framework for every distribution. Figure 1 shows a screenshot of the result page

of the analysis with an example dataset (provided in MOSAIC_SSD) containing censored data

and documenting the salinity tolerance of riverine macro-invertebrates[33] (hereinafter referred

to as the censored salinity dataset). The dataset contains 72-hrs LC50 values (lethal concentration

for 50% of the organisms) for 110 macro-invertebrate species from Australia. Data were

collected using rapid toxicity testing[34] and contain non-censored, right-censored and interval-
censored data. The result page shows a graphical representation of the censored data, the

distribution parameters, HCp computed for various interesting values of p and the bootstrap

confidence intervals within brackets. Figure 1 also shows the output of an SSD analysis with a

non censored dataset. It actually is a non-censored version of the salinity dataset described

earlier. The transformation from censored to non-censored dataset follows the customary

approach to censored data, which consists in discarding some type of data and transforming

others (more details in the next section). An analysis with non censored data follows identical

steps and yields results with the same outline, except that a traditional CDF is used to visualise

the data. The obvious difference between the outputs of the censored dataset and the non-
censored dataset is the representation of the CDF. For non-censored data, the CDF is represented

using the traditional Hazen plotting positions[1]. The choice of plotting positions remains
arbitrary and there is no perfect solution[1,24], so preference was given to the most standard approach. Representation of censored data CDF is far from evident. Building a CDF implies defining an ordering for the data. If obvious for non-censored data, such an ordering makes little sense for interval-censored data. They might be ranked according to the median of the interval, to the higher bound or the lower. Adding left or right-censored data complicates matter even more. Within fitdistrplus, the answer to this problem is to use the Turnbull estimate of the CDF, which is a non-parametric maximum likelihood estimator of the CDF[35]. This estimate can be obtained through an expectation-maximisation algorithm and yields the CDF which predicts the data with the highest probability. The Turnbull estimate is represented as a stepwise curve as on Figure 1 (top panel).

Finally, MOSAIC_SSD can be used as a stepping stone to perform further analysis with fitdistrplus. The last item on the MOSAIC_SSD result page is not shown on the screenshots. It is an R script offering the possibility to replicate the analysis using fitdistrplus, through a copy and paste operation in R. This script is intended as a stepping stone to using the complete fitdistrplus R-package. It can be adjusted by slightly changing some of the options. For instance, $HC_p$ for different values of $p$ can be computed, with an alternative distribution or a different fitting method. Moreover, this script ensures transparency and traceability of the results obtained through MOSAIC_SSD.
Added value of including censored data

Changing a few parameters in the R script provided within MOSAIC_SSD, it is possible to use *fitdistrplus* to investigate on several fundamental aspects of SSD, such as the influence of including censored data on the prediction. A customary approach when dealing with censored data is to discard or to transform it. More precisely, it is frequent to discard left or right-censored data and to take the middle of the interval-censored data as a single value. Two datasets were analysed to assess the effect of such data transformation on the predicted hazardous concentrations. In the censored salinity dataset mentioned earlier, out of 108 $LC_{50}$, 89 (82.4%) are censored, among which 60 (55.6%) are right-censored and 29 (26.8%) interval-censored. Most of the censored data resulted from the testing of rare species, for which the small number of individuals captured prevented the calculation of an $LC_{50}$ by fitting a concentration-effect model[33]. This extensive dataset was collected to be as representative as possible of the species found in nature[33]. Therefore, a first asset of taking censored data into account is to abstain from discarding or altering the vast majority of the data. The resulting SSD is therefore more representative of the community it aims to describe. Moreover, using only non-censored data in the analysis introduces a strong selection bias towards abundant species. This is particularly problematic, when some rare species are likely to be among those that the environmental manager wishes to protect by carrying out an SSD analysis. The second dataset was published by Koyama et al.[36], and contains vertebral deformity susceptibilities of marine fishes exposed to trifluralin (hereinafter referred to as the *censored trifluralin* dataset). The measured endpoint are 96-hrs $LC_{50}$ on 10 species. Four of the $LC_{50}$ are censored, among which two are right-censored and two are left-censored. On this dataset, the obvious advantage of taking censored data into
account is that the SSD can be fitted on 10 species, whereas discarding the censored data reduces
the size of the dataset to six species only. This is below the minimum recommendation of ECHA
(of 10, preferably 15\textsuperscript{[37]}). A non-censored version of the two datasets (hereinafter referred to as
the transformed salinity and transformed trifluralin datasets) was obtained following the habitual
procedure of discarding the right or left-censored data and taking the middle of the interval-
censored data. Fitting the lognormal distribution on the censored and transformed versions of the
datasets showed that discarding censored data had an adverse effect on the predicted $\text{HC}_5$
(Figure 2). For the salinity dataset, discarding left-censored data induced a clear upward bias for
the cumulative curve and a therefore greater $\text{HC}_5$ (Figure 2 left). The estimates for the $\text{HC}_5$
were: 9.85 g.L$^{-1}$[8.38; 11.80] for the censored dataset and 7.98 g.L$^{-1}$[6.63; 9.93] for the
transformed dataset, respectively. An unnecessary high hazardous concentration might seem a
harmless error, since it is more protective to use the transformed salinity dataset. However, that
incorrectly low value might motivate the use of costly decontamination measures at a specific
location, when efforts could be spared and distributed elsewhere.

The influence of censored data is dataset-dependent and the bias could be in the opposite
direction. This is illustrated on the trifluralin dataset (Figure 2 right). Fitting the log-normal
distribution yielded the following estimates for the $\text{HC}_5$:

\[
2.4 \times 10^{-3} \text{mg.L}^{-1}[4.7 \times 10^{-5}; 2.6 \times 10^{-2}] \quad \text{for the censored dataset and}
\]

\[
1.7 \times 10^{-2} \text{mg.L}^{-1}[8.9 \times 10^{-3}; 4.3 \times 10^{-2}] \quad \text{for the transformed dataset, respectively.}
\]

Discarding the censored data led to underestimate the variability in the community sampled by
the tested species, resulting in a smaller $\text{HC}_5$. Therefore, the width of the distribution was
underestimated and the fifth percentile had a larger value. On the trifluralin dataset, discarding the censored data led to an underestimation of the trifluralin real toxicity and its potential hazard to the environment. Another striking differentiation was that the span of the confidence interval was much larger when censored data were included in the SSD. It reveals that a possible effect of transforming censored datasets is to severely underestimate the width of the confidence interval and to give overconfident predictions on the hazardous concentrations.

Discussion

In this paper, we reviewed the general approach to fit an SSD to sensitivity data and explained how it was possible to use maximum likelihood to include censored data in SSD. We presented MOSAIC_SSD, a web-tool which enables any user to perform an SSD analysis including censored data with few very simple steps. MOSAIC_SSD is an interface to a more versatile tool, the R package fitdistrplus[10] and presents only few options to simplify the use. We supported the methodological approach behind MOSAIC_SSD with several arguments and showed the added value of including censored data into the SSD. Discarding or transforming censored data has been shown to alter the results of the SSD analysis. Using MOSAIC_SSD is a convenient way to take censored data into account in the fitting of an SSD. Moreover, the sound general statistical approach is also an asset to perform any sort of SSD. Considering the choice of a distribution, MOSAIC_SSD provides by default two standard distributions, the log-normal and log-logistic, but it encourages the use of alternative distributions by providing a stepping stone to using the R package fitdistrplus. The question "which distribution best fits a dataset?" cannot have a general answer and must be addressed by testing several options. Therefore, the possibility to try multiple distributions is a valuable asset. For instance, a user might wish to fit a
distribution that best describes the tails of the dataset, because determining a HC₅ is an extreme quantile estimation problem. In that case, a heavy tailed distribution such as Weibull or exponential is appropriate.

In selecting a distribution, it is important not to pick a distribution with too many parameters. One of the easily accessible software for SSD is BurrliOZ[19], which fits the Burr III distribution using maximum likelihood and computes confidence intervals using bootstrap. The Burr III distribution is very flexible[13], but it contains one parameter more than the log-normal or log-logistic distributions. Fitting of a distribution with many parameters requires a lot of data and the Burr III distribution is likely to suffer from strong structural correlation among the parameters[13]. Therefore, convergence can be difficult and the estimates produced are not very reliable. However, BurrliOZ is currently being developed to fit the log-logistic distribution on small datasets and to provide a comparison between at least the log-logistic and the Burr III distribution for larger datasets[3].

MOSAIC_SSD, easily accessible and user-friendly, can encourage the inclusion of censored data in SSD analysis in order to better use all the data at hand. We did not address all the methodological issues relating to the SSD approach but tried to improve the existing methods, with the aim to make the most of the available data given the cost of collecting them. There remain interrogations as to what might happen if the proportion of censored data is too great and the dataset is small. It is not possible to test this situation thoroughly, for there are many ways to censor data and no trivial way to choose between them. A good practice would be to consider the span of the confidence interval around the hazardous concentration of interest and decide if the dataset is adequate for predicting such concentrations.
or if more data need to be collected. Taking censored data into account would therefore be crucial to have a precise assessment of the confidence interval, and not an artificially reduced estimation as in the trifluralin dataset.

We mentioned that censored data might represent an important part of any dataset and that MOSAIC_SSD could be profitably used on many occasions. However, this work could have a more general scope, since fundamentally all data with a confidence interval could be considered as interval-censored data. Indeed, the confidence interval around an EC_{50} or any CEC estimate can be considered as the range which has a 95% probability of containing the real value and be reported as an interval-censored data. Using the confidence intervals on the CECs as censored data provides a basic way to propagate the uncertainty on the CEC into the SSD, a fundamental problem of SSD\[3\] which is seldom addressed\[38\].

Moreover, LOEC (lowest observed effect concentration) data, which are often reported, are indeed left-censored data. The only information LOEC carries is that the NOEC lies below this concentration\[39\]. Therefore, the SSD approach we propose, which includes censored data, would allow ecotoxicologists to better use the available experimental data used to calculate the NOEC.

However, we reached the limits of a traditional SSD based on CEC's and still discarded a lot of information. Indeed, a CEC is only a summary of a full concentration-effect curve. This summary sets aside several aspects of the response of a species to a pollutant, such as the slope of the curve. This slopes describes whether the species is gradually affected or there is a sudden drastic effect. It is possible to include all the information present in the experimental concentration-effect curve in the SSD by building a hierarchical model of SSD. This hierarchy
would model the joint probability of all the parameters describing a concentration-effect curve, not only the CEC in the classical SSD[40]. Moreover, this would also take proper account of the uncertainty on the species response modelling and to propagate uncertainty into the SSD.

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Figure 1: Screenshot of the result page of MOSAIC_SSD on the salinity censored dataset. Top shows the output of MOSAIC_SSD on the salinity dataset, bottom shows the output on a non-censored dataset obtained from a transformation of the salinity dataset.

Figure 2: Fitted and empirical cumulative distribution and the $H_{C5}$ for the salinity dataset (left) and the trifluralin dataset (right). The dotted line corresponds to a potentially affected fraction of 5%. Vertical arrows indicate the $H_{C5}$. Only the region around the $H_{C5}$ is represented. The blue line is for the censored dataset, the red for the transformed dataset. A log-normal distribution was fitted on both datasets.